DOUBLING ALGORITHM FOR THE DISCRETIZED BETHE-SALPETER EIGENVALUE PROBLEM

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Abstract. The discretized Bethe-Salpeter eigenvalue problem arises in the Green’s function evaluation in many body physics and quantum chemistry. discretization leads to a matrix eigenvalue problem for \( H \in \mathbb{C}^{2n\times2n} \) with a Hamiltonian-like structure. After an appropriate transformation of \( H \) to a standard symplectic form, the structure-preserving doubling algorithm, originally for algebraic Riccati equations, is extended for the discretized Bethe-Salpeter eigenvalue problem. Potential breakdowns of the algorithm, due to the ill condition or singularity of certain matrices, can be avoided with a double-Cayley transform or a three-recursion remedy. A detailed convergence analysis is conducted for the proposed algorithm, especially on the benign effects of the double-Cayley transform. Numerical results are presented to demonstrate the efficiency and structure-preserving nature of the algorithm.

Key words. Bethe-Salpeter eigenvalue problem, Cayley transform, doubling algorithm

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1. Introduction. The Bethe-Salpeter equation (BSE) \([28]\) arises in the Green’s function evaluation in many body physics, which is the state-of-art model to describe electronic excitation and molecule absorption \([6, 13, 14, 19, 20, 21, 22, 23, 24, 25, 26, 27, 31, 32]\). In the quantum chemistry and material science communities, the optical absorption spectrum of the BSE is an important and powerful tool for the characterization of different materials. In particular, the comparison of the computed and measured spectra helps to interpret experimental data and validate corresponding theories and models. It is generally known that good agreement between the theory and the experimental data can only be achieved by taking into account the interacting electron-hole pairs or excitons. This is the case for the BSE which is derived from the coupling of the electrons and their corresponding holes.

After discretization, the BSE becomes the Bethe-Salpeter eigenvalue problem (BS-EVP):

\[
H x = \begin{bmatrix} A & B \\ -B^T & -A \end{bmatrix} x = \lambda x, \tag{1.1}
\]

for \( x \neq 0 \), where \( A, B \in \mathbb{C}^{n\times n} \) satisfy \( A^H = A, B^T = B \). Here \((\cdot)^H\) and \((\cdot)^T\) denote the conjugate transpose and the transpose of matrices, respectively. It can be shown \([4]\) that any eigenvalue \( \lambda \) comes in quadruplets \( \{\pm \lambda, \pm \bar{X}\} \) (except for the degenerate cases when \( \lambda \) is purely real or imaginary, or zero). Further details on the BS-EVP can be found in \([3, 5, 29]\) and the references therein.

In principle, all possible excitation energies and absorption spectra are sought although some excitations are more probable than others. The associated likelihood is measured by the spectral density or the density of states of \( H \), defined as the number

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of eigenvalues per unit energy interval:

\[ \phi(\omega) = \frac{1}{2n} \sum_{j=1}^{2n} \delta(\omega - \lambda_j), \]

where \( \delta \) is the Dirac-delta function and \( \lambda_j \in \lambda(H) \), the spectrum of \( H \). Also of interest is the optical absorption spectrum:

\[ \epsilon^+(\omega) = \sum_{j=1}^{n} \frac{(d^H x_j)(y^H d_j)}{y_j^H x_j} \delta(\omega - \lambda_j), \]

where \( x_j \) and \( y_j \) are, respectively, the right- and left-eigenvectors corresponding to \( \lambda_j > 0 \), and \( d_r \) and \( d_l \) are the dipole vectors. Evidently, to estimate these quantities, we require all the eigenvalues \( \lambda_j \) and the associated eigenvectors \( x_j \) and \( y_j \). To complicate computations further, \( A \) and \( B \) are often high in dimensions (for systems with many occupied and unoccupied states) and generally dense.

In spite of the significance of the BS-EVP (1.1), only a few publications exist on its numerical solution, all under additional assumptions. Some remarkable discoveries have been made in [3, 5, 29] under the condition that \( \Gamma H \) is positive definite with \( \Gamma = \text{diag}(I_n, -I_n) \). Few general and efficient methods have been proposed to solve the BS-EVP (1.1). All methods proposed in [3, 5, 29] are designed for the linear response eigenvalue problem, under the extra assumptions that \( A, B \in \mathbb{R}^{n \times n} \) and \( A \pm B \) are symmetric positive definite. Low-rank or tensor approximations [3, 5] have been applied to handle the high computational demand but these techniques require additional structures on \( H \). Based on the equivalence of the BS-EVP and a real Hamiltonian eigenvalue problem, Shao et al. [29] put forward an efficient parallel approach to compute the eigenpairs corresponding to all the positive eigenvalues. Remarkable contributions have also been made for the numerical solution of the related linear response eigenvalue problem [1, 2].

**Contributions.** We solve the general BS-EVP (1.1), without assuming \( \Gamma H \) being positive definite. We propose a doubling algorithm (DA) for the BS-EVP in two recursions. To deal with potential breakdowns, we design the double-Cayley transform (DCT) and a three-recursion remedy. The DCT reverses at worst two steps of the DA if there exist some complex eigenvalues and not at all if all eigenvalues are real. In the rare occasions that the DCT fails, the more expensive three-recursion remedy can be applied, without changing the convergence radius. Our DA preserves the special structure of the eigen-pairs.

**Organization.** Some preliminaries are presented in Section 2 and our method is developed in Section 3. We present some illustrative numerical results in Section 4 before the conclusions in Section 5. The Appendix contains two technical lemmas.

2. Preliminaries. We denote the column space, the null space, the spectrum and the set of singular values by \( \mathcal{R}(\cdot), \mathcal{N}(\cdot), \lambda(\cdot) \) and \( \sigma(\cdot) \) respectively. By \( M \oplus N \) or \( \text{diag}(M, N) \), we denote \( \begin{bmatrix} M & 0 \\ 0 & N \end{bmatrix} \). Similarly, we define \( \bigoplus_j M_j \). The MATLAB expression \( M(k:l, s:t) \) denotes the submatrix of \( M \) containing elements in rows \( k \) to \( l \) and columns \( s \) to \( t \). Also, the \( i \)th column of the identity matrix \( I \) is \( e_i \) and

\[ J \equiv \begin{bmatrix} -I_n \\ I_n \end{bmatrix}, \quad \Gamma \equiv \begin{bmatrix} I_n \\ -I_n \end{bmatrix}, \quad \Pi \equiv \begin{bmatrix} I_n \end{bmatrix}. \]
Definition 1. The matrix pair \((M, L)\) with \(M, L \in \mathbb{C}^{2n \times 2n}\) is a symplectic pair if and only if \(M J M^T = L J L^T\).

Definition 2. The matrix pair \((M, L)\) is in the first standard symplectic form (SSF-1) if and only if

\[
M = \begin{bmatrix} E & 0 \\ F & I_n \end{bmatrix}, \quad L = \begin{bmatrix} I_n & K \\ 0 & E^T \end{bmatrix},
\]

with \(E, F \equiv F^T, K \equiv K^T \in \mathbb{C}^{n \times n}\).

Definition 3. Let \(M, L \in \mathbb{C}^{2n \times 2n}\) and denote \(\mathcal{N}(M, L) = \{[M_s, L_s] : M_s, L_s \in \mathbb{C}^{2n \times 2n}, \text{rank}([M_s, L_s]) = 2n, [M_s, L_s][L^T, -M^T]^T = 0\}\), which is nonempty. The action \((M, L) \mapsto (\tilde{M}, \tilde{L}) = (M, M, L, L)\) is called a doubling transformation of \((M, L)\) for some \([M_s, L_s] \in \mathcal{N}(M, L)\).

Next we consider the properties of the doubling transformation.

Lemma 4. ([18, Theorem 2.1]) Let \((\tilde{M}, \tilde{L})\) be the result of a doubling transformation of \((M, L)\), where \(M, L, \tilde{M}, \tilde{L} \in \mathbb{C}^{2n \times 2n}\), we have

1. \((\tilde{M}, \tilde{L})\) is a symplectic pair provided that \((M, L)\) is one; and
2. if \(MU = LUR\) and \(MVS = LV\) for some \(U, V \in \mathbb{C}^{2n \times l}\) and \(R, S \in \mathbb{C}^{l \times l}\), then \(\tilde{M}U = LUR^2\) and \(\tilde{M}VS^2 = LV\).

In other words, doubling transformations preserve symplecticity and deflating subspaces as well as square eigenvalues of matrix pairs.

Lemma 5. It holds that \(H\Pi = -\Pi H^T\) and \(\Gamma H \Gamma = H^T\).

Proof. It can be verified directly.

Lemma 6. Assume that \(HZ = ZS\) with \(Z \in \mathbb{C}^{2n \times l}\) and \(S \in \mathbb{C}^{l \times l}\), then we have \(H(\Pi Z) = (\Pi Z)(-S)\) and \((Z^H \Gamma)H = S^H(Z^H \Gamma)\).

Proof. The results directly follow from Lemma 5.

If \(S\) in Lemma 6 possesses the spectrum \(\lambda(S) = \{\lambda_1, \ldots, \lambda_l\}\) (repeated \(l\) times), Lemmas 5 and 6 imply that \(-\lambda, \bar{\lambda}\) and \(-\bar{\lambda}\) are also the eigenvalues of \(H\) with the same algebraic and geometric multiplicities. Provided that \(HX_j = X_j S_j\) with \(X_j \in \mathbb{C}^{2n \times l_j}\) and \(S_j \in \mathbb{C}^{l_j \times l_j}\) for \(j = 1, 2\), Lemma 6 further implies that \((X^H_1 \Gamma X_1)S_1 = X^H_1 \Gamma H X_1 = S^H_2(X^H_2 \Gamma X_2)\) and \((X^H_2 \Pi \Gamma)X_1 S_1 = (X^H_2 \Pi \Gamma)H X_1 = (-S^H_2)(X^H_2 \Pi \Gamma X_2)\), or equivalently

\[
(X^H_2 \Gamma X_1)S_1 - S^H_2(X^H_2 \Gamma X_1) = 0 = (X^H_2 \Pi \Gamma X_2)S_1 + S^H_2(X^H_2 \Pi \Gamma X_2).
\]

Apparently, when \(\lambda(S_1) \cap \lambda(S_2) = \emptyset\), we have \(X^H_1 \Gamma X_1 = 0\); when \(\lambda(S_1) \cap \lambda(-S_2) = \emptyset\), we have \(X^H_2 \Pi \Gamma X_1 = 0\). By Lemmas 5 and 6, we can then deduce the eigen-decomposition result of \(H\) for the convergence proof.

Temporarily assume that there is no purely imaginary nor zero eigenvalues for \(H\), \(\lambda_j \neq \lambda_k\) for \(j \neq k\) and

\[
\lambda(H) = \{\lambda_1, \ldots, \lambda_l, \bar{\lambda}_1, \ldots, \bar{\lambda}_l, -\lambda_1, \ldots, -\lambda_l, \ldots, \\
\lambda_{s_1}, \ldots, \lambda_{s_l}, \bar{\lambda}_{s_1}, \ldots, \bar{\lambda}_{s_l}, -\lambda_{s_1}, \ldots, -\lambda_{s_l}, \\
\lambda_{s_1+1}, \ldots, \lambda_{s_{l+1}}, -\lambda_{s_1+1}, \ldots, -\lambda_{s_{l+1}}, \lambda_{l_1}, \ldots, \lambda_{l_s}, -\lambda_{l_1}, \ldots, -\lambda_{l_s}\},
\]
where \( \lambda_j \in \mathbb{C} \) with (i) \( \Re(\lambda_j) \Im(\lambda_j) \neq 0 \) and \( \Re(\lambda_j) < 0 \) for \( j = 1, \ldots, s \), and (ii) \( \Im(\lambda_j) = 0 \) and \( \lambda_j < 0 \) for \( j = s + 1, \ldots, t \). Subsequently, we have the following result.

