THE HAMILTONIAN EXTENDED KRYLOV SUBSPACE METHOD*

PETER BENNER†, HEIKE FAßBENDER‡, AND MICHEL-NIKLAS SENN‡

Abstract. An algorithm for constructing a J-orthogonal basis of the extended Krylov subspace $\mathcal{K}_{r,s} = \text{range}\{u, Hu, H^2u, \ldots, H^{2r-1}u, H^{-1}u, H^{-2}u, \ldots, H^{-2s}u\}$, where $H \in \mathbb{R}^{2n\times 2n}$ is a large (and sparse) Hamiltonian matrix is derived (for $r = s+1$ or $r = s$). Surprisingly, this allows for short recurrences involving at most five previously generated basis vectors. Projecting H onto the subspace $\mathcal{K}_{r,s}$ yields a small Hamiltonian matrix. The resulting HEKS algorithm may be used in order to approximate $f(H)u$ where f is a function which maps the Hamiltonian matrix H to, e.g., a (skew-)Hamiltonian or symplectic matrix. Numerical experiments illustrate that approximating $f(H)u$ with the HEKS algorithm is competitive for some functions compared to the use of other (structure-preserving) Krylov subspace methods.

Key words. (Extended) Krylov Subspace, Hamiltonian, Symplectic, Matrix Function Evaluation.

AMS subject classifications. 65F25, 65F50, 65F60, 15A23.

1. Introduction. Let $H \in \mathbb{R}^{2n\times 2n}$ be a nonsingular (large-scale) Hamiltonian matrix, that is $J_nH = (J_nH)^T$, where $J_n = \left[\begin{smallmatrix} 0 & I_n \\ -I_n & 0 \end{smallmatrix}\right] \in \mathbb{R}^{2n\times 2n}$ and I_n is the $n \times n$ identity matrix. We are interested in computing a J-orthogonal basis of the extended Krylov subspace

$$\mathcal{K}_{r,s} := \mathcal{K}_{2r}(H, u) + \mathcal{K}_{2s}(H^{-1}, H^{-1}u) = \text{range}\{u, Hu, H^2u, \ldots, H^{2r-1}u, H^{-1}u, H^{-2}u, \ldots, H^{-2s}u\}, \tag{1.1}$$

where $u \in \mathbb{R}^{2n}$ and either $r = s+1$ or $r = s$. That is, assuming

$$\dim \mathcal{K}_{2r}(H, u) = 2r \quad \text{and} \quad \dim \mathcal{K}_{2s}(H^{-1}, H^{-1}u) = 2s,$$

we are looking for a matrix $S_{r+s} \in \mathbb{R}^{2n\times 2(r+s)}$ with J-orthonormal columns ($S_{r+s}^T J_n S_{r+s} = J_{r+s}$) such that the columns of S_{r+s} span the same subspace as $\mathcal{K}_{2r}(H, u) + \mathcal{K}_{2s}(H^{-1}, H^{-1}u)$.

Extended Krylov subspaces

$$\text{range}\{b, A^{-1}b, Ab, A^{-2}b, A^2b, \ldots, A^{-k}b, A^kb\} = \mathcal{K}_k(A, b) + \mathcal{K}_k(A^{-1}, A^{-1}b)$$

for general nonsingular matrices $A \in \mathbb{C}^{n\times n}$ and a vector $b \in \mathbb{C}^n$ have been used for the numerical approximation of $f(A)b$ for a function f and a large matrix A at least since the late 1990s mainly inspired by [7, 15]. In case an orthogonal matrix V has been constructed such that $\text{range}(V) = \mathcal{K}_k(A, b) + \mathcal{K}_k(A^{-1}, A^{-1}b)$, an approximation to $f(A)b$ can be obtained as

$$f(A)b \approx Vf(V^TAV)V^Tb. \tag{1.2}$$

More on functions of matrices, the computation of $f(A)b$ and the approximation of $f(a)b$ via Krylov subspace methods can be found in the all-encompassing monograph [14].

*Received by the editors on Month/Day/Year. Accepted for publication on Month/Day/Year. Handling Editor: Name of Handling Editor. Corresponding Author: Heike Faßbender

†Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstr. 1, 39106 Magdeburg, Germany (benner@mpi-magdeburg.mpg.de)

‡ Institute for Numerical Analysis, TU Braunschweig, Universitätsplatz 2, 38106 Braunschweig, Germany (h.fassbender@tu-braunschweig.de, m.senn@tu-braunschweig.de)

The idea of constructing a J-orthogonal basis for the extended Krylov subspace $\mathcal{K}_{r,s}$ (1.1) has first been considered in [20] in the context of approximating $\exp(H)u$. The Hamiltonian Extended Krylov Subspace (short HEKS) method presented in [20] is a straightforward adaption of the algorithm for computing an orthogonal basis of an extended Krylov subspace described in [15]. Our main finding in this paper is the observation that the HEKS algorithm allows for a short recurrence to generate S_{r+s}.

We will explore the use of an J-orthogonal basis S_{r+s} of the extended Krylov subspace $\mathcal{K}_{r,s}$ (1.1) for approximating $f(H)u$ for a (large-scale) Hamiltonian matrix H and a vector $u \in \mathbb{R}^{2n}$. Following the idea from (1.2) we have

$$f(H)u \approx S_{r+s} f(H_{r+s}) J_{r+s}^T S_{r+s}^T J_n u$$

where $H_{r+s} = J_{r+s}^T S_{r+s}^T J_n H S_{r+s} \in \mathbb{R}^{2(r+s)\times 2(r+s)}$ is a Hamiltonian matrix. That is, we can preserve the rich structural information inherent to the Hamiltonian structure of the matrix H. This would not be possible by computing a standard (orthogonal) basis $V \in \mathbb{R}^{2n\times 2(r+s)}$ of $\mathcal{K}_{r,s}$ as the matrix product $V^T H V$ will in general not be a Hamiltonian matrix even if H is Hamiltonian. Hence, the HEKS algorithm may be used in particular in order to approximate $f(H)u$ where f is a function which maps the Hamiltonian matrix H to a structured matrix such as a (skew-)Hamiltonian or symplectic matrix. Such a structure-preserving approximation of $f(H)u$ is, e.g., important in the context of symplectic exponential integrators for Hamiltonian systems, see, e.g., [8, 10, 19, 20]. A structure-preserving approximation of $f(H)u$ may also be computed using, e.g., an J-orthogonal basis $\tilde{S}_{2k}$ of the standard Krylov subspace range$\{u, Hu, H^2u \ldots, H^{2k-1}u\}$. Such a basis can be generated by the Hamiltonian Lanczos method [4, 5, 22]. Both approaches will be compared later on.

The paper is structured as follows: Section 2 summarizes some basic well-known facts about Hamiltonian and J-orthogonal matrices. In Section 3 the general idea of generating the desired J-orthogonal basis S_{r+s} of (1.1) as proposed in [20] is sketched. Then, it is noted that the projected matrices $H_{r+s} = J_{r+s}^T S_{r+s}^T J_n H S_{r+s}$ and $J_{r+s}^T S_{r+s}^T J_n H^{-1} S_{r+s}$ have at most $10k$, resp. $10k+2$, nonzero entries. The details are given in Section 4 and in Section 5. The resulting efficient HEKS algorithm using short recursions is summarized in Section 6. The rather long and technical constructive proof for our claim is deferred to the Appendix A. In Section 7 the approximation of $f(H)u$ using the HEKS algorithm is compared to the approximation by the extended Krylov subspace method [16] and by the Hamiltonian Lanczos method [5].

2. Preliminaries. Here we list some properties of Hamiltonian and J-orthogonal matrices useful for the following discussion.

1. $J_n = \left[\begin{smallmatrix} 0 & I_n \\ -I_n & 0 \end{smallmatrix}\right] \in \mathbb{R}^{2n\times 2n}$ is orthogonal and skew-symmetric, $J_n^T = J_n^{-1} = -J_n$.
2. Let $H \in \mathbb{R}^{2n\times 2n}$. H is Hamiltonian if and only if there exist matrices E, $B = B^T$, $C = C^T \in \mathbb{R}^{n\times n}$ such that
$$H = \begin{bmatrix} E & B \\ C & -E^T \end{bmatrix}.$$
3. Let $H \in \mathbb{R}^{2n\times 2n}$ be a nonsingular Hamiltonian matrix. Then H^{-1} is Hamiltonian as well.
4. The eigenvalues of a Hamiltonian matrix H occur in pairs $\{\lambda, -\lambda\}$ if λ is real or purely imaginary, or in quadruples $\{\lambda, \overline{\lambda}, -\lambda, -\overline{\lambda}\}$ otherwise. That is, the spectrum of a Hamiltonian matrix is symmetric with respect to both the real and the imaginary axis.
5. A matrix $S \in \mathbb{R}^{2n\times 2n}$ is called *symplectic* if $S^T J_n S = J_n$. Its columns are *J-orthogonal*.
6. Let $S \in \mathbb{R}^{2n\times 2n}$ be a symplectic matrix. Then $S^{-1} = J_n^T S^T J_n$ is symplectic as well.
7. Let $H \in \mathbb{R}^{2n\times 2n}$ be a Hamiltonian matrix and $S \in \mathbb{R}^{2n\times 2n}$ be a symplectic matrix. Then $S^{-1}HS$ is a Hamiltonian matrix.

8. Let $S \in \mathbb{R}^{2n\times 2m}, m \leq n$, have J-orthogonal columns, $S^T J_n S = J_m$. Let $H \in \mathbb{R}^{2n\times 2n}$ be Hamiltonian.
   (a) The matrix $J_m^T S^T J_n$ is the left inverse of S, $J_m^T S^T J_n S = I_{2m}$.
   (b) The matrix $(J_m^T S^T J_n) H S$ is Hamiltonian.

Numerous further properties of the sets of these matrices (and their interplay) have been studied in the literature, see, e.g., [17] and the references therein. In particular, J_n induces a skew-symmetric bilinear form $\langle \cdot, \cdot \rangle_{J_n}$ on $\mathbb{R}^{2n}$ defined by $\langle x, y \rangle_{J_n} = y^T J_n x$ for $x, y \in \mathbb{R}^{2n}$. Hamiltonian matrices are skew-adjoint with respect to the bilinear form $\langle \cdot, \cdot \rangle_{J_n}$, while symplectic matrices are orthogonal with respect to $\langle \cdot, \cdot \rangle_{J_n}$. The $2n \times 2n$ symplectic matrices form a Lie group, the $2n \times 2n$ Hamiltonian matrices the associated Lie algebra.

Assume that a matrix $S_k = [V_k \quad W_k] \in \mathbb{R}^{2n\times 2k}$ with J-orthogonal columns is given with $V_k = [v_1 \ \ v_2 \ \ \cdots \ \ v_k]$ and $W_k = [w_1 \ \ w_2 \ \ \cdots \ \ w_k] \in \mathbb{R}^{2n\times k}$. Two additional vectors $x, J_n x \in \mathbb{R}^{2n}$ can be added to S_k to generate a matrix $S_{k+1} = [V_{k+1} \quad W_{k+1}] \in \mathbb{R}^{2n\times 2k+2}$ with J-orthogonal columns by J-orthogonalizing the vectors x and $J_n x$ against all column vectors v_j, w_j of S_k via

$$\begin{aligned} v_{k+1} &= x - S_k J_k^T S_k^T J_n x, \\ w_{k+1} &= (J_n v_{k+1}) - S_k J_k^T S_k^T J_n (J_n v_{k+1}), \quad w_{k+1} = w_{k+1}/(v_{k+1}^T J_n w_{k+1}). \end{aligned}$$

3. Idea of the HEKS Algorithm. Let a Hamiltonian matrix $H \in \mathbb{R}^{2n\times 2n}$ and a vector $u_1 \in \mathbb{R}^{2n}$, $\|u_1\|_2 = 2$, be given. Assume that $\dim \mathcal{K}_{2r}(H, u_1) = 2r$ and $\dim \mathcal{K}_{2s}(H^{-1}, H^{-1}u_1) = 2s$. The goal is to construct a matrix $S_{r+s} \in \mathbb{R}^{2n\times 2(r+s)}$ with J-orthonormal columns ($S_{r+s}^T J_n S_{r+s} = J_{r+s}$) such that the columns of S_{r+s} span the same subspace as $\mathcal{K}_{2r}(H, u_1) + \mathcal{K}_{2s}(H^{-1}, H^{-1}u_1)$.

In [20] it is suggested to construct the matrix S_{r+s} in the following way (assuming that no breakdown occurs):

1. We start with the two vectors in $\mathcal{K}_2(H, u_1)$ and construct

$$S_1 = \begin{bmatrix} u_1 \mid v_1 \end{bmatrix} \in \mathbb{R}^{2n\times 2}$$

   with $S_1^T J_n S_1 = J_1$ and $\operatorname{range}\{S_1\} = \mathcal{K}_2(H, u_1)$. This corresponds to the choice $r = 1, s = 0$.
2. Thereafter we take the two vectors in $\mathcal{K}_2(H^{-1}, H^{-1}u_1)$ and construct

$$S_2 = \begin{bmatrix} y_1 \quad u_1 \mid x_1 \quad v_1 \end{bmatrix} = \begin{bmatrix} Y_1 \quad U_1 \mid X_1 \quad V_1 \end{bmatrix} \in \mathbb{R}^{2n\times 4}$$

   with $S_2^T J_n S_2 = J_2$ and $\operatorname{range}\{S_2\} = \mathcal{K}_2(H, u_1) + \mathcal{K}_2(H^{-1}, H^{-1}u_1)$. This corresponds to the choice $r = s = 1$.

We proceed in this fashion by alternating between the subspaces $\mathcal{K}_{2r}(H, u_1)$ and $\mathcal{K}_{2s}(H^{-1}, H^{-1}u_1)$. Assume that a matrix

$$S_{2k} = \begin{bmatrix} Y_k \quad U_k \mid X_k \quad V_k \end{bmatrix} \in \mathbb{R}^{2n\times 4k}, \qquad Y_k, U_k, X_k, V_k \in \mathbb{R}^{2n\times k}$$

with J-orthonormal columns has been constructed such that its columns span the same space as $\mathcal{K}_{2k}(H, u_1) + \mathcal{K}_{2k}(H^{-1}, H^{-1}u_1)$. The following three steps are repeated until the desired symplectic basis has been generated:

(3) Construct u_{k+1} and v_{k+1} and set

$$S_{2k+1} = \begin{bmatrix} Y_k \quad U_k \quad u_{k+1} \mid X_k \quad V_k \quad v_{k+1} \end{bmatrix} = \begin{bmatrix} Y_k \quad U_{k+1} \mid X_k \quad V_{k+1} \end{bmatrix} \in \mathbb{R}^{2n\times 4k+2}$$

with

$$U_{k+1} = \begin{bmatrix} U_k & u_{k+1} \end{bmatrix}, V_{k+1} = \begin{bmatrix} V_k & v_{k+1} \end{bmatrix} \in \mathbb{R}^{2n \times k+1}$$

such that $S_{2k+1}^T J_n S_{2k+1} = J_{2k+1}$ and range$\{S_{2k+1}\} = \mathcal{K}_{2k+2}(H, u_1) + \mathcal{K}_{2k}(H^{-1}, H^{-1}u_1)$. The new vectors are added as the last column to the U, resp. V-matrix.

(4) Construct y_{k+1} and x_{k+1} and set

$$S_{2k+2} = \begin{bmatrix} y_{k+1} & Y_k & U_{k+1} \mid x_{k+1} & X_k & V_{k+1} \end{bmatrix} = \begin{bmatrix} Y_{k+1} & U_{k+1} \mid X_{k+1} & V_{k+1} \end{bmatrix} \in \mathbb{R}^{2n \times 4k+4}$$

with

$$Y_{k+1} = \begin{bmatrix} y_{k+1} & Y_k \end{bmatrix}, X_{k+1} = \begin{bmatrix} x_{k+1} & X_k \end{bmatrix} \in \mathbb{R}^{2n \times k+1}$$

such that $S_{2k+2}^T J_n S_{2k+2} = J_{2k+2}$ and range$\{S_{2k+2}\} = \mathcal{K}_{2k+2}(H, u_1) + \mathcal{K}_{2k+2}(H^{-1}, H^{-1}u_1)$. The new vectors are added as the first column to the Y, resp. X-matrix.

(5) Set $k = k + 1$.

