

HAMILTONIAN SQUARE ROOTS OF SKEW HAMILTONIAN QUATERNIONIC MATRICES*

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Abstract. Criteria for existence of Hamiltonian quaternionic matrices that are square roots of a given skew Hamiltonian quaternionic matrix are developed. The criteria are formulated in terms of respective canonical forms of skew Hamiltonian quaternionic matrices. The Hamiltonian property is understood with respect to either the quaternionic conjugation, or an involutory antiautomorphism of the quaternions which is different from the quaternionic conjugation. Many results are stated and proved in a more general framework of symmetric and skewsymmetric matrices with respect to an invertible matrix which is skewsymmetric relative to an involutory antiautomorphism.

Key words. Hamiltonian matrix, Skew Hamiltonian matrix, Quaternion, Square root.

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1. Introduction. Let F be the field of real numbers R , the field of complex numbers C , or the skew field of real quaternions H . Denote by $F^{m \times n}$ the set of $m \times n$ matrices with entries in F , considered (in case $F = H$) as both right and left quaternionic vector space.

Let $\phi : F \longrightarrow F$ be a continuous involutory antiautomorphism of F (note that an antiautomorphism is automatically continuous in case $F = R$ or $F = H$). In particular ϕ is the identity map if $F = R$, and either the identity map or the complex conjugation if $F = C$. For $A \in F^{m \times n}$, we denote by A_ϕ the $n \times m$ quaternionic matrix obtained by applying ϕ entrywise to the *transposed* matrix A^T . Thus, for ϕ the complex or quaternionic conjugation, A_ϕ is just the conjugate transpose A^* of A . Note the following algebraic properties:

- (a) $(\alpha A + \beta B)_\phi = A_\phi \phi(\alpha) + B_\phi \phi(\beta)$, $\alpha, \beta \in F$, $A, B \in F^{m \times n}$.
- (b) $(A\alpha + B\beta)_\phi = \phi(\alpha)A_\phi + \phi(\beta)B_\phi$, $\alpha, \beta \in F$, $A, B \in F^{m \times n}$.
- (c) $(AB)_\phi = B_\phi A_\phi$, $A \in F^{m \times n}$, $B \in F^{n \times p}$.
- (d) $(A_\phi)_\phi = A$, $A \in F^{m \times n}$.
- (e) If $A \in F^{n \times n}$ is invertible, then $(A_\phi)^{-1} = (A^{-1})_\phi$.

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We fix the $2n \times 2n$ matrix

$$K = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}. \quad (1.1)$$

Clearly, $K_\phi = -K = K^{-1}$. A matrix $A \in \mathbb{F}^{2n \times 2n}$ is said to be $(\mathbb{F}, \phi)$ -Hamiltonian if the equality $(KA)_\phi = KA$, or equivalently $KA = -A_\phi K$, holds. We will often use the abbreviated notation ϕ -Hamiltonian (with $\mathbb{F}$ understood from context) and analogous abbreviations in subsequent terminology. A matrix $W \in \mathbb{F}^{2n \times 2n}$ is said to be ϕ -skew Hamiltonian if the equality $(KW)_\phi = -KW$, or equivalently $KW = W_\phi K$, holds.

A matrix $U \in \mathbb{F}^{2n \times 2n}$ is said to be ϕ -symplectic if

$$U_\phi K U = K. \quad (1.2)$$

It is easy to verify that if U is ϕ -symplectic, then so are U_ϕ , U^{-1} ; also, if U, V are ϕ -symplectic, then so is UV . We provide details only for the verification that if U is ϕ -symplectic, then so is U_ϕ . Indeed, taking inverses in the equality $U_\phi K U = K$, we get

$$-K = K^{-1} = U^{-1} K^{-1} (U_\phi)^{-1} = -U^{-1} K (U_\phi)^{-1},$$

hence $U K U_\phi = K$, which proves that U_ϕ is H -symplectic.

Note that if A is ϕ -Hamiltonian, resp., ϕ -skew Hamiltonian, and U is ϕ -symplectic, then $U^{-1}AU$ is also ϕ -Hamiltonian or ϕ -skew Hamiltonian, as the case may be. Two matrices $X, Y \in \mathbb{F}^{n \times n}$ are said to be $\mathbb{F}$ -similar if $X = S^{-1}YS$ for some invertible matrix $S \in \mathbb{F}^{n \times n}$; if S is in addition ϕ -symplectic, we say that X and Y are ϕ -symplectically similar.

In this paper we give criteria for a ϕ -skew Hamiltonian matrix W to have a ϕ -Hamiltonian square root, in other words a ϕ -Hamiltonian matrix A such that $A^2 = W$ (it is easy to see that the square of every ϕ -Hamiltonian matrix is ϕ -skew Hamiltonian). We also give sufficient conditions for a related property of a ϕ -skew Hamiltonian matrix W , namely that every ϕ -skew Hamiltonian matrix W' which is similar to W , is also ϕ -symplectically similar. The conditions are given in terms of existence of a ϕ -Hamiltonian square roots of $\pm W$ and $\pm W'$. In several cases, we compare existence of ϕ -Hamiltonian square roots over the field of complex numbers with that over the quaternions. Many results are stated and proved in a more general framework where K is replaced by any invertible matrix H such that $H_\phi = -H$.

The answers are known in two cases:

- (I) $\mathbb{F} = \mathbb{R}$, with ϕ the identity map, i.e., $A_\phi = A^T$, the transpose of A .
- (II) $\mathbb{F} = \mathbb{C}$, with ϕ the identity map.

Theorem 1.1. *In cases (I) and (II), an $n \times n$ matrix W is ϕ -skew Hamiltonian if and only if $W = A^2$ for some ϕ -Hamiltonian matrix A .*

The “if” part is easily seen. The non-trivial “only if” part was proved in [8], [13]; see also [7].

Theorem 1.2. *In cases (I) and (II), if two ϕ -skew Hamiltonian matrices are F -similar, then they are (F, ϕ) -symplectically similar.*

The proof follows from a canonical form of ϕ -skew Hamiltonian matrices (see, e.g., [8], [15] for the real case), or using polar decomposition (see [13] for the complex case).