**Lemma 7.** Suppose that no purely imaginary nor zero eigenvalues exist for \( H \). Then there exist

\[
X = [X_1, Y_1, \cdots, X_s, Y_s; X_{s+1}, \cdots, X_t] \in \mathbb{C}^{2n \times n},
\]

\[
S = \text{diag}(S_1, R_1, \ldots, S_s, R_s; S_{s+1}, \ldots, S_t) \in \mathbb{C}^{n \times n}
\]

with \( X_j \in \mathbb{C}^{2n \times l_j}, S_j \in \mathbb{C}^{l_j \times l_j}, \lambda(S_j) = \{\lambda_j, \ldots, \lambda_j\} \) \((j = 1, \ldots, t)\), \( Y_j \in \mathbb{C}^{2n \times l_j}, R_j \in \mathbb{C}^{l_j \times l_j} \) and \( \lambda(R_j) = \{\overline{\lambda}_j, \ldots, \overline{\lambda}_j\} \) \((j = 1, \ldots, s)\), such that

\[
H[X, \Pi \overline{X}] = [X, \Pi \overline{X}] \text{diag}(S, -\overline{S}), \quad [X, \Pi \overline{X}]^H \Gamma[X, \Pi \overline{X}] = \text{diag}(D, -\overline{D}),
\]

where \( D = \text{diag}(D_1, \ldots, D_s; D_{s+1}, \ldots, D_t) \),

\[
D_j = \begin{bmatrix} 0 & X_j^H \Gamma Y_j \\ X_j^H \Gamma X_j & 0 \end{bmatrix} \in \mathbb{C}^{2l_j \times 2l_j} \quad (j = 1, \ldots, s),
\]

\[
D_j = X_j^H \Gamma X_j \in \mathbb{C}^{l_j \times l_j} \quad (j = s + 1, \ldots, t).
\]

Obviously, \( D \) (in Lemma 7) is a nonsingular Hermitian matrix. Consequently, we can choose \( X \) which satisfies \([X, \Pi \overline{X}]^H \Gamma[X, \Pi \overline{X}] = \Gamma\). This leads to \( X^H \Gamma X = I_n \) and \( X^H \Gamma \Pi \overline{X} = 0 \), implying that \( X(1:n, 1:n) \in \mathbb{C}^{n \times n} \) is nonsingular with singular values no less than unity and \( X(1:n, 1:n)^T X(n+1:2n, 1:n) \) is complex symmetric.

Next consider the case when there exist some purely imaginary eigenvalues for \( H \). We further assume that the partial multiplicities (the sizes of the Jordan blocks) of \( H \) associated with the purely imaginary eigenvalues are all even. Let \( i \omega_1, \ldots, i \omega_q \) be the different purely imaginary eigenvalues with Jordan blocks \( J_{2p_{r,j}}(i \omega_j) \in \mathbb{C}^{2p_{r,j} \times 2p_{r,j}} \) for \( r = 1, \ldots, l_j \) and \( j = 1, \ldots, q \). Then there exist \( W_{r,j}, Z_{r,j} \in \mathbb{C}^{2n \times p_{r,j}} \) such that

\[
H \left[ W_{1,1}, Z_{1,1}; \cdots; W_{1,q}, Z_{1,q}; \cdots; W_{t,j}, Z_{t,j} \right] = \left[ W_{1,1}, Z_{1,1}; \cdots; W_{1,q}, Z_{1,q}; \cdots; W_{t,j}, Z_{t,j} \right] \cdot \left[ \bigoplus_{j=1}^{q} \bigoplus_{r=1}^{l_j} J_{2p_{r,j}}(i \omega_j) \right].
\]

With \( X \in \mathbb{C}^{2n \times n_1} \) and \( S \in \mathbb{C}^{n_1 \times n_1} \) and by Lemma 7, we obtain

\[
H \left[ X, W_\omega, \Pi \overline{X}, Z_\omega \right] = \left[ X, W_\omega, \Pi \overline{X}, Z_\omega \right] \tilde{S}, \quad (2.1)
\]

where \( n_1 + \sum_{j=1}^{q} \sum_{r=1}^{l_j} p_{r,j} = n \), and

\[
W_\omega = \left[ W_{1,1}, \cdots, W_{1,q}; \cdots; W_{t,j}, \cdots, W_{t,q} \right],
\]

\[
Z_\omega = \left[ Z_{1,1}, \cdots, Z_{1,q}; \cdots; Z_{t,j}, \cdots, Z_{t,q} \right],
\]

\[
J_\omega = \bigoplus_{j=1}^{q} \bigoplus_{r=1}^{l_j} J_{p_{r,j}}(i \omega_j), \quad \Omega_\omega = \bigoplus_{j=1}^{q} \bigoplus_{r=1}^{l_j} e_{p_{r,j}} e_1^T,
\]

\[
J_{2p_{r,j}}(i \omega_j) = \begin{bmatrix} J_{p_{r,j}}(i \omega_j) & e_{p_{r,j}} e_1^T \\ 0 & J_{p_{r,j}}(i \omega_j) \end{bmatrix}, \quad \tilde{S} = \begin{bmatrix} S & -\Omega_\omega \\ J_\omega & \Omega_\omega \end{bmatrix}.
\]
3. Doubling Algorithm. We now generalize the structure-preserving doubling algorithm (SDA) in [7, 8, 16, 17] to the DA for the BS-EVP.

3.1. Initial Symplectic Pencil. We transform \( H \) to a symplectic pair \((M, L)\) in the SSF-1 à la Cayley.

**Lemma 8.** For \( \alpha \in \mathbb{R} \), the matrix pair \((H + \alpha I_{2n}, H - \alpha I_{2n})\) is symplectic.

**Proof.** The result can be deduced from \((HJ)^T = HJ\). \(\square\)

**Theorem 9.** Select \( \alpha \in \mathbb{R} \) such that both \( \alpha I_n - A \) and \( R \equiv I_n - (\alpha I_n - A)^{-1}B(\alpha I_n - A)^{-1}B \) are nonsingular. There exists a nonsingular matrix \( G \in \mathbb{C}^{2n \times 2n} \) such that \([G(H + \alpha I_n), G(H - \alpha I_n)]\) is a symplectic pair in SSF-1, with

\[
M_\alpha \triangleq G(H + \alpha I_n) = \begin{bmatrix} E_\alpha & 0 \\ F_\alpha & I_n \end{bmatrix}, \quad L_\alpha \triangleq G(H - \alpha I_n) = \begin{bmatrix} I_n & \overline{F}_\alpha \\ 0 & \overline{E}_\alpha \end{bmatrix},
\]

where \( E_\alpha, F_\alpha \in \mathbb{C}^{n \times n} \) satisfy \( E_\alpha^H = E_\alpha \) and \( F_\alpha^T = F_\alpha \).

**Proof.** Let \( H_\pm \equiv H \pm \alpha I_{2n}, \ A_\pm \equiv A \pm \alpha I_n \),

\[ G_1 = \begin{bmatrix} A_\pm^{-1} & 0 \\ BA_\pm^{-1} & I_n \end{bmatrix}, \quad G_2 = \begin{bmatrix} I_n & A_\pm^{-1}BR^{-1}\overline{A}_\pm^{-1} \\ 0 & -R^{-1}\overline{A}_\pm^{-1} \end{bmatrix}, \]

and \( G = G_2G_1 \). We obtain

\[ G_1H_+ = \begin{bmatrix} A_\pm^{-1}A_+ & A_\pm^{-1}B \\ 2\alpha BA_\pm^{-1} & -\overline{A}_R \end{bmatrix}, \quad G_2G_1H_+ = \begin{bmatrix} E_\alpha & 0 \\ F_\alpha & I_n \end{bmatrix}, \]

\[ G_1H_- = \begin{bmatrix} I_n & A_\pm^{-1}B \\ 0 & -\overline{A}_R - 2\alpha I_n \end{bmatrix}, \quad G_2G_1H_- = \begin{bmatrix} I_n & \overline{F}_\alpha \\ 0 & \overline{E}_\alpha \end{bmatrix}, \]

with

\[
E_\alpha = I_n + 2\alpha \overline{R}^{-1}A_\pm^{-1}, \quad F_\alpha = -2\alpha \overline{A}_\pm^{-1}B\overline{R}^{-1}A_\pm^{-1}.
\]

Furthermore, since \( A^H = A \) and \( B^T = B \), we have

\[
E_\alpha^H = I_n + 2\alpha A_\pm^{-1}R^{-T} = I_n + 2\alpha (A_\pm^{-1} - B\overline{A}_\pm^{-1}B)^{-1} = E_\alpha,
\]

\[
F_\alpha^T = -2\alpha \overline{A}_\pm^{-1}(I_n - \overline{B}A_\pm^{-1}B\overline{A}_\pm^{-1})^{-1}B\overline{A}_\pm^{-1} = F_\alpha,
\]

i.e., \( E_\alpha \) and \( F_\alpha \) are Hermitian and complex symmetric, respectively. Lastly, we have

\[
(GH_\pm)J(GH_\pm)^T = \begin{bmatrix} E_\alpha \\ -\overline{E}_\alpha \end{bmatrix},
\]

implying that \([G(H + \alpha I_n), G(H - \alpha I_n)]\) is a symplectic pair in SSF-1. \(\square\)

The following lemma summarizes the eigen-structure of \((M_\alpha, L_\alpha)\) in relation to that of \(H\), neglecting the simple proof.

**Lemma 10.** Let

\[
H[X_1^T, X_2^T]^T = [X_1^T, X_2^T]^T S
\]

for some \( X_1, X_2 \in \mathbb{C}^{n \times l} \), \( S \in \mathbb{C}^{l \times l} \) and \( \alpha \notin \lambda(H) \), then we have

\[
M_\alpha[X_1^T, X_2^T]^T = L_\alpha[X_1^T, X_2^T]^T S_\alpha,
\]

with \( S_\alpha \equiv (S - \alpha I_l)^{-1}(S + \alpha I_l) \), where \( S_\alpha - \alpha I_l \) is nonsingular.
Intrinsically, the DA proposed below requires both $E_\alpha$ and $I_n - F_\alpha \overline{A}$ to be nonsingular. Lemma 11 and Theorems 12 and 13 below indicate that a small $\alpha$ could achieve such a goal. Moreover, for $\lambda \in \lambda(H)$, we have $(\lambda + \alpha)/(\lambda - \alpha) \in \lambda(S_\alpha)$. For the efficiency of the DA, we desire a small $|\alpha|$ for $\Re(\lambda) < 0$. Hence when $|\alpha| \geq \rho(H)$ (the spectral radius of $H$), we desire $|\alpha|$ to be minimized.

**Lemma 11.** Let $\alpha > \|H\|_F$, then $\alpha I_n - A$ is positive definite and $R \equiv I_n - (\alpha I_n - \overline{A})^{-1}B$ is nonsingular, with $\|R^{-1}\|_2 \leq [1 - \|(\alpha I_n - A)^{-1}\|_2^2 \|B\|^2_2]^{-1}$.

**Proof.** When $\|A\|_F < \|H\|_F < \alpha$, $\alpha I_n - A$ is positive definite Hermitian. Since $\alpha > \|H\|_F \geq \|A\|_F + \|B\|_F$, we have $(\alpha - \omega_1)^{-1} \leq (\alpha - \|A\|_F)^{-1} < \|B\|_F^{-1}$ with $\omega_1$ being the largest eigenvalue of $A$. In addition, with $\|(\alpha I_n - A)^{-1}\|_2 = (\alpha - \omega_1)^{-1}$, we have $\|(\alpha I_n - A)^{-1}\|_2 B_2 \leq \|(\alpha I_n - A)^{-1}\|_2 \|B\|_2 = (\alpha - \omega_1)^{-1} \|B\|_2 < 1$. This implies $\|(\alpha I_n - A)^{-1}\|_2 \|B\|^2_2 < 1$ and our results.

**Theorem 12.** As defined in (3.2), $E_\alpha$ is nonsingular when $\alpha > \|H\|_F$.

**Proof.** Denote the largest and smallest eigenvalues of $A$ by $\omega_1$ and $\omega_n$, respectively. With $\alpha > \|H\|_F$, we have $\|\alpha I_n - A\|_2 = \alpha - \omega_n$ and $\|(\alpha I_n - \overline{A})^{-1}\|_2 = (\alpha - \omega_1)^{-1}$, yielding $\|(\alpha I_n - A) - B(\alpha I_n - \overline{A})^{-1}B\|_2 \leq (\alpha - \omega_n) + (\alpha - \omega_1)^{-1} \|B\|^2_2$. We also have

$$\frac{\alpha^2 - \|A\|^2_2}{2} = (\alpha + \frac{\omega_n - \omega_1}{2})^2 + \frac{(\omega_1 + \omega_n)^2}{4} + \|B\|^2_2 < -\frac{(\alpha + \omega_n - \omega_1)^2}{2}.$$

As $\alpha^2 > \|H\|^2_2 = 2(\|B\|^2_2 + \|A\|^2_2)$, we obtain

$$\frac{\alpha^2 - \|A\|^2_2}{2} - \frac{(\alpha + \omega_n - \omega_1)^2}{2} < 0.$$

This implies $(\alpha - \omega_n)(\alpha - \omega_1) + \|B\|^2_2 - 2\alpha(\alpha - \omega_1) < 0$. We deduce $\|(\alpha I_n - A) - B(\alpha I_n - \overline{A})^{-1}B\|_2 < 2\alpha$, thus $2\alpha \notin \lambda\{(\alpha I_n - A) - B(\alpha I_n - \overline{A})^{-1}B\}$. Therefore, $E_\alpha = I_n - 2\alpha \left[(\alpha I_n - A) - B(\alpha I_n - \overline{A})^{-1}B\right]^{-1}$ is nonsingular. 

Complementing Theorem 12, we have $\lambda(E_\alpha)$ lies outside $[0, 2]$ when $\alpha > \|H\|_F$ because the moduli of all eigenvalues of $[(\alpha I_n - A) - B(\alpha I_n - \overline{A})^{-1}B]^{-1}$ are greater than $(2\alpha)^{-1}$.