We refrain from restating the algorithm given in [20] which implements the approach stated above in a straightforward way using long recurrences. As usual, a Krylov recurrence of the form

$$HS_{2k} = S_{2k}H_{2k} + \text{ some rest term},$$

for $r = s = k$ and

$$HS_{2k+1} = S_{2k+1}H_{2k+1} + \text{some rest term}$$

for $r = s + 1 = k$ holds, where $H_{2k} = J_{2k}^T S_{2k}^T J_n H S_{2k} \in \mathbb{R}^{4k \times 4k}$ and $H_{2k+1} = J_{2k+1}^T S_{2k+1}^T J_n H S_{2k+1} \in \mathbb{R}^{4k+2 \times 4k+2}$ are Hamiltonian matrices. In the next two sections we describe the very special forms of the projected matrices H_{2k} and H_{2k+1} as well as $J_{2k}^T S_{2k}^T J_n H^{-1} S_{2k}$ and $J_{2k+1}^T S_{2k+1}^T J_n H^{-1} S_{2k+1}$. These matrices have at most $10k$, resp. $10k + 2$, nonzero entries. A constructive proof for our claim is given in Appendix A, while the resulting efficient HEKS algorithm using short recursions is summarized in Section 6.

4. Projection $J_{r+s}^T S_{r+s}^T J_n H S_{r+s}$ of the Hamiltonian matrix H.

Assume that

$$S_{r+s} = \begin{bmatrix} Y_s & U_r \mid X_s & V_r \end{bmatrix}, \qquad Y_s, X_s \in \mathbb{R}^{2n \times s}, \quad U_r, V_r \in \mathbb{R}^{2n \times r},$$

with J-orthogonal columns has been constructed with the HEKS algorithm (as before, we assume that $r = s$ or $r = s + 1$). Then the projected Hamiltonian matrix

$$H_{r+s} = J_{r+s}^T S_{r+s}^T J_n H S_{r+s} \in \mathbb{R}^{2(r+s) \times 2(r+s)}$$

has a very special form with at most $2r + 8s$ nonzero entries. Let us first note that

$$H_{r+s} = \begin{bmatrix} -X_s^T J_n H Y_s & -X_s^T J_n H U_r & -X_s^T J_n H X_s & -X_s^T J_n H V_r \\ -V_r^T J_n H Y_s & -V_r^T J_n H U_r & -V_r^T J_n H X_s & -V_r^T J_n H V_r \\ Y_s^T J_n H Y_s & Y_s^T J_n H U_r & Y_s^T J_n H X_s & Y_s^T J_n H V_r \\ U_r^T J_n H Y_s & U_r^T J_n H U_r & U_r^T J_n H X_s & U_r^T J_n H V_r \end{bmatrix},$$

where the blocks are of size either $s \times s$, $r \times r$, $s \times r$, or $r \times s$. As will be proven in Appendix A, ten of these blocks are zero, three are diagonal (denoted by $\Delta_s, \Theta_r, \Lambda_s$), one symmetric tridiagonal (denoted by T_r) and two anti-bidiagonal (denoted by B_{sr}), i.e.,

$$H_{r+s} = \begin{bmatrix} 0 & 0 & \Lambda_s & B_{sr} \\ 0 & 0 & B_{sr}^T & T_r \\ \Delta_s & 0 & 0 & 0 \\ 0 & \Theta_r & 0 & 0 \end{bmatrix} \tag{4.3}$$

with

$$\Delta_s = \operatorname{diag}(\delta_s, \ldots, \delta_1) \in \mathbb{R}^{s \times s}, \qquad T_r = \begin{bmatrix} \alpha_1 & \beta_2 & & \\ \beta_2 & \ddots & \ddots & \\ & \ddots & \ddots & \beta_r \\ & & \beta_r & \alpha_r \end{bmatrix} \in \mathbb{R}^{r \times r},$$
$$\Theta_r = \operatorname{diag}(\vartheta_1, \ldots, \vartheta_r) \in \mathbb{R}^{r \times r},$$
$$\Lambda_s = \operatorname{diag}(\lambda_s, \ldots, \lambda_1) \in \mathbb{R}^{s \times s},$$

and either

$$B_{r-1,r} = \begin{bmatrix} & & & \gamma_{r-1} & \mu_r \\ & & \iddots & \mu_{r-1} & \\ & \iddots & \iddots & & \\ \gamma_1 & \mu_2 & & & \end{bmatrix} \in \mathbb{R}^{r-1 \times r} \qquad \text{if} \quad r = s+1,$$

or

$$B_{rr} = \begin{bmatrix} & & & \gamma_r \\ & & \iddots & \mu_r \\ & \iddots & \iddots & \\ \gamma_1 & \mu_2 & & \end{bmatrix} \in \mathbb{R}^{r \times r} \qquad \text{if} \quad r = s.$$

In particular, it holds for $j = 1, \ldots, s$

$$\delta_j = y_j^T J_n H y_j, \qquad \lambda_j = -x_j^T J_n H x_j,$$

and for $j = 1, \ldots, r$

$$\vartheta_j = u_j^T J_n H u_j, \qquad \alpha_j = -v_j^T J_n H v_j, \qquad \gamma_j = -x_j^T J_n H v_j,$$

and for $j = 2, \ldots, r$

$$\beta_j = -v_j^T J_n H v_{j-1} \qquad\qquad \mu_j = -x_{j-1}^T J_n H v_j.$$

We summarize this in the following theorem.

THEOREM 4.1. *Let $H \in \mathbb{R}^{2n \times 2n}$ be a Hamiltonian matrix. Let $r + s = n$ and either $r = s + 1$ or $r = s$. Then in case the procedure described in Section 3 does not break down for $u_1 \in \mathbb{R}^{2n}$ with $\|u_1\|_2 = 1$ there exists a symplectic matrix $S \in \mathbb{R}^{2n \times 2n}$ such that $Se_{s+1} = u_1$,*

$$\operatorname{range}\{S\} = \mathcal{K}_{2r}(H, u_1) + \mathcal{K}_{2s}(H^{-1}, H^{-1}u_1),$$

and

$$S^{-1}HS = H_{r+s}$$

with $H_{r+s} = H_n$ as in (4.3).

Proof. A constructive proof is given in Section A. □

REMARK 4.2. *In case the Hamiltonian matrix H can be written in the form $H = JK$ with the symmetric matrix K and K is positive definit, all inner products of the form $w^T JHw$ and $w^T JH^{-1}w$ are negative, as $w^T JHw = w^T JJKw = -w^T Kw < 0$ and as with K its inverse is symmetric and positive definite. Thus, in this case, all δ_j and ϑ_j are negative, while all λ_j and α_j are positive. Such Hamiltonian matrices have been considered in [1, 2].*

Theorem 4.1 implies

$$H \begin{bmatrix} Y_k & U_k & X_k & V_k \end{bmatrix} = S \left[\begin{array}{c|c||c|c} 0 & 0 & 0 & 0 \\ 0 & 0 & \Lambda_k & B_{kk} \\ \hline 0 & 0 & B_{kk}^T & T_k \\ 0 & 0 & \mu_{k+1} e_1^T & \beta_{k+1} e_k^T \\ 0 & 0 & 0 & 0 \\ \hline\hline 0 & 0 & 0 & 0 \\ \Delta_k & 0 & 0 & 0 \\ \hline 0 & \Theta_k & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array}\right].$$

From this, we obtain the HEKS-recursion for $r = s = k$

$$HS_{2k} = S_{2k} H_{2k} + \mu_{k+1} u_{k+1} e_{2k+1}^T + \beta_{k+1} u_{k+1} e_{4k}^T, \tag{4.4}$$

while for $r = s + 1 = k + 1$ we have

$$HS_{2k+1} = S_{2k+1} H_{2k+1} + (\gamma_{k+1} y_{k+1} + \beta_{k+2} u_{k+2}) e_{4k+2}^T. \tag{4.5}$$

5. Projection $J_{r+s}^T S_{r+s}^T J_n H^{-1} S_{r+s}$ of the Hamiltonian matrix H^{-1}. Assume that Theorem 4.1 holds. As $H_n = S^{-1} H S \in \mathbb{R}^{2n\times 2n}$ is Hamiltonian, its inverse $H_n^{-1} = S^{-1} H^{-1} S$ is Hamiltonian as well. Not only H_n has a nice sparse structure (4.3), but also its inverse. From that we can derive the special forms of $J_{2k}^T S_{2k}^T J_n H^{-1} S_{2k}$ and $J_{2k+1}^T S_{2k+1}^T J_n H^{-1} S_{2k+1}$.

Let $S = S_n = \begin{bmatrix} Y_s & U_r \mid X_s & V_r \end{bmatrix} \in \mathbb{R}^{2n\times 2n}$, $Y_s, X_s \in \mathbb{R}^{2n\times s}$, $U_r, V_r \in \mathbb{R}^{2n\times r}$, where $r + s = n$ and either $r = s$ or $r = s + 1$. Due to $S_n^{-1} = J_n^T S_n^T J_n$, we have

$$\begin{aligned} H_n^{-1} &= \begin{bmatrix} -X_s^T J_n H^{-1} Y_s & -X_s^T J_n H^{-1} U_r & -X_s^T J_n H^{-1} X_s & -X_s^T J_n H^{-1} V_r \\ -V_r^T J_n H^{-1} Y_s & -V_r^T J_n H^{-1} U_r & -V_r^T J_n H^{-1} X_s & -V_r^T J_n H^{-1} V_r \\ Y_s^T J_n H^{-1} Y_s & Y_s^T J_n H^{-1} U_r & Y_s^T J_n H^{-1} X_s & Y_s^T J_n H^{-1} V_r \\ U_r^T J_n H^{-1} Y_s & U_r^T J_n H^{-1} U_r & U_r^T J_n H^{-1} X_s & U_r^T J_n H^{-1} V_r \end{bmatrix} \\ &= \begin{bmatrix} 0 & 0 & \Delta_s^{-1} & 0 \\ 0 & 0 & 0 & \Theta_r^{-1} \\ E_s & G_{sr} & 0 & 0 \\ G_{sr}^T & F_r & 0 & 0 \end{bmatrix} \end{aligned}$$

with $E_s \in \mathbb{R}^{s\times s}$, $F_r \in \mathbb{R}^{r\times r}$, $G_{sr} \in \mathbb{R}^{s\times r}$ such that

$$\begin{bmatrix} \Lambda_s & B_{sr} \\ B_{sr}^T & T_r \end{bmatrix} \begin{bmatrix} E_s & G_{sr} \\ G_{sr}^T & F_r \end{bmatrix} = I$$

holds and $\Delta_s, \Theta_r, \Lambda_s, T_r, B_{sr}$ from (4.3). The matrices E_s, F_r and G_{sr} have a special structure like Λ_s, T_r and B_{sr}: F_r is diagonal, G_{sr} anti-bidiagonal as B_{sr} and E_s is symmetric tridiagonal;

$$F_r = \operatorname{diag}(f_{11}, f_{22}, \ldots, f_{rr}), \qquad E_s = \begin{bmatrix} e_{ss} & e_{s-1,s} & & \\ e_{s-1,s} & \ddots & \ddots & \\ & \ddots & \ddots & e_{12} \\ & & e_{12} & e_{11} \end{bmatrix} = E_s^T,$$

and either

$$G_{r-1,r} = \begin{bmatrix} & & & g_{r-1,r-1} & g_{r-1,r} \\ & & \iddots & g_{r-2,r-1} & \\ & g_{22} & \iddots & & \\ g_{11} & g_{12} & & & \end{bmatrix} \in \mathbb{R}^{r-1\times r} \qquad \text{if} \quad r = s+1,$$

or

$$G_{rr} = \begin{bmatrix} & & & g_{rr} \\ & & \iddots & g_{r-1,r} \\ & g_{22} & \iddots & \\ g_{11} & g_{12} & & \end{bmatrix} \in \mathbb{R}^{r\times r} \qquad \text{if} \quad r = s.$$

Next, the projected matrices $J_{2k}^T S_{2k}^T J_n H^{-1} S_{2k}$ and $J_{2k+1}^T S_{2k+1}^T J_n H^{-1} S_{2k+1}$ will be described. Let

$$\mathfrak{E}_j = \begin{bmatrix} I_j \\ 0 \end{bmatrix} \in \mathbb{R}^{r\times j}, \qquad \mathfrak{F}_\ell = \begin{bmatrix} 0 \\ I_\ell \end{bmatrix} \in \mathbb{R}^{s\times \ell}, \qquad \mathfrak{T}_{\ell j} = \begin{bmatrix} \mathfrak{F}_\ell & & & \\ & \mathfrak{E}_j & & \\ & & \mathfrak{F}_\ell & \\ & & & \mathfrak{E}_j \end{bmatrix} \in \mathbb{R}^{2n\times 2(\ell+j)}$$

for $j \leq r$, $\ell \leq s$. Thus, for $2k \leq n$ it holds

$$S_n \mathfrak{T}_{kk} = S_{2k} \in \mathbb{R}^{2n\times 4k} \qquad \text{and} \qquad S_n \mathfrak{T}_{k,k+1} = S_{2k+1} \in \mathbb{R}^{2n\times 4k+2},$$

as well as

$$\begin{aligned} S_n J_n \mathfrak{T}_{kk} &= \begin{bmatrix} -X_k & -V_k & Y_k & U_k \end{bmatrix} = S_{2k} J_{2k} \in \mathbb{R}^{2n\times 4k}, \\ S_n J_n \mathfrak{T}_{k,k+1} &= \begin{bmatrix} -X_k & -V_{k+1} & Y_k & U_{k+1} \end{bmatrix} = S_{2k+1} J_{2k+1} \in \mathbb{R}^{2n\times 4k+2}. \end{aligned}$$

Hence, we obtain

$$\begin{aligned} J_{2k}^T S_{2k}^T J_n H^{-1} S_{2k} &= \mathfrak{T}_{kk}^T J_n^T S_n^T J_n H^{-1} S_n \mathfrak{T}_{kk} = \mathfrak{T}_{kk}^T H_n^{-1} \mathfrak{T}_{kk} = \mathfrak{T}_{kk}^T \begin{bmatrix} 0 & 0 & \Delta_s^{-1} & 0 \\ 0 & 0 & 0 & \Theta_r^{-1} \\ E_s & G_{sr} & 0 & 0 \\ G_{sr}^T & F_r & 0 & 0 \end{bmatrix} \mathfrak{T}_{kk} \\ &= \begin{bmatrix} 0 & 0 & \mathfrak{F}_k^T \Delta_s^{-1} \mathfrak{F}_k & 0 \\ 0 & 0 & 0 & \mathfrak{E}_k^T \Theta_r^{-1} \mathfrak{E}_k \\ \mathfrak{F}_k^T E_s \mathfrak{F}_k & \mathfrak{F}_k^T G_{sr} \mathfrak{E}_k & 0 & 0 \\ \mathfrak{E}_k^T G_{sr}^T \mathfrak{F}_k & \mathfrak{E}_k^T F_r \mathfrak{E}_k & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & \Delta_k^{-1} & 0 \\ 0 & 0 & 0 & \Theta_k^{-1} \\ E_k & G_{kk} & 0 & 0 \\ G_{kk}^T & F_k & 0 & 0 \end{bmatrix} \end{aligned} \tag{5.6}$$

and

$$J_{2k+1}^T S_{2k+1}^T J_n H^{-1} S_{2k+1} = \mathfrak{T}_{k,k+1}^T J_n^T S_n^T J_n H^{-1} S_n \mathfrak{T}_{k,k+1} = \begin{bmatrix} 0 & 0 & \Delta_k^{-1} & 0 \\ 0 & 0 & 0 & \Theta_{k+1}^{-1} \\ E_k & G_{k,k+1} & 0 & 0 \\ G_{k,k+1}^T & F_{k+1} & 0 & 0 \end{bmatrix}. \tag{5.7}$$

The HEKS-recurrences for H^{-1} are given by

$$H^{-1} S_{2k} = S_{2k} \left(J_{2k}^T S_{2k}^T J_n H^{-1} S_{2k} \right) + (e_{2k,2k+1} x_{2k+1} + g_{2k,2k+1} v_{2k+1}) e_1^T \tag{5.8}$$

and

$$H^{-1}S_{2k+1} = S_{2k+1}\left(J_{2k+1}^T S_{2k+1}^T J_n H^{-1} S_{2k+1}\right) + x_{2k+1}(e_{2k,2k+1}e_1^T + g_{2k+1,2k+1}e_{2k+1}^T). \tag{5.9}$$

6. HEKS Algorithm. The HEKS algorithm is summarized in Fig. 1. The algorithm as given assumes that no breakdown occurs. Clearly, any division by zero will result in a serious breakdown. As can be seen from (4.4) a lucky breakdown occurs in case $\mu_{k+1} = \beta_{k+1} = 0$ or $u_{k+1} = 0$, as range$\{S_{2k}\} = \mathcal{K}_{2k}(H, u_1) + \mathcal{K}_{2k}(H^{-1}, H^{-1}u_1)$ is H-invariant. Moreover, (4.5) shows that in case $\gamma_{k+1} = \beta_{k+2} = 0$, a lucky breakdown occurs, as range$\{S_{2k+1}\} = \mathcal{K}_{2k+2}(H, u_1) + \mathcal{K}_{2k}(H^{-1}, H^{-1}u_1)$ is H-invariant. Similarly, lucky breakdown can be read off of (5.8) and (5.9) resulting in an H^{-1}-invariant subspace.