Thus, in the present paper we focus on the complex case with ϕ the complex conjugation (in this case, for the problem of existence of ϕ -Hamiltonian square roots only a minor modification of known results is required), and on the quaternionic case (which is essentially new).

The following notation for standard matrices will be used throughout: Jordan blocks

$$J_m(\lambda) = \begin{bmatrix} \lambda & 1 & 0 & \cdots & 0 \\ 0 & \lambda & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & 0 \\ \vdots & \vdots & & \lambda & 1 \\ 0 & 0 & \cdots & 0 & \lambda \end{bmatrix} \in \mathbb{H}^{m \times m}, \quad \lambda \in \mathbb{H}.$$

Standard real symmetric matrices:

$$F_m = \begin{bmatrix} 0 & \cdots & \cdots & 0 & 1 \\ \vdots & & & 1 & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & 1 & & & \vdots \\ 1 & 0 & \cdots & \cdots & 0 \end{bmatrix} = F_m^{-1} \in \mathbb{R}^{m \times m}, \quad (1.3)$$

$$G_m = \begin{bmatrix} 0 & \cdots & \cdots & 1 & 0 \\ \vdots & & & 0 & 0 \\ \vdots & & \ddots & \vdots & \\ 1 & 0 & & \vdots & \\ 0 & 0 & \cdots & \cdots & 0 \end{bmatrix} = \begin{bmatrix} F_{m-1} & 0 \\ 0 & 0 \end{bmatrix} \in \mathbb{R}^{m \times m}. \quad (1.4)$$

2. Complex case with ϕ the complex conjugation. In this section we consider the case

(III) $F = \mathbb{C}$, and ϕ is the complex conjugation,

which is more involved than cases (I) and (II). Both Theorems 1.1 and 1.2 generally fail. In this case, to obtain criteria for ϕ -skew Hamiltonian matrices to possess properties described in Theorems 1.1 and 1.2, we need to recall some material related to matrices with respect to indefinite inner products in $\mathbb{C}^{n \times n}$; [11] is a general reference on this topic.

Throughout the rest of this section we fix an invertible hermitian matrix $H \in \mathbb{C}^{n \times n}$. A matrix $A \in \mathbb{C}^{n \times n}$ is said to be *H-selfadjoint* if $HA = A^*H$, and *H-unitary* if $A^*HA = H$. Recall the well known canonical form for *H*-selfadjoint matrices, or more precisely, of the pairs (A, H) ; for convenience of reference, we include in the next theorem also the real case, restricting it to the situation when all eigenvalues are real:

Proposition 2.1. (A) *Let $A \in \mathbb{C}^{n \times n}$ be *H*-selfadjoint. Then there exists an invertible matrix $S \in \mathbb{C}^{n \times n}$ such that $S^{-1}AS$ and $S_\phi HS$ have the form*

$$S_\phi HS = \eta_1 F_{m_1} \oplus \cdots \oplus \eta_p F_{m_p} \oplus F_{2\ell_1} \oplus \cdots \oplus F_{2\ell_q}, \quad (2.1)$$

$$S^{-1}AS = J_{m_1}(\gamma_1) \oplus \cdots \oplus J_{m_p}(\gamma_p) \oplus \left[\begin{array}{cc} J_{\ell_1}(\alpha_1) & 0 \\ 0 & J_{\ell_1}(\overline{\alpha_1}) \end{array} \right] \oplus \cdots \oplus \left[\begin{array}{cc} J_{\ell_q}(\alpha_q) & 0 \\ 0 & J_{\ell_q}(\overline{\alpha_q}) \end{array} \right], \quad (2.2)$$

where $\eta_1, \dots, \eta_p$ are signs ± 1 , the complex numbers $\alpha_1, \dots, \alpha_q$ have positive imaginary part, and $\gamma_1, \dots, \gamma_p$ are real.

The form (2.2) is uniquely determined by A and H , up to a simultaneous permutation of the constituent blocks.

(B) *If, in addition, A and H are real and all eigenvalues of A are real, then the matrix S in part (A) can be chosen to be real as well (obviously, the parts $\oplus_{j=1}^q F_{2\ell_j}$ and $\oplus_{j=1}^q \left[\begin{array}{cc} J_{\ell_j}(\alpha_j) & 0 \\ 0 & J_{\ell_j}(\overline{\alpha_j}) \end{array} \right]$ are then absent in (2.2)).*

The signs $\eta_1, \dots, \eta_p$ in Theorem 2.2 form the *sign characteristic* of the pair (A, H) . Thus, the sign characteristic attaches a sign 1 or -1 to every partial multiplicity corresponding to a real eigenvalue of A .

The following description of the sign characteristic (the second description, see [10], [11]) will be useful. Let $A \in \mathbb{C}^{n \times n}$ be *H*-selfadjoint, let λ_0 be a fixed real eigenvalue of A , and let $\Psi_1 \subseteq \mathbb{C}^n$ be the subspace spanned by the eigenvectors of A

corresponding to λ_0 . For $x \in \Psi_1 \setminus 0$, denote by $\nu(x)$ the maximal length of a Jordan chain of A beginning with the eigenvector x . In other words, there exists a chain of $\nu(x)$ vectors $y_1 = x, y_2, \dots, y_{\nu(x)}$ such that

$$(A - \lambda_0 I)y_j = y_{j-1} \quad \text{for } j = 2, 3, \dots, \nu(x), \quad (A - \lambda_0 I)y_1 = 0,$$

(Jordan chain), and there is no chain of $\nu(x) + 1$ vectors with analogous properties. Let Ψ_i , $i = 1, 2, \dots, \gamma$ ($\gamma = \max\{\nu(x) \mid x \in \Psi_1 \setminus \{0\}\}$) be the subspace of Ψ_1 spanned by all $x \in \Psi_1$ with $\nu(x) \geq i$. Then

$$\text{Ker}(A - \lambda_0 I) = \Psi_1 \supseteq \Psi_2 \supseteq \dots \supseteq \Psi_\gamma.$$

