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STRUCTURE-PRESERVING ALGORITHMS FOR PALINDROMIC QUADRATIC EIGENVALUE PROBLEMS ARISING FROM VIBRATION OF FAST TRAINS*

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Abstract. In this paper, based on Patel's algorithm (1993), we propose a structure-preserving algorithm for solving palindromic quadratic eigenvalue problems (QEPs). We also show the relationship between the structure-preserving algorithm and the URV-based structure-preserving algorithm by Schröder (2007). For large sparse palindromic QEPs, we develop a generalized $\top$-skew-Hamiltonian implicitly restarted shift-and-invert Arnoldi algorithm for solving the resulting $\top$-skew-Hamiltonian pencils. Numerical experiments show that our proposed structure-preserving algorithms perform well on the palindromic QEP arising from a finite element model of high-speed trains and rails.

Key words. palindromic quadratic eigenvalue problem, $\top$-symplectic pencil, $\top$-skew-Hamiltonian pencil

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1. Introduction.

In this paper, we consider the palindromic quadratic eigenvalue problem (QEP) of the form

$$\mathcal{P}(\lambda)x \equiv (\lambda^2 A_1^\top + \lambda A_0 + A_1)x = 0, \tag{1.1}$$

where $\lambda \in \mathbb{C}$, $x \in \mathbb{C}^n \backslash \{0\}$ and $A_1, A_0 \in \mathbb{C}^{n\times n}$ with $A_0^\top = A_0$. Note that the superscript "$\top$" denotes the complex transpose. The scalar λ and the nonzero vector x in (1.1) are the eigenvalue and the associated eigenvector of $\mathcal{P}(\lambda)$, respectively. The underlying matrix polynomial $\mathcal{P}(\lambda)$ has the property that reversing the order of the coefficients, followed by taking the transpose, leads back to the original matrix polynomial, which explains the word "palindromic." Consequently, taking the transpose of (1.1), we easily see that the eigenvalues of $\mathcal{P}(\lambda)$ satisfy the "symplectic" property; that is, they are paired with respect to the unit circle, containing both an eigenvalue λ and its reciprocal $1/\lambda$ (with 0 and ∞ considered to be reciprocal).

The palindromic QEP (1.1) was first raised in the study of the vibration in the structural analysis for fast trains in Germany [3, 4], associated with the company SFE GmbH in Berlin. Existing fast train systems, like the Japanese Shinkansen, the French TGV, and the German ICE, are being modernized and expanded. Vibration is produced from the interaction between the wheels of a train and the rails underneath. Due to the ever increasing speed (currently up to 300 km/hr) of modern trains, the study of its vibration becomes an important task. Research does not only contribute

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towards the increased comfort of passengers, in terms of lower noise and vibration levels. More importantly, the safety in the operation of the trains will be improved, and the operational and construction costs will be optimized [4, 5, 12, 13]. In addition, innovative designs of railway bridges, embedded rail structures, and train suspension systems require accurate resolution of the vibration.

A standard approach for solving the palindromic QEP (1.1) is to transform it into a $2n \times 2n$ linear eigenvalue problem

$$\begin{bmatrix} 0 & I \\ A_1 & A_0 \end{bmatrix} \begin{bmatrix} x \\ \lambda x \end{bmatrix} = \lambda \begin{bmatrix} I & 0 \\ 0 & -A_1^\top \end{bmatrix} \begin{bmatrix} x \\ \lambda x \end{bmatrix} \tag{1.2}$$

and compute its generalized Schur form (see [23]). However, the symplectic property of the eigenvalues of (1.1) is not preserved by computation, generally, producing large numerical errors ([5]). Recently, some pioneering work [4, 12, 13] proposed a good linearization which linearizes the palindromic QEP (1.1) into the form $\lambda Z^\top + Z$, which preserves symplecticity to some extent, and suggested some structure-preserving solution methods. This leads to a vast improvement over previous approaches. Later, a QR-like algorithm [19] and a Jacobi-type method [4] combined with the Laub trick, a preprocessing step of the generalized Schur form [11], have been developed for solving the palindromic linear pencil $\lambda Z^\top + Z$. However, the latter method works well, only if there are no eigenvalues near ± 1. The Jacobi method typically needs about $O(n^3 \log(n))$ flops and the QR-like algorithm is of $O(n^4)$ flops. Recently, a URV-decomposition-based structured method of cubic complexity was developed in [20] to solve the palindromic linear pencil $\lambda Z^\top + Z$, producing eigenvalues which are paired to working precision. In section 3, we will show that the URV-based method [20] is mathematically equivalent to applying the structure-preserving algorithm in section 2 to the enlarged $2n \times 2n$ palindromic quadratic pencil $\zeta^2 Z^\top + \zeta 0 + Z$ (with $\zeta^2 = \lambda$). On the other hand, a structure-preserving doubling algorithm was developed in [1] via the computation of a solvent of a nonlinear matrix equation associated with (1.1). The numerical results show much promise but the convergence theory holds only when the algorithm does not break down.

As mentioned before, the linearization (1.2) generally cannot preserve the symplectic structure. Fortunately, the special linearization for (1.1) (see [1] or [10])

$$(\mathcal{M} - \lambda \mathcal{L}) z \equiv \left(\begin{bmatrix} A_1 & 0 \\ -A_0 & -I \end{bmatrix} - \lambda \begin{bmatrix} 0 & I \\ A_1^\top & 0 \end{bmatrix} \right) \begin{bmatrix} x \\ y \end{bmatrix} = 0 \tag{1.3}$$

obtained by setting $y = \frac{1}{\lambda} A_1 x$ and multiplying the second equation of (1.3) by λ satisfies

$$\mathcal{M} \mathcal{J} \mathcal{M}^\top = \mathcal{L} \mathcal{J} \mathcal{L}^\top, \tag{1.4}$$

where $\mathcal{J} \equiv \mathcal{J}_{2n}$ is the $2n \times 2n$ matrix $\left[\begin{smallmatrix} 0 & I_n \\ -I_n & 0 \end{smallmatrix}\right]$. In other words, the pencil $\mathcal{M} - \lambda \mathcal{L}$ or the matrix pair $(\mathcal{M}, \mathcal{L})$ in (1.3) preserves the symplectic structure of (1.4) and is said to be $\top$-symplectic.

For a real matrix pair $(\mathcal{M}, \mathcal{L})$ satisfying (1.4), a structure-preserving $(\mathcal{S} + \mathcal{S}^{-1})$-transform for the computation of all its eigenvalues is proposed by [9] and a numerically stable algorithm for reducing the transformed pair to a block triangular condensed form by using only orthogonal transformations was developed by Patel [16]. It is perfectly suitable for the $\top$-symplectic pair, but not applicable to the complex conjugate symplectic pair (i.e., $\mathcal{M}\mathcal{J}\mathcal{M}^H = \mathcal{L}\mathcal{J}\mathcal{L}^H$). In this paper, we adapt Patel's approach to solve the $\top$-symplectic pencil in (1.3) resulting from the palindromic QEP (1.1). Only unitary transformations are used and the symplectic structure is fully preserved, which make the method attractive. It is worth mentioning that the $(\mathcal{S}+\mathcal{S}^{-1})$-transform is, in general, a nonlinear transform as in solving the discrete-time optimal control problem [9, 16]. However, the special form in (1.3) leads to a linear $(\mathcal{S}+\mathcal{S}^{-1})$-transform without involving any matrix multiplication.

In some applications, the matrices A_1 and A_0 in (1.1) (and hence $\mathcal{M}$ and $\mathcal{L}$ in (1.3)) can be large and sparse and only the eigenvalues in a specified region are required. To accomplish this, the shift-and-invert (implicitly restarted) Arnoldi algorithm [7, 17, 21] is one of the most widely used standard techniques for computing selected eigenvalues of the large sparse matrix pencil $\mathcal{M}-\lambda\mathcal{L}$. In this approach, the corresponding shifted and inverted matrix is reduced to a Hessenberg form which no longer has the desirable symplectic structure.

Mehrmann and Watkins [15] developed a structure-preserving skew-Hamiltonian, isotropic, implicitly restarted shift-and-invert Arnoldi algorithm (SHIRA) for the computation of eigenpairs of a large sparse real skew-Hamiltonian/Hamiltonian pencil by transforming the pencils to a skew-Hamiltonian operator. In fact, SHIRA can be straightforwardly extended to solve a skew-Hamiltonian/Hamiltonian pencil in the complex transpose case (not in the complex conjugate case), referred to as $\top$SHIRA. We first transform the $\top$-symplectic pencil to a $\top$-skew-Hamiltonian eigenvalue problem by using the $(\mathcal{S}+\mathcal{S}^{-1})$-transform, then $\top$SHIRA is applied to the resulting $\top$-skew-Hamiltonian matrix. On the other hand, to avoid explicitly forming the $\top$-skew-Hamiltonian matrix in the above transformation, we also develop a generalized $\top$-skew-Hamiltonian implicitly restarted shift-and-invert Arnoldi algorithm (G$\top$SHIRA) for solving the $\top$-skew-Hamiltonian pencil resulting from the $(\mathcal{S}+\mathcal{S}^{-1})$-transform of the symplectic pencil $\mathcal{M}-\lambda\mathcal{L}$.

We introduce some definitions that will be used frequently in this paper.

Definition 1.1.

(i) *A matrix* $\mathcal{A}\in\mathbb{C}^{n\times n}$ *is called $\top$-symmetric or $\top$-skew-symmetric if it satisfies* $\mathcal{A}^\top=\mathcal{A}$ *or* $\mathcal{A}^\top=-\mathcal{A}$*, respectively.*

(ii) *A matrix* $\mathcal{U}\in\mathbb{C}^{2n\times 2n}$ *is called $\top$-symplectic if* $\mathcal{U}^\top\mathcal{J}\mathcal{U}=\mathcal{J}$*; a pencil* $\mathcal{M}-\lambda\mathcal{L}\in\mathbb{C}^{2n\times 2n}$ *or the matrix pair* $(\mathcal{M},\mathcal{L})$ *is called $\top$-symplectic if* $\mathcal{M}\mathcal{J}\mathcal{M}^\top=\mathcal{L}\mathcal{J}\mathcal{L}^\top$.

(iii) *A matrix* $\mathcal{H}\in\mathbb{C}^{2n\times 2n}$ *is called $\top$-Hamiltonian or $\top$-skew-Hamiltonian if it satisfies* $(\mathcal{H}\mathcal{J})^\top=\mathcal{H}\mathcal{J}$ *or* $(\mathcal{H}\mathcal{J})^\top=-\mathcal{H}\mathcal{J}$*, respectively.*

(iv) *A pencil* $\mathcal{K}-\lambda\mathcal{N}\in\mathbb{C}^{2n\times 2n}$ *or the matrix pair* $(\mathcal{K},\mathcal{N})$ *is called $\top$-skew-Hamiltonian if* $\mathcal{K}$ *and* $\mathcal{N}$ *are $\top$-skew-Hamiltonian.*

(v) *Let* $X,Y\in\mathbb{C}^{2n\times m}(1\le m\le n)$*;* X *is called $\top$-isotropic if* $X^\top\mathcal{J}X=0_m$*; and* X *and* Y *are called $\top$-bi-isotropic if* $X^\top\mathcal{J}Y=0_m$.

Throughout this paper, $A^\top$ and A^H denote the transpose and conjugate transpose of a matrix A, respectively. We denote the $m\times n$ zero matrix by $0_{m,n}$, and the zero and identity matrices of order n by 0_n and I_n, respectively. The ith column of I_n is denoted by e_i. We adopt the following MATLAB notations: $v(i:j)$ denotes the subvector of the vector v that consists of the ith to the jth entries of v. $A(i:j,k:\ell)$ denotes the submatrix of the matrix A that consists of the intersection of the rows i to j and the columns k to ℓ. $A(i:j,:)$ and $A(:,k:\ell)$ select the rows i to j and the columns k to ℓ, respectively, of A.

The paper is organized as follows. In section 2, we briefly present the structure-preserving algorithm based on Patel's method [16] for solving palindromic QEPs. In section 3, we show the relationship between the structure-preserving algorithm and the URV-based structured method proposed by Schröder [20]. In section 4, based on the SHIRA developed in [15], we introduce the ⊤-skew-Hamiltonian implicitly-restarted shift-and-invert Arnoldi algorithm (⊤SHIRA) for solving the resulting ⊤-skew-Hamiltonian matrix. In section 5, a generalized ⊤-skew-Hamiltonian implicitly-restarted shift-and-invert Arnoldi algorithm (G⊤SHIRA) for solving the resulting ⊤-skew-Hamiltonian pencils is developed. We present some numerical results of the proposed algorithms, using examples from a finite element model of fast trains [1], in section 6. Conclusions are given in section 7.

2. Structure-preserving algorithm I.

We adapt Patel's algorithm [16] applying to the $(\mathcal{S}+\mathcal{S}^{-1})$-transform of a ⊤-symplectic matrix pair for the computation of all its eigenpairs. Let $(\mathcal{M},\mathcal{L})$ be a ⊤-symplectic pair. The $(\mathcal{S}+\mathcal{S}^{-1})$-transform $(\mathcal{M}_s,\mathcal{L}_s)$ of $(\mathcal{M},\mathcal{L})$ is defined by (see [9])

$$\mathcal{M}_s \equiv \mathcal{M}\mathcal{J}\mathcal{L}^\top + \mathcal{L}\mathcal{J}\mathcal{M}^\top, \qquad \mathcal{L}_s \equiv \mathcal{L}\mathcal{J}\mathcal{L}^\top. \tag{2.1}$$

We first give the relationship between eigenpairs of a ⊤-symplectic pencil and its $(\mathcal{S}+\mathcal{S}^{-1})$-transform.

Theorem 2.1. *Let $(\mathcal{M},\mathcal{L})$ be a ⊤-symplectic pair and $(\mathcal{M}_s,\mathcal{L}_s)$ be its $(\mathcal{S}+\mathcal{S}^{-1})$-transform. Then*

(i) *μ is a double eigenvalue of $(\mathcal{M}_s,\mathcal{L}_s)$ if and only if $\nu, \frac{1}{\nu}$ are eigenvalues of $(\mathcal{M},\mathcal{L})$, where $\nu, \frac{1}{\nu}$ are two roots of the quadratic equation $\lambda + \frac{1}{\lambda} = \mu$.*

(ii) *Let x and y be linearly independent eigenvectors of $(\mathcal{L}^\top,\mathcal{M}^\top)$ corresponding to ν and $\frac{1}{\nu}$, respectively, i.e., $(\mathcal{L}^\top - \nu\mathcal{M}^\top)x = 0$ and $(\mathcal{L}^\top - \frac{1}{\nu}\mathcal{M}^\top)y = 0$. Then x and y are two linearly independent eigenvectors of $(\mathcal{M}_s,\mathcal{L}_s)$ corresponding to $\mu = \nu + \frac{1}{\nu}$.*

(iii) *Furthermore, from (ii), if $z_s = \alpha x + \beta y$ (with $\alpha\beta \neq 0$) is an eigenvector of $(\mathcal{M}_s,\mathcal{L}_s)$ corresponding to $\mu = \nu + \frac{1}{\nu}\,(\mu \neq \pm 2)$, i.e., $(\mathcal{M}_s - \mu\mathcal{L}_s)z_s = 0$, then $\mathcal{J}(\mathcal{L}^\top - \frac{1}{\nu}\mathcal{M}^\top)z_s$ and $\mathcal{J}(\mathcal{L}^\top - \nu\mathcal{M}^\top)z_s$ are the eigenvectors of $(\mathcal{M},\mathcal{L})$ corresponding to ν and $\frac{1}{\nu}$, respectively.*

Proof.