In case the Hamiltonian matrix H can be written in the form $H = JK$ with a symmetric positive definite matrix K, all inner products of the form $w^T JHw$ and $w^T JH^{-1}w$ are negative (see Remark 4.2). Hence, most scalars by which is divided in Algorithm 1 are nonzero and do not cause breakdown.

Implemented efficiently such that each matrix-vector product as well as each linear solve is computed only once, the algorithm requires (for adding 4 vectors) in the for-loop

- 4 matrix-vector-multiplications with H,
- 3 linear solves with H (efficiently implemented in the form $(JH)x = (Jb)$ making use of the symmetry of JH),
- 14 scalar products.

Any multiplication of a vector w by J_n should be implemented by rearranging the upper and the lower part of the vector w. That is, let $w = \left[\begin{smallmatrix} w_1 \\ w_2 \end{smallmatrix}\right]$, then $J_n w = \left[\begin{smallmatrix} w_2 \\ -w_1 \end{smallmatrix}\right]$.

Without some form of re-J-orthogonalization the HEKS algorithm suffers from the same numerical difficulties as any other Krylov subspace method.

7. Numerical Experiments. In this section, we demonstrate experimentally that the HEKS algorithm may be useful for approximating $f(H)u$ for a (large-scale) Hamiltonian matrix $H \in \mathbb{R}^{2n\times 2n}$ and a vector $u \in \mathbb{R}^{2n}$, $\|u\|_2 = 1$, via

$$f(H)u \approx \widetilde{S} f(\widetilde{H}) J_{2\ell}^T \widetilde{S}^T J_n u \tag{7.10}$$

with the $2n \times 2\ell$ J-orthogonal matrix $\widetilde{S}$ and the $2\ell \times 2\ell$ Hamiltonian matrix $\widetilde{H} = J_{2\ell}^T \widetilde{S}^T J_n H \widetilde{S}$. We consider two methods to construct $\widetilde{S}$:

- the HEKS method (Algorithm 1) which generates a J-orthogonal matrix $\widetilde{S}$ such that range$(\widetilde{S}) = \mathcal{K}_{r,s}$ with $r = s = \frac{\ell}{2}$ or $r - 1 = s = \frac{\ell-1}{2}$, depending on whether ℓ is even or odd. Then $f(H)u$ can be approximated via $\widetilde{S} f(\widetilde{H}) e_{s+1}$ (as due to the construction $J_{2\ell}^T \widetilde{S}^T J_n u = e_{s+1}$),
- the Hamiltonian Lanczos method (HamL) [5, 4, 22] which generates a J-orthogonal matrix $\widetilde{S}$ such that range$(\widetilde{S}) = \mathcal{K}_{2\ell}(H, u)$. Then $f(H)u$ can be approximated via $\widetilde{S} f(\widetilde{H}) e_1$ (as due to the construction $J_{2\ell}^T \widetilde{S}^T J_n u = e_1$).

These methods are compared to the corresponding unstructured methods

- the extended Krylov subspace method (EKSM) [15],
- the standard Arnoldi method [9],

Algorithm 1 HEKS with short recurrences

Require: Hamiltonian matrix $H \in \mathbb{R}^{2n\times 2n}$, $u_1 \in \mathbb{R}^{2n}$ with $\|u_1\|_2 = 1$

Ensure: a) $S_{2k} = [y_k \ \cdots \ y_1 \ u_1 \ \cdots \ u_k \mid x_k \ \cdots \ x_1 \ v_1 \ \cdots \ v_k \in \mathbb{R}^{2n\times 4k}$ with $S_{2k}^T J_n S_{2k} = J_{2k}$ and $H_{2k} = J_{2k} S_{2k}^T J_n H S_{2k}$ as in (4.3)

b) parameters $\lambda_j, \delta_j, \alpha_j, \gamma_j, \vartheta_j$ for $j = 1, \ldots, k$ and β_j, μ_j for $j = 2, \ldots, k$ which determine H_{2k}

(for $S_{2k+1} \in \mathbb{R}^{2n\times 4k+2}$ the algorithm needs to be modified appropriately)

$u_1 = u_1/\|u_1\|_2$ ▷ Set up $S_1 = [u_1 \mid v_1]$
$\vartheta_1 = u_1^T J_n H u_1$
$v_1 = H u_1/\vartheta_1$
$f_{11} = u_1^T J_n H^{-1} u_1$ ▷ Set up $S_2 = [y_1 \ u_1 \mid x_1 \ v_1]$
$w_x = H^{-1} u_1 - f_{11} v_1$
$x_1 = w_x/\|w_x\|_2$
$y_1 = H^{-1} x_1 / x_1^T J_n H^{-1} x_1$
$\lambda_1 = -x_1^T J_n H x_1$ and $\delta_1 = y_1^T J_n H y_1$
$\alpha_1 = -v_1^T J_n H v_1$ and $\gamma_1 = -x_1^T J_n H v_1$ ▷ Set up $S_3 = [y_1 \ u_1 \ u_2 \mid x_1 \ v_1 \ v_2]$
$w_u = H v_1 - \gamma_1 y_1 - \alpha_1 u_1$
$u_2 = w_u/\|w_u\|_2$
$\vartheta_2 = u_2^T J_n H u_2$
$v_2 = H u_2/\vartheta_2$
$e_{11} = y_1^T J_n H^{-1} y_1$ ▷ Set up $S_4 = [y_2 \ y_1 \ u_1 \ u_2 \mid x_2 \ x_1 \ v_1 \ v_2]$
$g_{11} = y_1^T J_n H^{-1} u_1$, and $g_{12} = y_1^T J_n H^{-1} u_2$
$w_x = H^{-1} y_1 - e_{11} x_1 - g_{11} v_1 - g_{12} v_2$
$x_2 = w_x/\|w_x\|_2$
$y_2 = H^{-1} x_2 / (H^{-1} x_2)^T J_n x_2$
$\lambda_2 = -x_2^T J_n H x_2$ and $\delta_2 = y_2^T J_n H y_2$
for $j = 3, 4, \ldots, k$ **do**
    $\alpha_{j-1} = -v_{j-1}^T J_n H v_{j-1}$ and $\beta_{j-1} = -v_{j-1}^T J_n H v_{j-2}$ ▷ Set up S_{2j-1}
    $\gamma_{j-1} = -x_{j-1}^T J_n H v_{j-1}$ and $\mu_{j-1} = -x_{j-2}^T J_n H v_{j-1}$
    $w_u = H v_{j-1} - \gamma_{j-1} y_{j-1} - \mu_{j-1} y_{j-2} - \beta_{j-1} u_{j-2} - \alpha_{j-1} u_{j-1}$
    $u_j = w_u/\|w_u\|_2$
    $\vartheta_j = u_j^T J_n H u_j$
    $v_j = H u_j/\vartheta_j$
    $g_{j-1,j-1} = y_{j-1}^T J_n H^{-1} u_{j-1}$ and $g_{j-1,j} = y_{j-1}^T J_n H^{-1} u_j$ ▷ Set up S_{2j}
    $e_{j-1,j-1} = y_{j-1}^T J_n H^{-1} y_{j-1}$ and $e_{j-2,j-1} = y_{j-1}^T J_n H^{-1} y_{j-2}$
    $w_x = H^{-1} y_{j-1} - e_{j-1,j-1} x_{j-1} - e_{j-2,j-1} x_{j-2} - g_{j-1,j-1} v_{j-1} - g_{j-1,j} v_j$
    $x_j = w_x/\|w_x\|_2$
    $y_j = H^{-1} x_j / (H^{-1} x_j)^T J_n x_j$
    $\lambda_j = -x_j^T J_n H x_j$ and $\delta_j = y_j^T J_n H y_j$
end for
$\alpha_k = -v_k^T J_n H v_k$ and $\beta_k = -v_k^T J_n H v_{k-1}$
$\gamma_k = -x_k^T J_n H v_k$ and $\mu_k = -x_{k-1}^T J_n H v_k$

which generate an orthogonal matrix Q such that either range$(Q) = \mathcal{K}_{r,s}$ or [range$(Q) = \mathcal{K}_{2\ell}(H, u)$. Then $f(H)u$ can be approximated via $Qf(Q^T HQ)e_1$ (as by construction, $Q^T u = e_1$ holds).

Only functions f which map H to a structured matrix are dealt with. In particular, we consider

- $f(H) = \exp(H)$: the exponential function of a Hamiltonian matrix is a symplectic matrix [11],
- $f(H) = \cos(H)$: $\cos(H)$ is a skew-Hamiltonian matrix (as a sum of even powers of H),
- $f(H) = \operatorname{sign}(H)$: $\operatorname{sign}(H)$ is a Hamiltonian matrix [18]. The matrix sign function is defined for any matrix $X \in \mathbb{C}^{n\times n}$ having no pure imaginary eigenvalues by $\operatorname{sign}(X) = X(X^2)^{-\frac{1}{2}}$ [13, 14]. An equivalent definition is $\operatorname{sign}(X) = T\operatorname{diag}(-I_p, I_q)T^{-1}$, where the Jordan decomposition of $X = T\operatorname{diag}(J_1, J_2)T^{-1}$ is such that the p eigenvalues of J_1 are assumed to lie in the open left half-plane, while the q eigenvalues of J_2 lie in the open right half-plane. The Newton iteration $S_0 = X$, $S_{k+1} = \frac{1}{2}(X_k + X_k^{-1})$ converges quadratically to $\operatorname{sign}(X)$ [21].

Utilizing HEKS or HamL, the projected matrix $\widetilde{H}$ is Hamiltonian again, so that $f(\widetilde{H})$ has the same structure as $f(H)$, while the projected matrix Q^THQ as well as $f(Q^THQ)$ obtained via EKSM and Arnoldi have no particular structure. Such a structure-preserving approximation of $f(H)u$ is, e.g., important in the context of symplectic exponential integrators for Hamiltonian systems, see, e.g., [8, 10, 19, 20].

All experiments are performed in MATLAB R2021b on an Intel(R) Core(TM) i7-8565U CPU @ 1.80GHz 1.99 GHz with 16GB RAM. Our MATLAB implementation employs the standard MATLAB function `expm` and `funm(H,@cos)` as well as `signm` from the Matrix Computation Toolbox [12]. The experimental code used to generate the results presented in the following subsection can be found at [3]. All algorithms are run to yield a 1000×30 matrix whose columns span the corresponding (extended) Krylov subspace. All methods are implemented using full re-(J)-orthogonalization. The accuracy of the approximation for HEKS and HamL is measured in terms of the relative error $\|f(H)u - \widetilde{S}f(\widetilde{H})J_{2\ell}^T\widetilde{S}^TJ_nu\|_2/\|f(H)u\|_2$, while $\|f(H)u - Qf(Q^THQ)Q^Tu\|_2/\|f(H)u\|_2$ is used for EKSM and Arnoldi.

7.1. Example 1. Inspired by [15, Example 4.1], our first test matrix is a diagonal Hamiltonian matrix $H_1 = \operatorname{diag}(D, -D)$ with a diagonal 500×500 real matrix D whose eigenvalues are log-uniformly distributed in the interval $[10^{-1}, 1]$. EKSM will preserve the symmetry of H, while HEKS and HL will not.

In Fig. 1, the relative accuracy of all four methods is displayed, using a random starting vector x (plots in the two leftmost columns) as well as a starting vector of all ones (plots in the two rightmost columns). The Hamiltonian Lanczos method and the Arnoldi method perform alike just as the HEKS algorithm and the EKS method. For the functions exp and cos the HEKS approximation makes significant progress only every other iteration step (that is, whenever the columns of $\widetilde{S}$ span $\mathcal{K}_{k,k-1}$). The same holds for the EKSM approximation of $\cos(H)x$ and $\cos(H)e$, but not for the approximation of $\exp(H)x$ and $\exp(H)e$. The HEKS algorithm adds the vectors from $\mathcal{K}_{r,s}$ in a different order than EKSM: HEKS alternates between adding two vectors from $\mathcal{K}_{2k}(H, u)$ and adding two vectors from $\mathcal{K}_{2k}(H^{-1}, H^{-1}u)$, while EKSM alternates between adding one vector from $\mathcal{K}_{2k}(H, u)$ and adding one from $\mathcal{K}_{2k}(H^{-1}, H^{-1}u)$ (for $u = x$ or $u = e$). Thus, the columns of $\widetilde{S}$ and Q span the same subspace only every other step. Adding vectors from $\mathcal{K}_{2k}(H^{-1}, H^{-1}u)$ does not seem to be relevant for the HEKS approximations $\exp(H)u$ and $\cos(H)u$ as well for the EKSM approximation of $\cos(H)u$. For the EKSM approximation of $\exp(H)u$ some convergence progress can be observed in every iteration step, but the overall convergence is similar to that of the HEKS approximation. In summary, the use of an extended Krylov subspace does not improve the convergence for these examples compared to the approximations computed using the Arnoldi method or the Hamiltonian Lanczos method. The latter two methods converge about twice as fast as the first two.

But for the matrix sign function, the two methods based on the extended Krylov subspace converge

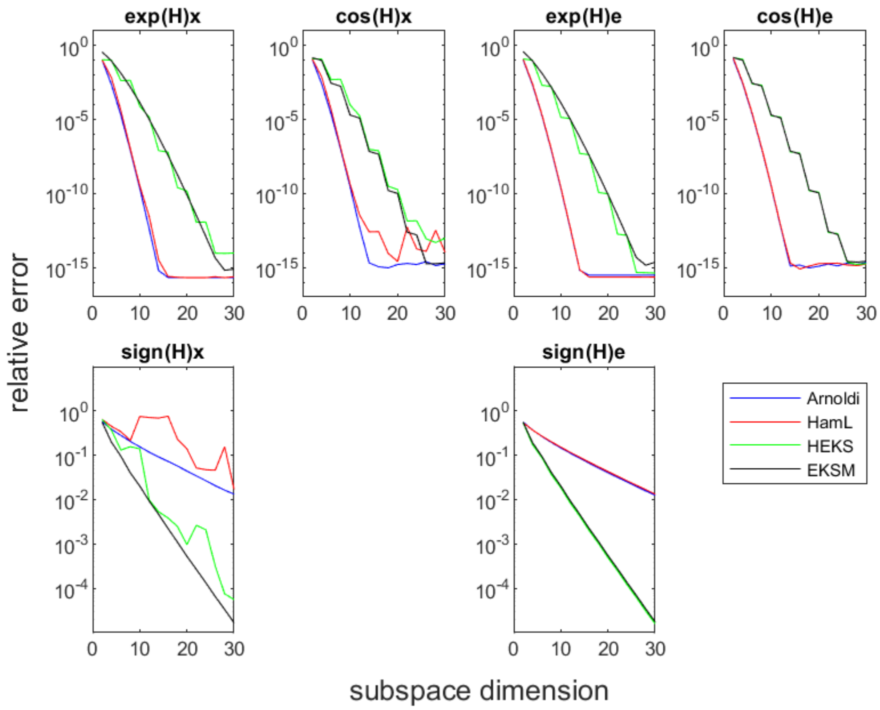

Figure 1. *Diagonal Hamiltonian matrix* $H_1 = \mathrm{diag}(A, -A)$ *with* `A = diag(logspace(-1,0,500));`*, two different choices of the starting vector* `x = randn(1000,1)` *and* `e = ones(1000,1)`

faster than the other two. They do make progress in every iteration step. It is clearly beneficial to use an extended Krylov subspace here.

The HEKS algorithm requires 34 matrix-vector-multiplications with H, 21 linear solves with H and 104 scalar products to construct the 1000×30 matrix $\widetilde{S}$. In contrast, the ESKM requires 15 matrix-vector-multiplications with H, 14 linear solves with H and 493 scalar products. As H in this example is diagonal, the linear solves and matrix-vector multiplications require less arithmetic operations than scalar products. Hence, the HEKS algorithm is faster than EKSM and requires less storage. Of course, the situation will change for more practically relevant examples with a more complex sparsity pattern. But it remains to note that there is a big difference in the number of scalar products to be performed, which is not due to the matrix structure but the difference of the short-term Lanczos-style and long-term Arnoldi-style recursions in the non-symmetric case.