Proposition 2.2. ([10], [11]) For $i = 1, \dots, \gamma$, let

$$f_i(x, y) = (x, Hy^{(i)}), \quad x \in \Psi_i, \quad y \in \Psi_i \setminus \{0\},$$

where $y = y^{(1)}, y^{(2)}, \dots, y^{(i)}$ is a Jordan chain of A corresponding to a real eigenvalue λ_0 with the eigenvector y , and let $f_i(x, 0) = 0$. Then:

- (i) $f_i(x, y)$ does not depend on the choice of $y^{(2)}, \dots, y^{(i)}$, subject to the above properties;
- (ii) for some selfadjoint linear transformation $G_i : \Psi_i \rightarrow \Psi_i$, we have

$$f_i(x, y) = (x, G_i y), \quad x, y \in \Psi_i;$$

- (iii) for the transformation G_i of (ii), $\Psi_{i+1} = \text{Ker } G_i$ (by definition $\Psi_{\gamma+1} = \{0\}$);
- (iv) the number of positive (negative) eigenvalues of G_i , counting multiplicities, coincides with the number of positive (negative) signs in the sign characteristic of (A, H) corresponding to the Jordan blocks of size i associated with the eigenvalue λ_0 of A .

For later reference, we will also need the connections between the canonical form of (A, H) , where A is H -selfadjoint, and that of $(-A, H)$:

Proposition 2.3. If $\varepsilon_1, \dots, \varepsilon_s$ are the signs in the sign characteristic of (A, H) attached to the s equal partial multiplicities $m, \dots, m$ of the real eigenvalue γ of A , then $(-1)^{m-1}\varepsilon_1, \dots, (-1)^{m-1}\varepsilon_s$ are the signs in the sign characteristic of $(-A, H)$ attached to the s equal partial multiplicities $m, \dots, m$ of the eigenvalue $-\gamma$ of $-A$.

Proof. Note that we may assume without loss of generality that A and H are given by the canonical form (2.2). Then take advantage of the equalities

$$(\text{diag}(1, -1, 1, \dots, (-1)^{m-1}))(-J_m(\gamma))(\text{diag}(1, -1, 1, \dots, (-1)^{m-1})) = J_m(-\gamma),$$

$$(\text{diag}(1, -1, 1, \dots, (-1)^{m-1}))F_m(\text{diag}(1, -1, 1, \dots, (-1)^{m-1})) = (-1)^{m-1}F_m.$$

Alternatively, we may use [11, Theorem 7.4.1]. $\square$

A criterion for existence of an H -selfadjoint square root of an H -selfadjoint matrix runs as follows:

Theorem 2.4. *Let $H \in \mathbb{C}^{n \times n}$ be invertible hermitian matrix, and let $A \in \mathbb{C}^{n \times n}$ be H -selfadjoint. Then there exists an H -selfadjoint matrix $B \in \mathbb{C}^{n \times n}$ such that $B^2 = A$ if and only if the following two conditions (1) and (2) hold:*

- (1) *For each negative eigenvalue λ of A (if any) the part of the canonical form, as in Proposition 2.1, of (A, H) corresponding to λ can be presented in the form*

$$(A_1 \oplus \cdots \oplus A_m, H_1 \oplus \cdots \oplus H_m),$$

where, for $i = 1, 2, \dots, m$,

$$A_i = \begin{bmatrix} J_{k_i}(\lambda) & 0 \\ 0 & J_{k_i}(\lambda) \end{bmatrix}, \quad H_i = \begin{bmatrix} F_{k_i}(\lambda) & 0 \\ 0 & -F_{k_i}(\lambda) \end{bmatrix}.$$

- (2) *If zero is an eigenvalue of A , then the part of the canonical form of (A, H) corresponding to the zero eigenvalue can be presented in the form*

$$(B_0 \oplus B_1 \oplus \cdots \oplus B_p, L_0 \oplus L_1 \oplus \cdots \oplus L_p), \quad (2.3)$$

where

$$B_0 = 0_{\ell_0 \times \ell_0}, \quad L_0 = I_{r_0} \oplus -I_{s_0}, \quad r_0 + s_0 = \ell_0, \quad (2.4)$$

and for each $i = 1, 2, \dots, p$, the pair (B_i, L_i) is one of the following two forms:

$$B_i = \begin{bmatrix} J_{\ell_i}(0) & 0 \\ 0 & J_{\ell_i}(0) \end{bmatrix}, \quad L_i = \begin{bmatrix} F_{\ell_i} & 0 \\ 0 & -F_{\ell_i} \end{bmatrix}, \quad \ell_i > 1, \quad (2.5)$$

or

$$B_i = \begin{bmatrix} J_{\ell_i}(0) & 0 \\ 0 & J_{\ell_i-1}(0) \end{bmatrix}, \quad L_i = \varepsilon_i \begin{bmatrix} F_{\ell_i} & 0 \\ 0 & F_{\ell_i-1} \end{bmatrix}, \quad (2.6)$$

with $\ell_i > 1$ and $\varepsilon_i = \pm 1$.

Theorem 2.4 was proved in [2] for H -selfadjoint matrices of the form $H^{-1}X^*HX$, in the setting of H -polar decompositions (Theorem 4.4 in [2]). The proof for general H -selfadjoint matrices is exactly the same. Note that the conditions on the Jordan form of B in part (2) coincide with the well-known criteria that guarantee existence of a (complex) square root of B [9], [5], [23].