(i) As in [9], since $\mathcal{M}\mathcal{J}\mathcal{M}^\top = \mathcal{L}\mathcal{J}\mathcal{L}^\top$, by (2.1) it holds that

$$\begin{aligned}\mathcal{M}_s - \mu\mathcal{L}_s &= \mathcal{M}\mathcal{J}\mathcal{L}^\top + \mathcal{L}\mathcal{J}\mathcal{M}^\top - \left(\nu + \frac{1}{\nu}\right)\mathcal{L}\mathcal{J}\mathcal{L}^\top \\ &= (\mathcal{M} - \nu\mathcal{L})\mathcal{J}\left(\mathcal{L}^\top - \frac{1}{\nu}\mathcal{M}^\top\right) \\ &= \left(\mathcal{M} - \frac{1}{\nu}\mathcal{L}\right)\mathcal{J}(\mathcal{L}^\top - \nu\mathcal{M}^\top). \qquad (2.2)\end{aligned}$$

Hence (i) follows.

(ii) From the last two equations of (2.2), it follows that

$$(\mathcal{M}_s - \mu\mathcal{L}_s)\,x = \left(\mathcal{M} - \frac{1}{\nu}\mathcal{L}\right)\mathcal{J}(\mathcal{L}^\top - \nu\mathcal{M}^\top)\,x = 0,$$

and

$$(\mathcal{M}_s - \mu\mathcal{L}_s)\,y = (\mathcal{M} - \nu\mathcal{L})\mathcal{J}\left(\mathcal{L}^\top - \frac{1}{\nu}\mathcal{M}^\top\right)y = 0.$$

(iii) By applying the last two equations of (2.2) again, it remains to show only that $\mathcal{J}(\mathcal{L}^\top - \frac{1}{\nu}\mathcal{M}^\top)z_s \neq 0$ and $\mathcal{J}(\mathcal{L}^\top - \nu\mathcal{M}^\top)z_s \neq 0$. From (ii) we have

$$\mathcal{J}\left(\mathcal{L}^\top - \frac{1}{\nu}\mathcal{M}^\top\right)z_s = \mathcal{J}\left(\mathcal{L}^\top - \frac{1}{\nu}\mathcal{M}^\top\right)(\alpha x + \beta y) = \alpha\mathcal{J}\left(\mathcal{L}^\top - \frac{1}{\nu}\mathcal{M}^\top\right)x \neq 0.$$

Similarly,

$$\mathcal{J}(\mathcal{L}^\top - \nu\mathcal{M}^\top)z_s = \mathcal{J}(\mathcal{L}^\top - \nu\mathcal{M}^\top)(\alpha x + \beta y) = \beta\mathcal{J}(\mathcal{L}^\top - \nu\mathcal{M}^\top)y \neq 0. \qquad \square$$

THEOREM 2.2. *Let* $(\mathcal{M}, \mathcal{L})$ *be the* $\top$*-symplectic pair as in* (1.3) *and* $(\mathcal{M}_s, \mathcal{L}_s)$ *be its* $(\mathcal{S} + \mathcal{S}^{-1})$*-transform. If* $z_s = [z_1^\top, z_2^\top]^\top$ *with* $z_1, z_2 \in \mathbb{C}^n$ *is an eigenvector of* $(\mathcal{M}_s, \mathcal{L}_s)$ *corresponding to* $\mu = \nu + \frac{1}{\nu}$ $(\mu \neq \pm 2)$, *then* $z_1 + \frac{1}{\nu}z_2$ *and* $z_1 + \nu z_2$ *are eigenvectors of* $\mathcal{P}(\lambda)$ *in* (1.1) *corresponding to* ν *and* $\frac{1}{\nu}$, *respectively.*

Proof. From (iii) of Theorem 2.1 we compute

$$\left(\mathcal{J}\left(\mathcal{L}^\top - \frac{1}{\nu}\mathcal{M}^\top\right)z_s\right)(1:n) = z_1 + \frac{1}{\nu}z_2, \quad (\mathcal{J}(\mathcal{L}^\top - \nu\mathcal{M}^\top)z_s)(1:n) = z_1 + \nu z_2. \tag{2.3}$$

Then, from (1.3) and (2.3), it follows that $\mathcal{P}(\nu)(z_1 + \frac{1}{\nu}z_2) = 0$ and $\mathcal{P}(\frac{1}{\nu})(z_1 + \nu z_2) = 0$. $\square$

Note that from (1.3), we have

$$\begin{aligned}(\mathcal{M}_s, \mathcal{L}_s) &= (\mathcal{M}\mathcal{J}\mathcal{L}^\top + \mathcal{L}\mathcal{J}\mathcal{M}^\top, \mathcal{L}\mathcal{J}\mathcal{L}^\top) \\ &= \left(\begin{bmatrix} A_1 - A_1^\top & A_0 \\ -A_0 & A_1 - A_1^\top \end{bmatrix}, \begin{bmatrix} 0 & -A_1 \\ A_1^\top & 0 \end{bmatrix}\right) \\ &= \left(\begin{bmatrix} A_0 & A_1^\top - A_1 \\ A_1 - A_1^\top & A_0 \end{bmatrix}, \begin{bmatrix} -A_1 & 0 \\ 0 & -A_1^\top \end{bmatrix}\right)\mathcal{J} \\ &\equiv (\mathcal{K}, \mathcal{N})\mathcal{J}. \end{aligned} \tag{2.4}$$

From (2.4), if z is an eigenvector of $(\mathcal{K}, \mathcal{N})$ corresponding to μ, then $z_s = \mathcal{J}^\top z$ is the eigenvector of $(\mathcal{M}_s, \mathcal{L}_s)$ corresponding to the same μ.

Remark 2.1.

(i) The $(\mathcal{S} + \mathcal{S}^{-1})$-transform $(\mathcal{M}_s, \mathcal{L}_s)$ in (2.1) of a $\top$-symplectic pair, in general, is a nonlinear (quadratic) transformation. For instance, the $(\mathcal{S} + \mathcal{S}^{-1})$-transform of the symplectic pair of the form $(\mathcal{M}, \mathcal{L}) \equiv ([\begin{smallmatrix} A & 0 \\ -H & I \end{smallmatrix}], [\begin{smallmatrix} I & G \\ 0 & A^\top \end{smallmatrix}])$ with $H = H^\top$ and $G = G^\top$ arisen from discrete-time optimal control problems produces a quadratic $(\mathcal{S} + \mathcal{S}^{-1})$-transform which involves matrix multiplications and is not backward stable. However, the special form of the $\top$-symplectic pair $(\mathcal{M}, \mathcal{L})$ in (1.3) leads to a linear $(\mathcal{S} + \mathcal{S}^{-1})$-transform as in (2.4) and does not involve any matrix multiplication.

(ii) The eigenvectors of $\mathcal{P}(\lambda)$ corresponding to ν and $1/\nu$ can be obtained from the eigenvectors of $(\mathcal{K}, \mathcal{N})$ directly (see Theorem 2.2), not requiring us to solve any linear system or perform any matrix-vector multiplications.

It is easily seen that $\mathcal{K}$ and $\mathcal{N}$ in (2.4) are both $\top$-skew-Hamiltonian. Patel [16] introduced two types of transformations that preserve the skew-Hamiltonian structure. The first type involves similarity transformations on $\mathcal{K}$ and $\mathcal{N}$, respectively, using Given rotations $G_0(i, c, \bar{s}) := G(i, n+i, c, \bar{s})$. The second type involves equivalence transformations on $\mathcal{K}$ and $\mathcal{N}$, respectively, by the left transformation $Q_0^\top := (U^\top \oplus V^\top)$ and the right transformation $Z_0 := (V \oplus U)$, where the unitary

$U, V \in \mathbb{C}^{n\times n}$ represent the application of Givens rotations. One can easily verify that the new transforming $\mathcal{K}$ and $\mathcal{N}$ are still $\top$-skew-Hamiltonian.

Based on Patel's approach [16] with these two types of transformations, we may reduce $(\mathcal{K}, \mathcal{N})$ to a block triangular structure; that is,

$$\mathcal{K} := Q^\top \mathcal{K} Z = \begin{bmatrix} K_{11} & K_{12} \\ 0 & K_{11}^\top \end{bmatrix}, \qquad \mathcal{N} := Q^\top \mathcal{N} Z = \begin{bmatrix} N_{11} & N_{12} \\ 0 & N_{11}^\top \end{bmatrix}, \tag{2.5}$$

where $K_{11} \in \mathbb{C}^{n\times n}$ is upper Hessenberg, $N_{11} \in \mathbb{C}^{n\times n}$ is upper triangular, and Q, Z are unitary satisfying

$$Q = \mathcal{J}^\top Z \mathcal{J}. \tag{2.6}$$

From (2.5), we see that the pair (K_{11}, N_{11}) contains half of the eigenvalues of $(\mathcal{K}, \mathcal{N})$. We then apply the QZ algorithm to (K_{11}, N_{11}) for computing all eigenpairs $\{(\mu_i, y_i)\}_{i=1}^n$. Consequently, $\{(\mu_i, Z[\begin{smallmatrix} y_i \\ 0 \end{smallmatrix}])\}_{i=1}^n$ are n eigenpairs of $(\mathcal{K}, \mathcal{N})$. From (2.4), $\{(\mu_i, z_i(\equiv \mathcal{J}^\top Z[\begin{smallmatrix} y_i \\ 0 \end{smallmatrix}]))\}_{i=1}^n$ are eigenpairs of $(\mathcal{M}_s, \mathcal{L}_s)$. Finally, we compute all eigenvalues and the associated eigenvectors of $\mathcal{P}(\lambda)$ by Theorem 2.2.

ALGORITHM 2.1 (structure-preserving algorithm I (SA_I)).

Input: *A palindromic quadratic pencil* $\mathcal{P}(\lambda) \equiv \lambda^2 A_1^\top + \lambda A_0 + A_1$ *with* $A_0, A_1 \in \mathbb{C}^{n\times n}$ *and* $A_0^\top = A_0$.
Output: *All eigenvalues and eigenvectors of* $\mathcal{P}(\lambda)$.
Step 1. *Form the pair* $(\mathcal{K}, \mathcal{N})$ *as in* (2.4)*;*
Step 2. *Reduce* $(\mathcal{K}, \mathcal{N})$ *to block upper triangular forms in* (2.5) *using unitary transformations. (See a pseudocode in Appendix* A.1.*);*
Step 3. *Compute eigenpairs* $\{(\mu_i, y_i)\}_{i=1}^n$ *of* (K_{11}, N_{11}) *defined in* (2.5) *by using the QZ algorithm;*
Step 4. *Compute* $z_i = \mathcal{J}^\top Z[\begin{smallmatrix} y_i \\ 0 \end{smallmatrix}] \equiv [\begin{smallmatrix} z_{i1} \\ z_{i2} \end{smallmatrix}], i = 1, 2, \ldots, n$*;*
Step 5. *Compute eigenvalues* ν_i *and* $\frac{1}{\nu_i}$ *of* $\mathcal{P}(\lambda)$ *by solving* $\nu^2 - \mu_i \nu + 1 = 0$*; Compute eigenvectors* $x_{i1} \equiv z_{i1} + \frac{1}{\nu_i} z_{i2}$, $x_{i2} \equiv z_{i1} + \nu_i z_{i2}$ *corresponding to* $\nu_i, \frac{1}{\nu_i}$, *respectively, for* $i = 1, 2, \ldots, n$.

Remark 2.2. The SA_I requires approximately $27n^3$ flops for the eigenvalues, and an additional $23n^3$ flops for the eigenvectors. While the QZ algorithm is applied to $(\mathcal{M}, \mathcal{L})$ directly, it requires approximately $120n^3$ flops for the eigenvalues and an additional $\frac{260}{3}n^3$ flops for the eigenvectors. Here and hereafter a flop is a floating point multiplication and addition for complex numbers, which involves 6 real flops.

3. Structure-preserving algorithm II vs. URV-based method. Recently in [4, 12, 13], a "good" linearization of the palindromic quadratic pencil (1.1) was proposed:

$$\lambda Z^\top + Z \equiv \lambda \begin{bmatrix} A_1^\top & A_0 - A_1 \\ A_1^\top & A_1^\top \end{bmatrix} + \begin{bmatrix} A_1 & A_1 \\ A_0 - A_1^\top & A_1 \end{bmatrix}. \tag{3.1}$$

This preserves the "symplecticity" of the eigenvalues. In order to solve the palindromic linear eigenvalue problem of (3.1), we rewrite it into a new palindromic quadratic pencil

$$\mathcal{Q}(\zeta) \equiv \zeta^2 Z^\top + \zeta 0_{2n} + Z \tag{3.2}$$

with $\zeta^2 = \lambda$. We then apply the SA_I algorithm proposed in section 2 to solve the palindromic QEP of (3.2). As in (2.4), we form

$$\widetilde{\mathcal{K}} = \begin{bmatrix} 0 & Z^\top - Z \\ Z - Z^\top & 0 \end{bmatrix}, \quad \widetilde{\mathcal{N}} = \begin{bmatrix} -Z & 0 \\ 0 & -Z^\top \end{bmatrix}. \tag{3.3}$$

By (2.5) there are unitary $\mathcal{U}_a, \mathcal{V}_a \in \mathbb{C}^{4n\times 4n}$ with $\mathcal{U}_a = \mathcal{J}_{4n}^\top \mathcal{V}_a \mathcal{J}_{4n}$ such that

$$\mathcal{U}_a^\top \widetilde{\mathcal{K}} \mathcal{V}_a = \begin{bmatrix} K_{11}^a & K_{12}^a \\ 0 & (K_{11}^a)^\top \end{bmatrix}, \quad \mathcal{U}_a^\top \widetilde{\mathcal{N}} \mathcal{V}_a = \begin{bmatrix} N_{11}^a & N_{12}^a \\ 0 & (N_{11}^a)^\top \end{bmatrix}, \tag{3.4}$$

where $K_{11}^a \in \mathbb{C}^{2n\times 2n}$ is upper Hessenberg with $\{0, 2, \ldots, 2n-2\}$-diagonals being zeros, $N_{11}^a \in \mathbb{C}^{2n\times 2n}$ is upper triangular with $\{1, 3, \ldots, 2n-1\}$-diagonals being zeros, and K_{12}^a and $N_{12}^a \in \mathbb{C}^{2n\times 2n}$ are skew symmetric with $\{1, -1, \ldots, 2n-1, -(2n-1)\}$-diagonals and with $\{2, -2, \ldots, 2n-2, -(2n-2)\}$-diagonals, respectively, being zeros. Here the ℓ-diagonal of a matrix $A \equiv [a_{ij}]_{i,j=1}^n$ consists of the entries $\{a_{ij}\}$ with $j - i = \ell$. Note that the extra zeros in K_{11}^a, N_{11}^a, K_{12}^a, and N_{12}^a are obtained by performing some suitable permutations on the special forms of (3.3) without any calculation. (See Appendix A.2 for details.) Denote

$$\mathcal{P}_{2n} = [e_1, e_{n+1}, e_2, e_{n+2}, \ldots, e_n, e_{2n}]. \tag{3.5}$$