7.2. Example 2. As a second example we use the Hamiltonian matrix $H_2 = \begin{bmatrix} A & -G \\ -Q & -A^T \end{bmatrix} \in \mathbb{R}^{1998 \times 1998}$ from Example 15 of the collection of benchmark examples for the numerical solution of continuous-time algebraic Riccati equations [6]. The matrix has a complex spectrum with real and imaginary parts between -2 and 2.

Fig. 2 provides the same information as in Fig. 1. Our findings from the first example are confirmed. The Hamiltonian Lanczos method and the Arnoldi method perform alike just as the HEKS algorithm and the EKS method. For the functions exp and cos the first two methods converge faster than the latter two.

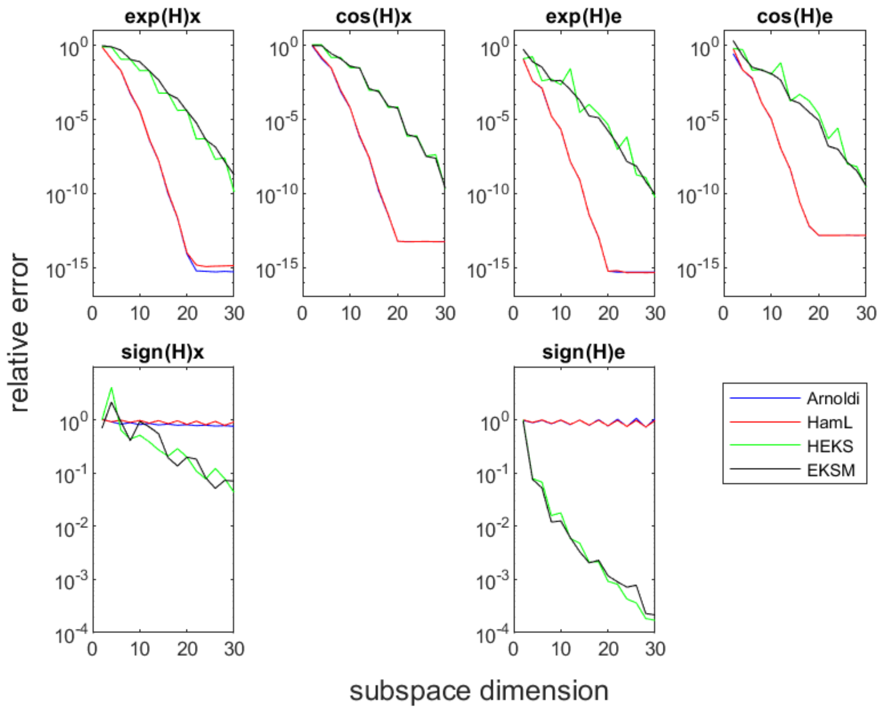

FIGURE 2. *Hamiltonian matrix H_2, two different choices of the starting vector* `x = randn(1998,1)` *and* `e = ones(1998,1)`

The use of the extended Krylov subspace does not result in faster convergence. But for the matrix sign function, the two method based on the extended Krylov subspace perform much better.

8. Concluding Remarks. The HEKS algorithm for computing a J-orthogonal basis of the extended Krylov subspace $\mathcal{K}_{r,s}$ (1.1) has been presented. Unlike the EKSM for generating an orthogonal basis of $\mathcal{K}_{r,r}$ it allows for short recurrences. The convergence analysis provide in [15] does not apply here as the field of values of a Hamiltonian matrix does not (strictly) lie in the right half-plane. Numerical experiments suggest that it may be useful to employ the HEKS algorithm for the approximation of the action of $f(H)$ on a vector u for Hamiltonian matrices H. The performance of the HEKS algorithm is similar to that of EKSM, but HEKS guarantees the structure-preserving projection of the Hamiltonian matrix which may be relevant for some applications.

Appendix A. Derivation of the HEKS Algorithm. This section is devoted to deriving short recurrences for the HEKS algorithm. We will follow the idea sketched in Section 3. First $S_1 \in \mathbb{R}^{2n\times 2}$ is constructed such that $S_1^TJ_nS_1 = J_1$ and the columns of S_1 span the same subspace as $\mathcal{K}_2(H, u_1)$ (that is, range$\{S_1\} = \mathcal{K}_2(H, u_1)$). Here $H \in \mathbb{R}^{2n\times 2n}$ is the Hamiltonian matrix under consideration and $u_1 \in \mathbb{R}^{2n}$ a given vector with $\|u_1\|_2 = 1$. Next $S_{2k} \in \mathbb{R}^{2n\times 4k}$ is constructed by extending S_{2k-1} by two columns such that $S_{2k}^TJ_nS_{2k} = J_{2k}$ and range$\{S_{2k}\} = \mathcal{K}_{2k}(H, u_1) + \mathcal{K}_{2k}(H^{-1}, H^{-1}u_1)$. Finally, $S_{2k+1} \in \mathbb{R}^{2n\times 4k+2}$ is constructed by extending S_{2k} by two columns such that $S_{2k+1}^TJ_nS_{2k+1} = J_{2k+1}$ and range$\{S_{2k+1}\} = \mathcal{K}_{2k+1}(H, u_1) + \mathcal{K}_{2k}(H^{-1}, H^{-1}u_1)$. In doing so, we will provide a proof that the projected matrices H_{2k} and H_{2k+1} as well as $J_{2k}^TS_{2k}^TJ_nH^{-1}S_{2k}$ and $J_{2k+1}^TS_{2k+1}^TJ_nH^{-1}S_{2k+1}$ are of the above given forms (4.3), (5.6) and

(5.7), resp.. In particular, we will prove Theorem 4.1. The assumption in Theorem 4.1 that no breakdown occurs in particular implies that in the following all assumptions on nonzero parameters must hold.

A.1. Step 1: range$\{S_1\} = \mathcal{K}_2(H, u_1)$**.** As u_1 satisfies $\|u_1\|_2 = 1$, there is nothing to do with the first vector in $\mathcal{K}_2(H, u_1)$. The second vector Hu_1 needs to J-orthogonalized against u_1. This is achieved by

$$v_1 = Hu_1/u_1^T J_n H u_1 = Hu_1/\vartheta_1 \tag{A.11}$$

assuming that $\vartheta_1 \neq 0$. Thus, the matrix $S_1 = [u_1 \mid v_1]$ has J-orthogonal columns by construction

$$S_1^T J_n S_1 = \begin{bmatrix} u_1^T J_n u_1 & u_1^T J_n v_1 \\ v_1^T J_n u_1 & v_1^T J_n v_1 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

as any vector is J-orthogonal to itself, $u_1^T J_n v_1 = u_1^T J_n H u_1 / u_1^T J_n H u_1 = 1$ and $v_1^T J_n u_1 = (u_1^T J_n^T v_1)^T = -(u_1^T J_n v_1)^T$.

A.1.1. The projected matrix $H_1 = J_1^T S_1^T J_n H S_1$**.** We will prove that

$$H_1 = J_1^T S_1^T J_n H S_1 = \begin{bmatrix} -v_1^T J_n H u_1 & -v_1^T J_n H v_1 \\ u_1^T J_n H u_1 & u_1^T J_n H v_1 \end{bmatrix} = \begin{bmatrix} 0 & \alpha_1 \\ \vartheta_1 & 0 \end{bmatrix} \tag{A.12}$$

holds. Due to (A.11) we have $Hu_1 = \vartheta_1 v_1$ and thus

$$v_1^T J_n H u_1 = \vartheta_1 \cdot v_1^T J_n v_1 = 0$$

as any vector is J-orthogonal to itself. The zero in position (2,2) follows from the zero in position $(1,1)$ as H as well as H_1 is Hamiltonian (or by noting that $0 = v_1^T J_n H u_1 = (v_1^T J_n H^T u_1)^T = u_1^T (J_n H)^T v_1 = u_1^T J_n H v_1 = 0$).

A.1.2. The projected matrix $J_1^T S_1^T J_n H^{-1} S_1$**.** Making use of the fact that $H^T J_n H^{-1} = -J_n$ as H is Hamiltonian ($(J_n H)^T = -H^T J_n = J_n H$), we have due to (A.11)

$$\vartheta_1 \cdot v_1^T J_n H^{-1} u_1 = (Hu_1)^T J_n H^{-1} u_1 = u_1^T H^T J_n H^{-1} u_1 = -u_1^T J_n u_1 = 0.$$

This implies $u_1^T J_n H^{-1} v_1 = 0$. Moreover, using (A.11) again

$$v_1^T J_n H^{-1} v_1 = (Hu_1)^T J_n H^{-1} (Hu_1)/\vartheta_1^2 = u_1^T H^T J_n u_1/\vartheta_1^2 = -u_1^T J_n H u_1/\vartheta_1^2 = -1/\vartheta_1.$$

Thus

$$J_1^T S_1^T J_n H^{-1} S_1 = \begin{bmatrix} -v_1^T J_n H^{-1} u_1 & -v_1^T J_n H^{-1} v_1 \\ u_1^T J_n H^{-1} u_1 & u_1^T J_n H^{-1} v_1 \end{bmatrix} = \begin{bmatrix} 0 & 1/\vartheta_1 \\ f_{11} & 0 \end{bmatrix}. \tag{A.13}$$

A.2. Step 2: range$\{S_2\} = \mathcal{K}_2(H, u_1) + \mathcal{K}_2(H^{-1}, H^{-1}u_1)$**.** Now the first vector from the Krylov subspace $\mathcal{K}_r(H^{-1}, H^{-1}u_1)$ is added to the symplectic basis by J-orthogonalization $H^{-1}u_1$ against u_1 and v_1. This is achieved by computing

$$w_x = (I - S_1 J_1^T S_1^T J_n) H^{-1} u_1,$$

and normalizing w_x to length 1, $x_1 = w_x/\|w_x\|_2$. Next the second vector from $\mathcal{K}_r(H^{-1}, H^{-1}u_1)$ needs to be added to the symplectic basis. This can be accomplished by J-orthogonalizing $H^{-1}x_1$ against u_1 and v_1

$$w_y = (I - S_1 J_1^T S_1^T J_n) H^{-1} x_1$$

and making sure that w_y is J-orthogonal against x_1 as well, $y_1 = w_y/w_y^T J x_1$. Here we assume that $\|w_x\|_2 \neq 0$ as well as $w_y^T J x_1 \neq 0$.

Collect the vectors into a matrix $S_2 = [y_1 \; u_1 \mid x_1 \; v_1] \in \mathbb{R}^{2n \times 4}$. By construction the columns of S_2 are J-orthogonal, that is

$$S_2^T J_n S_2 = J_2 \tag{A.14}$$

and

$$\mathrm{range}\{S_2\} = \mathcal{K}_2(H, u_1) + \mathcal{K}_2(H^{-1}, H^{-1}u_1).$$

Let us take a closer look at w_x and w_y. Making use of (A.13) we have

$$w_x = H^{-1}u_1 - [v_1 \;\; -u_1] \begin{bmatrix} u_1^T J_n H^{-1} u_1 \\ v_1^T J_n H^{-1} u_1 \end{bmatrix} = H^{-1}u_1 - [v_1 \;\; -u_1] \begin{bmatrix} f_{11} \\ 0 \end{bmatrix} = H^{-1}u_1 - f_{11} v_1.$$

Hence, with $\psi_1 = \|w_x\|_2$ we have

$$x_1 = \left(H^{-1}u_1 - f_{11}v_1\right)/\psi_1, \tag{A.15}$$

where, as already stated above, $\psi_1 \neq 0$ is assumed.

Next we turn our attention to w_y. We will make use of the fact that H^{-1} is Hamiltonian ($J_n H^{-1} = -H^{-T} J_n$) and $S_2^T J_n S_2 = J_2$. With (A.15) we see

$$u_1^T J_n H^{-1} x_1 = -(H^{-1}u_1)^T J_n x_1 = -(\psi_1 x_1 + f_{11} v_1)^T J_n x_1 = 0. \tag{A.16}$$

Similarly, it follows with (A.11) that

$$v_1^T J_n H^{-1} x_1 = -(H^{-1}v_1)^T J_n x_1 = u_1^T J_n x_1/\vartheta_1 = 0. \tag{A.17}$$

Hence,

$$w_y = H^{-1}x_1 - [v_1 \;\; -u_1] \begin{bmatrix} u_1^T J_n H^{-1} x_1 \\ v_1^T J_n H^{-1} x_1 \end{bmatrix} = H^{-1}x_1 - [v_1 \;\; -u_1] \begin{bmatrix} 0 \\ 0 \end{bmatrix} = H^{-1}x_1,$$

and

$$y_1 = H^{-1}x_1/\xi_1,$$

where we assume that

$$\xi_1 = (H^{-1}x_1)^T J_n x_1 = x_1^T H^{-T} J_n x_1 \neq 0. \tag{A.18}$$

Observe that

$$\delta_1 = y_1^T J_n H y_1 = \frac{1}{\xi_1^2} x_1^T H^{-T} J_n H H^{-1} x_1 = \frac{1}{\xi_1^2} x_1^T H^{-T} J_n x_1 = \frac{1}{\xi_1}. \tag{A.19}$$

Thus

$$y_1 = H^{-1}x_1/\xi_1 = \delta_1 H^{-1} x_1. \tag{A.20}$$

A.2.1. The projected matrix $H_2 = J_2^T S_2^T J_n H S_2$. We will see that the zero structure of $H_2 = J_2^T S_2^T J_n H S_2$ is given as follows:

$$H_2 = \left[\begin{array}{cc||cc} -x_1^T J_n H y_1 & -x_1^T J_n H u_1 & -x_1^T J_n H x_1 & -x_1^T J_n H v_1 \\ -v_1^T J_n H y_1 & -v_1^T J_n H u_1 & -v_1^T J_n H x_1 & -v_1^T J_n H v_1 \\ \hline\hline y_1^T J_n H y_1 & y_1^T J_n H u_1 & y_1^T J_n H x_1 & y_1^T J_n H v_1 \\ u_1^T J_n H y_1 & u_1^T J_n H u_1 & u_1^T J_n H x_1 & u_1^T J_n H v_1 \end{array}\right] = \left[\begin{array}{cc||cc} 0 & 0 & \lambda_1 & \gamma_1 \\ 0 & 0 & \gamma_1 & \alpha_1 \\ \hline\hline \delta_1 & 0 & 0 & 0 \\ 0 & \vartheta_1 & 0 & 0 \end{array}\right]. \tag{A.21}$$

The entries at the positions $(2,2),(4,2),(2,4)$ and $(4,4)$ (denoted in blue in (A.21)) are the same as in (A.12). Due to H and thus H_2 being Hamiltonian, we only need to prove the zero entries at the positions $(1,1),(1,2),(2,1)$ and $(3,2)$, the other zeros in (A.21) follow immediately.

Due to (A.11) we have $Hu_1 = \vartheta_1 v_1$. Thus, $x_1^T J_n H u_1 = \vartheta_1 \cdot x_1^T J_n v_1 = 0$ and $y_1^T J_n H u_1 = \vartheta_1 \cdot y_1^T J_n v_1 = 0$ due to (A.14). This gives the zero entries in the positions $(1,2)$ and $(3,2)$.

Due to (A.20) it follows with (A.14) for the entry $(2,1)$

$$v_1^T J_n H y_1 = \delta_1 v_1^T J_n H H^{-1} x_1 = \delta_1 v_1^T J_n x_1 = 0.$$

Moreover, in a similar way for the entry $(1,1)$ we have

$$x_1^T J_n H y_1 = \delta_1 x_1^T J_n H H^{-1} x_1 = \delta_1 x_1^T J_n x_1 = 0.$$

Hence, (A.21) holds.