**Theorem 13.** Assume that $\alpha > \varrho\|H\|_F + \frac{1}{2}(\varrho - 1)^{-1}\|B\|^2_2$ with $\varrho > 1$. Then $\|F_{\alpha}\|_2 < 1$ with $F_\alpha$ defined in (3.2).

**Proof.** Let $\omega_1$ be the largest eigenvalue of $A$. Then it holds that

$$\|\lambda I_n - A\|_2 = (\alpha - \omega_1)^{-1}, \quad \|F_{\alpha}\|_2 \leq \frac{2\alpha\|B\|^2_2}{(\alpha - \omega_1)^2 - \|B\|^2_2}.$$

We shall show that $\|B\|^2_2 / [(\alpha - \omega_1)^2 - \|B\|^2_2]$, in the right-hand-side of the inequality above, is bounded strictly from above by $(2\alpha)^{-1}$ when $\alpha > \varrho\|H\|_F + \frac{1}{2}(\varrho - 1)^{-1}\|B\|^2_2$, or equivalently

$$(\alpha - \omega_1)^2 - 2\alpha\|B\|^2_2 - \|B\|^2_2 > 0.$$  \(\text{(3.4)}\)

If $\|B\|^2_2 + \omega_1 \leq 0$, (3.4) is apparently valid. When $\|B\|^2_2 + \omega_1 > 0$ and considering the left-hand-side of (3.4) as a quadratic in $\alpha$, (3.4) holds if and only if $\alpha > \|B\|^2_2 + \omega_1 +$
demonstrates that when $\tilde{\eta} > 0$ and $\eta_1 \equiv 1/(2\eta^2)$, from the equality

$$
\sqrt{2} \|B\|_2 (\|B\|_2 + \omega_1) \quad \text{with} \quad \eta > 0 \quad \text{and} \quad \eta_1 \equiv 1/(2\eta^2),
$$

we deduce that

$$
\|B\|_2 + \omega_1 + \sqrt{2} \|B\|_2 (\|B\|_2 + \omega_1) = \left[ \eta \sqrt{\|B\|_2 \|B\|_2 + \eta_1 (\|B\|_2 + \omega_1)} \right]^2 - \eta^2 \|B\|_2 - \eta_1 (\|B\|_2 + \omega_1),
$$

and the imaginary axis is known.

With $\eta^2 = \frac{1}{2} (\varrho - 1)^{-1}$, we get $\eta^2 \|B\|_2 + (1 + \eta_1) (\|B\|_2 + \omega_1) < \alpha$, thus our result. \(\square\)

Theorem 13 demonstrates that when $\varrho$ is chosen as some moderate real positive scalar, such as $\sqrt{2}$, then the corresponding lower bound will be a good candidate for the initial $\alpha$. Additionally, when the condition in Theorem 13 is satisfied, $E_\alpha$ and $I_n - F_\alpha^T \alpha$ are nonsingular.

Although Theorems 12 and 13 show that a small $\alpha$ is sufficient for $E_\alpha$ and $I_n - F_\alpha^T \alpha$ to be nonsingular, the minimization of $|(\lambda + \alpha)/(\lambda - \alpha)|$ for an optimal $\alpha$ deserves further consideration, for the fast convergence of the DA. For the optimal $\alpha$, [11] proposed some remarkable techniques for the suboptimal solution

$$
\alpha_{\text{opt}} := \arg\min_{\alpha > 0} \max_{\Re(\lambda) < 0} \left| \frac{\xi + \alpha}{\xi - \alpha} \right|,
$$

where $D$ being an interval, a disk, an ellipse or a rectangle, [11, Theorem 2.1] considers the suboptimal solution $\alpha_{\text{opt}}$. The technique can be applied to (3.1) for a suboptimal $\alpha$ when the distance between $\{\lambda \in \lambda(H) : \Re(\lambda) < 0\}$ and the imaginary axis is known.

From now on, we will always assume $\alpha > 0$ such that $\alpha I_{2n} - H, \alpha I_n - A, I_n - (\alpha I_n - \overline{A})^{-1} B \alpha (I_n - A)^{-1} B$ and $E_\alpha$ are nonsingular and also assume that $1 \notin \sigma(F_\alpha)$ (before the discussion in Section 3.3).

3.2. Algorithm. We now construct a new symplectic pair by applying the doubling action to a given symplectic pair $(M, L)$ in SSF-1 in (3.1); i.e., for $E^H = E, F^T = F \in \mathbb{C}^{n \times n}$, we have

$$
M = \begin{bmatrix} E & 0 \\ F & I_n \end{bmatrix}, \quad L = \begin{bmatrix} I_n & F^T \\ 0 & E \end{bmatrix}, \quad \text{(3.5)}
$$

Theorem 14. For $M, L$ in (3.5) with $1 \notin \sigma(F)$, there exists $[M_*, L_*] \in \mathcal{N}(M, L)$ such that $(\tilde{M}, \tilde{L}) = ([M_*], L_*), \text{from the doubling transformation of } (M, L), \text{is a symplectic pair in SSF-1}. \text{Furthermore}, [\tilde{M}, \tilde{L}] \text{retains the SSF-1}:

$$
\tilde{M} = \begin{bmatrix} \tilde{E} & 0 \\ \tilde{F} & I_n \end{bmatrix}, \quad \tilde{L} = \begin{bmatrix} I_n & \tilde{F} \\ 0 & \tilde{E} \end{bmatrix},
$$

with $\tilde{E}^H = \tilde{E}, \tilde{F}^T = \tilde{F} \in \mathbb{C}^{n \times n}$.
Proof. Let

\[
M_\alpha = \begin{bmatrix}
E + E\overline{F}(I_n - F\overline{F})^{-1}F & 0 \\
\overline{E}(I_n - F\overline{F})^{-1}F & I_n
\end{bmatrix}, \quad L_\alpha = \begin{bmatrix} I_n & E\overline{F}(I_n - F\overline{F})^{-1} \\
0 & \overline{E}(I_n - F\overline{F})^{-1} \end{bmatrix}.
\]

We have rank([\(M_\alpha, L_\alpha\)]) = 2n and

\[
M_\alpha L = \begin{bmatrix}
E(I_n - F\overline{F})^{-1}E & E\overline{F}(I_n - F\overline{F})^{-1} \\
\overline{E}(I_n - F\overline{F})^{-1}E & E(I_n - F\overline{F})^{-1} \end{bmatrix} = L_\alpha M,
\]

implying that \([M_\alpha, L_\alpha] \in \mathcal{N}(M, L)\). Routine manipulations yield

\[
M_\alpha M = \begin{bmatrix}
E(I_n - F\overline{F})^{-1}E & 0 \\
F + E\overline{F}(I_n - F\overline{F})^{-1}E & I_n
\end{bmatrix}, \quad L_\alpha L = \begin{bmatrix} I_n & F + E\overline{F}(I_n - F\overline{F})^{-1}E \\
0 & \overline{E}(I_n - F\overline{F})^{-1} \end{bmatrix}.
\]

With \(\hat{E} = E(I_n - F\overline{F})^{-1}E\) and \(\hat{F} = F + E\overline{F}(I_n - F\overline{F})^{-1}E\), the result follows. \(\square\)

If we initially take \(M_0 = M_\alpha\) and \(L_0 = L_\alpha\) from (3.1)), indicating that \(E_0 = E_\alpha\) and \(F_0 = F_\alpha\) (specified in (3.2)), then successive doubling transformations in Theorem 14 produce a sequence of symplectic pairs \((M_k, L_k)\) provided that \((I_n - T_kF_k)\) are nonsingular for \(k \geq 0\). Specifically, we have a well-defined doubling iteration, provided that \(1 \notin \sigma(F_k)\): (for \(k = 0, 1, \ldots\))

\[
E_{k+1} = E_k(I_n - T_kF_k)^{-1}E_k, \quad F_{k+1} = F_k + E_kF_k(I_n - T_kF_k)^{-1}E_k. \tag{3.6}
\]

Assuming (3.3) with \(S_\alpha \equiv (S - \alpha I_1)^{-1}(S + \alpha I_1)\), Lemmas 4 and 10 imply

\[
M_k \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = L_k \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \begin{bmatrix} S_{\alpha}^{2k} \\ \end{bmatrix}, \quad M_k = \begin{bmatrix} E_k & 0 \\ F_k & I_n \end{bmatrix}, \quad \tilde{L}_k = \begin{bmatrix} I_n & \tilde{T}_k \\ 0 & \tilde{E}_k \end{bmatrix}. \tag{3.7}
\]

The DA in (3.6) has two iterative formulae for \(E_k\) and \(F_k\). Interestingly, the SDAs for Riccati equations and quadratic palindromic eigenvalue problems [7, 8, 9] have three, those for nonsymmetric algebraic Riccati equations [16, 17] have four, while the PDA for the linear palindromic eigenvalue problem [15] has one.

**Convergence.** We next consider the convergence of the DA. Without loss of generality, we assume for the moment that \(1 \notin \sigma(F_k)\) for all \(k = 0, 1, \ldots\). For the case that \(1 \in \sigma(F_k)\) for some \(k\), Theorem 20 below essentially demonstrates that the following convergence result still hold. We also require the technical assumption that \(X_1\) and \([X_1, \Psi_{11}]\), respectively, are nonsingular in Theorems 15 and 16 below.

**Theorem 15.** Assume that \(H\) possesses no purely imaginary eigenvalue and \(H[X_1^T, X_2^T]^T = [X_1^T, X_2^T]^TS\) with \(X_1, X_2, S \in \mathbb{C}^{n \times n}\), where \(\lambda(S)\) is in the interior of the left half plane. Then for \(\{E_k\}\) and \(\{F_k\}\) generated by (3.6), we have \(\lim_{k \to \infty} E_k = 0\) and \(\lim_{k \to \infty} F_k = -X_2X_1^{-1}\), both converging quadratically.

**Proof.** Let \(S_\alpha \equiv (S - \alpha I_1)^{-1}(S + \alpha I_1)\). Note that the spectral radius of \(S_\alpha\) is less than 1 when \(\alpha > 0\). The proof is similar to that of [18, Corollary 3.2]. \(\square\)

The following theorem illustrates the linear convergence of the proposed DA when some purely imaginary eigenvalues exist.

Let the Jordan decompositions of \(J_{2p_{r,j}}(i\omega_j + \alpha)[J_{2p_{r,j}}(i\omega_j - \alpha)]^{-1}\) be \(J_{2p_{r,j}}(i\omega_j + \alpha)[J_{2p_{r,j}}(i\omega_j - \alpha)]^{-1} = Q_{r,j}J_{2p_{r,j}}(e^{i\theta_j})Q_{r,j}^{-1}\) for \(r = 1, \ldots, l_j\) and \(j = 8\).
1, \cdots, q. Denote \( W_\omega = [W_{1,\omega}^T, W_{2,\omega}^T]^T \), \( Z_\omega = [Z_{1,\omega}^T, Z_{2,\omega}^T]^T \), \( Q_{r,j} = \begin{bmatrix} Q_{r,j}^{(11)} & Q_{r,j}^{(12)} \\ Q_{r,j}^{(21)} & Q_{r,j}^{(22)} \end{bmatrix} \)
and, for \( s', t' = 1, 2 \),
\[
Q^{(s', t')} := \bigoplus_{j=1}^{q} \bigoplus_{r=1}^{l_j} Q_{r,j}^{(s', t')}
\]
\[
\Psi_{11} \equiv W_{1,\omega}Q^{(11)} + Z_{1,\omega}Q^{(21)}, \quad \Psi_{21} \equiv W_{2,\omega}Q^{(11)} + Z_{2,\omega}Q^{(21)}.
\]

**Theorem 16.** Assume that the partial multiplicities of \( H \) associated with the purely imaginary eigenvalues are all even, and \( H \) has the eigen-decomposition specified in (2.1). Writing \( X = [X_1^T, X_2^T]^T \), provided that \([X_1, \Psi_{11}]\) is nonsingular, we then have \( \lim_{k \to \infty} E_k = 0 \) and \( \lim_{k \to \infty} F_k = [X_2, \Psi_{21}][X_1, \Psi_{11}]^{-1} \), both converging linearly.