Observe that the presentation (2.3) - (2.6) of the part of the canonical form of (A, H) corresponding to the eigenvalue zero need not be unique. For example, if

$$A = J_3(0) \oplus J_3(0) \oplus J_2(0) \oplus J_2(0),$$

$$H = F_3 \oplus (-F_3) \oplus F_2 \oplus (-F_2),$$

then one can form presentation (2.5), (2.6) in two ways:

$$B_1 = J_3(0) \oplus J_3(0), \quad B_2 = J_2(0) \oplus J_2(0), \quad H_1 = F_3 \oplus (-F_3), \quad H_2 = F_2 \oplus (-F_2),$$

and

$$B_1 = J_3(0) \oplus J_2(0), \quad B_2 = J_3(0) \oplus J_2(0), \quad H_1 = F_3 \oplus F_2, \quad H_2 = (-F_3) \oplus (-F_2).$$

Example 2.5. Let

$$A = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad H_1 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad H_2 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}.$$

Clearly, A is H_1 -selfadjoint and H_2 -selfadjoint. According to Theorem 2.4, there exists an H_1 -selfadjoint square root of A , and there does not exist an H_2 -selfadjoint square root of A . Indeed, all square roots $X \in \mathbb{C}^{3 \times 3}$ of A have the form

$$X = \begin{bmatrix} 0 & a & b \\ 0 & 0 & 0 \\ 0 & b^{-1} & 0 \end{bmatrix}, \quad a \in \mathbb{C}, \quad b \in \mathbb{C} \setminus \{0\},$$

as one can check by a straightforward algebra, taking advantage of the equalities $XA = 0$ and $X^2 = A$. Clearly, X is H_1 -selfadjoint if and only if a is real and $|b| = 1$, whereas the condition of H_2 -selfadjointness of X leads to the contradictory equality $|b| = -1$.

Corollary 2.6. (a) *If an H -selfadjoint matrix A has no real nonpositive eigenvalues, then A has an H -selfadjoint square root.*

(b) *Assume that invertible H -selfadjoint matrices A and B are such that each of the four matrices $\pm A$, $\pm B$ has an H -selfadjoint square root. Then A and B are $\mathbb{C}$ -similar if and only if A and B are H -unitarily similar, i.e., $A = U^{-1}BU$ for some H -unitary U .*

Proof. Part (a) is obvious from Theorem 2.4.

We prove the part (b). The “if” part being trivial, we focus on the “only if” part. Suppose A and B are $\mathbb{C}$ -similar. By Proposition 2.3 and Theorem 2.4, we see that

the canonical forms of (A, H) and (B, H) are essentially the same, i.e., may differ only in the order of the blocks: For every real eigenvalue λ of A (and therefore also of B), and for every positive integer k , the number of signs $+$ (resp., signs $-$) in the sign characteristic of (A, H) corresponding to Jordan blocks of size $k \times k$ with the eigenvalue λ , is equal to that in the sign characteristic of (B, H) . Now the uniqueness part of Proposition 2.1 yields the H -unitary similarity of A and B . $\square$

The hypothesis in Corollary 2.6 that A and B are invertible is essential as the following example shows: Let

$$A = -B = J_2(0) \oplus J_1(0) \oplus J_1(0), \quad H = F_2 \oplus F_1 \oplus -F_1.$$

Then the canonical form of the pair (B, H) is

$$(J_2(0) \oplus J_1(0) \oplus J_1(0), (-F_2) \oplus F_1 \oplus -F_1)$$

(cf. Proposition 2.3), in other words, there exists an invertible (complex) matrix S such that

$$S^{-1}BS = J_2(0) \oplus J_1(0) \oplus J_1(0), \quad S^*HS = (-F_2) \oplus F_1 \oplus (-F_1).$$

By Theorem 2.4, both A and B have H -selfadjoint square roots, in fact,

$$\begin{bmatrix} 0 & b & \pm 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & \pm 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}^2 = A, \quad \begin{bmatrix} 0 & b & 0 & \pm 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & \mp 1 & 0 & 0 \end{bmatrix}^2 = B,$$

where b is an arbitrary real number. Although A and B are evidently similar, they are not H -unitarily similar, because the pairs (A, H) and (B, H) have essentially different canonical forms.

Theorem 2.4 and Corollary 2.6 can be now applied to complex ϕ -Hamiltonian and ϕ -skew Hamiltonian matrices, where ϕ is the complex conjugation. Let $\widehat{K} = iK$. Obviously, $\widehat{K}$ is hermitian and invertible. Clearly, a matrix $A \in \mathbb{C}^{n \times n}$ is ϕ -skew Hamiltonian if and only if A is $\widehat{K}$ -selfadjoint, and a matrix $W \in \mathbb{C}^{n \times n}$ is ϕ -Hamiltonian if and only if iW is $\widehat{K}$ -selfadjoint. Thus, Theorem 2.4 and Corollary 2.6 yield the following result:

Theorem 2.7. (a) *A ϕ -skew Hamiltonian matrix $A \in \mathbb{C}^{n \times n}$ has a complex ϕ -Hamiltonian square root if and only if the canonical form of the pair $(-A, iK)$, where $-A$ is iK -selfadjoint, satisfies conditions (1) and (2) of Theorem 2.4. In particular, if A has no real nonnegative eigenvalues, then there is a ϕ -Hamiltonian matrix $X \in \mathbb{C}^{n \times n}$ such that $X^2 = A$.*

(b) Assume that invertible ϕ -skew Hamiltonian matrices $A, B \in \mathbb{C}^{n \times n}$ are such that each of the four matrices $\pm A, \pm B$ has a ϕ -Hamiltonian square root. Then A and B are similar (with a complex similarity matrix) if and only if A and B are ϕ -symplectically similar.

Remark 2.8. Using Proposition 2.3 it is easy to see that the following three conditions are equivalent:

- (a) The pair $(-A, iK)$ satisfies conditions (1) and (2) of Theorem 2.4;
- (b) The pair $(-A, -iK)$ satisfies conditions (1) and (2) of Theorem 2.4;
- (c) The pair (A, iK) satisfies conditions (1) and (2) of Theorem 2.4 with “negative” replaced by “positive” in (1) and with $\begin{bmatrix} F_{\ell_i} & 0 \\ 0 & F_{\ell_i-1} \end{bmatrix}$ replaced by $\begin{bmatrix} F_{\ell_i} & 0 \\ 0 & -F_{\ell_i-1} \end{bmatrix}$ in (2).

Remark 2.9. Theorem 2.7 and Remark 2.8 are valid, with the same proof, in a more general framework where K is replaced by any invertible skewhermitian matrix.