A.2.2. The projected matrix $J_2^T S_2^T J_n H^{-1} S_2$. Some of the entries in $\tilde{H}_2 = J_2^T S_2^T J_n H^{-1} S_2$ (denoted in blue) are already known from (A.13),

$$\begin{aligned} \tilde{H}_2 &= \left[\begin{array}{cc|cc} -x_1^T J_n H^{-1} y_1 & -x_1^T J_n H^{-1} u_1 & -x_1^T J_n H^{-1} x_1 & -x_1^T J_n H^{-1} v_1 \\ -v_1^T J_n H^{-1} y_1 & -v_1^T J_n H^{-1} u_1 & -v_1^T J_n H^{-1} x_1 & -v_1^T J_n H^{-1} v_1 \\ \hline y_1^T J_n H^{-1} y_1 & y_1^T J_n H^{-1} u_1 & y_1^T J_n H^{-1} x_1 & y_1^T J_n H^{-1} v_1 \\ u_1^T J_n H^{-1} y_1 & u_1^T J_n H^{-1} u_1 & u_1^T J_n H^{-1} x_1 & u_1^T J_n H^{-1} v_1 \end{array}\right] \\ &= \left[\begin{array}{cc|cc} 0 & 0 & 1/\delta_1 & 0 \\ 0 & 0 & 0 & 1/\vartheta_1 \\ \hline e_{11} & g_{11} & 0 & 0 \\ g_{11} & f_{11} & 0 & 0 \end{array}\right]. \end{aligned} \tag{A.22}$$

The entry in position $(1,3)$ follows from (A.18) and (A.19), while the zero entries in the positions $(1,2)$, $(1,4)$, $(2,3)$ and $(4,3)$ have already been proven in (A.16) and (A.17).

It remains to consider the entries at the positions $(3,3)$ and $(3,4)$. Using (A.20) and (A.11) leads to

$$\begin{aligned} y_1^T J_n H^{-1} x_1 &= \delta_1 (H^{-1} x_1)^T J_n (H^{-1} x_1) = 0, \\ y_1^T J_n H^{-1} v_1 &= y_1^T J_n u_1 / \vartheta_1 = 0. \end{aligned}$$

Hence, (A.22) holds.

A.3. Step 3: $\text{range}\{S_3\} = \mathcal{K}_4(H, u_1) + \mathcal{K}_2(H^{-1}, H^{-1}u_1)$. In this step the next two vectors $H^2 u_1$ and $H^3 u_1$ from $\mathcal{K}_4(H, u_1)$ are added to the symplectic basis. We start by J-orthogonalizing Hv_1 against the columns of S_2

$$w_u = (I - S_2 J_2^T S_2^T J_n) H v_1 = H v_1 - [x_1 \quad v_1 \quad -y_1 \quad -u_1] \begin{bmatrix} y_1^T J_n H v_1 \\ u_1^T J_n H v_1 \\ x_1^T J_n H v_1 \\ v_1^T J_n H v_1 \end{bmatrix}$$

$$= H v_1 - [x_1 \quad v_1 \quad -y_1 \quad -u_1] \begin{bmatrix} 0 \\ 0 \\ -\gamma_1 \\ -\alpha_1 \end{bmatrix} = H v_1 - \gamma_1 y_1 - \alpha_1 u_1 \tag{A.23}$$

where (A.21) gives that the first two entries of the last vector are zero. Normalizing w_u to length 1 gives u_2

$$u_2 = w_u / \chi_2, \tag{A.24}$$

where it is assumed that $\chi_2 = \|w_u\|_2 \neq 0$.

This step is finalized by J-orthogonalizing $H u_2$ against the columns of S_2:

$$w_v = (I - S_2 J_2^T S_2^T J_n) H u_2 = H u_2 - [x_1 \quad v_1 \quad -y_1 \quad -u_1] \begin{bmatrix} y_1^T J_n H u_2 \\ u_1^T J_n H u_2 \\ x_1^T J_n H u_2 \\ v_1^T J_n H u_2 \end{bmatrix}.$$

All entries of the last vector are zero. The first two zeros follow as $H^{-T} J_n H = -J_n$ with (A.20) and (A.11):

$$y_1^T J_n H u_2 / \delta_1 = (H^{-1} x_1)^T J_n H u_2 = -x_1^T J_n u_2 = 0,$$
$$u_1^T J_n H u_2 / \vartheta_1 = (H^{-1} v_1)^T J_n H u_2 = -v_1^T J_n u_2 = 0$$

by construction of u_2. The last zero follows as H is Hamiltonian with (A.23),

$$v_1^T J_n H u_2 = v_1^T (J_n H)^T u_2 = -(H v_1)^T J_n u_2 = -(\chi_2 u_2 + \gamma_1 y_1 + \alpha_1 u_1)^T J_n u_2 = 0$$

again due to the construction of u_2. With this and (A.15) we have for the next to last entry

$$\psi_1 \cdot x_1^T J_n H u_2 = (H^{-1} u_1 + f_{11} v_1)^T J_n H u_2 = -u_1^T J_n u_2 + f_{11} v_1^T J_n H u_2 = 0.$$

Thus the expression for w_v simplifies to

$$w_v = H u_2.$$

Normalizing w_v by $\vartheta_2 = u_2^T J_n H u_2$ to make sure it is J-orthogonal to u_2 as well yields

$$v_2 = H u_2 / \vartheta_2.$$

Let

$$S_3 = [y_1 \ u_1 \ u_2 \mid x_1 \ v_1 \ v_2] \in \mathbb{R}^{2n \times 6}.$$

Then by construction

$$S_3^T J_n S_3 = J_3 \tag{A.25}$$

and

$$\operatorname{range}\{S_3\} = \mathcal{K}_4(H, u_1) + \mathcal{K}_2(H^{-1}, H^{-1} u_1).$$

A.3.1. The projected matrix $H_3 = J_3^T S_3^T J_n H S_3$. Some of the entries (denoted in blue) in $H_3 = J_3^T S_3^T J_n H S_3$ are already known from (A.21)

$$H_3 = \left[\begin{array}{c|c|c||c|c|c} 0 & 0 & -x_1^T J_n H u_2 & \lambda_1 & \gamma_1 & -x_1^T J_n H v_2 \\ \hline 0 & 0 & -v_1^T J_n H u_2 & \gamma_1 & \alpha_1 & -v_1^T J_n H v_2 \\ -v_2^T J_n H y_1 & -v_2^T J_n H u_1 & -v_2^T J_n H u_2 & -v_2^T J_n H x_1 & -v_2^T J_n H v_1 & -v_2^T J_n H v_2 \\ \hline\hline \delta_1 & 0 & y_1^T J_n H u_2 & 0 & 0 & y_1^T J_n H v_2 \\ \hline 0 & \vartheta_1 & u_1^T J_n H u_2 & 0 & 0 & u_1^T J_n H v_2 \\ u_2^T J_n H y_1 & u_2^T J_n H u_1 & u_2^T J_n H u_2 & u_2^T J_n H x_1 & u_2^T J_n H v_1 & u_2^T J_n H v_2 \end{array}\right]$$

$$= \left[\begin{array}{c|c|c||c|c|c} 0 & 0 & 0 & \lambda_1 & \gamma_1 & \mu_2 \\ \hline 0 & 0 & 0 & \gamma_1 & \alpha_1 & \beta_2 \\ 0 & 0 & 0 & \mu_2 & \beta_2 & \alpha_2 \\ \hline\hline \delta_1 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & \vartheta_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \vartheta_2 & 0 & 0 & 0 \end{array}\right]. \tag{A.26}$$

The zeros in the third column (and hence the zeros in the last row) follow with $Hu_2 = \vartheta_2 v_2$ due to (A.25). Moreover, we have with (A.20) and (A.11)

$$v_2^T J_n H y_1 = \delta_1 v_2^T J_n x_1 = 0,$$
$$v_2^T J_n H u_1 = \vartheta_1 v_2^T J_n v_1 = 0$$

making again use of (A.25). Hence, (A.26) holds.

A.3.2. The projected matrix $J_3^T S_3^T J_n H^{-1} S_3$. Some of the entries in $\tilde{H}_3 = J_3^T S_3^T J_n H^{-1} S_3$ (denoted in blue) are already known from (A.22)

$$\tilde{H}_3 = \left[\begin{array}{ccc|ccc} 0 & 0 & -x_1^T J_n H^{-1} u_2 & 1/\delta_1 & 0 & -x_1^T J_n H^{-1} v_2 \\ 0 & 0 & -v_1^T J_n H^{-1} u_2 & 0 & 1/\vartheta_1 & -v_1^T J_n H^{-1} v_2 \\ -v_2^T J_n H^{-1} y_1 & -v_2^T J_n H^{-1} u_1 & -v_2^T J_n H^{-1} u_2 & -v_2^T J_n H^{-1} x_1 & -v_2^T J_n H^{-1} v_1 & -v_2^T J_n H^{-1} v_2 \\ \hline e_{11} & g_{11} & y_1^T J_n H^{-1} u_2 & 0 & 0 & y_1^T J_n H^{-1} v_2 \\ g_{11} & f_{11} & u_1^T J_n H^{-1} u_2 & 0 & 0 & u_1^T J_n H^{-1} v_2 \\ u_2^T J_n H^{-1} y_1 & u_2^T J_n H^{-1} u_1 & u_2^T J_n H^{-1} u_2 & u_2^T J_n H^{-1} x_1 & u_2^T J_n H^{-1} v_1 & u_2^T J_n H^{-1} v_2 \end{array}\right]$$

$$= \left[\begin{array}{ccc|ccc} 0 & 0 & 0 & 1/\delta_1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/\vartheta_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/\vartheta_2 \\ \hline e_{11} & g_{11} & g_{12} & 0 & 0 & 0 \\ g_{11} & f_{11} & 0 & 0 & 0 & 0 \\ g_{12} & 0 & f_{22} & 0 & 0 & 0 \end{array}\right]. \tag{A.27}$$

It remains to show that the five entries $v_2^T J_n H^{-1} z$ for $z = x_1, v_1, y_1, u_1, u_2$ as well as the three entries $z^T J_n H^{-1} u_2$ for $z = v_1, x_1, u_1$ are zero. Moreover, we need to show that $-v_2^T J_n H^{-1} v_2 = 1/\vartheta_2$.

Most of these relations follow from $H^T J_n H^{-T} = -J_n$ and due to $Hu_j = \vartheta_j v_j, j = 1, 2$. Making use of (A.25) in the last equality of each equation we have

$$\vartheta_1 \cdot v_1^T J_n H^{-1} u_2 = u_1^T H^T J_n H^{-1} u_2 = -u_1^T J_n u_2 = 0,$$
$$\vartheta_2 \cdot v_2^T J_n H^{-1} v_2 = u_2^T H^T J_n H^{-1} v_2 = -u_2^T J_n v_2 = -1,$$

and for $z = x_1, v_1, y_1, u_1, u_2$

$$\vartheta_2 \cdot v_2^T J_n H^{-1} z = u_2^T H^T J_n H^{-1} z = -u_2^T J_n z = 0.$$

Thus, $-v_2^T J_n H^{-1} v_2 = 1/\vartheta_2$ and the five entries in the $(1,1)$ (and the $(2,2)$) block of $\tilde{H}_3$ are zero.

The derivation of the final two zero entries needs a slightly more involved derivation. Due to (A.24), (A.25) and (A.22) we have

$$\begin{aligned}\chi_2 \cdot x_1^T J_n H^{-1} u_2 &= x_1^T J_n H^{-1}(Hv_1 - \gamma_1 y_1 - \alpha_1 u_1)\\ &= x_1^T J_n v_1 - \gamma_1 x_1^T J_n H^{-1} y_1 - \alpha_1 x_1^T J_n H^{-1} u_1 = 0,\end{aligned}$$

while due to H^{-1} being Hamiltonian, (A.15) and (A.25) we get

$$u_1^T J_n H^{-1} u_2 = (H^{-1} u_1)^T J_n u_2 = (\psi_1 x_1 + f_{11} v_1)^T J_n u_2 = 0.$$

Hence, (A.27) holds.

A.4. Step 4: $\mathrm{range}\{S_4\} = \mathcal{K}_4(H, u_1) + \mathcal{K}_4(H^{-1}, H^{-1}u_1)$**.** In this step the next two vectors $H^{-3}u_1$ and $H^{-4}u_1$ from $\mathcal{K}_4(H^{-1}, H^{-1}u_1)$ are added to the symplectic basis. We start by J-orthogonalizing $H^{-1}y_1$ against the columns of S_3

$$\begin{aligned} w_x = (I - S_3 J_3^T S_3^T J_n) H^{-1} y_1 &= H^{-1} y_1 - [x_1 \;\; V_2 \mid -y_1 \;\; -U_2] \begin{bmatrix} y_1^T J_n H^{-1} y_1 \\ U_2^T J_n H^{-1} y_1 \\ x_1^T J_n H^{-1} y_1 \\ V_2^T J_n H^{-1} y_1 \end{bmatrix} \\ &= H^{-1} y_1 - [x_1 \;\; V_2 \mid -y_1 \;\; -U_2] \begin{bmatrix} e_{11} \\ g_{11} \\ g_{12} \\ 0 \\ 0 \\ 0 \end{bmatrix} = H^{-1} y_1 - e_{11} x_1 - g_{11} v_1 - g_{12} v_2 \end{aligned}$$

due to (A.27).

Normalizing w_x to length 1 gives

$$x_2 = w_x / \psi_2, \tag{A.28}$$

where we assume that $\psi_2 = \|w_x\|_2 \neq 0$.

This step is finalized by J-orthogonalizing $H^{-1}x_2$ against the columns of S_3

$$w_y = (I - S_3 J_3^T S_3^T J_n) H^{-1} x_2 = H^{-1} x_2 - [x_1 \;\; V_2 \mid -y_1 \;\; -U_2] \begin{bmatrix} y_1^T J_n H^{-1} x_2 \\ U_2^T J_n H^{-1} x_2 \\ x_1^T J_n H^{-1} x_2 \\ V_2^T J_n H^{-1} x_2 \end{bmatrix}. \tag{A.29}$$

All entries $z^T J_n H^{-1} x_2 = -(H^{-1}z)^T J_n x_2$ in the last vector are zero. As $Hu_i = \vartheta_i v_i$, $i = 1, 2$, for the last two entries we have

$$\begin{aligned}\vartheta_1 \cdot (H^{-1} v_1)^T J_n x_2 &= u_1^T J_n x_2 = 0,\\ \vartheta_2 \cdot (H^{-1} v_2)^T J_n x_2 &= u_2^T J_n x_2 = 0\end{aligned}$$

by construction of x_2 as a vector J-orthogonal to all columns of S_3. Next, we use (A.28), (A.20) and (A.15) to see

$$\begin{aligned}
(H^{-1}y_1)^T J_n x_2 &= (\psi_2 x_2 - e_{11}x_1 - g_{11}v_1 - g_{12}v_2)^T J_n x_2 = 0,\\
(H^{-1}x_1)^T J_n x_2 &= \xi_1 y_1^T J_n x_2 = 0,\\
(H^{-1}u_1)^T J_n x_2 &= (\psi_1 x_1 - f_{11}v_1)^T J_n x_2 = 0
\end{aligned}$$

again by construction of x_2 as a vector J-orthogonal to all columns of S_3. With this and (A.24), it follows that

$$\chi_2 \cdot (H^{-1}u_2)^T J_n x_2 = (v_1 - \gamma_1 H^{-1}y_1 - \alpha_1 H^{-1}u_1)^T J_n x_2 = 0.$$

Thus,

$$y_2 = H^{-1}x_2/\xi_2,$$

where we assume that

$$\xi_2 = (H^{-1}x_2)^T J_n x_2 = x_2^T H^{-T} J_n x_2 \neq 0. \tag{A.30}$$

With the same argument as in (A.19) we see that

$$\delta_2 = y_2^T J_n H y_2 = \frac{1}{\xi_2^2}(H^{-1}x_2)^T J_n H H^{-1} x_2 = \frac{1}{\xi_2}.$$

Thus

$$y_2 = H^{-1}x_2/\xi_2 = \delta_2 H^{-1} x_2. \tag{A.31}$$

Let

$$S_4 = [y_2\ y_1\ u_1\ u_2 \mid x_2\ x_1\ v_1\ v_2] \in \mathbb{R}^{2n\times 8}.$$

Then by construction

$$S_4^T J_n S_4 = J_4 \tag{A.32}$$

and

$$\operatorname{range}\{S_4\} = \mathcal{K}_4(H, u_1) + \mathcal{K}_4(H^{-1}, H^{-1}u_1).$$

A.4.1. The projected matrix $H_4 = J_4^T S_4^T J_n H S_4$. Some of the entries in $H_4 = J_4^T S_4^T J_n H S_4$ (denoted in blue) are already known from (A.26)

$$H_4 = \left[\begin{array}{cc|cc||cc|cc}
-x_2^T J_n H y_2 & -x_2^T J_n H y_1 & -x_2^T J_n H u_1 & -x_2^T J_n H u_2 & -x_2^T J_n H x_2 & -x_2^T J_n H x_1 & -x_2^T J_n H v_1 & -x_2^T J_n H v_2\\
-x_1^T J_n H y_2 & 0 & 0 & 0 & -x_1^T J_n H x_2 & \lambda_1 & \gamma_1 & \mu_2\\
\hline
-v_1^T J_n H y_2 & 0 & 0 & 0 & -v_1^T J_n H x_2 & \gamma_1 & \alpha_1 & \beta_2\\
-v_2^T J_n H y_2 & 0 & 0 & 0 & -v_2^T J_n H x_2 & \mu_2 & \beta_2 & \alpha_2\\
\hline\hline
y_2^T J_n H y_2 & y_2^T J_n H y_1 & y_2^T J_n H u_1 & y_2^T J_n H u_2 & y_2^T J_n H x_2 & y_2^T J_n H x_1 & y_2^T J_n H v_1 & y_2^T J_n H v_2\\
y_1^T J_n H y_2 & \delta_1 & 0 & 0 & y_1^T J_n H x_2 & 0 & 0 & 0\\
\hline
u_1^T J_n H y_2 & 0 & \vartheta_1 & 0 & u_1^T J_n H x_2 & 0 & 0 & 0\\
u_2^T J_n H y_2 & 0 & 0 & \vartheta_2 & u_2^T J_n H x_2 & 0 & 0 & 0
\end{array}\right]$$

We will show that

$$
H_4 = \left[\begin{array}{cc|cc||cc|cc}
0 & 0 & 0 & 0 & \lambda_2 & 0 & 0 & \gamma_2 \\
0 & 0 & 0 & 0 & 0 & \lambda_1 & \gamma_1 & \mu_2 \\
\hline
0 & 0 & 0 & 0 & 0 & \gamma_1 & \alpha_1 & \beta_2 \\
0 & 0 & 0 & 0 & \gamma_2 & \mu_2 & \beta_2 & \alpha_2 \\
\hline\hline
\delta_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \delta_1 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & \vartheta_1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \vartheta_2 & 0 & 0 & 0 & 0
\end{array}\right]. \tag{A.33}
$$

Let us consider the entries in the first column of (A.33). We make use of (A.31) and obtain

$$z^T J_n H y_2 = \delta_2 z^T J_n x_2.$$

For $z = x_1, x_2, v_1, v_2, y_1, u_1, u_2$ we have $z^T J_n x_2 = 0$ due to (A.32), while, $y_2^T J_n x_2 = 1$. Thus $y_2^T J_n H y_2 = \delta_2$. Moreover, the other 7 entries in the first column are zero. This implies that the other 7 entries in the fifth row are zero as well.