**Proof.** By (2.1) and Lemmas 4 and 10, we have
\[
M_k \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \begin{bmatrix} W_{1,\omega} & \bar{X}_1 \\ W_{2,\omega} & \bar{X}_1 \end{bmatrix} \begin{bmatrix} Z_{1,\omega} \\ Z_{2,\omega} \end{bmatrix} = L_k \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \begin{bmatrix} W_{1,\omega} & \bar{X}_1 \\ W_{2,\omega} & \bar{X}_1 \end{bmatrix} \begin{bmatrix} Z_{1,\omega} \\ Z_{2,\omega} \end{bmatrix} \bar{S}_\alpha^{k}, \tag{3.8}
\]
where \( \bar{S}_\alpha = (\bar{S} + \alpha I)(\bar{S} - \alpha I)^{-1} \) with \( \bar{S} \) from (2.1). Let \( \Pi_\omega \) be the permutation matrix satisfying
\[
\Pi_\omega \text{diag} \left\{ S_i, -\bar{S}; \bigoplus_{j=1}^{q} \bigoplus_{r=1}^{l_j} J_{2p_r, i}(i\omega_j) \right\} \Pi_\omega^T = \bar{S},
\]
and denote \( D \equiv \text{diag} \{ I_{n_1}, I_{n_1}; \bigoplus_{j=1}^{q} \bigoplus_{r=1}^{l_j} Q_{r,j} \} \), \( J_{\omega, \theta} = \bigoplus_{j=1}^{q} \bigoplus_{r=1}^{l_j} J_{p_r, i}(\omega_j) \), and \( S_\alpha := (S + \alpha I)(S - \alpha I)^{-1} \), it holds that
\[
\bar{S}_\alpha = \left( \Pi_\omega D \Pi_\omega^T \right) \begin{bmatrix} S_\alpha & \Omega_\omega \\ J_{\omega, \theta} & S_\alpha^{-1} \Omega_\omega \end{bmatrix} \left( \Pi_\omega D^{-1} \Pi_\omega^T \right).
\]
This further implies
\[
\bar{S}_\alpha^{2k} = \left( \Pi_\omega D \Pi_\omega^T \right) \begin{bmatrix} S_\alpha^{2k} & \Omega_\omega, \theta, k \\ J_{\omega, \theta}^{2k} & S_\alpha^{-2k} \end{bmatrix} \left( \Pi_\omega D^{-1} \Pi_\omega^T \right) \tag{3.9}
\]
with \( \Omega_\omega, \theta, k = \bigoplus_{j=1}^{q} \bigoplus_{r=1}^{l_j} J_{2p_r, i}(\omega_j)(1 : p_r, i + 1 : 2p_r) \). By (3.8) and (3.9) we have
\[
M_k \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \begin{bmatrix} W_{1,\omega} & \bar{X}_1 \\ W_{2,\omega} & \bar{X}_1 \end{bmatrix} \begin{bmatrix} Z_{1,\omega} \\ Z_{2,\omega} \end{bmatrix} \left( \Pi_\omega D \Pi_\omega^T \right) = L_k \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \begin{bmatrix} W_{1,\omega} & \bar{X}_1 \\ W_{2,\omega} & \bar{X}_1 \end{bmatrix} \begin{bmatrix} Z_{1,\omega} \\ Z_{2,\omega} \end{bmatrix} \left( \Pi_\omega D^{-1} \Pi_\omega^T \right)
\]
\[
\begin{bmatrix} S_\alpha^{2k} & J_{\omega, \theta}^{2k} \\ J_{\omega, \theta}^{2k} & S_\alpha^{-2k} \end{bmatrix} \begin{bmatrix} \Omega_\omega, \theta, k \\ \Omega_\omega, \theta, k \end{bmatrix}.
\]
Similar to the proof of [12, Theorem 4.2], we obtain the result.
Next assume that we have acquired a symplectic pair \((M_k, L_k)\) with \(\|E_k\|_F < u\), where \(u\) is some small tolerance. The question is then how to compute the eigenvalues and eigenvectors of \(H\) from \(E_k\) and \(F_k\). Without loss of generality, we just show the details for the case that no purely imaginary eigenvalues exist.

Denote the error \(Z_k \equiv F_k + X_1 X_1^{-1}\) (Theorem 15 and (3.6) suggest \(\|Z_k\|_F < u\)), where \(X_1, X_2 \in \mathbb{C}^{n \times n}\) satisfy \(H [X_1^T, X_2^T]^T = [X_1^T, X_2^T] S\) with \(\lambda(S) \subseteq \mathbb{C}_-\), we have

\[
H \begin{bmatrix} I_n & 0 \\ -F_k \\ \end{bmatrix} = \begin{bmatrix} I_n \\ -F_k \\ \end{bmatrix} X_1 S X_1^{-1} + \begin{bmatrix} 0 \\ Z_k \\ \end{bmatrix} X_1 S X_1^{-1} - H \begin{bmatrix} 0 \\ Z_k \\ \end{bmatrix}. \tag{3.10}
\]

Pre- and post-multiplying \([I_n, -F_k^H]\) and \((I_n + F_k^H F_k)^{-1}\), respectively, to both sides of (3.10), we obtain

\[
(I_n + F_k^H F_k) X_1 S X_1^{-1} (I_n + F_k^H F_k)^{-1} = \left\{ \begin{bmatrix} I_n & -F_k^H \end{bmatrix} H \begin{bmatrix} I_n & -F_k^T \end{bmatrix} + (F_k^H Z_k X_1 S X_1^{-1} + B Z_k + F_k^H A Z_k) \right\} (I_n + F_k^H F_k)^{-1}.
\]

Accordingly, we can take the eigenvalues of \(H_k \equiv [I_n, -F_k^H] H [I_n, -F_k^T]^T (I_n + F_k^H F_k)^{-1}\) to approximate \(\lambda(S)\) (the stable subspectrum of \(H\)). By the generalized Bauer-Fike theorem \([30]\), when the eigenvalues \(\lambda_p(S)\) have Jordan blocks of maximum size \(m\), there exists an eigenvalue \(\lambda_q(H_k)\) such that

\[
\frac{|\lambda_p(S) - \lambda_q(H_k)|^m}{|1 + |\lambda_p(S) - \lambda_q(H_k)||^m - 1|} \leq \| (F_k^H Z_k X_1 S X_1^{-1} + B Z_k + F_k^H A Z_k) (I_n + F_k^H F_k)^{-1} \|_2 \leq \| F_k^H Z_k X_1 S X_1^{-1} + B Z_k + F_k^H A Z_k \|_2,
\]

for some \(\Upsilon > 0\) associated with \(S\). Consequently, we can approximate \(\lambda(S)\) by \(\lambda(H_k)\).

### 3.3. Double-Cayley Transform.

When \(1 \in \sigma(F_{k_0})\) for some \(k_0 > 1\) (or the condition in Theorem 14 is violated), we cannot construct the new symplectic pair \((M_{k_0+1}, L_{k_0+1})\) via the doubling transformation in (3.6). In this section, we divert the DA from this potential interruption using a DCT. We shall also prove the efficiency of the technique, not requiring a restart with a new \(\alpha\). It is worthwhile to point that the DCT may be applied when \(I - F_{k_0} F_{k_0}\) is ill-conditioned. In practice, we may set a tolerance \(u\) and once the singular values of \(F_{k_0}\) satisfy \(\frac{\min_{\sigma \in \sigma(F_{k_0})} |\sigma - 1|}{\max_{\sigma \in \sigma(F_{k_0})} |\sigma - 1|} < u\), the DCT is then applied.

We require the following results firstly.

**Lemma 17.** Assume that the doubling iteration (3.6) does not break off for all \(k < k_0\). If \(E_{k_0}\) is nonsingular, so are \(E_k\) \((0 < k \leq k_0)\).

**Proof.** This directly follows from \(E_{k+1} = E_k (I_n - F_k F_k)^{-1} E_k\) in (3.6).

Obviously, Lemma 17 suggests that \(M_{k_0}\) and \(L_{k_0}\), defined in (3.7), are both nonsingular and so is

\[
L_{k_0}^{-1} M_{k_0} = \begin{bmatrix} E_{k_0} - F_{k_0} F_{k_0}^{-1} F_{k_0} & -F_{k_0} F_{k_0}^{-1} \\ F_{k_0}^{-1} F_{k_0} & F_{k_0}^{-1} \end{bmatrix}.
\]

Since \(L_{k_0}^{-1} M_{k_0} [X_1^T, X_2^T]^T = [X_1^T, X_2^T]^T S_{\alpha k_0}^{\pm}\), the fact that \(\{0, \alpha\} \not\subset \lambda(H)\) implies \(L_{k_0}^{-1} M_{k_0} \pm I_{2n}\) are nonsingular. Consequently, we have the following theorem.
Theorem 18. Let \( \vartheta \in \{-1, 1\} \) and \( \beta \in \mathbb{R} \). Provided that \( \vartheta \notin \lambda(E_{k_0}) \), then

(a) \( Z = \partial I_n - E_{k_0} + \vartheta F_{k_0}(\vartheta \overline{E}_{k_0} - I_n)^{-1}F_{k_0} \) is nonsingular;

(b) \( (\hat{H} + \beta \vartheta I_{2n})[X_1^T, X_2^T]^T = (\hat{H} - \beta \vartheta I_{2n})[X_1^T, X_2^T]^T(\partial S_{\alpha}^{2k_0}) \) with \( \hat{A} = \beta \vartheta I_n - 2\beta Z^{-1}, \hat{B} = (\beta I_n - \partial \hat{A})F_{k_0}(F_{k_0} - \vartheta I_n)^{-1} \) and \( \hat{H} = \begin{bmatrix} \hat{A} & \hat{B} \\ -\hat{B} & -\hat{A} \end{bmatrix} \) and \( \hat{A} \) is Hermitian and \( \hat{B} \) is symmetric.

Proof. For (a) with \( \vartheta \notin \lambda(E_{k_0}) \), \( E_{k_0} - \vartheta I_n \) is nonsingular and so is

\[
K \triangleq \begin{bmatrix}
I_n & F_{k_0}(I_n - \vartheta \overline{E}_{k_0})^{-1} \\
0 & (\overline{E}_{k_0} - \vartheta I_n)^{-1}
\end{bmatrix}.
\]

In addition, pre-multiplying \( L_{k_0}^{-1}M_{k_0} \) by \( K \) gives

\[
K(L_{k_0}^{-1}M_{k_0} - \vartheta I_{2n}) = \begin{bmatrix}
E_{k_0} - \vartheta I_n + \vartheta F_{k_0}(I_n - \vartheta \overline{E}_{k_0})^{-1}F_{k_0} & 0 \\
(I_n - \vartheta \overline{E}_{k_0})^{-1}F_{k_0} & I_n
\end{bmatrix},
\]

implying that \( Z = \vartheta I_n - E_{k_0} + \vartheta F_{k_0}(\vartheta \overline{E}_{k_0} - I_n)^{-1}F_{k_0} \) is nonsingular.

For (b), manipulations show that \( \hat{H} = \beta \vartheta(\partial L_{k_0}^{-1}M_{k_0} - \vartheta I_n)^{-1}(\partial L_{k_0}^{-1}M_{k_0} + \vartheta I_n) \).

Then \( M_{k_0} [X_1^T, X_2^T]^T = L_{k_0} [X_1^T, X_2^T]^T S_{\alpha}^{2k_0} \) implies

\[
(L_{k_0}^{-1}M_{k_0} - \vartheta I_{2n})^{-1}(L_{k_0}^{-1}M_{k_0} + \vartheta I_{2n})[X_1^T, X_2^T]^T = [X_1^T, X_2^T]^T S_{\alpha}^{2k_0} (S_{\alpha}^{2k_0} - \vartheta I_{2n})^{-1}(S_{\alpha}^{2k_0} + \vartheta I_{2n})
\]

leading to \( \hat{H}[X_1^T, X_2^T]^T = [X_1^T, X_2^T]^T \partial (S_{\alpha}^{2k_0} - \vartheta I_{2n})^{-1}(S_{\alpha}^{2k_0} + \vartheta I_{2n}) \). Consequently, the result follows from the resulting equalities

\[
(\hat{H} + \beta \vartheta I_{2n})[X_1^T, X_2^T]^T = [X_1^T, X_2^T]^T(\partial S_{\alpha}^{2k_0} - \vartheta I_{2n})^{-1}(S_{\alpha}^{2k_0} + \vartheta I_{2n})
\]

For (c), \( \hat{A}^T = \hat{A} \) directly follows from its definition and the facts that \( E_{k_0}^{\dagger} = E_{k_0} \) and \( F_{k_0}^T = F_{k_0} \). For the symmetry of \( \hat{B} \), observe that

\[
\hat{B} = 2\beta \vartheta Z^{-1}F_{k_0}(E_{k_0} - \vartheta I_n)^{-1}
\]

\[
= 2\beta \vartheta(E_{k_0} - \vartheta I_n)^{-1}[I_n + \vartheta F_{k_0}(\vartheta \overline{E}_{k_0} - I_n)^{-1}F_{k_0}(\vartheta I_n - E_{k_0})^{-1}]^{-1}F_{k_0}(\vartheta I_n - E_{k_0})^{-1}
\]

\[
= 2\beta \vartheta(E_{k_0} - \vartheta I_n)^{-1}F_{k_0}[I_n + \vartheta(\overline{E}_{k_0} - I_n)^{-1}F_{k_0}(\vartheta I_n - E_{k_0})^{-1}F_{k_0}]^{-1}(\vartheta I_n - E_{k_0})^{-1}
\]

\[
= 2\beta \vartheta(E_{k_0} - \vartheta I_n)^{-1}F_{k_0}Z^{-1} = 2\beta \vartheta(E_{k_0} - \vartheta I_n)^{-1}F_{k_0}Z^{-1} = B^T.
\]

The proof is complete. \( \square \)

Theorem 18 implies \( \hat{H}[X_1^T, X_2^T]^T = \beta \vartheta[X_1^T, X_2^T]^T(S_{\alpha}^{2k_0} + \vartheta I_{2n})(S_{\alpha}^{2k_0} - \vartheta I_{2n})^{-1} \), hence each eigenvalue \( \lambda \) of \( H \) corresponds to an eigenvalue \( \mu \) of \( \hat{H} \):

\[
\mu = f(\lambda) \triangleq \beta \vartheta \cdot \frac{(\lambda + \alpha)^{2k_0} + \vartheta(\lambda - \alpha)^{2k_0}}{(\lambda + \alpha)^{2k_0} - \vartheta(\lambda - \alpha)^{2k_0}}.
\]

More specifically, for \( \lambda \in \lambda(H) \), we have

\[
\begin{cases}
\{ \mu, \overline{\mu} = f(\overline{\lambda}) \}, & -\mu = f(-\lambda), \quad -\overline{\mu} = f(-\overline{\lambda}) \subseteq \lambda(\hat{H}) \quad \text{if } \mathfrak{R}(\lambda) \overline{\mathfrak{R}}(\lambda) \neq 0; \\
\{ \mu, \overline{\mu} = f(-\lambda) \} \subseteq \lambda(\hat{H}) \quad \text{if } \mathfrak{R}(\lambda) = 0; \\
\{ \mu, \overline{\mu} = f(\overline{\lambda}) \} \subseteq \lambda(\hat{H}) \quad \text{if } \mathfrak{R}(\lambda) = 0.
\end{cases}
\]
In addition, \( \mu \in \lambda(\hat{H}) \) is purely imaginary if \( \lambda \in \lambda(H) \) is so. Equivalently, there exists no purely imaginary eigenvalues for \( \hat{H} \) when there is none for \( H \).