Let

$$\mathcal{U}^\top = \begin{bmatrix} \mathcal{P}_{2n}^\top & 0 \\ 0 & \mathcal{P}_{2n}^\top \end{bmatrix} \mathcal{U}_a^\top, \quad \mathcal{V} = \mathcal{V}_a \begin{bmatrix} \mathcal{P}_{2n} & 0 \\ 0 & \mathcal{P}_{2n} \end{bmatrix}. \tag{3.6}$$

Then we have

$$\mathcal{U}^\top \widetilde{\mathcal{K}} \mathcal{V} = \left[\begin{array}{cc|cc} 0 & R_1 & T_1 & 0 \\ R_2 & 0 & 0 & -T_2 \\ \hline 0 & 0 & 0 & R_2^\top \\ 0 & 0 & R_1^\top & 0 \end{array}\right], \tag{3.7a}$$

$$\mathcal{U}^\top \widetilde{\mathcal{N}} \mathcal{V} = \left[\begin{array}{cc|cc} R_3 & 0 & 0 & -T_3 \\ 0 & R_4 & T_3^\top & 0 \\ \hline 0 & 0 & R_3^\top & 0 \\ 0 & 0 & 0 & R_4^\top \end{array}\right], \tag{3.7b}$$

where $R_1 \in \mathbb{C}^{n\times n}$ is upper Hessenberg, $R_2, R_3, R_4 \in \mathbb{C}^{n\times n}$ are upper triangular, $T_1, T_2 \in \mathbb{C}^{n\times n}$ are skew symmetric, and $T_3 \in \mathbb{C}^{n\times n}$. From (3.7), we see that in order to compute the eigenvalues and the eigenvectors of $(\widetilde{\mathcal{K}}, \widetilde{\mathcal{N}})$ it suffices to compute those of the matrix pair

$$(R_1 R_4^{-1} R_2, R_3). \tag{3.8}$$

We apply the periodic QZ algorithm [2, 18] to the matrix pair in (3.8) without forming the product explicitly, which gives the n eigenpairs $\{(\gamma_i, y_i)\}_{i=1}^n$, where $y_i \in \mathbb{C}^n$. Let $\mu_i = \sqrt{\gamma_i}$ (one branch of the square root of γ_i), $\eta_i := \mu_i R_1^{-1} R_3 y_i$, and $\widetilde{y}_i = [y_i^\top, \eta_i^\top]^\top$. It follows that $\{(\mu_i, \widetilde{z}_i(\equiv \mathcal{V}[\begin{smallmatrix}\widetilde{y}_i \\ 0\end{smallmatrix}]))\}_{i=1}^n$ are n eigenpairs of $(\widetilde{\mathcal{K}}, \widetilde{\mathcal{N}})$. Write $\widetilde{z}_i = [\widetilde{z}_{i1}^\top, \widetilde{z}_{i2}^\top]^\top$ and solve ν_i and $\frac{1}{\nu_i}$ for $\nu^2 + (2 - \mu_i^2)\nu + 1 = 0$. By Theorem 2.2 and (3.1), we compute the eigenvectors

$$x_{i1} = \widetilde{x}_{i1}(1:n) + \widetilde{x}_{i1}(n+1:2n), \quad x_{i2} = \widetilde{x}_{i2}(1:n) + \widetilde{x}_{i2}(n+1:2n) \tag{3.9a}$$

of $\mathcal{P}(\lambda)$ corresponding to ν_i and $\frac{1}{\nu_i}$, respectively, where

$$\widetilde{x}_{i1} := \widetilde{z}_{i2} - \frac{1}{\sqrt{\nu_i}}\widetilde{z}_{i1}, \quad \widetilde{x}_{i2} := \widetilde{z}_{i2} - \sqrt{\nu_i}\widetilde{z}_{i1}. \tag{3.9b}$$

ALGORITHM 3.1 (structure-preserving algorithm II (SA_II)).

Input: *A palindromic quadratic pencil* $\mathcal{P}(\lambda) \equiv \lambda^2 A_1^\top + \lambda A_0 + A_1$ *with* $A_0, A_1 \in \mathbb{C}^{n\times n}$ *and* $A_0^\top = A_0$.
Output: *All eigenvalues and eigenvectors of* $\mathcal{P}(\lambda)$.
Step 1. *Form the pair* $(\widetilde{\mathcal{K}}, \widetilde{\mathcal{N}})$ *as in* (3.3);
Step 2. *Reduce* $(\widetilde{\mathcal{K}}, \widetilde{\mathcal{N}})$ *to block upper triangular forms as in* (3.7) *using unitary transformations of* (3.4)–(3.6);
Step 3. *Compute eigenpairs* $\{(\gamma_i, y_i)\}_{i=1}^n$ *of* $(R_1R_4^{-1}R_2, R_3)$ *in* (3.8) *by the periodic QZ algorithm* [18];
Step 4. *Compute* $\widetilde{z}_i = \mathcal{V}[\begin{smallmatrix}\widetilde{y}_i\\0\end{smallmatrix}] \equiv [\begin{smallmatrix}\widetilde{z}_{i1}\\ \widetilde{z}_{i2}\end{smallmatrix}]$, *where* $\widetilde{y}_i = [\begin{smallmatrix}I_n\\ \sqrt{\gamma_i}R_1^{-1}R_3\end{smallmatrix}]y_i$ *for* $i = 1, 2, \ldots, n$;
Step 5. *Compute* ν_i *and* $\frac{1}{\nu_i}$ *by solving* $\nu^2 + (2-\gamma_i)\nu + 1 = 0$; *Compute eigenvectors* x_{i1} *and* x_{i2} *of* $\mathcal{P}(\lambda)$ *as in* (3.9a) *corresponding to* $\nu_i, \frac{1}{\nu_i}$, *respectively, for* $i = 1, 2, \ldots, n$.

Remark 3.1.

(i) In Step 3, since R_1, R_4, R_2, and R_3 are already in Hessenberg-triangular form, the first step in the periodic QZ algorithm is not needed.

(ii) The SA_II requires $62n^3$ flops for the eigenvalues, and an additional $23n^3$ flops for the eigenvectors.

Recently a URV-decomposition-based structured method was proposed in [20] for solving the palindromic linear pencil (3.1). From [20] there are unitary $U, V \in \mathbb{C}^{2n\times 2n}$ such that

$$U^\top Z V = \begin{bmatrix} 0 & \widehat{R}_4^\top \Pi_n \\ \Pi_n \widehat{R}_3 & \Pi_n \widehat{T}_3 \Pi_n \end{bmatrix}, \quad V^\top (Z - Z^\top) V = \begin{bmatrix} 0 & -\widehat{R}_2^\top \Pi_n \\ \Pi_n \widehat{R}_2 & \Pi_n \widehat{T}_2 \Pi_n \end{bmatrix} \tag{3.10a}$$

and

$$U^\top (Z^\top - Z) U = \begin{bmatrix} 0 & -\widehat{R}_1^\top \Pi_n \\ \Pi_n \widehat{R}_1 & \Pi_n \widehat{T}_1 \Pi_n \end{bmatrix}, \tag{3.10b}$$

where $\Pi_n = [e_n, \ldots, e_1]$, $\widehat{R}_1 \in \mathbb{C}^{n\times n}$ is upper Hessenberg, $\widehat{R}_2, \widehat{R}_3, \widehat{R}_4 \in \mathbb{C}^{n\times n}$ are upper triangular, $\widehat{T}_1, \widehat{T}_2 \in \mathbb{C}^{n\times n}$ are skew symmetric, and $\widehat{T}_3 \in \mathbb{C}^{n\times n}$. Define

$$\mathcal{U}_0^\top := \left[\begin{array}{cc|cc} 0 & \Pi_n & 0 & 0 \\ 0 & 0 & 0 & \Pi_n \\ \hline 0 & 0 & I_n & 0 \\ -I_n & 0 & 0 & 0 \end{array}\right] \begin{bmatrix} U^\top & 0 \\ 0 & V^\top \end{bmatrix}, \quad \mathcal{V}_0 := \mathcal{J}_{4n}^\top \mathcal{U}_0 \mathcal{J}_{4n}. \tag{3.11}$$

Then it is easily seen that $\mathcal{U}_0^H \widetilde{\mathcal{K}} \mathcal{V}_0$ and $\mathcal{U}_0^H \widetilde{\mathcal{N}} \mathcal{V}_0$ have the same forms as in (3.7) with "\hat" being over all submatrices. Furthermore, if we define

$$\mathcal{U}_b^\top = \begin{bmatrix} \mathcal{P}_{2n} & 0 \\ 0 & \mathcal{P}_{2n} \end{bmatrix} \mathcal{U}_0^\top, \quad \mathcal{V}_b := \mathcal{J}_{4n}^\top \mathcal{U}_b \mathcal{J}_{4n}, \tag{3.12}$$

then we have

$$\mathcal{U}_b^H \widetilde{\mathcal{K}} \mathcal{V}_b = \begin{bmatrix} K_{11}^b & K_{12}^b \\ 0 & (K_{11}^b)^\top \end{bmatrix}, \quad \mathcal{U}_b^H \widetilde{\mathcal{N}} \mathcal{V}_b = \begin{bmatrix} N_{11}^b & N_{12}^b \\ 0 & (N_{11}^b)^\top \end{bmatrix}, \tag{3.13}$$

where $K_{11}^b, K_{12}^b, N_{11}^b$, and N_{12}^b are of the same forms as in (3.4).

THEOREM 3.1. *If K_{11}^a and K_{11}^b are unreduced, and N_{11}^a and N_{11}^b are nonsingular (see* (3.4) *and* (3.13)*), then the SA_II is mathematically equivalent to the URV-based structured method.*

Proof. Denote $\mathcal{V}_a := [\mathcal{V}_1^a, \mathcal{V}_2^a]$ with $\mathcal{V}_i^a \in \mathbb{C}^{4n\times 2n} (i = 1, 2)$. Since $\mathcal{U}_a = \mathcal{J}_{4n}^\top \mathcal{V}_a \mathcal{J}_{4n}$, it holds that $\mathcal{U}_a = [\mathcal{J}_{4n}\mathcal{V}_2^a, -\mathcal{J}_{4n}\mathcal{V}_1^a]$. From (3.4), it follows that

$$\widetilde{\mathcal{K}}\mathcal{V}_1^a = \mathcal{J}_{4n}\mathcal{V}_2^a K_{11}^a, \quad \widetilde{\mathcal{N}}\mathcal{V}_1^a = \mathcal{J}_{4n}\mathcal{V}_2^a N_{11}^a. \tag{3.14}$$

This implies that

$$\widetilde{\mathcal{K}}\mathcal{V}_1^a = \widetilde{\mathcal{N}}\mathcal{V}_1^a (N_{11}^a)^{-1} K_{11}^a. \tag{3.15}$$

Since the first columns of $\mathcal{V}_1^a$ and $\mathcal{V}_1^b$ ($\mathcal{V}_b \equiv [\mathcal{V}_1^b, \mathcal{V}_2^b]$) are both e_1, by applying the implicit Q-theorem to (3.15), the matrices $\mathcal{U}_a$ and $\mathcal{V}_a$ are uniquely determined, and $\mathcal{U}_a = \mathcal{U}_b$ and $\mathcal{V}_a = \mathcal{V}_b$. ∎

4. ⊤-skew-Hamiltonian Arnoldi method.

Based on SHIRA [15], in this section we briefly introduce the structure-preserving ⊤-skew-Hamiltonian Arnoldi algorithm to compute the desired eigenpairs of a ⊤-skew-Hamiltonian $\mathcal{B}$.

As in (2.4), using the $(\mathcal{S} + \mathcal{S}^{-1})$-transform, we transform $\mathcal{M} - \lambda\mathcal{L}$ of (1.3) into a ⊤-skew-Hamiltonian pencil $\mathcal{K} - \mu\mathcal{N}$ by

$$\mathcal{K} - \mu\mathcal{N} \equiv \left[(\mathcal{L}\mathcal{J}\mathcal{M}^\top + \mathcal{M}\mathcal{J}\mathcal{L}^\top) - \mu\mathcal{L}\mathcal{J}\mathcal{L}^\top\right]\mathcal{J}^\top. \tag{4.1}$$

Next, we derive the shift-invert transformation of $\mathcal{K} - \mu\mathcal{N}$. Let $\lambda_0 \notin \sigma(\mathcal{M}, \mathcal{L})$. Then, from Theorem 2.2(i), we have $\mu_0 \equiv \lambda_0 + \frac{1}{\lambda_0} \notin \sigma(\mathcal{K}, \mathcal{N})$. Define the shift-invert transformation $\widehat{\mathcal{K}} - \widehat{\mu}\widehat{\mathcal{N}}$ for $\mathcal{K} - \mu\mathcal{N}$ with $\widehat{\mu} = \frac{1}{\mu - \mu_0}$ and

$$\widehat{\mathcal{K}} \equiv -\lambda_0\mathcal{N} = -\lambda_0\mathcal{L}\mathcal{J}\mathcal{L}^\top\mathcal{J}^\top = \lambda_0 \begin{bmatrix} A_1^\top & 0 \\ 0 & A_1 \end{bmatrix}, \tag{4.2a}$$

$$\widehat{\mathcal{N}} \equiv -\lambda_0(\mathcal{K} - \mu_0\mathcal{N}) = -\lambda_0(\mathcal{L}\mathcal{J}\mathcal{M}^\top + \mathcal{M}\mathcal{J}\mathcal{L}^\top - \mu_0\mathcal{L}\mathcal{J}\mathcal{L}^\top)\mathcal{J}^\top. \tag{4.2b}$$

Substituting $\mu_0 = \lambda_0 + \frac{1}{\lambda_0}$ into (4.2b), $\widehat{\mathcal{N}}$ can be factorized as

$$\begin{aligned} \widehat{\mathcal{N}} &= -\lambda_0 \left(\mathcal{L}\mathcal{J}\mathcal{M}^\top + \mathcal{M}\mathcal{J}\mathcal{L}^\top - \left(\lambda_0 + \frac{1}{\lambda_0}\right)\mathcal{L}\mathcal{J}\mathcal{L}^\top\right)\mathcal{J}^\top \\ &= (\mathcal{M} - \lambda_0\mathcal{L})\,\mathcal{J}\left(\mathcal{M}^\top - \lambda_0\mathcal{L}^\top\right)\mathcal{J}^\top \equiv \mathcal{N}_1\mathcal{N}_2, \end{aligned} \tag{4.3}$$

where

$$\mathcal{N}_1 = \mathcal{M} - \lambda_0\mathcal{L}, \quad \mathcal{N}_2 = \mathcal{J}(\mathcal{M}^\top - \lambda_0\mathcal{L}^\top)\mathcal{J}^\top \tag{4.4}$$

are nonsingular and satisfy $\mathcal{N}_2^\top\mathcal{J} = \mathcal{J}\mathcal{N}_1$. The generalized eigenvalue problem $\widehat{\mathcal{K}}z = \widehat{\mu}\widehat{\mathcal{N}}z$ is then equivalent to the eigenvalue problem $\mathcal{B}y = \widehat{\mu}y$, where $y = \mathcal{N}_2 z$ and

$$\mathcal{B} \equiv \mathcal{N}_1^{-1}\widehat{\mathcal{K}}\mathcal{N}_2^{-1}. \tag{4.5}$$

Using the facts that $\widehat{\mathcal{K}}\mathcal{J} = \mathcal{J}\widehat{\mathcal{K}}^\top$ and $\mathcal{N}_2^\top \mathcal{J} = \mathcal{J}\mathcal{N}_1$, we find that $\mathcal{B}$ satisfies

$$\mathcal{J}\mathcal{B}^\top = \mathcal{J}\mathcal{N}_2^{-\top}\widehat{\mathcal{K}}^\top \mathcal{N}_1^{-\top} = \mathcal{N}_1^{-1}\mathcal{J}\widehat{\mathcal{K}}^\top \mathcal{N}_1^{-\top} = \mathcal{N}_1^{-1}\widehat{\mathcal{K}}\mathcal{J}\mathcal{N}_1^{-\top} = \mathcal{N}_1^{-1}\widehat{\mathcal{K}}\mathcal{N}_2^{-1}\mathcal{J} = \mathcal{B}\mathcal{J},$$

and hence $\mathcal{B}$ is again $\top$-skew-Hamiltonian.