For the entries $x_2^T J_n H z$ for $z = y_1, u_1, u_2$, in the first row we note that

$$\psi_2 \cdot x_2^T J_n H z = (H^{-1} y_1 - e_{11} x_1 - g_{11} v_1 - g_{12} v_2)^T J_n H z = -y_1^T J_n z - (e_{11} x_1 + g_{11} v_1 + g_{12} v_2)^T J_n H z = 0$$

due to (A.28), (A.32) and (A.26). These zeros imply zeros in the positions $(6,5), (7,5)$ and $(8,5)$.

It remains to consider the two entries at the positions $(1,6)$ and $(1,7)$. With (A.15) it follows that

$$\psi_1 \cdot x_2^T J_n H x_1 = x_2^T J_n H (H^{-1} u_1 - f_{11} v_1) = x_2^T J_n u_1 - f_{11} x_2^T J_n H v_1 = -f_{11} x_2^T J_n H v_1$$

due to (A.32). Thus, the entry at position $(1,6)$ is zero if and only if the entry at position $(1,7)$ is zero. For the entry at position $(1,7)$ we have with (A.24) and (A.23)

$$x_2^T J_n H v_1 = x_2^T J_n (\chi_2 u_2 + \gamma_1 y_1 \alpha_1 u_1) = 0$$

due to (A.32). Hence, (A.33) holds.

A.4.2. The projected matrix $J_4^T S_4^T J_n H^{-1} S_4$. Some of the entries in $\tilde{H}_4 = J_4^T S_4^T J_n H^{-1} S_4$ (denoted in blue) are already known from (A.27),

$$
\left[\begin{array}{cccc|cccc}
-x_2^T J_n H^{-1} y_2 & 0 & 0 & 0 & -x_2^T J_n H^{-1} x_2 & 0 & 0 & 0 \\
-x_1^T J_n H^{-1} y_2 & 0 & 0 & 0 & 0 & 1/\delta_1 & 0 & 0 \\
-v_1^T J_n H^{-1} y_2 & 0 & 0 & 0 & 0 & 0 & 1/\vartheta_1 & 0 \\
-v_2^T J_n H^{-1} y_2 & 0 & 0 & 0 & 0 & 0 & 0 & 1/\vartheta_2 \\
\hline
y_2^T J_n H^{-1} y_2 & y_2^T J_n H^{-1} y_1 & y_2^T J_n H^{-1} u_1 & y_2^T J_n H^{-1} u_2 & y_2^T J_n H^{-1} x_2 & y_2^T J_n H^{-1} x_1 & y_2^T J_n H^{-1} v_1 & y_2^T J_n H^{-1} v_2 \\
y_1^T J_n H^{-1} y_2 & e_{11} & g_{11} & g_{12} & 0 & 0 & 0 & 0 \\
u_1^T J_n H^{-1} y_2 & g_{11} & f_{11} & 0 & 0 & 0 & 0 & 0 \\
u_2^T J_n H^{-1} y_2 & g_{12} & 0 & f_{22} & 0 & 0 & 0 & 0
\end{array}\right]
$$

$$
= \left[\begin{array}{cc|cc||cc|cc}
0 & 0 & 0 & 0 & 1/\delta_2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1/\delta_1 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 1/\vartheta_1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/\vartheta_2 \\
\hline\hline
e_{22} & e_{12} & g_{12} & g_{22} & 0 & 0 & 0 & 0 \\
e_{12} & e_{11} & g_{11} & g_{12} & 0 & 0 & 0 & 0 \\
\hline
g_{12} & g_{11} & f_{11} & 0 & 0 & 0 & 0 & 0 \\
g_{22} & g_{12} & 0 & f_{22} & 0 & 0 & 0 & 0
\end{array}\right]. \tag{A.34}
$$

In addition, most of the ones in the 5th column (denoted in red) and hence in the first row are known from the derivations concerning (A.29).

Let us consider the remaining entries in the first row. As H^{-1} is Hamiltonian and due to (A.30), we have

$$x_2^T J_n H^{-1} x_2 = x_2^T (J_n H^{-1})^T x_2 = -(H^{-1}x_2)^T J_n x_2 = -\xi_2 = -1/\delta_2.$$

Due to (A.31) and (A.32) it follows that

$$\xi_2 \cdot y_2^T J_n H^{-1} x_2 = y_2^T J_n y_2 = 0.$$

Finally, we consider the three remaining entries in the first column,

$$z^T J_n H^{-1} y_2 = -(H^{-1}z)^T J_n y_2$$

for $z = x_1, v_1, v_2$. Due to $\vartheta_i H^{-1} v_i = u_i$ for $i = 1, 2$, we obtain with (A.32)

$$\vartheta_i \cdot (H^{-1}v_i)^T J_n y_2 = u_i^T J_n y_2 = 0,$$

while with (A.20) we have

$$\delta_1 \cdot (H^{-1}x_1)^T J_n y_2 = y_1^T J_n y_2 = 0.$$

Hence, (A.34) holds.

A.5. Step 5: $\mathrm{range}\{S_5\} = \mathcal{K}_6(H, u_1) + \mathcal{K}_4(H^{-1}, H^{-1}u_1)$ **and Step 6:** $\mathrm{range}\{S_6\} = \mathcal{K}_6(H, u_1) + \mathcal{K}_6(H^{-1}, H^{-1}u_1)$**.** We refrain from stating Steps 5 and 6 explicitly even so u_2 and x_2 are not displaying the general form of u_k and x_k. This can only be seen from u_3 and x_3 which would be derived in Steps 5 and 6. As the derivations which lead to u_3 and x_3 are the same as in the general case for deriving u_{k+1} and x_{k+1}, we directly proceed to the general case assuming that Algorithm 1 holds up to step k.

A.6. Step 2k+1: $\mathrm{range}\{S_{2k+1}\} = \mathcal{K}_{2k+2}(H, u_1) + \mathcal{K}_{2k}(H^{-1}, H^{-1}u_1)$**.** Assume that we have constructed

$$S_{2k} = [y_k \ \cdots \ y_1 \ u_1 \ \cdots \ u_k \mid x_k \ \cdots \ x_1 \ v_1 \ \cdots \ v_k] = [Y_k \ U_k \mid X_k \ V_k] \in \mathbb{R}^{2n \times 4k}$$

such that $S_{2k}^T J n S_{2k} = J_{2k}$,

$$H_{2k} = J_{2k}^T S_{2k}^T J_n H S_{2k} = \begin{bmatrix} -X_k^T J_n H Y_k & -X_k^T J_n H U_k & -X_k^T J_n H X_k & -X_k^T J_n H V_k \\ -V_k^T J_n H Y_k & -V_k^T J_n H U_k & -V_k^T J_n H X_k & -V_k^T J_n H V_k \\ Y_k^T J_n H Y_k & Y_k^T J_n H U_k & Y_k^T J_n H X_k & Y_k^T J_n H V_k \\ U_k^T J_n H Y_k & U_k^T J_n H U_k & U_k^T J_n H X_k & U_k^T J_n H V_k \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0 & \Lambda_k & B_{kk} \\ 0 & 0 & B_{kk}^T & T_k \\ \Delta_k & 0 & 0 & 0 \\ 0 & \Theta_k & 0 & 0 \end{bmatrix} \tag{A.35}$$

as in (4.3) ($r = s = k$),

$$\tilde{H}_{2k} = J_{2k}^T S_{2k}^T J_n H^{-1} S_{2k} = \begin{bmatrix} -X_k^T J_n H^{-1} Y_k & -X_k^T J_n H^{-1} U_k & -X_k^T J_n H^{-1} X_k & -X_k^T J_n H^{-1} V_k \\ -V_k^T J_n H^{-1} Y_k & -V_k^T J_n H^{-1} U_k & -V_k^T J_n H^{-1} X_k & -V_k^T J_n H^{-1} V_k \\ Y_k^T J_n H^{-1} Y_k & Y_k^T J_n H^{-1} U_k & Y_k^T J_n H^{-1} X_k & Y_k^T J_n H^{-1} V_k \\ U_k^T J_n H^{-1} Y_k & U_k^T J_n H^{-1} U_k & U_k^T J_n H^{-1} X_k & U_k^T J_n H^{-1} V_k \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0 & \Delta_k^{-1} & 0 \\ 0 & 0 & 0 & \Theta_k^{-1} \\ E_k & G_{kk} & 0 & 0 \\ G_{kk}^T & F_k & 0 & 0 \end{bmatrix} \tag{A.36}$$

as in (5.6) and

$$\operatorname{range}\{S_{2k}\} = \mathcal{K}_{2k}(H, u_1) + \mathcal{K}_{2k}(H^{-1}, H^{-1}u_1).$$

The computational steps can be found in Algorithm 1.

In this step the next two vectors $H^{2k}u_1$ and $H^{2k+1}u_1$ from $\mathcal{K}_{2k+2}(H, u_1)$ are added to the symplectic basis. Due to the previous construction, this is achieved by first considering Hv_k. J-orthogonalizing Hv_k against the columns of S_{2k} yields

$$\begin{aligned} w_u = (I - S_{2k}J_2^T S_{2k}^T J_n)Hv_k &= Hv_k - [X_k \quad V_k \quad -Y_k \quad -U_k] \begin{bmatrix} Y_k^T J_n H v_k \\ U_k^T J_n H v_k \\ X_k^T J_n H v_k \\ V_k^T J_n H v_k \end{bmatrix} \\ &= Hv_k - \gamma_k y_k - \mu_k y_{k-1} - \beta_k u_{k-1} - \alpha_k u_k \end{aligned}$$

as due to (A.35)

$$Y_k^T J_n H v_k = 0, \qquad U_k^T J_n H v_k = 0,$$

$$X_k^T J_n H v_k = \begin{bmatrix} -\gamma_k \\ -\mu_k \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \qquad V_k^T J_n H v_k = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ -\beta_k \\ -\alpha_k \end{bmatrix}.$$

Normalizing w_u to length 1 gives

$$u_{k+1} = w_u / \chi_{k+1}, \tag{A.37}$$

where it is assumed that $\chi_{k+1} = \|w_u\|_2 \neq 0$.

This step is finalized by J-orthogonalizing Hu_{k+1} against the columns of S_{2k}

$$w_v = (I - S_{2k}J_{2k}^T S_{2k}^T J_n)Hu_{k+1} = Hu_{k+1} - [X_k \quad V_k \quad -Y_k \quad -U_k] \begin{bmatrix} Y_k^T J_n H u_{k+1} \\ U_k^T J_n H u_{k+1} \\ X_k^T J_n H u_{k+1} \\ V_k^T J_n H u_{k+1} \end{bmatrix}.$$

All entries of the last vector are zero. The zeros in the first two blocks $Y_k^T J_n H u_{k+1}$ and $U_k^T J_n H u_{k+1}$ can be seen by using $y_j = \delta_j H^{-1} x_j$ and $u_j = \vartheta_j H^{-1} v_j$ for $j = 1, \dots, k$ as well as $H^{-T} J_n H = -J_n$:

$$\begin{aligned} y_j^T J_n H u_{k+1}/\delta_j &= (H^{-1}x_j)^T J_n H u_{k+1} = -x_j^T J_n u_{k+1} = 0, \\ u_j^T J_n H u_{k+1}/\vartheta_j &= (H^{-1}v_j)^T J_n H u_{k+1} = -v_j^T J_n u_{k+1} = 0, \end{aligned}$$

due to the construction of u_{k+1} as J-orthogonal against all columns of S_{2k}.

The zeros in the last block $V_k^T J_n H v_k$ follow as H is Hamiltonian and with

$$\chi_j u_j = H v_j - \gamma_j y_j - \mu_j y_{j-1} - \beta_j u_{j-1} - \alpha_j u_j$$

for $j = 1, \dots, k$, (where we set $\beta_1 = \mu_1 = 0$ and $y_0 = u_0 = 0$)

$$\begin{aligned} v_j^T J_n H u_{k+1} &= v_j^T (J_n H)^T u_{k+1} = -(H v_j)^T J_n u_{k+1} \\ &= -(\chi_j u_j + \gamma_j y_j + \mu_j y_{j-1} + \beta_j u_{j-1} + \alpha_j u_j)^T J_n u_{k+1} = 0, \end{aligned} \tag{A.38}$$

again due to the construction of u_{k+1} as J-orthogonal against all columns of S_{2k}.

With this we can show that the entries of the next to last block $X_k^T J_n H v_k$ are all zero. First, with $\psi_1 x_1 = H^{-1} u_1 - f_{11} v_1$ and $H^{-T} J_n H = -J_n$ we have

$$\begin{aligned} \psi_1 \cdot x_1^T J_n H u_{k+1} &= (H^{-1}u_1 - f_{11}v_1)^T J_n H u_{k+1} = u_1^T H^{-T} J_n H u_{k+1} - f_{11} v_1 J_n H u_{k+1} \\ &= -u_1^T J_n u_{k+1} - f_{11} v_1 J_n H u_{k+1} = 0 \end{aligned} \tag{A.39}$$

due to the construction of u_{k+1} as J-orthogonal against all columns of S_{2k} and due to (A.38). Next, we use

$$\psi_{j+1} x_{j+1} = H^{-1} y_j - e_{jj} x_j - e_{j-1,j} x_{j-1} - g_{jj} v_j - g_{j1,j+1} v_{j+1} \tag{A.40}$$

for $j = 1, \dots, k-1$ (where we set $e_{01} = 0$ and $x_0 = 0$, see Lines 16 and 29 of Algorithm 1) for the other entries of the next to last block

$$\begin{aligned} \psi_{j+1} \cdot x_{j+1}^T J_n H u_{k+1} &= -(e_{jj} x_j + e_{j-1,j} x_{j-1} + g_{jj} v_j + g_{j,j+1} v_{j+1})^T J_n H u_{k+1} + y_j^T H^{-T} J_n H u_{k+1} \\ &= -(e_{jj} x_j + e_{j-1,j} x_{j-1})^T J_n H u_{k+1} - y_j^T J_n u_{k+1} \end{aligned}$$

as $v_j^T J_n H u_{k+1} = 0$ due to (A.38). Clearly, $y_j^T J_n u_{k+1} = 0$ by construction of u_{k+1}. Thus, it remains to consider

$$\psi_{j+1} \cdot x_{j+1}^T J_n H u_{k+1} = -(e_{jj} x_j + e_{j-1,j} x_{j-1})^T J_n H u_{k+1}.$$

For $j = 1$ we have with $x_0 = 0$ and (A.39) that $\psi_2 \cdot x_2^T J_n H u_{k+1} = 0$. With this, we get $\psi_3 \cdot x_3^T J_n H u_{k+1} = 0$, and, continuing in this fashion,

$$\psi_{j+1} \cdot x_{j+1}^T J_n H u_{k+1} = 0.$$

Thus the expression for w_v simplifies to

$$w_v = H u_{k+1}.$$

Normalizing w_v by $\vartheta_{k+1} = u_{k+1}^T J_n H u_{k+1}$ to make sure it is J-orthogonal to u_{k+1} yields

$$v_{k+1} = H u_{k+1} / \vartheta_{k+1}. \tag{A.41}$$

Let $S_{2k+1} = [y_k \ \cdots \ y_1 \ u_1 \ \cdots \ u_{k+1} \mid x_k \ \cdots \ x_1 \ v_1 \ \cdots \ v_{k+1}] = [Y_k \ U_{k+1} \mid X_k \ V_{k+1}] \in \mathbb{R}^{2n \times 4k+2}$. Then by construction

$$S_{2k+1}^T J_n S_{2k+1} = J_{2k+1} \tag{A.42}$$

and $\text{range}\{S_{2k+1}\} = \mathcal{K}_{2k+2}(H, u_1) + \mathcal{K}_{2k}(H^{-1}, H^{-1}u_1)$.