3. Quaternionic case, ϕ a nonstandard involutory antiautomorphism.

From now on in this paper we assume that $\mathbb{F} = \mathbb{H}$. The standard quaternionic units are denoted by i, j, k with the standard multiplication table. The complex field will be thought of as embedded in $\mathbb{H}$ using i as the complex imaginary unit; thus, $\mathbb{C} = \text{Span}_{\mathbb{R}}\{1, i\}$, where we denote by $\text{Span}_{\mathbb{R}} X$ the real vector space generated by a subset X of $\mathbb{H}$.

In this section we further assume that the fixed involutory antiautomorphism (in short, *iaa*) ϕ of $\mathbb{H}$ is nonstandard, i.e., different from the quaternionic conjugation. (The case when ϕ is the quaternionic conjugation will be considered in the next section.) In this case there are exactly two quaternions β such that $\phi(\beta) = -\beta$ and $|\beta| = 1$; in fact, one of them is the negative of the other, and moreover $\beta^2 = -1$. We fix one of them, denoted β , throughout this section. We denote by $\text{Inv}(\phi)$ the set of all quaternions fixed by ϕ ; $\text{Inv}(\phi)$ is a three-dimensional real vector space spanned by $1, \alpha_1, \alpha_2$, where $\alpha_1, \alpha_2 \in \mathbb{H}$ are certain square roots of -1 . (For these and other well-known properties of *iaa*'s see, for example, [1], [16], or [17].)

Let $H \in \mathbb{H}^{n \times n}$ be an invertible matrix which is also ϕ -skewsymmetric, i.e., such that

$$H_{\phi} = -H. \quad (3.1)$$

The matrix H will be fixed throughout this section.

A matrix $A \in \mathbb{H}^{n \times n}$ is said to be H -symmetric if the equality $HA = A_{\phi}H$ holds. In turn, the equality $HA = A_{\phi}H$ is equivalent to $(HA)_{\phi} = -HA$. Also, a matrix

$A \in \mathbb{H}^{n \times n}$ is said to be H -skewsymmetric if the equality $(HA)_\phi = HA$ holds.

In this section we will develop criteria for existence of H -skewsymmetric square roots of H -symmetric matrices. In the particular case when H is given by (1.1), a matrix is ϕ -skew Hamiltonian if and only if it is H -symmetric, and a matrix is ϕ -Hamiltonian if and only if it is H -skewsymmetric. Thus, as a particular case, criteria for existence of ϕ -Hamiltonian square roots of ϕ -skew Hamiltonian matrices will be obtained (however, we will not formulate these particular cases separately).

3.1. Preliminaries: Canonical forms. It is easy to see that A is H -symmetric if and only if $S^{-1}AS$ is $S_\phi HS$ -symmetric, for any invertible matrix $S \in \mathbb{H}^{n \times n}$. Canonical form under this action is given next.

Proposition 3.1. *Let $H = -H_\phi \in \mathbb{H}^{n \times n}$ be an invertible matrix, and let A be H -symmetric. Then there exists an invertible matrix S such that the matrices $S^{-1}AS$ and $S_\phi HS$ have the form*

$$S_\phi HS = \eta_1 \beta F_{m_1} \oplus \cdots \oplus \eta_p \beta F_{m_p} \oplus \left[\begin{array}{cc} 0 & F_{\ell_1} \\ -F_{\ell_1} & 0 \end{array} \right] \oplus \cdots \oplus \left[\begin{array}{cc} 0 & F_{\ell_q} \\ -F_{\ell_q} & 0 \end{array} \right] \quad (3.2)$$

$$S^{-1}AS = J_{m_1}(\gamma_1) \oplus \cdots \oplus J_{m_p}(\gamma_p) \oplus \left[\begin{array}{cc} J_{\ell_1}(\alpha_1) & 0 \\ 0 & J_{\ell_1}(\alpha_1) \end{array} \right] \oplus \cdots \oplus \left[\begin{array}{cc} J_{\ell_q}(\alpha_q) & 0 \\ 0 & J_{\ell_q}(\alpha_q) \end{array} \right], \quad (3.3)$$

where $\eta_1, \dots, \eta_p$ are signs ± 1 , the quaternions $\alpha_1, \dots, \alpha_q \in \text{Inv}(\phi) \setminus \mathbb{R}$, and $\gamma_1, \dots, \gamma_p$ are real.

Moreover, the form (3.3) is unique up to permutations of the diagonal blocks, and up to replacements of each α_j by a similar quaternion $\beta_j \in \text{Inv}(\phi)$.

Several versions of the canonical form are available in the literature, some more explicit than others, see, e. g., [3], [6], [12], [21], [4]; often, the canonical forms for H -symmetric matrices are derived from canonical forms for pairs of ϕ -skewsymmetric quaternionic matrices. In this form, Proposition 3.1 was proved with full details in [17].

Next, a canonical form for matrices that are H -skewsymmetric is given. First, we describe the primitive forms:

- (α) $L = \kappa \beta F_k$, $A = \beta J_k(0)$, where $\kappa = 1$ if k is even, and $\kappa = \pm 1$ if k is odd;
 (β)

$$L = \left[\begin{array}{cc} 0 & F_\ell \\ -F_\ell & 0 \end{array} \right], \quad A = \left[\begin{array}{cc} -J_\ell(\alpha) & 0 \\ 0 & J_\ell(\alpha) \end{array} \right],$$

where $\alpha \in \text{Inv}(\phi)$, $\Re(\alpha) > 0$.

(γ) $L = \delta\beta F_s$, $A = \beta J_s(\tau)$, where $\delta = \pm 1$ and τ is a negative real number.

Proposition 3.2. *Let $A \in \mathbb{H}^{n \times n}$ be H -skewsymmetric, where $H \in \mathbb{H}^{n \times n}$ is invertible and ϕ -skewsymmetric. Then there exists an invertible quaternionic matrix S such that $S_\phi HS$ and $S^{-1}AS$ have the following block diagonal form:*

$$S_\phi HS = L_1 \oplus L_2 \oplus \cdots \oplus L_m, \quad S^{-1}AS = A_1 \oplus A_2 \oplus \cdots \oplus A_m, \quad (3.4)$$

where each pair (L_i, A_i) has one of the forms (α) , (β) , (γ) . Moreover, the form (3.4) is uniquely determined by the pair (H, A) , up to a permutation of blocks and up to a replacement of each α in the form (β) with a similar quaternion α' such that $\phi(\alpha') = \alpha'$.