We now define the Krylov matrix with respect to u_1 and j $(1 \le j \le n)$ by

$$K_j \equiv K_j[\mathcal{B}, u_1] = [u_1, \mathcal{B}u_1, \ldots, \mathcal{B}^{j-1}u_1] \tag{4.6}$$

and state two useful theorems from [15]. Note that these theorems are slightly different from the originals, but the proofs are almost identical to the ones in [15].

THEOREM 4.1 (see [15]). *Let $\mathcal{B} \in \mathbb{C}^{2n\times 2n}$ be $\top$-skew-Hamiltonian and $K_j \equiv K_j[\mathcal{B}, u_1]$ $(1 \le j \le n)$ be a Krylov matrix with rank$(K_j) = j$. Then span(K_j) is $\top$-isotropic and if $K_j = U_j\widehat{R}_j$ is a QR-factorization, then*

$$\mathcal{B}U_j = U_j\widehat{H}_j + \widehat{u}_{j+1}e_j^\top, \tag{4.7}$$

where $\widehat{H}_j \in \mathbb{C}^{j\times j}$ is unreduced upper Hessenberg, $U_j \in \mathbb{C}^{2n\times j}$ is orthonormal and $\top$-isotropic, and $\widehat{u}_{j+1} \in \mathbb{C}^{2n}$ is a suitable vector such that

$$U_j^H \widehat{u}_{j+1} = 0 \quad \text{and} \quad U_j^\top \mathcal{J}\widehat{u}_{j+1} = 0. \tag{4.8}$$

THEOREM 4.2 (see [15]). *Let $\mathcal{B} \in \mathbb{C}^{2n\times 2n}$ be $\top$-skew-Hamiltonian. If rank $(K_n[\mathcal{B}, u_1]) = n$, then there is a unitary $\top$-symplectic matrix $\mathcal{U}$ with $\mathcal{U}e_1 = u_1$ such that*

$$\mathcal{U}^H\mathcal{B}\mathcal{U} = \begin{bmatrix} \widehat{H}_n & \widehat{N}_n \\ 0 & \widehat{H}_n^\top \end{bmatrix}, \tag{4.9}$$

where $\widehat{H}_n$ is unreduced upper Hessenberg and $\widehat{N}_n$ is $\top$-skew-symmetric.

Based on Theorem 4.2, the jth step of the Arnoldi process is given by

$$\widehat{h}_{j+1,j}u_{j+1} = \mathcal{B}u_j - \sum_{i=1}^{j} \widehat{h}_{ij}u_i, \tag{4.10}$$

where $\widehat{h}_{ij} = u_i^H\mathcal{B}u_j$, $i = 1, \ldots, j$, and $\widehat{h}_{j+1,j} > 0$ is chosen so that $\|u_{j+1}\|_2 = 1$. In order to ensure that the space span$\{u_1, \ldots, u_{j+1}\}$ is $\top$-isotropic to working precision, the jth step of the $\top$-isotropic Arnoldi process is modified by

$$\widehat{h}_{j+1,j}u_{j+1} = \mathcal{B}u_j - \sum_{i=1}^{j} \widehat{h}_{ij}u_i - \sum_{i=1}^{j} \widehat{t}_{ij}\mathcal{J}\bar{u}_i, \tag{4.11}$$

where $\widehat{h}_{ij} = u_i^H\mathcal{B}u_j$, $\widehat{t}_{ij} = -u_i^\top\mathcal{J}\mathcal{B}u_j$, $i = 1, \ldots, j$, and $\widehat{h}_{j+1,j} > 0$ is chosen so that $\|u_{j+1}\|_2 = 1$. We present the $\top$SHIRA-method.

ALGORITHM 4.1 ($\top$SHIRA).

> **Input:** $\top$-*skew-Hamiltonian matrix* $\mathcal{B}$ *with starting vector* u_1.
> **Output:** U_ℓ *and upper Hessenberg matrix* $\widehat{H}_\ell$ *with* $\mathcal{B}U_\ell = U_\ell \widehat{H}_\ell$, $U_\ell^H U_\ell = I_\ell$ *and* $U_\ell^\top \mathcal{J} U_\ell = 0$.
> *Use* (4.11) *with starting vector* u_1 *to generate the* ℓ*th step of the* $\top$-*isotropic Arnoldi factorization:*
> $$\mathcal{B}U_\ell = U_\ell \widehat{H}_\ell + \widehat{h}_{\ell+1,\ell} u_{\ell+1} e_\ell^\top.$$
> *For* $k = 1, 2, \ldots,$ *until wanted* ℓ *eigenpairs of* $\mathcal{B}$ *are convergent,*
> *Use* (4.11) *to extend the* ℓ*th step of the* $\top$-*isotropic Arnoldi factorization to the* $(\ell+p)$*th step of the* $\top$-*isotropic Arnoldi factorization:*
> $$\mathcal{B}U_{\ell+p} = U_{\ell+p} \widehat{H}_{\ell+p} + \widehat{h}_{\ell+p+1,\ell+p} u_{\ell+p+1} e_{\ell+p}^\top.$$
> *Use standard implicitly restarted step for the Arnoldi algorithm* [8] *to reform a new* ℓ*th step of the* $\top$-*isotropic Arnoldi factorization.*
> *End*

Remark 4.1.

(i) $\widehat{h}_{\ell+1,\ell}$ is set to zero if $|\widehat{h}_{\ell+1,\ell}| < tol(|\widehat{h}_{\ell,\ell}| + |\widehat{h}_{\ell+1,\ell+1}|)$ for some stopping tolerance "tol."

(ii) Let (θ_i, v_i) be an eigenpair of $\widehat{H}_\ell$, i.e., $\widehat{H}_\ell v_i = \theta_i v_i$. Let $y_i = U_\ell v_i$ be the Ritz vector of $\mathcal{B}$ corresponding to the Ritz value θ_i. Then from (4.7) and (4.8), we have

$$\begin{aligned}
&\|\mathcal{B}y_i - \theta_i y_i\|_2 = \|\mathcal{B}U_\ell v_i - \theta_i U_\ell v_i\|_2 \\
&= \|(U_\ell \widehat{H}_\ell + \widehat{u}_{\ell+1,\ell} e_\ell^\top) v_i - \theta_i U_\ell v_i\|_2 \\
&= \|U_\ell(\widehat{H}_\ell v_i - \theta_i v_i) + \widehat{h}_{\ell+1,\ell}(e_\ell^\top v_i) u_{\ell+1}\|_2 \\
&= |\widehat{h}_{\ell+1,\ell}||e_\ell^\top v_i|.
\end{aligned}$$

5. Generalized $\top$-skew-Hamiltonian Arnoldi method. We now consider the generalized eigenvalue problem $\widehat{\mathcal{K}} z = \widehat{\mu}\widehat{\mathcal{N}} z$, where $\widehat{\mathcal{K}}$ and $\widehat{\mathcal{N}}$ are $\top$-skew-Hamiltonian given in (4.2). Based on the reduction method [16], $\widehat{\mathcal{K}} - \widehat{\mu}\widehat{\mathcal{N}}$ can be reduced to block triangular condensed forms

$$\mathcal{V}^\top(\widehat{\mathcal{K}} - \widehat{\mu}\widehat{\mathcal{N}})\mathcal{U} = \begin{bmatrix} K_{11} & K_{12} \\ 0 & K_{11}^\top \end{bmatrix} - \widehat{\mu} \begin{bmatrix} N_{11} & N_{12} \\ 0 & N_{11}^\top \end{bmatrix}, \tag{5.1}$$

where $K_{11}, N_{11} \in \mathbb{C}^{n\times n}$ are, respectively, upper Hessenberg and upper triangular, and $\mathcal{V}$ and $\mathcal{U} \in \mathbb{C}^{2n\times 2n}$ are unitary satisfying

$$\mathcal{V} = \mathcal{J}^\top \mathcal{U} \mathcal{J}. \tag{5.2}$$

In order to solve a large sparse product or a periodic eigenvalue problem, recently, a product (or a periodic) Arnoldi process and a product Krylov process were, respectively, proposed by Kressner's book [6, section 4.2.5] and Watkins' book [24, section 9.10]. Using the result of Theorem 4.1, we adopt the idea of the periodic Arnoldi process [6, section 4.2.5] to develop a generalized $\top$-skew-Hamiltonian algorithm which preserves the structure of (5.1) for the computation of the desired eigenpairs of $\widehat{\mathcal{K}} z = \widehat{\mu}\widehat{\mathcal{N}} z$.

THEOREM 5.1. *Let* $\mathcal{B} \equiv \mathcal{N}_1^{-1}\widehat{\mathcal{K}}\mathcal{N}_2^{-1}$ *be* $\top$-*skew-Hamiltonian defined in* (4.5). *Let* $\widehat{\mathcal{N}} = \mathcal{N}_1\mathcal{N}_2$ *and* $K_j \equiv K_j[\mathcal{B}, u_1]$ *be the Krylov matrix with rank*$(K_j) = j$. *If*

$$\mathcal{N}_2^{-1} K_j = Z_j R_{2,j} \quad \text{and} \quad \mathcal{N}_1 K_j = Y_j R_{1,j} \tag{5.3}$$

are QR-factorizations, where $Z_j, Y_j \in \mathbb{C}^{2n\times j}$ are orthonormal and $R_{2,j}, R_{1,j}$ are nonsingular upper triangular, then we have

$$\widehat{\mathcal{K}} Z_j = Y_j H_j + \widehat{y}_{j+1} e_j^\top \tag{5.4}$$

and

$$\widehat{\mathcal{N}} Z_j = Y_j R_j, \tag{5.5}$$

where $H_j \in \mathbb{C}^{j\times j}$ is unreduced upper Hessenberg, $R_j \in \mathbb{C}^{j\times j}$ is nonsingular upper triangular, and Y_j and Z_j are $\top$-bi-isotropic such that

$$Y_j^H \widehat{y}_{j+1} = 0 \quad \text{and} \quad Z_j^\top \mathcal{J} \widehat{y}_{j+1} = 0 \tag{5.6}$$

for a suitable $\widehat{y}_{j+1} \in \mathbb{C}^{2n}$.

Proof. Let $K_j = U_j \widehat{R}_j$ be the QR-factorization of K_j with $\widehat{R}_j$ being nonsingular upper triangular. From Theorem 4.1, it follows that

$$\mathcal{N}_1^{-1} \widehat{\mathcal{K}} \mathcal{N}_2^{-1} U_j = U_j \widehat{H}_j + \widehat{u}_{j+1} e_j^\top. \tag{5.7}$$

Substituting (5.3) into (5.7) we obtain

$$\begin{aligned}
\widehat{\mathcal{K}} Z_j &= \widehat{\mathcal{K}} \mathcal{N}_2^{-1} K_j R_{2,j}^{-1} = \widehat{\mathcal{K}} \mathcal{N}_2^{-1} U_j \widehat{R}_j R_{2,j}^{-1} \\
&= (\mathcal{N}_1 U_j \widehat{H}_j + \mathcal{N}_1 \widehat{u}_{j+1} e_j^\top) \widehat{R}_j R_{2,j}^{-1} \\
&= Y_j (R_{1,j} \widehat{R}_j^{-1} \widehat{H}_j \widehat{R}_j R_{2,j}^{-1}) + \gamma_j Y_j Y_j^H \mathcal{N}_1 \widehat{u}_{j+1} e_j^\top + \gamma_j (I - Y_j Y_j^H) \mathcal{N}_1 \widehat{u}_{j+1} e_j^\top \\
&= Y_j H_j + \widehat{y}_{j+1} e_j^\top, \qquad (5.8)
\end{aligned}$$

where $\gamma_j = e_j^\top \widehat{R}_j R_{2,j}^{-1} e_j$,

$$H_j = R_{1,j} \widehat{R}_j^{-1} \widehat{H}_j \widehat{R}_j R_{2,j}^{-1} + \gamma_j Y_j^H \mathcal{N}_1 \widehat{u}_{j+1} e_j^\top, \tag{5.9}$$

and

$$\widehat{y}_{j+1} = \gamma_j (I - Y_j Y_j^H) \mathcal{N}_1 \widehat{u}_{j+1}. \tag{5.10}$$

Since $\widehat{R}_j$, $R_{1,j}$, and $R_{2,j}$ are nonsingular upper triangular, and $\widehat{H}_j$ is unreduced upper Hessenberg, from (5.9) it follows that H_j is unreduced upper Hessenberg. Clearly, it holds that $Y_j^H \widehat{y}_{j+1} = 0$ by (5.10).

On the other hand, from (5.3), we also have

$$\widehat{\mathcal{N}} Z_j = \mathcal{N}_1 \mathcal{N}_2 Z_j = \mathcal{N}_1 K_j R_{2,j}^{-1} = Y_j R_{1,j} R_{2,j}^{-1} \equiv Y_j R_j,$$

where $R_j = R_{1,j} R_{2,j}^{-1}$ is nonsingular and upper triangular.

We now show that Y_j and Z_j are $\top$-bi-isotropic. By the fact that $\mathcal{N}_2^\top \mathcal{J} = \mathcal{J} \mathcal{N}_1$ and (5.3), it holds that

$$Y_j^\top \mathcal{J} Z_j = R_{1,j}^{-\top} K_j^\top (\mathcal{N}_1^\top \mathcal{J} \mathcal{N}_2^{-1}) K_j R_{2,j}^{-1} = R_{1,j}^{-\top} K_j^\top \mathcal{J} K_j R_{2,j}^{-1} = 0. \tag{5.11}$$

From (5.8) and (5.10), we have

$$Z_j^\top \mathcal{J} \widehat{y}_{j+1} e_j^\top = Z_j^\top \mathcal{J} (\widehat{\mathcal{K}} Z_j - Y_j H_j) = Z_j^\top \mathcal{J} \widehat{\mathcal{K}} Z_j,$$

which is $\top$-skew-symmetric. This implies that $Z_j^\top \mathcal{J} \widehat{y}_{j+1} = 0$. $\square$

THEOREM 5.2. *Let $\mathcal{B} = \mathcal{N}_1^{-1}\widehat{\mathcal{K}}\mathcal{N}_2^{-1}$ be $\top$-skew-Hamiltonian defined in* (4.5) *and $\widehat{\mathcal{N}} = \mathcal{N}_1\mathcal{N}_2$. If rank$(K_n[\mathcal{B}, u_1]) = n$, then there are unitary matrices $\mathcal{U}$ and $\mathcal{V}$ satisfying* (5.2) *and $\mathcal{V}e_1 = \mathcal{N}_1 u_1/\|\mathcal{N}_1 u_1\|_2$ such that*

$$\mathcal{V}^\top \widehat{\mathcal{K}}\mathcal{U} = \begin{bmatrix} H_n & S_n \\ 0 & H_n^\top \end{bmatrix}, \quad \mathcal{V}^\top \widehat{\mathcal{N}}\mathcal{U} = \begin{bmatrix} R_n & T_n \\ 0 & R_n^\top \end{bmatrix}, \tag{5.12}$$

where H_n is unreduced upper Hessenberg, R_n is nonsingular upper triangular, and S_n and T_n are $\top$-skew-symmetric.