Next select \( \gamma \in \mathbb{R} \) with \( \gamma I_n - \hat{A} \) and \( I_n - (\gamma I_n - \hat{A})^{-1} \hat{B}(\gamma I_n - \hat{A})^{-1} \hat{B} \) being nonsingular. Theorem 9 could then be applied to \( \hat{A} \) and \( \hat{B} \), which are defined in Theorem 18, to obtain a new SSF-1 derived from \( H \). Thus, we have

\[
M_{k_0+1} \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = L_{k_0+1} \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \left[ \beta \vartheta (\alpha_{k_0}^2 + \vartheta I) (\alpha_{k_0}^2 - \vartheta I)^{-1} + \gamma I \right] \cdot \left[ \beta \vartheta (\alpha_{k_0}^2 + \vartheta I) (\alpha_{k_0}^2 - \vartheta I)^{-1} - \gamma I \right]^{-1},
\]

with

\[
M_{k_0+1} = \begin{bmatrix} E_{k_0+1} & 0 \\ F_{k_0+1} & I_n \end{bmatrix}, \quad L_{k_0+1} = \begin{bmatrix} I_n & \overline{F}_{k_0+1} \\ 0 & \overline{E}_{k_0+1} \end{bmatrix},
\]

\[
E_{k_0+1} = I_n - 2\gamma \left[ (\gamma I_n - \hat{A}) - \hat{B}(\gamma I_n - \hat{A})^{-1} \hat{B} \right]^{-1},
\]

\[
F_{k_0+1} = -2\gamma (\gamma I_n - \hat{A})^{-1} \hat{B} \left[ (\gamma I_n - \hat{A}) - \hat{B}(\gamma I_n - \hat{A})^{-1} \hat{B} \right]^{-1}.
\]

We call the above transform from \((M_{k_0}, L_{k_0})\) to \((M_{k_0+1}, L_{k_0+1})\), both symplectic, a DCT. Accordingly, with \( \delta_{\lambda} \triangleq (\lambda + \alpha)(\lambda - \alpha)^{-1}, |\delta_{\lambda}| < 1 \) and \( \varpi \triangleq (\beta - \vartheta \gamma)(\beta \vartheta + \gamma)^{-1} \), an eigenvalue \( \mu \) of \( \hat{H} \) (in (3.11)) would be transformed into an eigenvalue \( \nu \) of \((M_{k_0+1}, L_{k_0+1})\) via the following formula: (for \( \lambda \in \lambda(H) \))

\[
\nu \equiv \varrho(\mu) = \frac{\mu + \gamma}{\mu - \gamma}.
\]

One may consider the condition number of \( I_n - \overline{F}_{k_0+1} F_{k_0+1} \), or equivalently, the difference between 1 and \( \sigma(F_{k_0}) \). Obviously, \( \sigma(F_{k_0}) \) depends on \( \gamma \). Without loss of generality we assume \( \vartheta = 1 \), then with \( \gamma = \beta(\kappa_{k_0}^2 + 1)(\kappa_{k_0}^2 - 1)^{-1} \) (with \( \kappa \) to be specified), we have

\[
F_{k_0+1} = \frac{-\kappa_{k_0}^2 + 1}{\kappa_{k_0}^2 - 1} \left( \frac{Z}{\kappa_{k_0}^2 - 1} + I_n \right)^{-1} F_{k_0}(E_{k_0} - I_n)^{-1}
\]

\[
\cdot \left[ \left( \frac{Z}{\kappa_{k_0}^2 - 1} + I_n \right) - \overline{F}_{k_0}(E_{k_0} - I_n)^{-1} \left( \frac{Z}{\kappa_{k_0}^2 - 1} + I_n \right)^{-1} F_{k_0}(E_{k_0} - I_n)^{-1} \right]^{-1} Z.
\]

Thus we can choose some \( \kappa \) to make \( I_n - \overline{F}_{k_0+1} F_{k_0+1} \) well conditioned. We leave the issue of an optimal \( \kappa \) or \( \gamma \) for the future, while making random choices in our numerical experiments. Theorem 20 and Corollary 21 below illustrate that \( \kappa \) characterizes the convergence rate and does not have to be large.

With \( \gamma > 0 \) and \( \Re(\mu) < 0 \), we have \(|\nu(\mu)| < 1\). The following lemma reveals more.

**Lemma 19.** Provided that \( \vartheta, \gamma > 0 \), then each \( \nu \) corresponding to a non-purely imaginary eigenvalue \( \lambda \in \lambda(H) \) with \( \Re(\lambda) < 0 \) satisfies \(|\nu| < 1\).
Proof. Let \( \xi + i \eta = \phi = \delta_\lambda^{2k_0} \), we then have \(|\phi| = |\delta_\lambda|^{2k_0} \) and \(|\xi| \leq |\delta_\lambda|^{2k_0} \).
Consequently, from the definition of \( \nu \) we deduce that
\[
|\nu|^2 = \frac{(\xi^2 + \eta^2)(\beta \theta + \gamma)^2 + (\beta - \vartheta \gamma)^2 + 2 \delta \xi (\beta^2 - \gamma^2)}{(\beta \theta + \gamma)^2 + (\beta - \vartheta \gamma)^2 (\xi^2 + \eta^2) + 2 \delta \xi (\beta^2 - \gamma^2)}
\]
\[
= \frac{|\delta_\lambda|^{2k_0+1} + 2 \xi \varpi + \varpi^2}{|\delta_\lambda|^{2k_0+1} \varpi^2 + 2 \xi \varpi + 1}.
\]
(3.12)
Since \( \vartheta \beta, \gamma > 0 \) and the function defined in (3.12) is (i) monotone nondecreasing with respect to \( \xi \) when \( \beta > \vartheta \gamma \) or (ii) monotone non-increasing otherwise, we obtain
\[
|\nu|^2 \leq \begin{cases}
\frac{|\delta_\lambda|^{2k_0} (|\delta_\lambda|^{2k_0} + 2 \varpi) + \varpi^2}{|\delta_\lambda|^{2k_0} (2 \varpi + |\delta_\lambda|^{2k_0} \varpi^2) + 1}, & \text{if } \beta > \vartheta \gamma; \\
\frac{|\delta_\lambda|^{2k_0} (|\delta_\lambda|^{2k_0} - 2 \varpi) + \varpi^2}{|\delta_\lambda|^{2k_0} (-2 \varpi + |\delta_\lambda|^{2k_0} \varpi^2) + 1}, & \text{if } \beta < \vartheta \gamma;
\end{cases}
\]
which is equivalent to
\[
|\nu|^2 \leq \frac{|\delta_\lambda|^{2k_0}(|\delta_\lambda|^{2k_0} + 2|\varpi|) + \varpi^2}{|\delta_\lambda|^{2k_0} (2|\varpi| + |\delta_\lambda|^{2k_0} \varpi^2) + 1} = \left( \frac{|\delta_\lambda|^{2k_0} + |\varpi|}{|\delta_\lambda|^{2k_0} |\varpi| + 1} \right)^2.
\]
Obviously, \(|\delta_\lambda|^{2k_0} + |\varpi|(|\delta_\lambda|^{2k_0} |\varpi| + 1)^{-1} < 1 \) from \(|\varpi| = |\beta - \vartheta \gamma|/(\vartheta \beta + \gamma) < 1 \) and \(|\delta_\lambda| < 1 \), thus the result follows.

Lemma 19 demonstrates that for \( \lambda \in \lambda(H) \) satisfying \( \Re(\lambda) \neq 0 \), the DCT maps half of these \( \lambda \) to some values inside of the unit circle and the other half outside. Next we consider the detailed relationship between \( \nu \) and \( \varrho = \delta_\lambda^{2k_0} \), which is vital for the convergence of the DA coupled with the DCT.

Obviously, when \( \vartheta \beta, \gamma > 0 \), we have \(|\varpi| < 1 \). Taking \( \gamma = \beta(\kappa^{2k_0} + \varrho)(\vartheta \kappa^{2k_0} - 1)^{-1} > 0 \) with \( \kappa > 1 \), we obtain \( \varpi = -\kappa^{-2k_0} \) and
\[
\nu = \varrho \frac{|\delta_\lambda|^{2k_0-1} - \kappa^{-2k_0-1}}{|\delta_\lambda|^{2k_0-1} - \kappa^{-2k_0-1}},
\]
\[
\delta_\lambda^{2k_0-1} + \kappa^{-2k_0-1}.
\]
Denote \( \xi + i \eta = \delta_\lambda^{2k_0-1} \) and define
\[
\phi = \arctan \delta_\lambda^{2k_0-1}
\]
\[
= \frac{1}{2} \ln \frac{(\lambda - \alpha)^{2k_0-1} + (\alpha + \lambda)^{2k_0-1}}{(\lambda - \alpha)^{2k_0-1} - (\alpha + \lambda)^{2k_0-1}} + \frac{i}{2} \arg \frac{(\lambda - \alpha)^{2k_0-1} + (\lambda + \alpha)^{2k_0-1}}{(\lambda - \alpha)^{2k_0-1} - (\alpha + \lambda)^{2k_0-1}},
\]
\[
\psi = \arctanh \kappa^{-2k_0-1} = \frac{1}{2} \left[ \ln(1 + \sqrt{|\varpi|}) - \ln(1 - \sqrt{|\varpi|}) \right].
\]
We deduce that
\[
\arg \left[ \frac{(\lambda - \alpha)^{2k_0-1} + (\alpha + \lambda)^{2k_0-1}}{(\lambda - \alpha)^{2k_0-1} - (\alpha + \lambda)^{2k_0-1}} \right] = \arctan \frac{2 \eta}{1 - \xi^2 - \eta^2} \in \left( -\frac{\pi}{2}, \frac{\pi}{2} \right).
\]
Specifically, \( \arg \left[ \frac{(\lambda - \alpha)^{2k_0-1} + (\alpha + \lambda)^{2k_0-1}}{(\lambda - \alpha)^{2k_0-1} - (\alpha + \lambda)^{2k_0-1}} \right] = 0 \) when \( \lambda \in \mathbb{R} \). Moreover, by the definitions of \( \phi \) and \( \psi \), routine manipulations show that
\[
\nu = \varrho \tanh(\phi - \psi) \tanh(\phi + \psi)
\]
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with

$$\phi \pm \psi = \frac{1}{2} \ln \left[ \frac{\sqrt{\gamma + \vartheta \beta + \sqrt{\vartheta \gamma - \beta}} + \sqrt{\vartheta \gamma - \beta}}{\sqrt{\gamma + \vartheta \beta + \sqrt{\vartheta \gamma - \beta}}} \right] \sqrt{(1 + \xi)^2 + \eta^2} + \frac{i}{2} \arctan \frac{2\eta}{1 - \xi^2 - \eta^2}.$$ 

Under the assumptions in Lemma 19, the following theorem gives a sharp bound for those $|\nu|$ corresponding to $\lambda$ which satisfies $3(\lambda) \neq 0$ and $|\delta| < 1$.

**Theorem 20.** Assume that $\lambda$ is not a purely imaginary eigenvalue of $H$, $\vartheta \beta > 0$ and $\kappa \geq 2$. Then we have $|\nu| \leq \max \left\{ |\delta|^{2^k_0 - 2}, \kappa^{-2^k_0 - 2} \right\}$.