As with Proposition 3.1, several equivalent versions of the canonical form of H -skew-symmetric matrices are known; we mention here only the books [3], [4]; usually, they are derived from the canonical forms for pairs of quaternionic matrices, where one matrix is ϕ -symmetric and the other one is ϕ -skewsymmetric. A detailed proof of the canonical form as in Proposition 3.2 can be found in [18].

3.2. Main results. A criterion for existence of a quaternionic H -skewsymmetric square roots of H -symmetric matrices is given in the following theorem:

Theorem 3.3. *Let $H \in \mathbb{H}^{n \times n}$ be an invertible skewsymmetric matrix, and let $A \in \mathbb{H}^{n \times n}$ be H -symmetric. Then there exists an H -skewsymmetric matrix $B \in \mathbb{H}^{n \times n}$ such that $B^2 = A$ if and only if the following two conditions (1) and (2) hold:*

- (1) *For each positive eigenvalue λ of A (if any) the part of the canonical form, as in Proposition 3.1, of (A, H) corresponding to λ can be presented in the form*

$$(A_1 \oplus \cdots \oplus A_m, H_1 \oplus \cdots \oplus H_m),$$

where, for $i = 1, 2, \dots, m$,

$$A_i = \begin{bmatrix} J_{k_i}(\lambda) & 0 \\ 0 & J_{k_i}(\lambda) \end{bmatrix}, \quad H_i = \begin{bmatrix} \beta F_{k_i} & 0 \\ 0 & -\beta F_{k_i} \end{bmatrix}.$$

- (2) *If zero is an eigenvalue of A , then the part of the canonical form of (A, H) corresponding to the zero eigenvalue can be presented in the form*

$$(B_0 \oplus B_1 \oplus \cdots \oplus B_p, L_0 \oplus L_1 \oplus \cdots \oplus L_p), \quad (3.5)$$

where

$$B_0 = 0_{\ell_0 \times \ell_0}, \quad L_0 = \beta I_{r_0} \oplus -\beta I_{s_0}, \quad r_0 + s_0 = \ell_0, \quad (3.6)$$

and for each $i = 1, 2, \dots, p$, the pair (B_i, L_i) is one of the following two forms:

$$B_i = \begin{bmatrix} J_{\ell_i}(0) & 0 \\ 0 & J_{\ell_i}(0) \end{bmatrix}, \quad L_i = \begin{bmatrix} \beta F_{\ell_i}(\lambda) & 0 \\ 0 & -\beta F_{\ell_i}(\lambda) \end{bmatrix}, \quad \ell_i > 1, \quad (3.7)$$

or

$$B_i = \begin{bmatrix} J_{\ell_i}(0) & 0 \\ 0 & J_{\ell_i-1}(0) \end{bmatrix}, \quad L_i = \varepsilon_i \begin{bmatrix} \beta F_{\ell_i}(\lambda) & 0 \\ 0 & -\beta F_{\ell_i-1}(\lambda) \end{bmatrix}, \quad (3.8)$$

with $\ell_i > 1$ and $\varepsilon_i = \pm 1$.

We single out a particular case of Theorem 3.3 and a corollary that expresses the property of some H -symmetric matrices for which similarity is equivalent to H -symplectic similarity, in terms of existence of H -skewsymmetric square roots:

Corollary 3.4. (1) *If an H -symmetric matrix $A \in \mathbb{H}^{n \times n}$ has no nonnegative real eigenvalues then A admits quaternionic H -skewsymmetric square roots.*

(2) *Assume that invertible H -symmetric matrices $A, B \in \mathbb{H}^{n \times n}$ are such that each of the four matrices $\pm A, \pm B$ admits H -skewsymmetric square roots. Then A and B are $\mathbb{H}$ -similar if and only if A and B are H -symplectically similar, i. e.,*

$$A = U^{-1}BU \quad (3.9)$$

for some $U \in \mathbb{H}^{n \times n}$ such that $U_\phi H U = H$.

Proof. Part (1) follows immediately from Theorem 3.3. For part (2), assume that A and B are similar. The hypotheses on A and B , together with Theorem 3.3 imply that the pairs (A, H) and (B, H) have the same canonical form as set forth in Proposition 3.1. Thus,

$$(S_1)_\phi H S_1 = (S_2)_\phi H S_2, \quad S_1^{-1} A S_1 = S_2^{-1} B S_2$$

for some invertible $S_1, S_2 \in \mathbb{H}^{n \times n}$. Then (3.9) is satisfied with $U = S_2 S_1^{-1}$. $\square$

By combining Theorem 3.3 with Theorem 2.7 and Remark 2.8, the following comparison result is obtained (the “if” part there is trivial):

Corollary 3.5. *Let $H \in \mathbb{C}^{n \times n}$ be invertible skewhermitian matrix, and let $A \in \mathbb{C}^{n \times n}$ be H -symmetric in the sense of complex conjugation, in other words $HA = A^*H$. Let ϕ be the (unique) nonstandard iaa of $\mathbb{H}$ such that $\phi(i) = -i$. Then A admits quaternionic H -skewsymmetric square roots if and only if A admits complex H -skewsymmetric square roots, i. e., there exists a matrix $B \in \mathbb{C}^{n \times n}$ such that $B^2 = A$ and $HB = -B^*H$.*

The next subsection is devoted to the proof of Theorem 3.3.

3.3. Proof of Theorem 3.3. We start with a lemma. Recall that the *spectrum* $\sigma(X)$ of a quaternionic matrix $X \in \mathbb{H}^{m \times m}$ consists of all $\lambda \in \mathbb{H}$ (eigenvalues) such that $Ax = x\lambda$ holds for some nonzero vector $x \in \mathbb{H}^{m \times 1}$. Observe that if $\lambda \in \sigma(X)$, then also $\mu\lambda\mu^{-1} \in \sigma(X)$ for every nonzero $\mu \in \mathbb{H}$.