Proof. Applying Theorem 5.1 for $j = n$, we have $\widehat{y}_{n+1}$ being orthogonal to Y_n and $\mathcal{J}\bar{Z}_n$. This implies that $\widehat{y}_{n+1} = 0$. Then (5.4) and (5.5) become

$$\widehat{\mathcal{K}}Z_n = Y_n H_n \quad \text{and} \quad \widehat{\mathcal{N}}Z_n = Y_n R_n, \tag{5.13}$$

where H_n is unreduced upper Hessenberg and R_n is nonsingular upper triangular. Let $\mathcal{U} \equiv \begin{bmatrix} Z_n & -\mathcal{J}\bar{Y}_n \end{bmatrix}$, $\mathcal{V} \equiv \begin{bmatrix} Y_n & -\mathcal{J}\bar{Z}_n \end{bmatrix}$. Clearly,

$$Z_n^H Z_n = I_n, \quad Y_n^H Y_n = I_n, \quad \text{and} \quad Y_n^\top \mathcal{J} Z_n = 0_n. \tag{5.14}$$

Then $\mathcal{U}$ and $\mathcal{V}$ satisfy (5.2). Since $\widehat{\mathcal{K}}\mathcal{J}$ and $\widehat{\mathcal{N}}\mathcal{J}$ are $\top$-skew symmetric, from (5.13)–(5.14), (5.12) follows. ∎

Based on Theorem 5.2, we now introduce a generalized $\top$-isotropic Arnoldi process which produces $\top$-bi-isotropic matrices Z_j and Y_{j+1} at the jth step.

By the recursive definition of j, let us first assume that the $\top$-bi-isotropic matrices Z_{j-1} and Y_j satisfy (5.4) and (5.5) with $j := j-1$. That is, the $(j-1)$th step of the generalized $\top$-isotropic Arnoldi process generates

$$\widehat{\mathcal{N}}Z_{j-1} = Y_{j-1}R_{j-1}. \tag{5.15}$$

Now, we compare the jth columns of both sides in (5.5) which give

$$\widehat{\mathcal{N}}z_j = \sum_{i=1}^{j-1} r_{ij}y_i + r_{jj}y_j. \tag{5.16}$$

With (5.15), (5.16) it can be rewritten as

$$r_{jj}^{-1}z_j = \widehat{\mathcal{N}}^{-1}y_j - \sum_{i=1}^{j-1} \widehat{r}_{ij}z_i, \tag{5.17}$$

where

$$[\widehat{r}_{1j}, \ldots, \widehat{r}_{j-1,j}]^\top := -r_{jj}^{-1}R_{j-1}^{-1}[r_{1j}, \ldots, r_{j-1,j}]^\top. \tag{5.18}$$

Since $Z_j^H Z_j = I_j$, the coefficient $\widehat{r}_{ij}$ in (5.17) can be evaluated by

$$\widehat{r}_{ij} = z_j^H \widehat{\mathcal{N}}^{-1}y_j, \quad i = 1, \ldots, j-1, \tag{5.19}$$

and r_{jj} in (5.17) is chosen so that $\|z_j\|_2 = 1$. Substituting $[\widehat{r}_{1j}, \ldots, \widehat{r}_{j-1,j}]^\top$ of (5.19) into (5.18), we obtain the coefficient vector $[r_{1j}, \ldots, r_{j-1,j}]^\top$.

In exact arithmetic, z_j is orthogonal to $\mathcal{J}\bar{Y}_j$ automatically. As before, round-off errors cause $z_j^\top \mathcal{J} y_i$, $i = 1, \ldots, j$, to be tiny values. Thus, the jth step of the generalized $\top$-isotropic Arnoldi process for z_j should be modified by

$$r_{jj}^{-1} z_j = \widehat{\mathcal{N}}^{-1} y_j - \sum_{i=1}^{j-1} \widehat{r}_{ij} z_i - \sum_{i=1}^{j} s_{ij} \mathcal{J} \bar{y}_i, \tag{5.20a}$$

where

$$s_{ij} = y_i^\top \mathcal{J}^\top \left(\widehat{\mathcal{N}}^{-1} y_j - \sum_{i=1}^{j-1} \widehat{r}_{ij} z_i \right), \quad i = 1, \ldots, j. \tag{5.20b}$$

From (5.4), similar to (4.11), the jth step of the generalized $\top$-isotropic Arnoldi process for y_{j+1} is given by

$$h_{j+1,j} y_{j+1} = \widehat{\mathcal{K}} z_j - \sum_{i=1}^{j} h_{ij} y_i - \sum_{i=1}^{j} t_{ij} \mathcal{J} \bar{z}_i, \tag{5.21a}$$

where

$$h_{ij} = y_i^H \widehat{\mathcal{K}} z_j, \quad t_{ij} = z_i^\top \mathcal{J}^\top \widehat{\mathcal{K}} z_j, \quad i = 1, \ldots, j, \tag{5.21b}$$

and $h_{j+1,j} > 0$ is chosen so that $\|y_{j+1}\|_2 = 1$. Combing (5.20) and (5.21), we state the jth step of the generalized $\top$-isotropic Arnoldi process.

ALGORITHM 5.1 (the jth generalized $\top$-isotropic Arnoldi step).

Input: $\top$-*skew-Hamiltonian* $\widehat{\mathcal{K}}$ *and* $\widehat{\mathcal{N}}$, *upper triangular* $R(1:j-1, 1:j-1)$,
 $Y_j = [y_1, \ldots, y_j]$ *and* $Z_{j-1} = [z_1, \ldots, z_{j-1}]$ *with* $Y_j^H Y_j = I_j$,
 $Z_{j-1}^H Z_{j-1} = I_{j-1}$, *and* $Y_j^\top \mathcal{J} Z_{j-1} = 0$.
Output: $[h_{1,j}, \ldots, h_{j+1,j}]$, $R(1:j, 1:j)$, y_{j+1}, *and* z_j.
 Compute z_j *in* (5.20) *by using the modified Gram–Schmidt step:*
  Solve $\widehat{\mathcal{N}} z_j = y_j$;
  For $i = 1, \ldots, j-1$
   $\widehat{r}_{ij} = z_i^H z_j$, $z_j = z_j - \widehat{r}_{ij} z_i$
  End
  Set $R(j,j) := \|z_j\|_2^{-1}$, $z_j := R(j,j) z_j$, *and*
   $R(1:j-1, j) := -R(j,j) R(1:j-1, 1:j-1) [\widehat{r}_{1j}, \cdots, \widehat{r}_{j-1,j}]^\top$;
 Reorthogonalize z_j *to* $\mathcal{J}\bar{Y}_j$:
  For $i = 1, \ldots, j$
   $s_{ij} = y_i^\top \mathcal{J}^\top z_j$, $z_j = z_j - s_{ij} \mathcal{J} \bar{y}_i$
  End
 Compute y_{j+1} *in* (5.21):
  Compute $y_{j+1} = \widehat{\mathcal{K}} z_j$;
  For $i = 1, \ldots, j$
   $h_{ij} = y_i^H y_{j+1}$, $y_{j+1} = y_{j+1} - h_{ij} y_i$
  End
  Set $h_{j+1,j} := \|y_{j+1}\|_2$ *and* $y_{j+1} := y_{j+1}/h_{j+1,j} y_{j+1}$;
  For $i = 1, \ldots, j$
   $t_{ij} = z_i^\top \mathcal{J}^\top y_{j+1}$, $y_{j+1} = y_{j+1} - t_{ij} \mathcal{J} \bar{z}_i$
  End

5.1. Implicitly restart. We now derive the implicitly restarted step for the $(\ell+p)$th step of the generalized $\top$-isotropic Arnoldi process. Suppose we have computed the $(\ell+p)$th step of the generalized $\top$-isotropic Arnoldi factorization:

$$\widehat{\mathcal{K}} Z_{\ell+p} = Y_{\ell+p} H_{\ell+p} + h_{\ell+p+1,\ell+p} y_{\ell+p+1} e_{\ell+p}^{\top}, \tag{5.22}$$

$$\widehat{\mathcal{N}} Z_{\ell+p} = Y_{\ell+p} R_{\ell+p}. \tag{5.23}$$

Let $\{\lambda_1, \ldots, \lambda_\ell, \lambda_{\ell+1}, \ldots, \lambda_{\ell+p}\}$ be the eigenvalues of the matrix pair $(H_{\ell+p}, R_{\ell+p})$, where $\{\lambda_1, \ldots, \lambda_\ell\}$ are the wanted eigenvalues. Let Q_k and V_k for $k = 1, \ldots, p$ be unitary matrices computed by the implicit-QZ step [22, p. 147] for $(H_{\ell+p}, R_{\ell+p})$ with the single shift $\lambda_{\ell+k}$.

Let $\widehat{H}_{\ell+p} := Q_p^H \cdots Q_1^H H_{\ell+p} V_1 \cdots V_p$, $\widehat{R}_{\ell+p} := Q_p^H \cdots Q_1^H R_{\ell+p} V_1 \cdots V_p$, $\widehat{Y}_{\ell+p} := Y_{\ell+p} Q_1 \cdots Q_p$, and $\widehat{Z}_{\ell+p} := Z_{\ell+p} V_1 \cdots V_p$. Then $\widehat{H}_{\ell+p}$ and $\widehat{R}_{\ell+p}$ are upper Hessenberg and upper triangular, respectively, and $\widehat{Y}_{\ell+p}$ and $\widehat{Z}_{\ell+p}$ satisfy $\widehat{Y}_{\ell+p}^{\top} \mathcal{J} \widehat{Z}_{\ell+p} = 0$ because of $Y_{\ell+p}^{\top} \mathcal{J} Z_{\ell+p} = 0$. Multiplying (5.22) and (5.23) by $V_1 \cdots V_p$, we get

$$\widehat{\mathcal{K}} \widehat{Z}_{\ell+p} = \widehat{Y}_{\ell+p} \widehat{H}_{\ell+p} + h_{\ell+p+1,\ell+p} y_{\ell+p+1} e_{\ell+p}^{\top} V_1 \cdots V_p, \tag{5.24}$$

$$\widehat{\mathcal{N}} \widehat{Z}_{\ell+p} = \widehat{Y}_{\ell+p} \widehat{R}_{\ell+p}. \tag{5.25}$$

Since

$$e_{\ell+p}^{\top} V_1 = \alpha_{\ell+p} e_{\ell+p-1}^{\top} + \beta_{\ell+p} e_{\ell+p}^{\top},$$

by induction, the first $\ell - 1$ entries of $e_{\ell+p}^{\top} V_1 \cdots V_p$ are zero. Hence a new ℓth step of the generalized $\top$-isotropic Arnoldi factorization can be obtained by equating the first ℓ columns of (5.24) and (5.25):

$$\widehat{\mathcal{K}} \widehat{Z}_{\ell} = \widehat{Y}_{\ell} \widehat{H}_{\ell} + \widehat{h}_{\ell+p+1,\ell+p} y_{\ell+p+1} e_{\ell}^{\top},$$
$$\widehat{\mathcal{N}} \widehat{Z}_{\ell} = \widehat{Y}_{\ell} \widehat{R}_{\ell}.$$

We summarize the above processes in Algorithm 5.2.

ALGORITHM 5.2 (generalized implicitly restarted step).

> **Input:** *given* $(Y_{\ell+p}, y_{\ell+p+1}, Z_{\ell+p}, H_{\ell+p}, h_{\ell+p+1,\ell+p}, R_{\ell+p})$;
> **Output:** $(Y_\ell, y_{\ell+1}, Z_\ell, H_\ell, h_{\ell+1,\ell}, R_\ell)$ *formed a new* ℓ*th step of the generalized* $\top$*-isotropic Arnoldi factorization. The best* ℓ *eigenvalues are locked in* (H_ℓ, R_ℓ).
> **Sort** *the eigenvalues of* $(H_{\ell+p}, R_{\ell+p})$ *from best to worst according to the sorting criterion and take* $\{\lambda_{\ell+1}, \ldots, \lambda_{\ell+p}\}$ *to be the* p *worst eigenvalues.*
> **Set** $v := h_{\ell+p+1,\ell+p} e_{\ell+p}$;
> **For** $k = 1, \ldots, p$,
>   **Compute** *unitary matrices* Q_k *and* V_k *by the implicit-QZ step for* $(H_{\ell+p}, R_{\ell+p})$ *with the single shift* $\lambda_{\ell+k}$ *so that* $Q_k^H H_{\ell+p} V_k$ *and* $Q_k^H R_{\ell+p} V_k$ *are upper Hessenberg and upper triangular, respectively;*
>   **Update** $Y_{\ell+p} := Y_{\ell+p} Q_k$, $Z_{\ell+p} := Z_{\ell+p} V_k$, $H_{\ell+p} := Q_k^H H_{\ell+p} V_k$, $R_{\ell+p} := Q_k^H R_{\ell+p} V_k$, $v := Z_k^H v$;
> **End**
> **Set** $H_\ell = H_{\ell+p}(1:\ell, 1:\ell)$, $h_{\ell+1,\ell} := e_\ell^{\top} v$, $R_\ell = R_{\ell+p}(1:\ell, 1:\ell)$, $Y_\ell := Y_{\ell+p}(:, 1:\ell)$, $y_{\ell+1} := y_{\ell+p+1}$, $Z_\ell := Z_{\ell+p}(:, 1:\ell)$.

We now present the G⊤SHIRA.

ALGORITHM 5.3 (G⊤SHIRA).