**Proof.** With $\gamma = \beta \frac{\kappa^{2^k_0 + \theta}}{\vartheta \kappa^{2^k_0 - 1}}$ and $\cos \left( \arctan \frac{2\eta}{1 - \xi^2 - \eta^2} \right) > 0$, we have

$$\left\{ \begin{array}{ll}
\ln \left[ \frac{\sqrt{\gamma + \vartheta \beta + \sqrt{\vartheta \gamma - \beta}} + \sqrt{\vartheta \gamma - \beta}}{\sqrt{\gamma + \vartheta \beta + \sqrt{\vartheta \gamma - \beta}}} \right] \sqrt{(1 + \xi)^2 + \eta^2} \geq 0, & \text{if } \frac{(1 + \xi)^2 + \eta^2}{(1 - \xi^2 + \eta^2)} \geq 1; \\
\ln \left[ \frac{\sqrt{\gamma + \vartheta \beta + \sqrt{\vartheta \gamma - \beta}} + \sqrt{\vartheta \gamma - \beta}}{\sqrt{\gamma + \vartheta \beta + \sqrt{\vartheta \gamma - \beta}}} \right] \sqrt{(1 + \xi)^2 + \eta^2} < 0, & \text{otherwise}.
\end{array} \right.$$ 

From Lemma 25 and $|(1 + \xi)^2 + \eta^2|/(1 - \xi^2 + \eta^2)^{-1} \geq 1 \iff \xi \geq 0$, we obtain

$$|\nu| < \begin{cases} 
\cosh(\phi - \psi), & \text{if } \xi > 0; \\
\cosh(\phi + \psi), & \text{if } \xi < 0.
\end{cases}$$

Now assume that $\xi > 0$ and we consider two distinct cases.

(i) When

$$\sqrt{(1 - \xi)^2 + \eta^2} \leq \frac{\sqrt{\gamma + \vartheta \beta - \sqrt{\vartheta \gamma - \beta}} \sqrt{(1 + \xi)^2 + \eta^2}}{\sqrt{\gamma + \vartheta \beta + \sqrt{\vartheta \gamma - \beta}}} \frac{(1 + \xi)^2 + \eta^2}{(1 - \xi)^2 + \eta^2} < 1$$

or

$$\frac{\sqrt{\gamma + \vartheta \beta - \sqrt{\vartheta \gamma - \beta}} \sqrt{(1 + \xi)^2 + \eta^2}}{\sqrt{\gamma + \vartheta \beta + \sqrt{\vartheta \gamma - \beta}}} \frac{(1 + \xi)^2 + \eta^2}{(1 - \xi)^2 + \eta^2} \geq 1,$$

we have

$$\ln \left[ \frac{(1 - \xi)^2 + \eta^2}{(1 + \xi)^2 + \eta^2} \right] \leq \ln \left[ \frac{\sqrt{\gamma + \vartheta \beta - \sqrt{\vartheta \gamma - \beta}} \sqrt{(1 + \xi)^2 + \eta^2}}{\sqrt{\gamma + \vartheta \beta + \sqrt{\vartheta \gamma - \beta}}} \frac{(1 + \xi)^2 + \eta^2}{(1 - \xi)^2 + \eta^2} \right] < 0$$

or

$$0 \leq \ln \left[ \frac{\sqrt{\gamma + \vartheta \beta - \sqrt{\vartheta \gamma - \beta}} \sqrt{(1 + \xi)^2 + \eta^2}}{\sqrt{\gamma + \vartheta \beta + \sqrt{\vartheta \gamma - \beta}}} \frac{(1 + \xi)^2 + \eta^2}{(1 - \xi)^2 + \eta^2} \right] \leq \ln \left[ \frac{(1 + \xi)^2 + \eta^2}{(1 - \xi)^2 + \eta^2} \right].$$

Hence by (c) and (b) in Lemma 25, it is apparent that

$$|\nu|^2 < |\tanh(\phi - \psi)|^2$$

$$\leq \left| \tanh \left\{ \frac{1}{2} \ln \left[ \frac{(1 + \xi)^2 + \eta^2}{(1 - \xi)^2 + \eta^2} \right] + \frac{i}{2} \arctan \frac{2\eta}{1 - \xi^2 - \eta^2} \right\} \right|^2$$

$$= |\tanh(\phi)|^2 = |\delta_\lambda|^{2^k_0},$$

implying that $|\nu| < |\delta_\lambda|^{2^k_0 - 1}$. 14
(ii) When

\[
\frac{\sqrt{\gamma + \beta^2} - \sqrt{\delta^2 - \beta}}{\sqrt{\gamma + \beta^2} + \sqrt{\delta^2 - \beta}} \sqrt{(1 + \xi)^2 + \eta^2} < \sqrt{(1 - \xi)^2 + \eta^2} < 1,
\]

we define \( \tilde{\xi} + i\tilde{\eta} = \delta_{\lambda}^2 \) and without loss of generality assume that \( \tilde{\xi} > 0 \), which satisfies \( \tilde{\xi} > |\tilde{\eta}| \) for \( 0 < \xi = \tilde{\xi}^2 - \tilde{\eta}^2 \). Similar to (i), we obtain

\[
|\nu| < |\tanh(\phi - \psi)| = |\tanh(\tilde{\phi} - \tilde{\psi})| < |\tanh(\tilde{\phi} - \tilde{\psi})|,
\]

where \( \tilde{\phi} = \arctanh \delta_{\lambda}^2 \) and \( \tilde{\psi} = \arctanh \kappa^{-2\kappa_{0}^{-2}} \). Since \( \xi = \tilde{\xi}^2 - \tilde{\eta}^2 > 0 \) and \( |\tilde{\xi}|^2 + |\tilde{\eta}|^2 = |\delta_{\lambda}|^2 \), we have \( \xi^2 > \frac{1}{2} |\delta_{\lambda}|^2 \), leading to

\[
|\nu|^2 < |\tanh(\tilde{\phi} - \tilde{\psi})|^2
\]

\[
= \kappa^{-2\kappa_{0}^{-2}} - 1 + \frac{|\delta_{\lambda}|^2 \kappa_{0}^{-1} + 2\tilde{\xi}}{1 - |\delta_{\lambda}|^2 \kappa_{0}^{-1}} + \frac{|\delta_{\lambda}|^2 \kappa_{0}^{-1} - 2\tilde{\xi}}{1 - |\delta_{\lambda}|^2 \kappa_{0}^{-1}}.
\]

Since \( |\tanh(\tilde{\phi} - \tilde{\psi})|^2 \) is monotonically nonincreasing with respect to \( \tilde{\xi} \), taking \( \tilde{\xi} = \frac{1}{\sqrt{2}} |\delta_{\lambda}|^2 \) in the above formula yields

\[
|\nu|^2 < |\tanh(\tilde{\phi} - \tilde{\psi})|^2 < \frac{1 + |\delta_{\lambda}|^2 \kappa_{0}^{-1} - \sqrt{2} \kappa_{0}^{-2} |\delta_{\lambda}|^2 \kappa_{0}^{-2}}{1 - |\delta_{\lambda}|^2 \kappa_{0}^{-1} - \sqrt{2} \kappa_{0}^{-2} |\delta_{\lambda}|^2 \kappa_{0}^{-2}}
\]

\[
= \kappa^{-2\kappa_{0}^{-1}} \left[ \frac{(2 - 1/2 \kappa_{0}^{-2} |\delta_{\lambda}|^2 \kappa_{0}^{-1} - 1)^2 + 2 - 1/2 \kappa_{0}^{-1} |\delta_{\lambda}|^2 \kappa_{0}^{-1}}{(2 - 1/2 \kappa_{0}^{-2} |\delta_{\lambda}|^2 \kappa_{0}^{-1} - 1)^2 + 2 - 1/2 \kappa_{0}^{-1} |\delta_{\lambda}|^2 \kappa_{0}^{-1}} \right].
\]

(3.13)

\[
= |\delta_{\lambda}|^2 \kappa_{0}^{-1} \left[ \frac{(\kappa_{0}^{-2} - 2 - 1/2 |\delta_{\lambda}|^2 \kappa_{0}^{-1} - 1)^2 + 2 - 1/2 |\delta_{\lambda}|^2 \kappa_{0}^{-1}}{(\kappa_{0}^{-2} - 2 - 1/2 |\delta_{\lambda}|^2 \kappa_{0}^{-1} - 1)^2 + 2 - 1/2 |\delta_{\lambda}|^2 \kappa_{0}^{-1}} \right].
\]

(3.14)

Obviously for \( \kappa \geq 2 \), we obtain \( |\nu|^2 < |\tanh(\tilde{\phi} - \tilde{\psi})|^2 < 1/2 \). Hence, by Lemma 26, when either

(a) \( 2^{-1/2} (|\delta_{\lambda}| \kappa)^{2\kappa_{0}^{-2}} \leq \frac{1}{2} \), i.e., \( (|\delta_{\lambda}| \kappa)^{2\kappa_{0}^{-2}} \leq 1/\sqrt{2} \); or

(b) \( \frac{1}{2} < 2^{-1/2} (|\delta_{\lambda}| \kappa)^{2\kappa_{0}^{-2}} \leq 1 - 2^{-1/2} |\delta_{\lambda}|^2 \kappa_{0}^{-2} \), i.e.,

\[
(|\delta_{\lambda}| \kappa)^{2\kappa_{0}^{-2}} \geq 1/\sqrt{2}, \quad |\delta_{\lambda}|^2 \kappa_{0}^{-2} (\kappa_{0}^{-2} + \kappa_{0}^{-2}) \leq \sqrt{2},
\]

the quantity in the square brackets in (3.13) would be no greater than 1. This indicates that \( |\nu|^2 \leq \kappa^{-2\kappa_{0}^{-1}} \) or \( |\nu| < \kappa^{-2\kappa_{0}^{-2}} \).

When

\[
(|\delta_{\lambda}| \kappa)^{2\kappa_{0}^{-2}} \geq 1/\sqrt{2}, \quad |\delta_{\lambda}|^2 \kappa_{0}^{-2} (\kappa_{0}^{-2} + \kappa_{0}^{-2}) > \sqrt{2},
\]

which imply \( |\delta_{\lambda}|^2 \kappa_{0}^{-2} > \sqrt{2}/(\kappa_{0}^{-2} + \kappa_{0}^{-2}) \), we obtain

\[
|\delta_{\lambda}|^{2\kappa_{0}^{-2}} + |\delta_{\lambda}|^{-2\kappa_{0}^{-2}} < \frac{\sqrt{2} \kappa_{0}^{-2}}{\sqrt{2} \kappa_{0}^{-1} + 1} + \frac{\kappa_{0}^{-1} + 1}{\sqrt{2} \kappa_{0}^{-2}} < \kappa_{0}^{-2} \kappa_{0}^{-2},
\]

(3.15)
where the first ‘<’ follows from the fact that the function $f(x) = x + x^{-1}$ is monotonically decreasing when $x < 1$. Thus, the assumption $\kappa \geq 2$ and (3.15) together affirm that $2^{-1/2}\delta_\lambda L |\delta_\chi^2|^{2k_0-2} < 2^{-1}\kappa^{2k_0-2}$ and $2^{-1/2}\delta_\chi |\delta_\lambda |^{2k_0-2} \leq \kappa^{2k_0-2} - 2^{-1/2}|\delta_\lambda|^2|^{2k_0-2}$. Again using Lemma 26, we know that the quantity in the square brackets in (3.14) is no greater than 1, suggesting that the value of the right-hand-side of (3.14) will be no greater than $|\delta_\chi|^{2k_0-1}$, or equivalently $|\nu| < |\delta_\chi|^{2k_0-2}$.

Consequently, the result holds for the case when $\xi > 0$. The $\xi < 0$ case can be proved similarly and we omit the details.

For a real $\lambda \in \lambda(H)$, we can obtain a better result, with the power $2^{k_0-2}$ replaced by $2^{k_0}$ in the following corollary.

**Corollary 21.** Let $\kappa > 1$ and $\vartheta \beta, \alpha > 0$, then for $\lambda < 0$ ($\lambda \in \lambda(H)$), we have $|\nu| \leq \max\left\{ |\delta_\chi|^{2k_0}, \kappa^{-2k_0} \right\}$.

**Proof.** Let $\phi = \text{arctanh}(\delta_\chi^2)$, then $\phi = \frac{1}{2} \ln\left[ \frac{(\lambda-\alpha)^2 + (\lambda+\alpha)^2}{(\lambda-\alpha)^2 - (\lambda+\alpha)^2} \right] > 0$ since $\lambda < 0$, and $\psi = \text{arctanh}(-\kappa^{-2\phi}) = -\frac{1}{2} \ln\left( \frac{\kappa^{2\phi} - 1}{\kappa^{2\phi} + 1} \right) < 0$. From the definition of $\nu$, we have $\nu = \vartheta \tanh(\phi + \psi)$. Because $\tanh(\omega) = (e^\omega - e^{-\omega})/(e^\omega + e^{-\omega})^{-1}$, $\tanh(-\omega) = -\tanh(\omega)$ and $\tanh(\omega)$ is nondecreasing with respect to $\omega \in \mathbb{R}$, then when $\phi \geq |\psi|$ we have $0 \leq |\nu| = \tanh(\phi + \psi) \leq \tanh(\phi)$. Otherwise for $\phi < |\psi|$, we have $|\nu| = \tanh(-\psi - \phi) < \tanh(-\psi) = \kappa^{-2\phi}$. Hence, the result holds.