A.6.1. The projected matrix $H_{2k+1} = J_{2k+1}^T S_{2k+1}^T J_n H S_{2k+1}$. Most of the entries in $H_{2k+1} = J_{2k+1}^T S_{2k+1}^T J_n H S_{2k+1}$ (denoted in blue) are already known from H_{2k} (A.35)

$$H_{2k+1} = \left[\begin{array}{c|c|c||c|c|c}
0 & 0 & -X_k^T J_n H u_{k+1} & \Lambda_k & B_{kk} & -X_k^T J_n H v_{k+1} \\ \hline
0 & 0 & -V_k^T J_n H u_{k+1} & {B_{kk}}^T & T_k & -V_k^T J_n H v_{k+1} \\
-v_{k+1}^T J_n H Y_k & -v_{k+1}^T J_n H U_k & -v_{k+1}^T J_n H u_{k+1} & -v_{k+1}^T J_n H X_k & -v_{k+1}^T J_n H V_k & -v_{k+1}^T J_n H v_{k+1} \\ \hline\hline
\Delta_k & 0 & Y_k^T J_n H u_{k+1} & 0 & 0 & Y_k^T J_n H v_{k+1} \\ \hline
0 & \Theta_k & U_k^T J_n H u_{k+1} & 0 & 0 & U_k^T J_n H v_{k+1} \\
u_{k+1}^T J_n H Y_k & u_{k+1}^T J_n H U_k & u_{k+1}^T J_n H u_{k+1} & u_{k+1}^T J_n H X_k & u_{k+1}^T J_n H V_k & u_{k+1}^T J_n H v_{k+1}
\end{array}\right]$$

$$= \left[\begin{array}{c|c|c||c|c|c}
0 & 0 & 0 & \Lambda_k & B_{kk} & \begin{matrix}\mu_k \\ 0 \\ \vdots \\ 0\end{matrix} \\ \hline
0 & 0 & 0 & {B_{kk}}^T & T_k & \begin{matrix}0 \\ \vdots \\ 0 \\ \beta_{k+1}\end{matrix} \\
0 & 0 & 0 & \mu_k \; 0 \cdots 0 & 0 \cdots 0 \; \beta_{k+1} & \alpha_{k+1} \\ \hline\hline
\Delta_k & 0 & 0 & 0 & 0 & 0 \\ \hline
0 & \Theta_k & 0 & 0 & 0 & 0 \\
0 & 0 & \vartheta_{k+1} & 0 & 0 & 0
\end{array}\right] = \left[\begin{array}{c|c||c|c}
0 & 0 & \Lambda_k & B_{k,k+1} \\ \hline
0 & 0 & B_{k,k+1}^T & T_{k+1} \\ \hline\hline
\Delta_k & 0 & 0 & 0 \\ \hline
0 & \Theta_{k+1} & 0 & 0
\end{array}\right]. \tag{A.43}$$

The zeros in the third column (and hence in the last row) follow due to $Hu_{k+1} = \vartheta_{k+1} v_{k+1}$ and (A.42). The zeros in the first block $v_{k+1}^T J_n H Y_k$ of the third row follow due to $Hy_j = \delta_j x_j$, for $j = 1, \ldots, k$, the ones in the second block $v_{k+1}^T J_n H U_k$ due to $Hu_j = \vartheta_j v_j$, $j = 1, \ldots, k$. This also implies the zeros in the last row of the fourth and fifth block.

Moreover, we obtain

$$v_{k+1}^T J_n H V_{k-1} = 0$$

from

$$\chi_{j+1} u_{j+1} = H v_j - \gamma_j y_j - \mu_j y_{j-1} - \beta_j u_{j-1} - \alpha_j u_j \tag{A.44}$$

for $j = 1, \ldots, k-1$ (where we set $\beta_0 = \mu_0 = 0$ and $u_0 = y_0 = 0$, see Lines 11 and 24 in Algorithm 1) as

$$v_{k+1}^T J_n H v_j = v_{k+1}^T J_n (\psi_{j+1} u_{j+1} + \gamma_j y_j + \mu_j y_{j-1} + \beta_j u_{j-1} + \alpha_j u_j) = 0$$

due to the construction of v_{k+1} as J-orthogonal against all columns of S_{2k}. With this, $\psi_1 x_1 = H^{-1} u_1 - f_{11} v_1$ and the recurrence for x_j as in (A.40), we observe that

$$v_{k+1}^T J_n H X_{k-1} = 0$$

holds. This can be seen step by step. Due to (A.42) and $v_{k+1}^T J_n H V_{k-1} = 0$, we have

$$\psi_1 v_{k+1}^T J_n H x_1 = v_{k+1}^T J_n H (H^{-1} u_1 - f_{11} v_1) = v_{k+1}^T J_n u_1 - f_{11} v_{k+1}^T J_n H v_1 = 0,$$

and with this and (A.28) we have further

$$\psi_2 v_{k+1}^T J_n H x_2 = -v_{k+1}^T J_n y_1 - e_{11} v_{k+1}^T J_n H x_1 - g_{11} v_{k+1}^T J_n H v_1 - g_{12} v_{k+1}^T J_n H v_2 = 0.$$

In this fashion we continue with the expression for x_{j+1} as in Line 30 of Algorithm 1 to obtain for $j = 2, \ldots, k-2$

$$\begin{aligned}\psi_{j+1} v_{k+1}^T J_n H x_{j+1} = {} & -v_{k+1}^T J_n y_j - e_{jj} v_{k+1}^T J_n H x_j - e_{j-1,j} v_{k+1}^T J_n H x_{j-1} \\ & - g_{jj} v_{k+1}^T J_n H v_{j+1} - g_{j,j+1} v_{k+1}^T J_n H v_j = 0.\end{aligned}$$

Hence, (A.43) holds.

A.6.2. The projected matrix $J_{2k+1}^T S_{2k+1}^T J_n H^{-1} S_{2k+1}$. Most of the entries in

$$\tilde{H}_{2k+1} = J_{2k+1}^T S_{2k+1}^T J_n H^{-1} S_{2k+1}$$

(denoted in blue) are already known from (A.36)

$$\tilde{H}_{2k+1} = \left[\begin{array}{ccc|ccc} 0 & 0 & -X_k^T J_n H^{-1} u_{k+1} & \Delta_k^{-1} & 0 & -X_k^T J_n H^{-1} v_{k+1} \\ 0 & 0 & -V_k^T J_n H^{-1} u_{k+1} & 0 & {\Theta_k}^{-1} & -V_k^T J_n H^{-1} v_{k+1} \\ -v_{k+1}^T J_n H^{-1} Y_k & -v_{k+1}^T J_n H^{-1} U_k & -v_{k+1}^T J_n H^{-1} u_{k+1} & -v_{k+1}^T J_n H^{-1} X_k & -v_{k+1}^T J_n H^{-1} V_k & -v_{k+1}^T J_n H^{-1} v_{k+1} \\ \hline E_k & G_k & Y_k^T J_n H^{-1} u_{k+1} & 0 & 0 & Y_k^T J_n H^{-1} v_{k+1} \\ {G_k}^T & F_k & U_k^T J_n H^{-1} u_{k+1} & 0 & 0 & U_k^T J_n H^{-1} v_{k+1} \\ u_{k+1}^T J_n H^{-1} Y_k & u_{k+1}^T J_n H^{-1} U_k & u_{k+1}^T J_n H^{-1} u_{k+1} & u_{k+1}^T J_n H^{-1} X_k & u_{k+1}^T J_n H^{-1} V_k & u_{k+1}^T J_n H^{-1} v_{k+1} \end{array}\right]$$

(A.45)

$$= \left[\begin{array}{ccc|ccc} 0 & 0 & 0 & \Delta_k^{-1} & 0 & 0 \\ 0 & 0 & 0 & 0 & {\Theta_k}^{-1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/\vartheta_{k+1} \\ \hline E_k & G_k & \begin{matrix} g_{k,k+1} \\ 0 \\ \vdots \\ 0 \end{matrix} & 0 & 0 & 0 \\ {G_k}^T & F_k & 0 & 0 & 0 & 0 \\ g_{k,k+1}\ 0 \cdots 0 & 0 & f_{k+1,k+1} & 0 & 0 & 0 \end{array}\right] = \left[\begin{array}{cc|cc} 0 & 0 & \Delta_k^{-1} & 0 \\ 0 & 0 & 0 & \Theta_{k+1}^{-1} \\ \hline E_k & G_{k,k+1} & 0 & 0 \\ G_{k,k+1}^T & F_{k+1} & 0 & 0 \end{array}\right]$$

With (A.41) and $H^{-T} J_n H = -J_n$, we see that the entries $v_{k+1}^T J_n H^{-1} z$ in the third block row are zeros (despite the last entry)

$$\vartheta_1 \cdot v_{k+1}^T J_n H^{-1} z = u_{k+1}^T H^T J_n H^{-1} z = -u_{k+1}^T J_n z = 0 \tag{A.46}$$

for $z \in \{y_1, \ldots, y_k, u_1, \ldots, u_{k+1}, x_1, \ldots, x_k, v_1 \ldots, v_k\}$ due to the construction of u_{k+1} as J-orthogonal to all columns of S_{2k}. This implies the zeros in the last column of (A.45). For the last entry we have

$$-\vartheta_{k+1} \cdot v_{k+1}^T J_n H^{-1} v_{k+1} = -u_{k+1}^T H^T J_n H^{-1} v_{k+1} = u_{k+1}^T J_n v_{k+1} = 1.$$

Thus, $-v_{k+1}^T J_n H^{-1} v_{k+1} = 1/\vartheta_{k+1}$.

With (A.37) the entries in the upper part of the third column (as well as the entries in the fourth and fifth block of the last row) are zero as

$$\begin{aligned} \chi_{k+1} z^T J_n H^{-1} u_{k+1} &= z^T J_n H^{-1}(H v_k - \gamma_k y_k - \mu_k y_{k-1} - \beta_k u_{k-1} - \alpha_k u_k) \\ &= z^T J_n v_k - z^T J_n H^{-1}(\gamma_k y_k + \mu_k y_{k-1} + \beta_k u_{k-1} + \alpha_k u_k) = 0 \end{aligned}$$

for $z \in \{x_1, \ldots, x_k, v_1, \ldots, v_k\}$ due to (A.46) and (A.36).

The entries in $Y_{k-1}^T J_n H^{-1} u_{k+1}$ are zero as H^{-1} is Hamiltonian and (A.40) yield

$$\begin{aligned} y_j^T J_n H^{-1} u_{k+1} &= -(H^{-1} y_j)^T J_n u_{k+1} \\ &= -(\psi_{j+1} x_{j+1} - e_{jj} x_j - e_{j-1,j} x_{j-1} - g_{jj} v_j - g_{j,j+1} v_{j+1})^T J_n u_{k+1} = 0 \end{aligned} \tag{A.47}$$

for $j = 1, \ldots, k-1$ due to the construction of u_{k+1} as J-orthogonal to all columns of S_{2k}.

With this, we can show in a recursive manner that the entries in

$$U_{k-1}^T J_n H^{-1} u_{k+1} = -(H^{-1} U_{k-1})^T J_n u_{k+1}$$

are zero by making use of $\chi_1 u_1 = \psi_1 x_1 - f_{11} v_1$ and (A.44). First we obtain

$$\chi_1 \cdot (H^{-1}u_1)^T J_n u_{k+1} = (\psi_1 x_1 - f_{11} v_1)^T J_n u_{k+1} = 0 \tag{A.48}$$

due to the construction of u_{k+1} as J-orthogonal to all columns of S_{2k}. Next we observe

$$\chi_2 \cdot (H^{-1}u_2)^T J_n u_{k+1} = (v_1 - \gamma_1 H^{-1} y_1 - \alpha_1 H^{-1} u_1)^T J_n u_{k+1} = 0,$$

where the first term is zero as u_{k+1} is J-orthogonal to v_1, the second one due to (A.47) and the third term due to (A.48). Continuing in this fashion, we have

$$\begin{aligned}\chi_j \cdot (H^{-1}u_j)^T J_n u_{k+1} &= (v_{j-1} - \gamma_{j-1} H^{-1} y_{j-1} - \mu_{j-1} H^{-1} y_{j-2})^T J_n u_{k+1} \\ &\quad - (\beta_{j-2} H^{-1} u_{j-2} + \alpha_{j-1} H^{-1} u_{j-1})^T J_n u_{k+1} = 0\end{aligned}$$

where the first term is zero as u_{k+1} is J-orthogonal to v_{j-1}, the second and third one due to (A.47), and the fourth and fifth term due to the preceding observations.

Hence, (A.45) holds.

A.7. Step 2k+2: range$\{S_{2k+2}\} = \mathcal{K}_{2k+2}(H, u_1) + \mathcal{K}_{2k+2}(H^{-1}, H^{-1}u_1)$**.** Assume that we have constructed $S_{2k+1} = [Y_k \;\; U_{k+1} \mid X_k \;\; V_{k+1}] \in \mathbb{R}^{2n \times 4k+2}$ as in the previous section.

The two vectors $H^{-(2k+1)}u_1$ and $H^{-(2k+2)}u_1$ from $\mathcal{K}_{2k+2}(H^{-1}, H^{-1}u_1)$ are added to the symplectic basis. Due to the previous construction, this is achieved by constructing x_{k+1} from $H^{-1}y_k$ and y_{k+1} from $H^{-1}x_{k+1}$. First $H^{-1}y_k$ is J-orthogonalized against the columns of S_{2k+1}:

$$\begin{aligned} w_x &= (I - S_{2k+1} J_{2k+1}^T S_{2k+1}^T J_n) H^{-1} y_k = H^{-1} y_k - [X_k \;\; V_{k+1} \quad -Y_k \quad -U_{k+1}] \begin{bmatrix} Y_k^T J_n H^{-1} y_k \\ U_{k+1}^T J_n H^{-1} y_k \\ X_k^T J_n H^{-1} y_k \\ V_{k+1}^T J_n H^{-1} y_k \end{bmatrix} \\ &= H^{-1} y_k - e_{kk} x_k - e_{k-1,k} x_{k-1} - g_{kk} v_k - g_{k,k+1} v_{k+1} \end{aligned}$$

due to (A.45). Normalizing w_x to length 1 gives

$$x_{k+1} = w_x / \psi_{k+1}, \tag{A.49}$$

where we assume that $\psi_{k+1} = \|w_x\|_2 \neq 0$.