Input: ⊤*-skew-Hamiltonian matrices* $\widehat{\mathcal{K}}$ *and* $\widehat{\mathcal{N}}$ *with starting vector* y_1.
Output: Z_ℓ, Y_ℓ, *upper Hessenberg* H_ℓ, *and upper triangular* R_ℓ *with*

$$\widehat{\mathcal{K}} Z_\ell = Y_\ell H_\ell,\ \widehat{\mathcal{N}} Z_\ell = Y_\ell R_\ell, Y_\ell^H Y_\ell = I_\ell,\ Z_\ell^H Z_\ell = I_\ell, \text{ and } Y_\ell^\top \mathcal{J} Z_\ell = 0.$$

Use Algorithm 5.1 *with starting vector* y_1 *to generate an* ℓ*th step of the generalized* ⊤*-isotropic Arnoldi factorization:*

$$\widehat{\mathcal{K}} Z_\ell = Y_\ell H_\ell + h_{\ell+1,\ell} y_{\ell+1} e_\ell^\top,$$
$$\widehat{\mathcal{N}} Z_\ell = Y_\ell R_\ell.$$

For $k = 1, 2, \ldots,$ *until wanted* ℓ *eigenpairs of* $(\widehat{\mathcal{K}}, \widehat{\mathcal{N}})$ *are convergent,*

Use Algorithm 5.1 *to extend the* ℓ*th step of the generalized* ⊤*-isotropic Arnoldi factorization to the* $(\ell + p)$*th step of the generalized* ⊤*-isotropic Arnoldi factorization:*

$$\widehat{\mathcal{K}} Z_{\ell+p} = Y_{\ell+p} H_{\ell+p} + h_{\ell+p+1,\ell+p} y_{\ell+p+1} e_{\ell+p}^\top,$$
$$\widehat{\mathcal{N}} Z_{\ell+p} = Y_{\ell+p} R_{\ell+p}.$$

Use Algorithm 5.2 *to reform a new* ℓ*th step of the generalized* ⊤*-isotropic Arnoldi factorization.*

End

Remark 5.1.

(i) $h_{\ell+1,\ell}$ is set to zero if $|h_{\ell+1,\ell}| < tol(|h_{\ell,\ell}| + |h_{\ell+1,\ell+1}|)$ for some stopping tolerance "*tol*."

(ii) Let (θ_i, v_i) be an eigenpair of (H_ℓ, R_ℓ), i.e., $H_\ell v_i = \theta_i R_\ell v_i$, and let $z_i = Z_\ell v_i$ be a Ritz vector of the eigenproblem $\widehat{\mathcal{K}} z = \mu \widehat{\mathcal{N}} z$ corresponding to the Ritz value θ_i. Then from (5.4) and (5.5), we have

$$\begin{aligned} &\|\widehat{\mathcal{K}} z_i - \theta_i \widehat{\mathcal{N}} z_i\|_2 = \|\widehat{\mathcal{K}} Z_\ell v_i - \theta_i \widehat{\mathcal{N}} Z_\ell v_i\|_2 \\ &= \|(Y_\ell H_\ell + h_{\ell+1,\ell} y_{\ell+1} e_\ell^\top) v_i - \theta_i Y_\ell R_\ell v_i\|_2 \\ &= \|Y_\ell (H_\ell v_i - \theta_i R_\ell v_i) + h_{\ell+1,\ell}(e_\ell^\top v_i) y_{\ell+1}\|_2 \\ &= \|h_{\ell+1,\ell}(e_\ell^\top v_i) y_{\ell+1}\|_2 = |h_{\ell+1,\ell}||e_\ell^\top v_i|. \end{aligned}$$

6. Numerical study: Vibration of fast trains. In this section, we shall study the resonance phenomena of a railway track under high frequent excitation forces. We present numerical results of the vibration of fast trains to illustrate the performance of the proposed structure-preserving algorithms in sections 2–5. All numerical experiments are carried out using MATLAB 2006b with the machine precision $eps \approx 2.22 \times 10^{-16}$.

Research in the vibration of fast trains contributes to the safety of operations of high-speed trains as well as new designs of train bridges, embedded rail structures (ERS), and train suspension systems. Recently, the dynamic response of the vehicle-rail-bridge interaction system under different train speed was studied in [25] and a procedure for designing an optimal ERS was proposed in [14]. In both papers, the accurate numerical estimation to the resonance frequencies of the rail plays an important role. However, as mentioned by Ipsen in [5], the classical finite element packages fail to deliver correct resonance frequency for such problems. In this section, we would like to use our structure-preserving algorithms to solve the palindromic QEP (1.1) arising from the spectral modal analysis of rails under periodic excitation forces.

In the model of vibration of fast trains, we assume that the rail sections between consecutive sleeper bays are identical, the distance between consecutive wheels is the same, and the wheel loads are equal. The rail between two sleepers is modeled by a three-dimensional isotropic elastic solid with linear isoparametric tetrahedron finite elements. Figure 6.1 shows a three-dimensional rail model (see [1] for details).

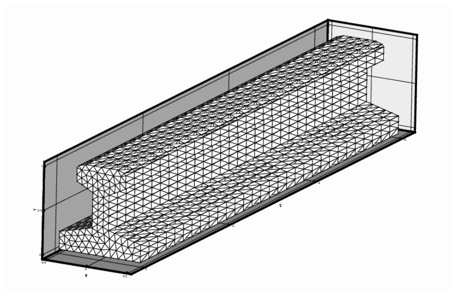

FIG. 6.1. *A three-dimensional rail model.*

Based on the ERS design [14], the external force is assumed to be periodic and the displacements of two boundary cross sections of the modeled rail are assumed to have a ratio λ, which is dependent on the excitation frequency of the external force. From the virtual work principle and strain-stress relationship, the governing equation for the displacement vector q involving viscous damping can be formulated by $Kq + D\dot{q} + M\ddot{q} = f(t)$, where K, D, and M from the finite element discretization on a uniform mesh satisfy the given boundary conditions. These matrices have the form

$$\begin{bmatrix} E_{11} & \widetilde{E}_{1,2:m-1}^{\top} & \frac{1}{\lambda}E_{m,m+1} \\ \widetilde{E}_{1,2:m-1} & \widetilde{E}_{2:m-1} & \widetilde{E}_{2:m-1,m}^{\top} \\ \lambda E_{m,m+1}^{\top} & \widetilde{E}_{2:m-1,m} & E_{m,m} \end{bmatrix}$$

in which $\widetilde{E}_{1,2:m-1}^{\top} = [E_{12}^{\top}, 0_n, \ldots, 0_n]$, $\widetilde{E}_{2:m-1,m} = [0_n, \ldots, 0_n, E_{m-1,m}]$, and $\widetilde{E}_{2:m-1} = \mathrm{tridiag}\big(E_{i-1,i}, E_{i,i}, E_{i,i+1}^{\top}\big)_{i=2}^{m-1}$ with $E_{ij} \in \mathbb{R}^{n\times n}$, $i, j = 1, \ldots, m+1$. (See [1] for details.) Furthermore, from the spectral modal analysis, we consider $q = \widetilde{x}e^{i\omega t}$, where ω is the frequency of the external force and $\widetilde{x}$ is the corresponding eigenmode. Consequently, we get the palindromic QEP

$$\left(\lambda^2 \widetilde{A}_1^{\top} + \lambda \widetilde{A}_0 + \widetilde{A}_1\right) \widetilde{x} = 0, \tag{6.1}$$

where

$$\left[\widetilde{A}_1\right]_{ij} = \begin{cases} K_{m,m+1} + i\omega D_{m,m+1} - \omega^2 M_{m,m+1} & (\text{if } \ i = m, j = 1), \\ 0 & \text{otherwise}, \end{cases}$$

$$\left[\widetilde{A}_0\right]_{ij} = \begin{cases} K_{i,j} + i\omega D_{i,j} - \omega^2 M_{i,j} & (\text{if } \ i - 1 \le j \le i + 1), \\ 0 & \text{otherwise}. \end{cases}$$

By consulting the preprocessing procedure (see [4] or [1]) for the deflation of all trivial zero and infinite eigenvalues of (6.1), we arrive to the deflated palindromic QEP

$$\left(\lambda^2 A_1^{\top} + \lambda A_0 + A_1\right) x = 0. \tag{6.2}$$

Example 6.1. We first consider the deflated palindromic QEP (6.2) for high-speed trains and rails. The size of A_0 and A_1 after deflation is $n = 303$, and the excitation frequency ω is chosen as 1000. The absolute values of the eigenvalues vary from 10^{-20} to 10^{20}.

We compute all eigenpairs of Example 6.1 by the SA_I, SA_II, and QZ algorithm. Note that as shown in section 3, SA_II and the URV-based method [20] are mathematically equivalent. In practice, we compare the backward error (relative residual (RRes)) of (1.1) by SA_II and the SKURV software [18]. Since SKURV gives only the eigenvalues, the associated eigenvectors are computed from (3.9) and (3.10) by inverse iteration. Numerical results show that the backward errors obtained by SA_II and SKURV for Example 6.1 are slightly different. Therefore, in the following computation, we adapt SA_II instead of the URV-method.

To measure the accuracy of an approximate eigenpair (λ, x) for (6.2), we use the RRes

$$\text{RRes} \equiv \frac{\|\lambda^2 A_1^\top x + \lambda A_0 x + A_1 x\|_2}{(|\lambda^2|\|A_1\|_F + |\lambda|\|A_0\|_F + \|A_1\|_F)\|x\|_2}. \tag{6.3}$$

As mentioned before, theoretically, the eigenvalues of (6.2) appear in pairs $(\lambda, \frac{1}{\lambda})$. So, if we sort the eigenvalues in the ascending order by modulus, the product of the ith and $(2n + 1 - i)$th sorted eigenvalues should be one. Therefore, we define the reciprocities of computed eigenvalues by

$$|\lambda_i \lambda_{2n+1-i} - 1|, \; i = 1, \ldots, n. \tag{6.4}$$

The RRes of the computed eigenpairs by the SA_I, SA_II, and QZ algorithm for the eigenvalues with absolute values in $[10^{-20}, 10^{20}]$ and $\omega = 1000$ are shown in Figure 6.2. For eigenvalues with small modulus, the SA_I performs much better than the SA_II and the QZ algorithm. For eigenvalues near the unit circle or with large modulus, all three algorithms have similar accuracy.

The important reciprocity property of eigenvalues is shown in Figure 6.3. Clearly, SA_I and SA_II preserve the essential reciprocity property as expected, while the QZ algorithm has only less than 12 pairs of computed eigenvalues near the unit circle with reciprocity near zero ($\approx 1.17 \times 10^{-12}$). The average and maximal values of all reciprocities are 0.220 and 1.006, respectively.

Next, we apply the SA_I, SA_II, and QZ algorithm to the palindromic QEP with various excitation frequency ω. Figure 6.4 shows the RRes of all computed eigenpairs with eigenvalues in $[10^{-20}, 10^{20}]$ by the three algorithms for 100 different ω's uniformly chosen from 50 to 5000. We see that the RRes of the SA_I are better than those of the SA_II and the QZ algorithm for all ω's.

Example 6.2. *We now consider the palindromic QEP* (6.1) *for high-speed trains and rails, with n, the size of A_0 and A_1, being* 5757.

Computational cost. Before showing our numerical results computed by the $\top$SHIRA and G$\top$SHIRA, we compare the computational costs of one step of the $\top$-isotropic Arnoldi process and the implicitly restarted step in each algorithm.

In one step of the $\top$SHIRA, it requires one matrix-vector product for $\mathcal{B}$, and $3j$ inner products and saxpy operations with vector length $2n$. Since $\mathcal{B} = \mathcal{N}_1^{-1}\widetilde{\mathcal{K}}\mathcal{N}_2^{-1}$, by the definitions of $\widetilde{\mathcal{K}}$ and $(\mathcal{N}_1, \mathcal{N}_2)$ in (4.2a) and (4.4), the matrix-vector of $\mathcal{B}$ requires solving 2 linear systems, 4 and 2 matrix-vector products for A_1 and A_0, respectively, and 6 saxpy operations with vector length n.

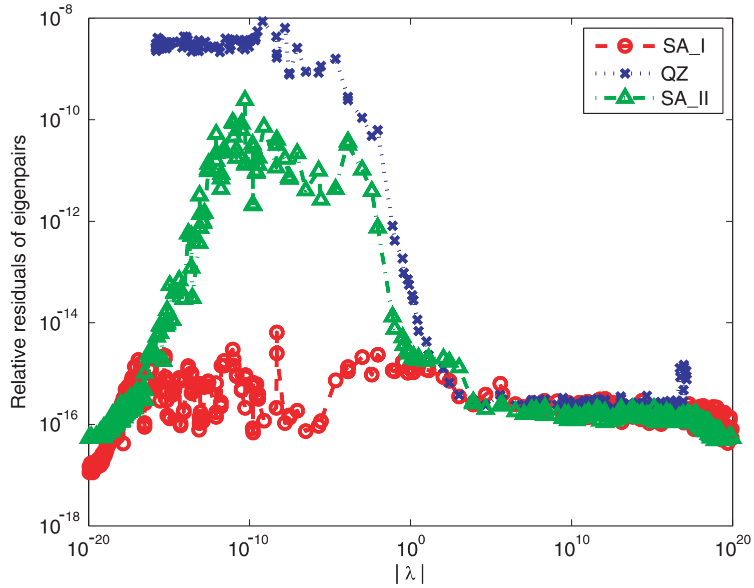

Fig. 6.2. *RRes of Example* 6.1 *($\omega = 1000$).*

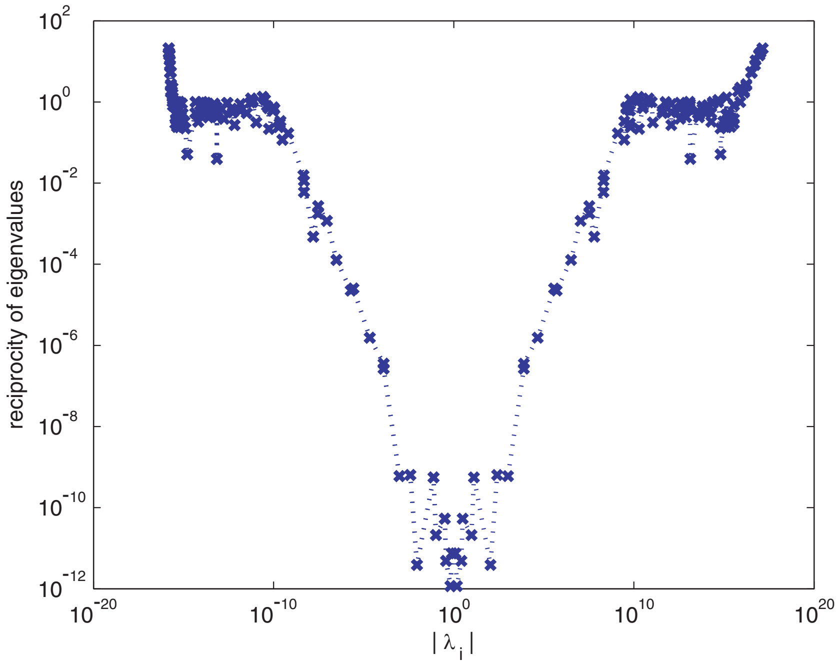

Fig. 6.3. *Reciprocities of computed eigenvalues produced by the QZ algorithm ($\omega = 1000$).*

In one step of the G⊤SHIRA, solving $\widetilde{z}_j$ requires solving 2 linear systems, 2 matrix-vector products of A_0 and A_1, and 6 saxpy operations with vector length n; computing z_j requires $2j - 1$ inner products and saxpy operations with vector length $2n$;

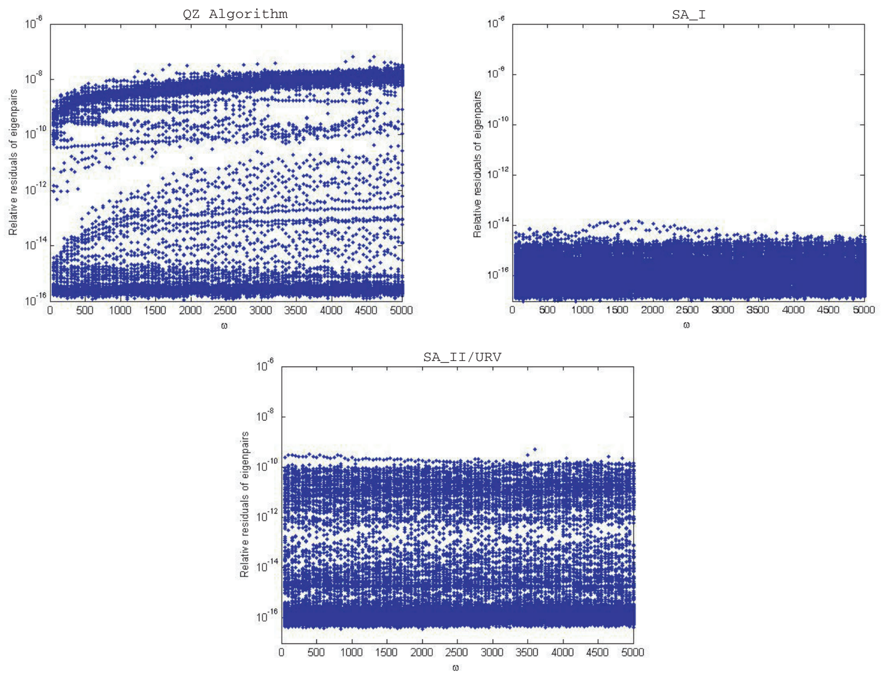

FIG. 6.4. *The RRes of eigenvalues vs. ω.*

TABLE 6.1
Computational cost of one step of the ⊤-isotropic Arnoldi process in the ⊤SHIRA and G⊤SHIRA algorithms.