To sum up, we propose the DCT to avoid the potential interruption of the DA caused by $1 \in \sigma(F_k_0)$ for some $k_0$. We have conducted a detailed analysis on the eigenvalue $\nu$ of the new pair $(M_{k_0+1}, L_{k_0+1})$, produces a sharp bound of $|\nu|$ in Theorem 20 relative to $|\delta_\chi|^{2k_0-2}$. Furthermore, Theorem 20 and Corollary 21 imply that a double-Cayley step reverses the convergence at worst by two steps in general and not at all when $\lambda$ is real. This guarantees the convergence of the DA when the DCT is only occasionally called for. Similar comments apply when there exist some singular value $\sigma \in \sigma(F_k_0)$ close to unity, meaning $I - T_k_0 F_k_0$ is ill-conditioned, and the double-Cayley remedy is applied.

Note that the DCT is applicable when $\vartheta \notin \lambda(E_{k_0})$ with $\vartheta \in \{-1, 1\}$. In the rare occasions when the condition is violated, the three-recursion remedy proposed in subsection 3.4 will be employed.

We construct an example to show the need for the DCT.

**Example 3.1.** Let $A = A^\dagger, B = B^\dagger \in \mathbb{C}^{5 \times 5}$ with

$$A = \begin{bmatrix} 0.6607 & 0.1299 - 0.1365 i & 0.0632 - 0.0086 i & -0.0341 - 0.0517 i & -0.0628 - 0.0446 i \\ 0.1299 + 0.1365 i & 0.2441 - 0.1293 - 0.1035 i & -0.0363 + 0.1567 i & 0.1042 + 0.1268 i \\ 0.0632 + 0.0086 i & -0.1293 + 0.1035 i & 0.6772 & 0.0236 + 0.0491 i & 0.0542 + 0.0113 i \\ -0.0341 + 0.0517 i & -0.0363 + 0.1567 i & 0.0236 - 0.0491 i & 0.6804 - 0.0326 + 0.0427 i \\ -0.0628 + 0.0446 i & 0.1042 - 0.1268 i & 0.0542 - 0.0113 i & -0.0326 - 0.0427 i & 0.6787 \end{bmatrix},$$

$$B = \begin{bmatrix} 0.5704 + 0.2081 i & -0.4605 - 0.0322 i & 0.1693 - 0.3006 i & -0.1181 + 0.4597 i & 0.2109 + 0.8779 i \\ 0.4605 + 0.0322 i & -0.5737 - 0.1759 i & -0.1520 + 0.0419 i & 0.1526 - 0.0408 i & 0.1452 - 0.2288 i \\ -0.0628 - 0.0446 i & 0.1526 - 0.0408 i & 0.4908 - 0.7534 i & 0.1880 - 0.0406 i & -0.1733 + 0.1743 i \\ 0.1693 + 0.3006 i & 0.1783 - 0.0406 i & -0.1783 - 0.6552 i & -0.5212 + 0.1871 i & 0.2109 + 0.8779 i \\ 0.2109 + 0.8779 i & -0.1522 + 0.2288 i & -0.1733 - 0.1743 i & -0.5212 + 0.1871 i & 0.2548 - 0.7032 i \end{bmatrix}.$$

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By setting $\alpha = 1$ and with the formulae in Theorem 9, we have $E_0 = E_\alpha$ and $F_0 = F_\alpha$:

$$E_0 = \begin{bmatrix} 1.2482 & 0.4505 & -0.4735i & 0.2193 + 0.0298i & -0.1182 - 0.1794i & -0.2179 - 0.0152i \\ 0.4505 + 0.4735i & -0.1966 & -0.4485 - 0.3591i & 0.1259 + 0.5435i & 0.3613 + 0.4371i \\ 0.2193 + 0.0298i & 0.1966 & 0.0817 + 0.1703i & 0.1880 + 0.6039i \\ -0.1182 + 0.1794i & -0.4485 - 0.3591i & 0.0817 - 0.1703i & 1.3166 & -0.1132 + 0.1482i \\ -0.2179 + 0.0152i & 0.3613 - 0.4371i & 0.1880 - 0.0391i & -0.1132 - 0.1482i & 1.3105 \\ \end{bmatrix},$$

$$F_0 = \begin{bmatrix} -1.0682 + 0.5623i & -0.8603 + 0.0680i & 0.3168 + 0.5662i & -0.2188 - 0.8623i & 0.3967 - 0.1673i \\ -0.8603 + 0.0680i & 0.0883 - 0.3226i & -0.2885 - 0.0846i & 0.2898 + 0.0828i & 0.2745 + 0.4354i \\ 0.3168 + 0.5662i & -0.2885 - 0.0846i & 0.9207 + 1.1403i & 0.3503 + 0.0768i & -0.3258 + 0.3298i \\ -0.2188 - 0.8623i & -0.2898 - 0.0828i & 0.3503 + 0.0765i & -0.3329 + 2.1301i & 0.9749 - 0.3506 \\ -0.3967 - 0.1673i & 0.2745 + 0.4354i & -0.3258 + 0.3298i & -0.9749 - 0.3516i & -0.4766 + 1.3105i \\ \end{bmatrix}. $$

Applying the DA to $E_0$ and $F_0$ for 5 iterations, we obtain:

$$E_5 = \begin{bmatrix} 1.5012 & -0.0992 + 0.1043i & -0.0483 + 0.0066i & 0.0260 + 0.0395i & 0.0480 + 0.034i \\ -0.0992 - 0.1043i & 1.8195 & 0.0988 + 0.0791i & 0.0277 - 0.1197i & -0.0796 - 0.0963i \\ -0.0483 - 0.0066i & 0.0988 - 0.0791i & 1.4886 & -0.01180 - 0.0375i & -0.0414 - 0.0086i \\ 0.0260 - 0.0395i & 0.0277 + 0.1197i & -0.0180 + 0.0375i & 1.4861 & 0.0249 - 0.0326i \\ 0.0480 - 0.034i & -0.0796 - 0.0963i & -0.0414 + 0.0086i & 0.0249 + 0.0326i & 1.4757 \\ \end{bmatrix},$$

$$F_5 = \begin{bmatrix} -0.9956 + 0.6352i & -0.7338 - 0.3015i & 0.2834 + 0.6319i & -0.1291 - 0.8499i & 0.4238 - 0.2379 \\ -0.7338 + 0.3015i & -0.5359 - 0.0786i & -0.3942 - 0.2753i & -0.4018 + 0.2612i & 0.3380 + 0.6318i \\ 0.2834 + 0.6319i & -0.3942 - 0.2753i & 0.9025 + 1.2990i & 0.2689 + 0.0968i & -0.3410 - 0.3895i \\ -0.1291 - 0.8499i & -0.4018 + 0.2612i & 0.2689 + 0.0968i & 0.2733 + 1.2440i & -0.8719 - 0.3476i \\ 0.4238 - 0.2379i & -0.3380 + 0.6318i & -0.3410 + 0.3895i & -0.8719 + 0.3476i & -0.4230 + 1.2123i \\ \end{bmatrix}. $$

The singular values [10] of $F_5$ are {1.9376, 1.9376, 1.9376, 1.9376, 1}. Hence, the next doubling step breaks down and the DCT is required to carry the DA forward.

### 3.4. Three-recursion remedy

This subsection is devoted to resolve the issue that the DCT fails. Especially, one may apply the three-recursion remedy from this section when two step reversions occur with some complex eigenvalues for $H$.

Let $Z = Z^T \in \mathbb{C}^{n \times n}$ (which may be chosen randomly) and $I_n + F_k Z$ be nonsingular. Write $P_k = (I_n + F_k Z)^{-1} E_k$, $G_k = (I_n + F_k Z)^{-1} F_k^T$ and $H_k = (F_k + Z) - E_k^T Z (I_n + F_k Z)^{-1} E_k$. The following lemma shows how we transform the two recursions for $E_k$ and $F_k$ to three.

**Lemma 22.** For the decomposition (2.1) it holds that

$$[P_k \ 0] \begin{bmatrix} I & 0 \\ H_k & I_n \end{bmatrix} [I \ -Z \ I_n] = X_2 \begin{bmatrix} W_{1,\omega} & X_2 & Z_{1,\omega} \end{bmatrix} X_1 \begin{bmatrix} W_{2,\omega} & X_1 & Z_{2,\omega} \end{bmatrix} \hat{S}^{Z^2_k}_{\alpha},$$

where $X_1, X_2, W_{1,\omega}, W_{2,\omega}, Z_{1,\omega}, Z_{2,\omega}$ and $\hat{S}^{Z^2_k}_{\alpha}$ are defined as in (3.8).

**Proof.** Define $\Phi = \begin{bmatrix} (I_n + F_k Z)^{-1} & 0 \\ -E_k^T Z (I_n + F_k Z)^{-1} & I_n \end{bmatrix}$, then we deduce that

$$\begin{bmatrix} E_k & 0 \\ F_k & I_n \end{bmatrix} \begin{bmatrix} I_n & 0 \\ Z & I_n \end{bmatrix} = \begin{bmatrix} P_k & 0 \\ H_k & I_n \end{bmatrix}, \quad \begin{bmatrix} I_n & G_k \\ 0 & P_k^T \end{bmatrix} \begin{bmatrix} I_n & 0 \\ Z & I_n \end{bmatrix} = \begin{bmatrix} I_n & G_k \\ 0 & P_k^T \end{bmatrix}.$$

With $\begin{bmatrix} I_n & 0 \\ Z & I_n \end{bmatrix}^{-1} = \begin{bmatrix} I_n & 0 \\ -Z & I_n \end{bmatrix}$, the result follows from (3.8). $\square$

Since $F_k^T = F_k$ and $Z^T = Z$, we have $G_k^T = G_k$ and $H_k^T = H_k$. Applying the doubling algorithms [18] for CARE and DARE, provided that $(I_n - G_{k+j-1} H_{k+j-1})^{-1}$
are well-defined for \( j \geq 1 \), we formulate the three recursions for \( P_{k+j}, G_{k+j} \) and \( H_{k+j} \) as below:

\[
P_{k+j} = P_{k+j-1}(I_n - G_{k+j-1} H_{k+j-1})^{-1} P_{k+j-1}, \\
G_{k+j} = G_{k+j-1} + P_{k+j-1}(I_n - G_{k+j-1} H_{k+j-1})^{-1} G_{k+j-1} P_{k+j-1}^T, \\
H_{k+j} = H_{k+j-1} + P_{k+j-1}^T H_{k+j-1}(I_n - G_{k+j-1} H_{k+j-1})^{-1} P_{k+j-1},
\]

where \( G_{k+j}^T = G_{k+j} \) and \( H_{k+j}^T = H_{k+j} \). It is worthwhile to point that when \( I_n - G_{k+j} H_{k+j} \) is singular or ill-conditioned, we can always randomly choose some other \( Z^T = Z \in \mathbb{C}^{n \times n} \) and construct \( \Psi \in \mathbb{C}^{2n \times 2n} \) such that

\[
\begin{bmatrix}
P_{k+j} & 0 \\
H_{k+j} & I_n
\end{bmatrix}
\begin{bmatrix}
I_n & 0 \\
Z & I_n
\end{bmatrix}
= \begin{bmatrix}
\tilde{P}_{k+j} & 0 \\
\tilde{H}_{k+j} & I_n
\end{bmatrix},
\begin{bmatrix}
I_n & G_{k+j} \\
0 & P_{k+j}^T
\end{bmatrix}
\begin{bmatrix}
I_n & 0 \\
Z & I_n
\end{bmatrix}
= \begin{bmatrix}
I_n & \tilde{G}_{k+j} \\
0 & \tilde{P}_{k+j}^T
\end{bmatrix}.
\]

Provided that \( I_n - G_{k+j} H_{k+j} \) are well-conditioned for all \( j \geq 0 \), the following two theorems demonstrate the convergence of the three recursions specified in (3.17).

**Theorem 23.** Upon the assumption in Theorem 15, it holds that \( \lim_{k \to \infty} P_k = 0 \) and \( \lim_{k \to \infty} H_k = Z - X_2 X_1^{-1} \), both converging quadratically.