This step is finalized by J-orthogonalizing $H^{-1}x_{k+1}$ against the columns of S_{2k+1}:

$$w_y = (I - S_{2k+1} J_{2k+1}^T S_{2k+1}^T J_n) H^{-1} x_{k+1} = H^{-1} x_{k+1} - [X_k \;\; V_{k+1} \mid -Y_k \;\; -U_{k+1}] \begin{bmatrix} Y_k^T J_n H^{-1} x_{k+1} \\ U_{k+1}^T J_n H^{-1} x_{k+1} \\ X_k^T J_n H^{-1} x_{k+1} \\ V_{k+1}^T J_n H^{-1} x_{k+1} \end{bmatrix}.$$

All entries $z^T J_n H^{-1} x_{k+1} = -(H^{-1}z)^T J_n x_{k+1}$ in the last vector are zero. In order to see this, let us first consider $z = v_j, j = 1, \ldots, k+1$. Due to $\vartheta_j v_j = H u_j$, we have immediately

$$(H^{-1} v_j)^T J_n x_{k+1} = -u_j^T J_n x_{k+1} / \vartheta_j = 0.$$

Next, we consider $z = x_j, j = 1, \dots, k$, and make use of $\xi_j y_j = H^{-1}x_j$ to obtain

$$(H^{-1}x_j)^T J_n x_{k+1} = \zeta_j y_j^T J_n x_{k+1} = 0.$$

Rewriting (A.40) in terms of $H^{-1}y_j$, the case $z = y_j, j = 1, \dots, k$ yields

$$(H^{-1}y_j)^T J_n x_{k+1} = (\psi_j x_j - e_{j-1,j-1}x_{j-1} - g_{j-1,j-1}v_{j-1} - g_{j-1,j}v_j)^T J_n x_{k+1} = 0.$$

Finally, for $z = u_j$ we obtain from (A.15)

$$(H^{-1}u_1)^T J_n x_{k+1} = (\psi_1 x_1 - f_{11}v_1)^T J_n x_{k+1} = 0,$$

from (A.24)

$$(H^{-1}u_2)^T J_n x_{k+1} = (v_1 + \gamma_1 H^{-1}y_1 + \alpha_1 H^{-1}u_1)^T J_n x_{k+1}/\chi_2 = 0,$$

and from (A.37)

$$(H^{-1}u_{j+1})^T J_n x_{k+1} = (v_j + \gamma_j H^{-1}y_j + \mu_j y_{j-1} + \beta_j u_{j-1} + \alpha_j H^{-1}u_j)^T J_n x_{k+1}/\chi_{j+1} = 0$$

for $j = 2, \dots, k$.

Thus,

$$y_{k+1} = H^{-1}x_{k+1}/\xi_{k+1} \tag{A.50}$$

where we assume that

$$\xi_{k+1} = (H^{-1}x_{k+1})^T J_n x_{k+1} = x_{k+1}^T H^{-T} J_n x_{k+1} \neq 0.$$

With the same argument as in (A.19) we see that

$$\delta_{k+1} = -\frac{1}{\xi_{k+1}}.$$

Let $S_{2k+2} = [y_{k+1}\ Y_k\ u_{k+1} \mid x_{k+1}\ X_k\ V_{k+1}] \in \mathbb{R}^{2n \times 4k+4}$. Then by construction $S_{2k+2}^T J_n S_{2k+2} = J_{2k+2}$ and range$\{S_{2k+2}\} = \mathcal{K}_{2k+2}(H, u_1) + \mathcal{K}_{2k+2}(H^{-1}, H^{-1}u_1)$.

A.7.1. The projected matrix $H_{2k+2} = J_{2k+2}^T S_{2k+2}^T J_n H S_{2k+2}$. Most of the entries in $H_{2k+2} = J_{2k+2}^T S_{2k+2}^T J_n H S_{2k+2}$ (denoted in blue) are already known from (A.43)

$$\left[\begin{array}{cc|c||cc|c}
-x_{k+1}^T J_n H y_{k+1} & -x_{k+1}^T J_n H Y_k & -x_{k+1}^T J_n H U_{k+1} & -x_{k+1}^T J_n H x_{k+1} & -x_{k+1}^T J_n H X_k & -x_{k+1}^T J_n H V_{k+1} \\
-X_k^T J_n H y_{k+1} & \color{blue}{0} & \color{blue}{0} & -X_k^T J_n H x_{k+1} & \color{blue}{\Lambda_k} & \color{blue}{B_{k,k+1}} \\
\hline
-V_{k+1}^T J_n H y_{k+1} & \color{blue}{0} & \color{blue}{0} & -V_{k+1}^T J_n H x_{k+1} & \color{blue}{B_{k,k+1}{}^T} & \color{blue}{T_{k+1}} \\
\hline\hline
y_{k+1}^T J_n H y_{k+1} & y_{k+1}^T J_n H Y_k & y_{k+1}^T J_n H U_{k+1} & y_{k+1}^T J_n H x_{k+1} & y_{k+1}^T J_n H X_k & y_{k+1}^T J_n H V_{k+1} \\
Y_k^T J_n H y_{k+1} & \color{blue}{\Delta_k} & \color{blue}{0} & Y_k^T J_n H x_{k+1} & \color{blue}{0} & \color{blue}{0} \\
\hline
U_{k+1}^T J_n H y_{k+1} & \color{blue}{0} & \color{blue}{\Theta_{k+1}} & U_{k+1}^T J_n H x_{k+1} & \color{blue}{0} & \color{blue}{0}
\end{array}\right]$$

$$= \left[\begin{array}{cc|c||cc|c}
0 & 0 & 0 & \lambda_{k+1} & 0 & 0 \cdots 0\ \gamma_{k+1} \\
0 & \color{blue}{0} & \color{blue}{0} & 0 & \color{blue}{\Lambda_k} & \color{blue}{B_{k,k+1}} \\
\hline
0 & \color{blue}{0} & \color{blue}{0} & \begin{smallmatrix} 0 \\ \vdots \\ 0 \\ \gamma_{k+1} \end{smallmatrix} & \color{blue}{B_{k,k+1}{}^T} & \color{blue}{T_{k+1}} \\
\hline\hline
\delta_{k+1} & 0 & 0 & 0 & 0 & 0 \\
0 & \color{blue}{\Delta_k} & \color{blue}{0} & 0 & \color{blue}{0} & \color{blue}{0} \\
\hline
0 & \color{blue}{0} & \color{blue}{\Theta_{k+1}} & 0 & \color{blue}{0} & \color{blue}{0}
\end{array}\right] = \left[\begin{array}{cc||cc}
0 & 0 & \Lambda_{k+1} & B_{k+1,k+1} \\
0 & 0 & B_{k1,k+1}^T & T_{k+1} \\
\hline\hline
\Delta_{k+1} & 0 & 0 & 0 \\
0 & \Theta_{k+1} & 0 & 0
\end{array}\right]. \tag{A.51}$$

Making use of (A.50) we obtain $z^T J_n H y_{k+1} = \delta_{k+1} z^T J_n x_{k+1} = 0$ for all but two of the entries in the first column, that is, for $z = x_1, \dots, x_{k+1},\ v_1,\ \dots,\ v_{k+1},\ y_1,\ \dots,\ y_k,\ u_1,\ \dots,\ u_{k+1}$. This gives the zeros in the fourth row as well.

For the entries $x_{k+1}^T J_n H z$ in the first row we note that with (A.49) and $H^{-T} J_n H = J^T$,

$$x_{k+1}^T J_n H z = \psi_{k+1} (H^{-1} y_k - e_{kk} x_k - e_{k-1,k} x_{k-1} - g_{k-1,k} v_{k+1} - g_{kk} v_k)^T J_n H z = 0$$

for $z = y_1, \dots, y_k, u_1, \dots, u_{k+1}, x_1, \dots, x_{k-2}, v_1, \dots, v_{k-2}$ due to (A.43) and $S_{2k-1}^T J_n S_{2k+1} = J_{2k+1}$. Next, with $H v_j = \chi_{j+1} u_{j+1} + \gamma_j y_j + \mu_j y_{j-1} + \beta_k u_{j-1} - \alpha_j u_j$ (A.44), it follows for $j = k-1, k, k-1$ that

$$x_{k+1}^T J_n H v_{k-2} = x_{k+1}^T J_n H v_{k-1} = x_{k+1}^T J_n H v_k = 0$$

as $S_{2k-1}^T J_n S_{2k+1} = J_{2k+1}$. With this and (A.49) we obtain three more zero entries

$$\psi_{k-2} x_{k+1}^T J_n H x_{k-2} = \psi_{k-1} x_{k+1}^T J_n H x_{k-1} = \psi_k x_{k+1}^T J_n H x_k = 0.$$

This gives the zeros in the fourth column as well.

Hence, (A.51) holds.

A.7.2. The projected matrix $J_{2k+2}^T S_{2k+2}^T J_n H^{-1} S_{2k+2}$. Most of the entries in

$$\tilde{H}_{2k+2} = J_{2k+2}^T S_{2k+2}^T J_n H^{-1} S_{2k+2}$$

(denoted in blue) are already known from (A.45),

$$\left[\begin{array}{ccc|ccc}
x_{k+1}^T J_n H^{-1} y_{k+1} & 0 & 0 & 1/\delta_{k+1} & 0 & 0 \\
X_k^T J_n H^{-1} y_{k+1} & 0 & 0 & 0 & {\Delta_k}^{-1} & 0 \\
V_{k+1}^T J_n H^{-1} y_{k+1} & 0 & 0 & 0 & 0 & {\Theta_{k+1}}^{-1} \\
\hline
-y_{k+1}^T J_n H^{-1} y_{k+1} & -y_{k+1}^T J_n H^{-1} Y_k & -y_{k+1}^T J_n H^{-1} U_{k+1} & -y_{k+1}^T J_n H^{-1} x_{k+1} & -y_{k+1}^T J_n H^{-1} X_k & -y_{k+1}^T J_n H^{-1} V_{k+1} \\
-Y_k^T J_n H^{-1} y_{k+1} & E_k & G_{k,k+1} & 0 & 0 & 0 \\
-U_{k+1}^T J_n H^{-1} y_{k+1} & {G_{k,k+1}}^T & F_{k+1} & 0 & 0 & 0
\end{array}\right]$$

(A.52)

$$= \left[\begin{array}{cc|c||cc|c}
0 & 0 & 0 & 1/\delta_{k+1} & 0 & 0 \\
0 & 0 & 0 & 0 & {\Delta_k}^{-1} & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & {\Theta_{k+1}}^{-1} \\
\hline\hline
\begin{array}{c} e_{k+1,k+1} \\ e_{k,k+1} \\ 0 \\ \vdots \\ 0 \end{array} & \begin{array}{c} e_{k,k+1}\ 0 \cdots 0 \\ E_k \end{array} & \begin{array}{c} 0 \cdots 0\ g_{k+1,k+1} \\ G_{k,k+1} \end{array} & 0 & 0 & 0 \\
\hline
\begin{array}{c} 0 \\ \vdots \\ 0 \\ g_{k+1,k+1} \end{array} & {G_{k,k+1}}^T & F_{k+1} & 0 & 0 & 0
\end{array}\right]$$

$$= \left[\begin{array}{cc||cc}
0 & 0 & \Delta_{k+1}^{-1} & 0 \\
0 & 0 & 0 & \Theta_{k+1}^{-1} \\
\hline\hline
E_{k+1} & G_{k+1,k+1} & 0 & 0 \\
G_{k+1,k+1}^T & F_{k+1} & 0 & 0
\end{array}\right]$$

All but one of the zeros in the first row (denoted in red) and the fourth column follow from the derivations in the previous section. Due to (A.50),

$$x_{k+1}^T J_n H^{-1} y_{k+1} = -(H^{-1} x_{k+1})^T J_n y_{k+1} = -\xi_{k+1} y_{k+1}^T J_n y_{k+1} = 0,$$

and the last zero in the first row/fourth columns follows.

Now, let us consider the first column. We have $X_k^T J_n H^{-1} y_{k+1} = 0$ as for $j = 1, \dots, k$

$$x_j^T J_n H^{-1} y_{k+1} = -(H^{-1} x_j)^T J_n y_{k+1} = -\xi_j y_j^T J_n y_{k+1} = 0,$$

and $V_{k+1}^T J_n H^{-1} y_{k+1} = 0$ as for $j = 1, \dots, k+1$

$$v_j^T J_n H^{-1} y_{k+1} = -(H^{-1} v_j)^T J_n y_{k+1} = -u_j^T J_n y_{k+1} / \vartheta_j = 0.$$

Next, observe that $Y_{k-1}^T J_n H^{-1} y_{k+1} = 0$ as for $j = 1, \dots, k-1$

$$y_j^T J_n H^{-1} y_{k+1} = \xi_j (H^{-1} x_j)^T J_n H^{-1} y_{k+1} = \xi_j x_j^T J_n y_{k+1} = 0.$$

Finally, making use of (A.44) we observe that $U_k^T J_n H^{-1} y_{k+1} = 0$ as for $j = 1, \dots, k$.

Hence, (A.52) holds.

REFERENCES

[1] P. Amodio. A symplectic lanczos-type algorithm to compute the eigenvalues of positive definite hamiltonian matrices. In Peter M. A. Sloot, David Abramson, Alexander V. Bogdanov, Yuriy E. Gorbachev, Jack J. Dongarra, and Albert Y. Zomaya, editors, *Computational Science — ICCS 2003*, pages 139–148, Berlin, Heidelberg, 2003. Springer Berlin Heidelberg.

[2] P. Amodio. On the computation of few eigenvalues of positive definite hamiltonian matrices. *Future Generation Computer Systems*, 22(4):403–411, 2006.

[3] H. Faßbender and M.-N. Senn, 2022. https://doi.org/10.5281/zenodo.6261078.

[4] P. Benner, H. Faßbender, and M. Stoll. A Hamiltonian Krylov–Schur-type method based on the symplectic Lanczos process. *Linear Algebra and its Applications*, 435(3):578 – 600, 2011.

[5] P. Benner and H. Faßbender. An implicitly restarted symplectic Lanczos method for the Hamiltonian eigenvalue problem. *Linear Algebra Appl.*, 263:75–111, 1997.

[6] P. Benner, A.J. Laub, and V. Mehrmann. A collection of benchmark examples for the numerical solution of algebraic Riccati equations I: Continuous-time case. Technical Report SPC 95_22, Fakultät für Mathematik, TU Chemnitz–Zwickau, 09107 Chemnitz, FRG, 1995. Available from `http://www.tu-chemnitz.de/sfb393/spc95pr.html`.

[7] V. Druskin and L. Knizhnerman. Extended Krylov subspaces: Approximation of the matrix square root and related functions. *SIAM Journal on Matrix Analysis and Applications*, 19(3):755–771, 1998.

[8] T. Eirola and A. Koskela. Krylov integrators for Hamiltonian systems. *BIT Numerical Mathematics*, 59(1):57–76, 2019.

[9] G. H. Golub and C. F. Van Loan. *Matrix computations. 4th ed.* Baltimore, MD: The Johns Hopkins University Press, 4th ed. edition, 2013.

[10] E. Hairer, C. Lubich, and G. Wanner. *Geometric Numerical Integration.* Springer Series in Computational Mathematics 31. Springer-Verlag Berlin Heidelberg, 2006.

[11] W. F. Harris and J. R. Cardoso. The exponential-mean-log-transference as a possible representation of the optical character of an average eye. *Ophthalmic and Physiological Optics*, 26(4):380–383, 2006.

[12] N. J. Higham. The Matrix Computation Toolbox. http://www.ma.man.ac.uk/~higham/mctoolbox.

[13] N. J. Higham. The matrix sign decomposition and its relation to the polar decomposition. *Linear Algebra Appl.*, 212-213:3–20, 1994.

[14] N. J. Higham. *Functions of matrices. Theory and computation.* Philadelphia, PA: Society for Industrial and Applied Mathematics (SIAM), 2008.

[15] L. Knizhnerman and V. Simoncini. A new investigation of the extended Krylov subspace method for matrix function evaluations. *Numerical Linear Algebra with Applications*, 17(4):615–638, 2010.

[16] L. Knizhnerman and V. Simoncini. Convergence analysis of the extended Krylov subspace method for the Lyapunov equation. *Numer. Math.*, 118(3):567–586, 2011.

[17] D. S. Mackey, N. Mackey, and F. Tisseur. Structured tools for structured matrices. *Electron. J. Linear Algebra*, 10:106–145, 2003.

[18] D. S. Mackey, N. Mackey, and F. Tisseur. Structured factorizations in scalar product spaces. *SIAM J. Matrix Anal. Appl.*, 27(3):821–850, 2006.

[19] L. Mei and X. Wu. Symplectic exponential Runge–Kutta methods for solving nonlinear Hamiltonian systems. *Journal of Computational Physics*, 338:567–584, 2017.

[20] S. Meister. Exponential symplectic integrators for Hamiltonian systems. Master's thesis, Fakultät für Mathematik, Technische Universität Chemnitz, Germany, 2011.

[21] J. D. Roberts. Linear model reduction and solution of the algebraic Riccati equation by use of the sign function. *International Journal of Control*, 32(4):677–687, 1980.

[22] D. S. Watkins. On Hamiltonian and symplectic Lanczos processes. *Linear Algebra Appl.*, 385:23–45, 2004.