	⊤SHIRA	G⊤SHIRA
Solving linear system	2	2
Matrix-vector product for A_1	4	4
Matrix-vector product for A_0	2	2
Inner products	$6j$	$8j-2$
Saxpy operations	$6j+6$	$8j+4$

computing y_{j+1} requires 2 matrix-vector products for A_1, and $2j$ inner products and saxpy operations with vector length $2n$.

We summarize the above computational costs in Table 6.1. The vector length of the inner products and saxpy operations in Table 6.1 is equal to n. On the other hand, the implicitly restarted steps in the ⊤SHIRA and G⊤SHIRA require $2(\ell+p-1)p$ and $4(\ell+p-1)p$ saxpy operations with vector length $2n$, respectively. Comparing one ⊤-isotropic Arnoldi step with one implicitly restarted step, the G⊤SHIRA algorithm is slightly more expensive than the ⊤SHIRA algorithm.

Accuracy of eigenpairs. We now compare the numerical results computed by the ⊤SHIRA and G⊤SHIRA algorithms. Here, $\lambda_{\omega,1},\ldots,\lambda_{\omega,10}$ denote target eigenvalues, and we set $\ell=10$, $p=20$ in the implicitly restarted step for each algorithm.

The RRes of $(\lambda_{\omega,i},x_i)$ and $(\frac{1}{\lambda_{\omega,i}},\widetilde{x}_i)$ for $i=1,\ldots,10$ are shown in Figure 6.5, where x_i and $\widetilde{x}_i$ are the corresponding computed eigenvectors. In (a) and (b) of Figure 6.5, we show those RRes for frequency $\omega=50$ and $\omega=2000$, respectively. The notations "Δ" and "×" denote the results computed by the ⊤SHIRA and G⊤SHIRA

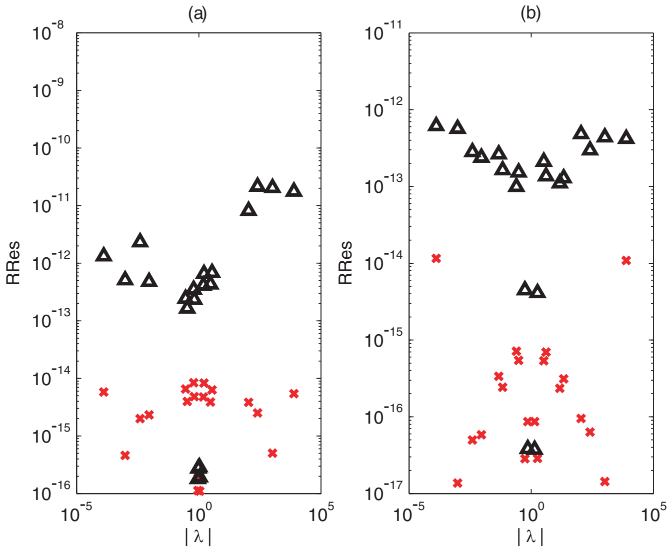

FIG. 6.5. *The RRes of the eigenpairs computed by the* ⊤*SHIRA and G*⊤*SHIRA algorithms. The notations "Δ" and "×" denote the results computed by the* ⊤*SHIRA and G*⊤*SHIRA algorithms, respectively. In* (a) *and* (b)*, the frequency* ω *is equal to* 50 *and* 2000*, respectively.*

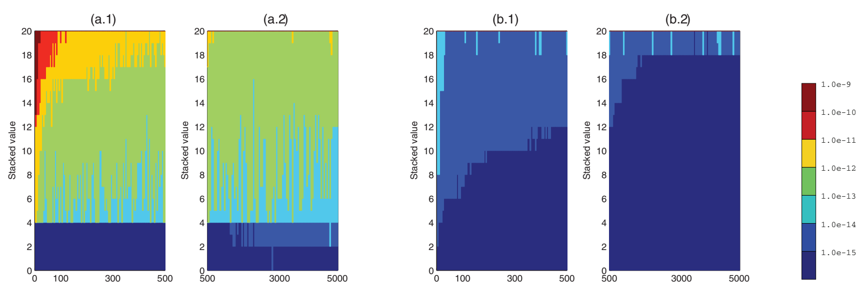

FIG. 6.6. *The stacked bars of* $\ell_{\omega,k}$ *for* $k = 1, \ldots, 7$ *with different* ω*. For each* ω*, all* $\ell_{\omega,k}$ *for* $k = 1, \ldots, 7$ *are stacked to form a vertical bar with ordering* $\ell_{\omega,1}, \ell_{\omega,2}, \ldots, \ell_{\omega,7}$*. Each bar is multicolored and the color corresponds to distinct* $\ell_{\omega,k}$*. The color bar in the right position shows the relationship between color and interval* I_k*, which corresponds to* $\ell_{\omega,k}$*. The results in* (a) *and* (b) *are computed by the* ⊤*SHIRA and G*⊤*SHIRA algorithms, respectively.*

algorithms, respectively. From these results, we see that the reciprocity property of the eigenvalues are preserved in both algorithms, but the accuracy of the eigenpairs computed by the G⊤SHIRA algorithm is obviously better than that by the ⊤SHIRA algorithm.

In order to give an overall comparison between the two algorithms, we compute the eigenpairs $(\lambda_{\omega,i}, x_i)$ and $(\frac{1}{\lambda_{\omega,i}}, \widetilde{x}_i)$ for $i = 1, \ldots, 10$ with $\omega = 5, 10, 15, \ldots, 500$ and $\omega = 550, 600, 650, \ldots, 5000$. We analyze the distribution of the corresponding 20 RRes with respect to ω. We partition the interval $(0, 10^{-9})$ into seven subintervals $\mathcal{I}_1 = (0, 10^{-15}]$, $\mathcal{I}_2 = (10^{-15}, 10^{-14}], \ldots, \mathcal{I}_7 = (10^{-10}, 10^{-9})$. For fixed ω, let $\ell_{\omega,k}$ be the number of the RRes which belongs to the interval $\mathcal{I}_k$ for $k = 1, \ldots, 7$. In Figure 6.6, for each ω, all $\ell_{\omega,k}$, $k = 1, \ldots, 7$, are stacked to form a vertical bar with ordering

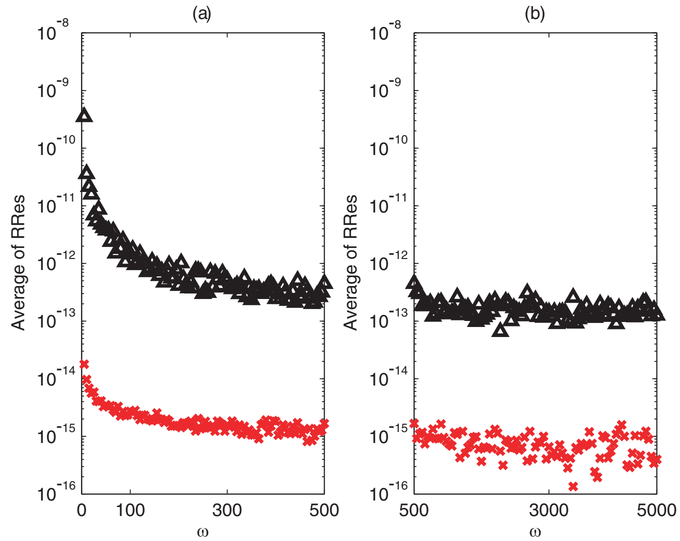

FIG. 6.7. *The average of RRes for the twelve eigenpairs computed by the* ⊤*SHIRA and* G⊤*SHIRA algorithms. The notations "Δ" and "×" denote the results computed by the* ⊤*SHIRA and* G⊤*SHIRA algorithms, respectively.*

$\ell_{\omega,1}, \ell_{\omega,2}, \ldots, \ell_{\omega,7}$. The bar height is 20 which is the sum of $\ell_{\omega,1}, \ldots, \ell_{\omega,7}$. Each bar is multicolored and the color corresponds to distinct $\ell_{\omega,k}$. The color bar in the right bottom position of Figure 6.6 shows the relationship between colors and intervals $\mathcal{I}_k$ corresponding to $\ell_{\omega,k}$. All stacked bars of $\ell_{\omega,k}$ $(k = 1, \ldots, 7)$ with $\omega = 5, 10, 15, \ldots, 500$ are shown in (a.1) and (b.1) of Figure 6.6 and those with $\omega = 550, 600, 650, \ldots, 5000$ are shown in (a.2) and (b.2) of Figure 6.6. The results in (a) and (b) of Figure 6.6 are computed by the ⊤SHIRA and the G⊤SHIRA algorithms, respectively.

In the above paragraph, we show the distribution of the RRes for different ω for the comparison of the accuracy of the target eigenpairs. From another point of view, we show the average of the RRes for the target eigenpairs with each ω in Figure 6.7. The notations "Δ" and "×" in Figure 6.7 denote the results computed by the ⊤SHIRA and G⊤SHIRA algorithms, respectively. From Figures 6.6 and 6.7, we can summarize that the accuracy of the eigenpairs computed by the G⊤SHIRA algorithm are obviously better than that of the ⊤SHIRA algorithm for all ω in $(0, 5000]$.

We now try to explain the different accuracies of the two algorithms. One important reason is that the ⊤SHIRA algorithm needs to solve a linear system in the extraction method of eigenvectors, while the G⊤SHIRA algorithm needs only vector additions. The accuracy of the extracted eigenvector will be reduced if the condition number of the linear system is large. On the other hand, Theorem A.1 in Appendix A.3 may help explain this phenomenon from the viewpoint of the minimal residual. The accuracy of the eigenpair computed by the G⊤SHIRA algorithm is better than that by the ⊤SHIRA algorithm, since the G⊤SHIRA algorithm is a generalized Arnoldi algorithm for $\widehat{\mathcal{K}}z = \widehat{\mu}\widehat{\mathcal{N}}z$, while the ⊤SHIRA algorithm is an Arnoldi algorithm for $\mathcal{N}_1^{-1}\widehat{\mathcal{K}}\mathcal{N}_2^{-1}y = \widehat{\mu}y$.

7. Conclusions. In this paper, we first transform a palindromic QEP to a ⊤-skew-Hamiltonian pencil by the $(S + S^{-1})$-transform. Then, we extend Patel's approach to solve the $\top$-skew-Hamiltonian pencil efficiently. We have also developed a structure-preserving generalized $\top$-skew-Hamiltonian implicitly restarted Arnoldi method (G$\top$SHIRA) for solving the large sparse $\top$-skew-Hamiltonian pencil. Numerical results show that the accuracy of desired eigenpairs computed by the G$\top$SHIRA is better than that computed by the classical $\top$SHIRA. The standard algorithms proposed in this paper are numerically stable for solving palindromic QEPs. In the future, we are motivated to develop structure-preserving algorithms for solving the antipalindromic QEP $\lambda^2 A_1^\top + \lambda A_0 - A_1$ with $A_0^\top = -A_0$, efficiently.

Appendix.

A.1. In this section we list pseudocodes of Step 2 in Algorithm 2.1.

In the following, givensl(α,β,i) returns a Givens rotation G such that $G[\begin{smallmatrix}\alpha\\ \beta\end{smallmatrix}] = \gamma e_i$ with $\gamma \in \mathbb{C}$; givensr(α,β,i) returns a Givens rotation G such that $[\alpha\ \beta]G = \gamma e_i^\top$ with $\gamma \in \mathbb{C}$. The functions qr(A) and ql(A) perform the standard QR and QL factorizations.

Step 2 *in Algorithm* 2.1. function $[\mathcal{K}, \mathcal{N}, Q, Z] = \mathsf{rbutf}(\mathcal{K}, \mathcal{N})$

Input: Matrices $\mathcal{K}, \mathcal{N}$ in the form (2.4).

Output: Unitary Q, Z and $\mathcal{K}, \mathcal{N}$ of the form (2.5), where $\mathcal{K}$ and $\mathcal{N}$ are overwritten by $Q\mathcal{K}Z$ and $Q\mathcal{N}Z$, respectively.