**Proof.** The results follow from the fact

\[
\begin{bmatrix}
P_k & 0 \\
H_k & I_n
\end{bmatrix}
\begin{bmatrix}
X_1 & \bar{X}_2 \\
X_2 - ZX_1 & \bar{X}_1 - Z \bar{X}_2
\end{bmatrix}
= \begin{bmatrix}
I_n & G_k \\
0 & P_k^T
\end{bmatrix}
\begin{bmatrix}
X_1 & \bar{X}_2 \\
X_2 - ZX_1 & \bar{X}_1 - Z \bar{X}_2
\end{bmatrix}
\begin{bmatrix}
S^2 & \bar{S}^{2e} \\
\bar{S}_e & S^{-2e}_e
\end{bmatrix}
\]

and \( \lim_{k \to \infty} S^2 = 0 \). We omit the details, as in [18, Corollary 3.2].

**Theorem 24.** Under the assumption in Theorem 16, it holds that \( \lim_{k \to \infty} P_k = 0 \) and \( \lim_{k \to \infty} H_k = Z - X_2 X_1^{-1} \), both converging linearly.

**Proof.** By (3.16) and similar to the proof of Theorem 16, we obtain the result.

**4. Numerical Results.** We illustrate the performance of the DA with some test examples, three of which from discretized Bethe-Salpeter equations and one generated by the \texttt{randn} command in MATLAB. We also apply \texttt{eig} in MATLAB (as in \texttt{eig}(H) and \texttt{eig}(GH, G)) and Algorithm 1 in [29] to the test examples for comparison. Computing \( \text{eig}(GH, G) \) is based on the equivalence of \( Hx = \lambda x \) and

\[
\begin{bmatrix}
A \\
B
\end{bmatrix} x = \lambda \begin{bmatrix}
I_n & 0 \\
0 & -I_n
\end{bmatrix} x.
\]

No DCT or three-recursion remedy was required. All algorithms are implemented in MATLAB 2012b on a 64-bit PC with an Intel Core i7 processor at 3.4 GHz and 8G RAM.

**Example 4.1.** We consider three examples from the discretized Bethe-Salpeter equations for naphthalene (C_{10}H_{8}), gallium arsenide (GaAs) and boron nitride (BN). The dimensions of the corresponding \( H \) associated with C_{10}H_{8}, GaAs and BN are respectively 64, 256 and 4608. All eigenpairs of \( H \) are computed.

Using \texttt{eig}(H) as the baseline for comparison, we present the relative accuracy of the computed eigenvalues and the execution time (eTime) of the other three algorithms, all averaged over 50 trials. For the relative accuracy, we compute prec =
\[ \log_{10} \left( \max_j |(\lambda_j - \tilde{\lambda}_j) / \lambda_j| \right) \] where \( \lambda_j \) and \( \tilde{\lambda}_j \) are the computed eigenvalues by the \texttt{eig}(H) command and one of the methods, respectively. The residuals

\[ \frac{\| H - [X, \Pi \Xi] \text{diag}(S, S)[X, \Pi \Xi]^{-1} F \|_F}{\| H \|_F}, \quad \frac{\| Y^H X - \Lambda \|_F}{\| H \|_F}, \]

respectively for the DA, \texttt{eig}(\Gamma^H, \Gamma) and \cite[Algorithm 1]{29} are displayed, with \( Y \) and \( X \) being respectively the left and right eigenvector matrices and \( \Lambda \) the diagonal matrix containing the eigenvalues of \( H \) (please refer to \cite{29} for details). Also, the numbers of iterations required for doubling averaged over 50 trails are presented. It is worthwhile to point out that for the DA all \( \alpha \)'s in the 50 trails are generated by the function \texttt{randn}. The results are tabulated in Table 1.

| C10Hs | DA algorithm 1 in \cite{29} \textbf{eig}(\Gamma H, \Gamma) |
|-------|-------------------------------------------------|
| prec  | \(-13.99\)                                      |
| residual | \(8.14 \times 10^{-16}\)                     |
| \(e\)Time | \(7.958 \times 10^{-1}\)                    |
| iteration | \(6.84\)                                       |
| GaAs  | \(-13.99\)                                      |
| residual | \(6.86 \times 10^{-16}\)                     |
| \(e\)Time | \(5.881 \times 10^{-1}\)                    |
| iteration | \(8.46\)                                       |
| BN    | \(-13.99\)                                      |
| residual | \(7.50 \times 10^{-16}\)                     |
| \(e\)Time | \(6.610 \times 10^{-1}\)                    |
| iteration | \(7.44\)                                       |

Table 1

Numerical results for Example 4.1

Table 1 demonstrates that all three methods produce comparable results in terms of the relative accuracy. The DA spends slightly more time than the other methods but produces more accurate solutions with smaller residuals.

**Example 4.2.** The test example, randomly generated by the command \texttt{randn} in MATLAB, is designed to illustrate the structure-preserving property of the DA, a distinct feature of our method. The defining matrices are

\[
H = \begin{bmatrix}
A & B \\
-B & -A
\end{bmatrix}, \quad A = \begin{bmatrix}
A_1 & A_2 \\
A_3
\end{bmatrix}, \quad B = \begin{bmatrix}
B_1 & B_2 \\
B_3
\end{bmatrix}
\]
with

\[
A_1 = \begin{bmatrix}
2.6361 & 1.0378 \times 10^1 & 5.0751 \times 10^{-2} \\
1.0378 \times 10^1 & 5.2431 \times 10^{-2} & -4.6067 \times 10^{-1} \\
5.0751 \times 10^{-2} & -4.6067 \times 10^{-1} & -1.6892 \times 10^{-2}
\end{bmatrix},
\]
\[
A_2 = \begin{bmatrix}
-4.0549 \times 10^{-1} & -3.7710 + 2.7569i \\
-3.7710 - 2.7569i & -4.0549 \times 10^{-1}
\end{bmatrix},
\]
\[
A_3 = \begin{bmatrix}
3.6378 \times 10^{-1} & 2.7293 \times 10^{-1} + 3.5908i \\
2.7293 \times 10^{-1} - 3.5908i & 3.6378 \times 10^{-1}
\end{bmatrix},
\]
\[
B_1 = \begin{bmatrix}
-2.6361 & -1.0375 \times 10^1 \\
-1.0375 \times 10^1 & -5.3457 \times 10^{-2} \\
-5.1181 \times 10^{-2} & 5.0988 \times 10^{-1}
\end{bmatrix},
\]
\[
B_2 = \begin{bmatrix}
1.2343 \times 10^{-1} - 3.8788i \times 10^{-1} & 3.7566 - 2.7464i \\
3.7566 - 2.7464i & 4.0704 \times 10^{-1} + 6.0156i \times 10^{-5}
\end{bmatrix},
\]
\[
B_3 = \begin{bmatrix}
3.6148 \times 10^{-1} - 5.5211i \times 10^{-2} & -2.7152 \times 10^{-1} - 3.5722i \\
-2.7152 \times 10^{-1} - 3.5722i & -3.6567 \times 10^{-1} + 5.9265i \times 10^{-5}
\end{bmatrix}.
\]

The spectrum of \( H \) is

\[
\lambda(H) = \{ \pm 4.1204 \times 10^{-3}, \pm 4.1204 \times 10^{-3}, \pm 4.1204 \times 10^{-3}, \\
\pm 4.0549 \times 10^{-1} \pm 5.9927i \times 10^{-5}, \pm 3.6378 \times 10^{-1} \pm 5.8959i \times 10^{-5} \}.
\]

Note that the algebraic and the geometric multiplicities of \( \pm 4.1204 \times 10^{-3} \) are 3 and 1, respectively. The DA, \( \text{eig}(H) \) and \( \text{eig}(\Gamma H, \Gamma) \) produce the eigenvalues \( \lambda_D, \lambda_E \) and \( \lambda_{Ge} \) respectively:

\[
\lambda_D = \{ \pm 4.1092 \times 10^{-3}, \pm 4.1092 \times 10^{-3}, \pm 4.1092 \times 10^{-3}, \\
\pm 4.0549 \times 10^{-1} \pm 5.9927i \times 10^{-5}, \pm 3.6378 \times 10^{-1} \pm 5.8959i \times 10^{-5} \},
\]
\[
\lambda_E = \{ 4.1137 \times 10^{-3} - 1.1615i \times 10^{-5}, 4.1136 \times 10^{-3} + 1.1614i \times 10^{-5}, \\
4.1338 \times 10^{-3} + 1.2681i \times 10^{-9}, -4.1136 \times 10^{-3} - 1.1649i \times 10^{-5}, \\
-4.1136 \times 10^{-3} - 1.1650i \times 10^{-5}, -4.1338 \times 10^{-3} - 1.3011i \times 10^{-9}, \\
\pm 4.0549 \times 10^{-1} \pm 5.9927i \times 10^{-5}, \pm 3.6378 \times 10^{-1} \pm 5.8959i \times 10^{-5} \},
\]
\[
\lambda_{Ge} = \{ 4.1272 \times 10^{-3} - 1.1919i \times 10^{-5}, 4.1272 \times 10^{-3} - 1.1919i \times 10^{-5}, \\
4.1272 \times 10^{-3} - 1.1919i \times 10^{-5}, -4.1272 \times 10^{-3} + 1.1851i \times 10^{-5}, \\
-4.1272 \times 10^{-3} + 1.1851i \times 10^{-5}, -4.1272 \times 10^{-3} + 1.1851i \times 10^{-5}, \\
\pm 4.0549 \times 10^{-1} \pm 5.9927i \times 10^{-5}, \pm 3.6378 \times 10^{-1} \pm 5.8959i \times 10^{-5} \}.
\]

Although all three methods produce computed eigenvalues of low relative accuracy, with \( \text{precDA} = -2.5680 \), \( \text{precEE} = -2.4862 \) and \( \text{precGe} = -2.4764 \), the DA preserves the distinct eigen-structure of \( H \). All eigenvalues from DA appear in quadruples \( \{ \lambda, -\lambda, -\lambda, \lambda \} \subseteq \lambda(H) \), unless when \( \Im(\lambda) = 0 \) then in pairs \( \{ \lambda, -\lambda \} \subseteq \lambda(H) \). The low accuracy (in the order of \( \pm 4.1204 \times 10^{-3} \)) of the computed eigenvalues from the methods can be attributed to the defective eigenvalues. Note that Algorithm 1 in [29] failed because the required assumption \( \Gamma H > 0 \) is not satisfied.

5. Conclusions. In this paper, we propose a doubling algorithm for the discretized Bethe-Salpeter eigenvalue problem, where the Hamiltonian-like matrix \( H \) is firstly transformed to a symplectic pair with special structure then \( E_k = E_k^H \) and \( F_k = F_k^H \) are computed iteratively. Theorems are proved on the quadratic convergence of the algorithm if no purely imaginary eigenvalues exist (and linear convergence otherwise). The simple double-Cayley transform is designed to deal with any potential
breakdown when 1 is in or close to $\sigma(F_k)$ for some $k$. We also prove that at most two steps of retrogression occur (for complex eigenvalues of $H$, but none for real ones). In addition, a three-recursion remedy is put forward when the double-Cayley transform fails. Numerical examples have been presented to illustrate the efficiency and the distinct structure-preserving nature of the doubling method. The optimal choice of $\alpha$ and the removal of the invertibility assumption of $X_1$ (or $[X_1, \Psi_{11}]$ if purely imaginary eigenvalues exist) will be left for future research.

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**Appendix A. Useful Lemmas.** The following lemmas are required in Section 3.

**Lemma 25.** Given $\omega, \zeta \in \mathbb{R}$, it holds that
(a) $|\tanh(-\omega + i\zeta)|^2 = |\tanh(\omega + i\zeta)|^2 = |e^{2\omega} + e^{-2\omega} - 2\cos(2\zeta)|[e^{2\omega} + e^{-2\omega} + 2\cos(2\zeta)]^{-1}$;
(b) $|\tanh(\omega + i\zeta)|^2 < 1$ when $\cos(2\zeta) > 0$; and
(c) for $\cos(2\zeta) > 0$, $|\tanh(\omega + i\zeta)|^2$ is monotonically nondecreasing with respect to $\omega$ when $\omega \geq 0$, and monotonically nonincreasing otherwise.

**Proof.** Simple computations lead to the two results (a) and (b), and we omit the details here. For (c), we have $\partial \tanh(\omega + i\zeta)/\partial \omega = [8(e^{2\omega} - e^{-2\omega})\cos(2\zeta)]/[e^{2\omega} + e^{-2\omega} + 2\cos(2\zeta)]^{-1}$. Since $\cos(2\zeta) > 0$, the result follows.

**Lemma 26.** Define $f(\xi) = (\xi - \tau)^2 + \xi^2$, then for $0 \leq \xi \leq \frac{\tau}{2}$, we have
(a) $f(\xi) = f(\tau - \xi)$;
(b) $f(\xi) \geq f(\eta) \geq \frac{\tau^2}{2}$ for all $\eta$ with $\frac{\tau}{2} \geq \eta \geq \xi$; and
(c) $f(\xi) \geq f(\eta) \geq \frac{1}{16}$ for all $\eta$ with $\tau - \xi \geq \eta \geq \frac{\tau}{2}$.

**Proof.** From the fact that $(\xi, \xi)$ and $(1 - \xi, 1 - \xi)$ are two symmetrical points with respect to the line $g(\omega) = -\omega + \tau$, the result follows with details omitted.

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