Lemma 3.6. *Let*

$$X = X_1 \oplus \cdots \oplus X_p \in \mathbb{H}^{m \times m}, \quad X_j \in \mathbb{H}^{m_j \times m_j}, \quad \text{for } j = 1, 2, \dots, p,$$

where $m = m_1 + \cdots + m_p$, and assume that

$$\sigma(X_j) \cap \sigma(X_k) = \emptyset, \quad \forall \quad j \neq k.$$

If $Y \in \mathbb{H}^{m \times m}$ commutes with X , then Y has the form

$$Y = Y_1 \oplus \cdots \oplus Y_p \in \mathbb{H}^{m \times m}, \quad Y_j \in \mathbb{H}^{m_j \times m_j}, \quad \text{for } j = 1, 2, \dots, p,$$

where $X_j Y_j = Y_j X_j$ for $j = 1, 2, \dots, p$.

The proof is easily reduced to the case of complex matrices (where the result is well known), by using the standard representation of quaternions as 2×2 complex matrices.

Proof of Theorem 3.3. In view of Proposition 3.1, without loss of generality we may (and do) assume that H and A are given by the right hand sides of (3.2) and (3.3), respectively. Since a square root of A obviously commutes with A , by Lemma 3.6 we may further assume that one of the following two cases hold: 1. $\sigma(A) = \{\gamma\}$, where γ is real; 2. $\sigma(A) = \{\mu\alpha\mu^{-1} : \mu \in \mathbb{H} \setminus \{0\}\}$, where α is a fixed nonreal quaternion.

Consider the first case. Then

$$H = \eta_1 \beta F_{m_1} \oplus \cdots \oplus \eta_s \beta F_{m_s}, \quad A = J_{m_1}(\gamma) \oplus \cdots \oplus J_{m_s}(\gamma),$$

where $\gamma \in \mathbb{R}$ and the η_j 's are signs ± 1 . Assume first that conditions (1) and (2) of Theorem 3.3 hold. We may identify the real vector space $\text{Span}_{\mathbb{R}}\{1, \beta\}$ spanned by 1 and β with $\mathbb{C}$, via identification of $i \in \mathbb{C}$ with β ; then ϕ acts as the complex conjugation on $\text{Span}_{\mathbb{R}}\{1, \beta\}$. Now the existence of H -skewsymmetric square root of A follows from Theorem 2.4 and Remark 2.8 (the equivalence of (a) and (c)); the H -skewsymmetric square root of A exists already in $\text{Span}_{\mathbb{R}}\{1, \beta\}$.

Conversely, suppose that there exists an H -skewsymmetric matrix B such that $B^2 = A$. We have to show that conditions (1) and (2) of Theorem 3.3 hold true. The conditions are vacuous if γ is negative; so assume $\gamma \geq 0$, and consider separately the

case when $\gamma > 0$ and the case when $\gamma = 0$. If $\gamma > 0$, then the canonical form for B (Proposition 3.2) shows that

$$S_\phi HS = \begin{bmatrix} 0 & F_{\ell_1} \\ -F_{\ell_1} & 0 \end{bmatrix} \oplus \cdots \oplus \begin{bmatrix} 0 & F_{\ell_s} \\ -F_{\ell_s} & 0 \end{bmatrix},$$

$$S^{-1}BS = \begin{bmatrix} -J_{\ell_1}(\alpha) & 0 \\ 0 & J_{\ell_1}(\alpha) \end{bmatrix} \oplus \cdots \oplus \begin{bmatrix} -J_{\ell_s}(\alpha) & 0 \\ 0 & J_{\ell_s}(\alpha) \end{bmatrix},$$

for some invertible $S \in \mathbb{H}^{n \times n}$, where α is the positive square root of γ . Then

$$S^{-1}AS = \begin{bmatrix} J_{\ell_1}(\alpha)^2 & 0 \\ 0 & J_{\ell_1}(\alpha)^2 \end{bmatrix} \oplus \cdots \oplus \begin{bmatrix} J_{\ell_s}(\alpha)^2 & 0 \\ 0 & J_{\ell_s}(\alpha)^2 \end{bmatrix},$$

and to complete the consideration of the case when $\gamma > 0$ we only need to exhibit an invertible matrix $T \in \mathbb{H}^{\ell \times \ell}$ such that

$$T^{-1} \begin{bmatrix} J_\ell(\alpha)^2 & 0 \\ 0 & J_\ell(\alpha)^2 \end{bmatrix} T = \begin{bmatrix} J_\ell(\gamma) & 0 \\ 0 & J_\ell(\gamma) \end{bmatrix}$$

and

$$T_\phi \begin{bmatrix} 0 & F_\ell \\ -F_\ell & 0 \end{bmatrix} T = \begin{bmatrix} \beta F_\ell & 0 \\ 0 & -\beta F_\ell \end{bmatrix}.$$

We take T in the form

$$T = \begin{bmatrix} X & X \\ \beta X & -\beta X \end{bmatrix},$$

where the matrix $X \in \mathbb{R}^{\ell \times \ell}$ satisfies the equalities

$$X^T F_\ell X = \frac{1}{2} F_\ell, \quad J_\ell(\alpha)^2 X = X J_\ell(\gamma). \quad (3.10)$$

We now proceed to show that there exists a (necessarily invertible) real matrix X satisfying (3.10). Indeed, the canonical form of the real F_ℓ -selfadjoint matrix $J_\ell(\alpha)^2$ (see, for example, [11], [14]) shows that there exists a real invertible matrix $\hat{X}$ such that

$$\hat{X}^T F_\ell \hat{X} = \varepsilon F_\ell, \quad J_\ell(\alpha)^2 \hat{X} = \hat{X} J_\ell(\gamma), \quad (3.11)$$

where $\varepsilon = \pm 1$. However, ε coincides with the sign of $e_1^T F_\ell y$, where $y \in \mathbb{R}^{\ell \times 1}$ is taken to satisfy the condition $(J_\ell(\alpha)^2 - \gamma I)^{\ell-1} y = e_1$. (See Proposition 2.2). We can take $y = \frac{1}{(2\alpha)^{\ell-1}} e_\ell$, so $e_1^T F_\ell y = \frac{1}{(2\alpha)^{\ell-1}}$, and therefore $\varepsilon = 1$. Now clearly $X = (\sqrt{2})^{-1} \hat{X}$ satisfies (3.10).