$[Q_1, R] \leftarrow \mathsf{qr}(\mathcal{N}(1:n, 1:n))$
$Q \leftarrow \mathrm{diag}(Q_1^H, I_n)$
$Z \leftarrow \mathrm{diag}(I_n, \bar{Q}_1)$
$\mathcal{K} \leftarrow Q\mathcal{K}Z$
$\mathcal{N} \leftarrow Q\mathcal{N}Z$
for $j = 1 : n-2$
  for $k = j+1 : n-1$
    % *annihilate* $\mathcal{K}(n+k, j)$ *by Givens rotation in* $(n+k, n+k+1)$ *plane*
    $G \leftarrow \mathsf{givensl}(\mathcal{K}(n+k, j), \mathcal{K}(n+k+1, j), 2)$
    $Q(n+k : n+k+1, :) \leftarrow GQ(n+k : n+k+1, :)$
    $\mathcal{K}(n+k : n+k+1, :) \leftarrow G\mathcal{K}(n+k : n+k+1, :)$
    $\mathcal{N}(n+k : n+k+1, :) \leftarrow G\mathcal{N}(n+k : n+k+1, :)$
    $Z(:, k : k+1) \leftarrow Z(:, k : k+1)G^\top$
    $\mathcal{K}(:, k : k+1) \leftarrow \mathcal{K}(:, k : k+1)G^\top$
    $\mathcal{N}(:, k : k+1) \leftarrow \mathcal{N}(:, k : k+1)G^\top$
    % *annihilate* $\mathcal{N}(k+1, k)$ *by Givens rotation in* $(k, k+1)$ *plane*
    $G \leftarrow \mathsf{givensl}(\mathcal{N}(k, k), \mathcal{N}(k+1, k), 1)$
    $Q(k : k+1, :) \leftarrow GQ(k : k+1, :)$
    $\mathcal{K}(k : k+1, :) \leftarrow G\mathcal{K}(k : k+1, :)$
    $\mathcal{N}(k : k+1, :) \leftarrow G\mathcal{N}(k : k+1, :)$
    $Z(:, n+k : n+k+1) \leftarrow Z(:, n+k : n+k+1)G^\top$
    $\mathcal{K}(:, n+k : n+k+1) \leftarrow \mathcal{K}(:, n+k : n+k+1)G^\top$
    $\mathcal{N}(:, n+k : n+k+1) \leftarrow \mathcal{N}(:, n+k : n+k+1)G^\top$
  end
  % *annihilate* $\mathcal{N}(2n, j)$ *by Givens rotation in* $(n, 2n)$ *plane*
  $G \leftarrow \mathsf{givensl}(\mathcal{N}(n, j), \mathcal{N}(2n, j), 1)$
  $Q([n\ 2n], :) \leftarrow GQ([n\ 2n], :)$
  $\mathcal{K}([n\ 2n], :) \leftarrow G\mathcal{K}([n\ 2n], :)$
  $\mathcal{N}([n\ 2n], :) \leftarrow G\mathcal{N}([n\ 2n], :)$
  $Z(:, [n\ 2n]) \leftarrow Z(:, [n\ 2n])G^H$
  $\mathcal{K}(:, [n\ 2n]) \leftarrow \mathcal{K}(:, [n\ 2n])G^H$

32: $\quad\mathcal{N}(:,[n\ 2n]) \leftarrow \mathcal{N}(:,[n\ 2n])G^H$
33: $\quad$**for** $k = n : -1 : j+2$
34: $\quad\quad$% *annihilate* $\mathcal{K}(k,j)$ *by Givens rotation in* $(k-1,k)$ *plane*
35: $\quad\quad G \leftarrow \mathsf{givensl}(\mathcal{K}(k-1,j), \mathcal{K}(k,j), 1)$
36: $\quad\quad Q(k-1:k,:) \leftarrow GQ(k-1:k,:)$
37: $\quad\quad \mathcal{K}(k-1:k,:) \leftarrow G\mathcal{K}(k-1:k,:)$
38: $\quad\quad \mathcal{N}(k-1:k,:) \leftarrow G\mathcal{N}(k-1:k,:)$
39: $\quad\quad Z(:,n+k-1:n+k) \leftarrow Z(:,n+k-1:n+k)G^\top$
40: $\quad\quad \mathcal{K}(:,n+k-1:n+k) \leftarrow \mathcal{K}(:,n+k-1:n+k)G^\top$
41: $\quad\quad \mathcal{N}(:,n+k-1:n+k) \leftarrow \mathcal{N}(:,n+k-1:n+k)G^\top$
42: $\quad\quad$% *annihilate* $\mathcal{N}(k,k-1)$ *by Givens rotation in* $(k-1,k)$ *plane*
43: $\quad\quad G \leftarrow \mathsf{givensr}(\mathcal{N}(k,k-1), \mathcal{N}(k,k), 2)$
44: $\quad\quad Q(n+k-1:n+k,:) \leftarrow G^\top Q(n+k-1:n+k,:)$
45: $\quad\quad \mathcal{K}(n+k-1:n+k,:) \leftarrow G^\top \mathcal{K}(n+k-1:n+k,:)$
46: $\quad\quad \mathcal{N}(n+k-1:n+k,:) \leftarrow G^\top \mathcal{N}(n+k-1:n+k,:)$
47: $\quad\quad Z(:,k-1:k) \leftarrow Z(:,k-1:k)G$
48: $\quad\quad \mathcal{K}(:,k-1:k) \leftarrow \mathcal{K}(:,k-1:k)G$
49: $\quad\quad \mathcal{N}(:,k-1:k) \leftarrow \mathcal{N}(:,k-1:k)G$
50: $\quad$**end**
51: **end**

A.2. To show the extra zeros of the subdiagonals of the submatrices in (3.4), let $\mathbb{H}_k$ and $\mathbb{T}_k$ be the sets of $k \times k$ upper Hessenberg and triangular matrices, respectively, and let $\mathbb{S}_{2k}$ be the set of $2k \times 2k$ $\top$-skew symmetric matrices. Denote

$$\mathbb{A}_{2k} = \left\{ A \in \mathbb{C}^{2k\times 2k} \middle| A \equiv P_{2k}^\top \left[\begin{array}{c|c} 0_k & \diagdown\!\!\!\bigtriangledown \\ \hline \bigtriangledown & 0_k \end{array}\right] P_{2k} \ \text{ with } \diagdown\!\!\!\bigtriangledown \in \mathbb{H}_k \ \text{ and } \bigtriangledown \in \mathbb{T}_k \right\}, \tag{A2.1}$$

where $P_{2k} = [e_1, e_{k+1}, e_2, e_{k+2}, \ldots, e_k, e_{2k}]$,

$$\mathbb{R}_{2k} = \left\{ R \in \mathbb{C}^{2k\times 2k} \middle| R \equiv P_{2k}^\top \left[\begin{array}{c|c} 0_k & \bigtriangledown \\ \hline \bigtriangledown & 0_k \end{array}\right] P_{2k} \ \text{ with } \bigtriangledown \in \mathbb{T}_k \right\}, \tag{A2.2}$$

$$\mathbb{B}_{2m,2k} = \{B \in \mathbb{C}^{2m\times 2k} | Be_1 = Be_3 = \cdots = Be_{2k-1} = 0\}, \tag{A2.3}$$

$$\widehat{\mathbb{B}}_{2m,2k} = \{\widehat{B} \in \mathbb{C}^{2m\times 2k} | \widehat{B}e_2 = \widehat{B}e_4 = \cdots = \widehat{B}e_{2k} = 0\}, \tag{A2.4}$$

$$\begin{aligned}\mathbb{C}_{2m\times 2k} = \{C \in \mathbb{C}^{2m\times 2k} | c_{ij} = 0, i = 1, \ldots, 2m, j = 1, \ldots, 2k \\ \text{and } \ (i,j) \neq (1,2k)\},\end{aligned} \tag{A2.5}$$

$$\begin{aligned}\mathbb{D}_{2k} = \{D \in \mathbb{C}^{2k\times 2k} | D \in \mathbb{S}_{2k} \ \text{ with } \ \{1,-1,3,-3,\ldots,2k-1,-(2k-1)\} \\ -\text{ diagonals being zeros}\},\end{aligned} \tag{A2.6}$$

$$\begin{aligned}\widehat{\mathbb{D}}_{2k} = \{\widehat{D} \in \mathbb{C}^{2k\times 2k} | \widehat{D} \in \mathbb{S}_{2k} \ \text{ with } \ \{2,-2,4,-4,\ldots,2k-2,-(2k-2)\} \\ -\text{ diagonals being zeros}\}.\end{aligned} \tag{A2.7}$$

After performing the first and second steps of the SA_I (i.e., Steps 07–50 in section A.1, for $j = 1$ and 2) on $(\widetilde{\mathcal{K}}, \widetilde{\mathcal{N}})$, it produces

$$K_{11}^{(2)} := \left[\begin{array}{cc|cccc} 0 & \times & 0 & \cdots & 0 \\ \times & 0 & \times & \cdots & \times \\ \hline 0 & \times & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & 0 \end{array}\right], \quad K_{12}^{(2)} := \left[\begin{array}{cc|ccc} 0 & 0 & \times & \cdots & \times \\ 0 & 0 & 0 & \cdots & 0 \\ \hline \times & 0 & & & \\ \vdots & \vdots & & G_{2n-2} & \\ \times & 0 & & & \end{array}\right], \tag{A2.8a}$$

(A2.8b) $$K_{21}^{(2)} := \left[\begin{array}{cc|ccc} 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ \hline 0 & 0 & & & \\ \vdots & \vdots & & H_{2n-2} & \\ 0 & 0 & & & \end{array}\right], \ K_{22}^{(2)} := (K_{11}^{(2)})^\top,$$

and

(A2.9a) $$N_{11}^{(2)} := \left[\begin{array}{cc|ccc} \times & 0 & \times & \cdots & \times \\ 0 & \times & 0 & \cdots & 0 \\ \hline 0 & 0 & & & \\ \vdots & \vdots & & T_{2n-2} & \\ 0 & 0 & & & \end{array}\right], \ N_{12}^{(2)} := \left[\begin{array}{cc|ccc} 0 & \times & 0 & \cdots & 0 \\ \times & 0 & \times & \cdots & \times \\ \hline 0 & \times & & & \\ \vdots & \vdots & & 0_{2n-2} & \\ 0 & \times & & & \end{array}\right],$$

(A2.9b) $$N_{21}^{(2)} := 0_{2n}, \quad N_{22}^{(2)} := (N_{11}^{(2)})^\top,$$

where G_{2n-2} and $H_{2n-2} \in \mathbb{S}_{2n-2}$ and $T_{2n-2} \in \mathbb{T}_{2n-2}$. Let $m = n - k$. Suppose after $2k$ steps (for $j = 1, 2, \ldots, 2k$) the SA_I gives

(A2.10a) $$K_{11}^{(2k)} := \begin{bmatrix} A_{2k} & B_{2m,2k}^\top \\ C_{2m,2k} & 0_{2m} \end{bmatrix}, \quad K_{12}^{(2k)} := \begin{bmatrix} D_{2k} & \widehat{B}_{2m,2k}^\top \\ \widehat{B}_{2m,2k} & G_{2m} \end{bmatrix},$$

(A2.10b) $$K_{21}^{(2k)} := \begin{bmatrix} 0_{2k} & 0_{2m,2k}^\top \\ 0_{2m,2k} & H_{2m} \end{bmatrix}, \quad K_{22}^{(2k)} := (K_{11}^{(2k)})^\top,$$

and

(A2.11a) $$N_{11}^{(2k)} := \begin{bmatrix} R_{2k} & \widehat{E}_{2m,2k}^\top \\ 0_{2m,2k} & T_{2m} \end{bmatrix}, \ N_{12}^{(2k)} := \begin{bmatrix} \widehat{D}_{2k} & E_{2m,2k}^\top \\ E_{2m,2k} & 0_{2m} \end{bmatrix},$$

(A2.11b) $$N_{21}^{(2k)} := 0_{2n}, \quad N_{22}^{(2k)} := (N_{11}^{(2k)})^\top,$$

where $A_{2k} \in \mathbb{A}_{2k}$, $R_{2k} \in \mathbb{R}_{2k}$, $C_{2m,2k} \in \mathbb{C}_{2m,2k}$, $B_{2m,2k}$, $E_{2m,2k} \in \mathbb{B}_{2m,2k}$, $\widehat{B}_{2m,2k}$, $\widehat{E}_{2m,2k} \in \widehat{\mathbb{B}}_{2m,2k}$, $D_{2k} \in \mathbb{D}_{2k}$, $\widehat{D}_{2k} \in \widehat{\mathbb{D}}_{2k}$, $G_{2m}, H_{2m} \in \mathbb{S}_{2m}$, and $T_{2m} \in \mathbb{T}_{2m}$.

By letting $k' = k+1$ and $m' = m-1$, we perform the SA_I for $j = 2k+1, 2k+1$ and obtain

(A2.12a) $$K_{11}^{(2k')} := \begin{bmatrix} A_{2k'} & B_{2m',2k'}^\top \\ C_{2m',2k'} & 0_{2m'} \end{bmatrix}, \quad K_{12}^{(2k')} := \begin{bmatrix} D_{2k'} & \widehat{B}_{2m',2k'}^\top \\ \widehat{B}_{2m',2k'} & G_{2m'} \end{bmatrix},$$

(A2.12b) $$K_{21}^{(2k')} := \begin{bmatrix} 0_{2k'} & 0_{2m',2k'}^\top \\ 0_{2m',2k'} & H_{2m'} \end{bmatrix}, \quad K_{22}^{(2k')} := (K_{11}^{(2k')})^\top,$$

and

(A2.13a) $$N_{11}^{(2k')} := \begin{bmatrix} R_{2k'} & \widehat{E}_{2m',2k'}^\top \\ 0_{2m',2k'} & T_{2m'} \end{bmatrix}, \ N_{12}^{(2k')} := \begin{bmatrix} \widehat{D}_{2k'} & E_{2m',2k'}^\top \\ E_{2m',2k'} & 0_{2m'} \end{bmatrix},$$

(A2.13b) $$N_{21}^{(2k')} := 0_{2n}, \quad N_{22}^{(2k')} := (N_{11}^{(2k')})^\top,$$

where the subblocks in (A2.12)–(A2.13) have the same forms as in (A2.10)–(A2.11) by replacing k and m by k' and m', respectively, and satisfy

$$A_{2k} = \Phi_{2k}^\top A_{2k'} \Phi_{2k}, \quad D_{2k} = \Phi_{2k}^\top D_{2k} \Phi_{2k}, \tag{A2.14a}$$

$$R_{2k} = \Phi_{2k}^\top R_{2k'} \Phi_{2k}, \quad \widehat{D}_{2k} = \Phi_{2k}^\top \widehat{D}_{2k'} \Phi_{2k}, \tag{A2.14b}$$

where $\Phi_{2k} = [e_1, \ldots, e_{2k}]$ with $e_i \in \mathbb{C}^{2k'}, i = 1, \ldots, 2k$. By the inductive process above, (3.4) holds with $k' = n$ in (A2.12)–(A2.13) and with the superscript "a" in (3.4) being $(2n)$. ☐

A.3. THEOREM A.1. *Let $V \in \mathbb{C}^{n\times r}$ be a unitary matrix and $A, B \in \mathbb{C}^{n\times n}$. Then*

$$\|AV - BVC\|_2 \geq \|AV - BVP\|_2 \qquad \textit{for all } C \in \mathbb{C}^{r\times r},$$

where $P = (V^H B^H BV)^{-1}(V^H B^H AV)$, or equivalently, $P = (U^H BV)^{-1}(U^H AV)$, where $BV = US$ is the QR factorization of BV.

Proof. Since

$$\begin{aligned} -C^H V^H B^H BVP &= -C^H V^H B^H BV(V^H B^H BV)^{-1}(V^H B^H AV) \\ &= -C^H V^H B^H AV, \end{aligned}$$

it follows that

$$\begin{aligned} &(V^H A^H - C^H V^H B^H)(AV - BVC) \\ &= V^H A^H AV - C^H V^H B^H AV - V^H A^H BVC + C^H V^H B^H BVC \\ &= V^H A^H AV + (P^H - C^H)V^H B^H BV(P - C) - P^H V^H B^H BVP \\ &= (V^H A^H - P^H V^H B^H)(AV - BVP) + (P^H - C^H)V^H B^H BV(P - C). \end{aligned}$$

Obviously, $(P^H - C^H)V^H B^H BV(P - C)$ is semidefinite. Then by Weyl's theorem, we have

$$\lambda_j((AV - BVC)^H(AV - BVC)) \geq \lambda_j((AV - BVP)^H(AV - BVP)), \; j = 1, \ldots, n.$$

Hence

$$\|AV - BVC\|_2 \geq \|AV - BVP\|_2,$$

since $\|G\|_2^2 = \lambda\max(G^H G)$. ☐

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