Finally, consider the case $\gamma = 0$. Since B is H -skewsymmetric, by Proposition 3.2 we have

$$S_\phi HS = \beta F_{2k_1} \oplus \cdots \oplus \beta F_{2k_r} \bigoplus \kappa_1 \beta F_{2\ell_1-1} \oplus \cdots \oplus \kappa_s \beta F_{2\ell_s-1},$$

$$S^{-1}BS = \beta J_{2k_1}(0) \oplus \cdots \oplus \beta J_{2k_s}(0) \bigoplus \beta J_{2\ell_1-1}(0) \oplus \cdots \oplus \beta J_{2\ell_s-1}(0),$$

where $S \in \mathbb{H}^{n \times n}$ is invertible, and where the k_j 's and ℓ_j 's are positive integers and the κ_j 's are signs ± 1 . To verify that condition (2) of Theorem 3.3 holds true, all what we need to show is the following two claims:

Claim 3.7. *There exists an invertible matrix $T \in \mathbb{R}^{2k \times 2k}$ such that*

$$T_\phi(\beta F_{2k})T = \begin{bmatrix} \beta F_k & 0 \\ 0 & -\beta F_k \end{bmatrix}, \quad T^{-1}(\beta J_{2k}(0))^2 T = \begin{bmatrix} J_k(0) & 0 \\ 0 & J_k(0) \end{bmatrix}, \quad (3.12)$$

where k is a positive integer.

Claim 3.8. *There exists an invertible matrix $T \in \mathbb{R}^{(2\ell-1) \times (2\ell-1)}$ such that*

$$T_\phi(\beta F_{2\ell-1})T = (-1)^\ell \begin{bmatrix} \beta F_\ell & 0 \\ 0 & -\beta F_{\ell-1} \end{bmatrix}$$

and

$$T^{-1}(\beta J_{2\ell-1}(0))^2 T = \begin{bmatrix} J_\ell(0) & 0 \\ 0 & J_{\ell-1}(0) \end{bmatrix},$$

where $\ell > 1$ is an integer.

Consider first Claim 3.7. Since the real matrix $-J_{2k}(0)^2$ is F_{2k} -selfadjoint, and the Jordan form of $-J_{2k}(0)^2$ is $J_k(0) \oplus J_k(0)$, by Proposition 2.1(B) there exists an invertible $T \in \mathbb{R}^{2k \times 2k}$ such that

$$T_\phi F_{2k} T = (\varepsilon_1 F_k) \oplus (\varepsilon_2 F_k), \quad T^{-1}(-J_{2k}(0)^2)T = J_k(0) \oplus J_k(0),$$

where $\varepsilon_j = \pm 1$. To determine ε_j , $j = 1, 2$, we use Proposition 2.2. In the notation of that theorem, we have $\gamma = k$,

$$\Psi_1 = \cdots = \Psi_\gamma = \text{Span}\{e_1, e_2\},$$

and, choosing the orthonormal basis $\{e_1, e_2\}$, the selfadjoint linear transformation $G_\gamma : \Psi_\gamma \longrightarrow \Psi_\gamma$ is represented by the 2×2 hermitian matrix $\widehat{G}$. The matrix $\widehat{G}$ is defined by the property that

$$[c^* \ d^*] \widehat{G} \begin{bmatrix} a \\ b \end{bmatrix} = \langle ae_1 + be_2, F_{2k}((-1)^{k-1}ce_{2k-1} + (-1)^{k-1}de_{2k}) \rangle, \quad a, b, c, d \in \mathbb{C}. \quad (3.13)$$

We denote here by $\langle x, y \rangle = y^*x$, $x, y \in \mathbb{C}^{2k}$, the standard inner product in $\mathbb{C}^{2k}$. To obtain formula (3.13), we took advantage of the equality

$$(-J_{2k}(0)^2)^{k-1}((-1)^{k-1}ce_{2k-1} + (-1)^{k-1}de_{2k}) = ce_1 + de_2.$$

The right hand side in (3.13) is easily computed to be

$$\begin{bmatrix} d^* & c^* \end{bmatrix} \begin{bmatrix} (-1)^{k-1} & 0 \\ 0 & (-1)^{k-1} \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix},$$

so

$$\widehat{G} = \begin{bmatrix} 0 & (-1)^{k-1} \\ (-1)^{k-1} & 0 \end{bmatrix},$$

the matrix $\widehat{G}$ has one positive and one negative eigenvalue, and we may take $\varepsilon_1 = 1$, $\varepsilon_2 = -1$. This proves Claim 3.7.

Claim 3.8 is proved by using analogous considerations, again taking advantage of Proposition 2.1(B) and Proposition 2.2. There exists an invertible $T \in \mathbb{R}^{(2\ell-1) \times (2\ell-1)}$ such that

$$T_\phi F_{2\ell-1} T = (\varepsilon_1 F_\ell) \oplus (\varepsilon_2 F_{\ell-1}), \quad T^{-1}(-J_{2\ell-1}(0)^2)T = J_\ell(0) \oplus J_{\ell-1}(0),$$

where $\varepsilon_j = \pm 1$. In the notation of Proposition 2.2, we have $\gamma = \ell$,

$$\Psi_1 = \cdots = \Psi_{\gamma-1} = \text{Span}\{e_1, e_2\}, \quad \Psi_\gamma = \text{Span}\{e_1\}.$$

The selfadjoint linear transformation $G_{\gamma-1}$ is represented (with respect to the basis $\{e_1, e_2\}$) by the matrix $\widehat{G}_{\gamma-1}$ defined by

$$\begin{bmatrix} c^* & d^* \end{bmatrix} \widehat{G}_{\gamma-1} \begin{bmatrix} a \\ b \end{bmatrix} = \langle ae_1 + be_2, F_{2\ell-1}((-1)^\ell ce_{2\ell-3} + (-1)^\ell de_{2\ell-2}) \rangle, \quad a, b, c, d \in \mathbb{C}. \quad (3.14)$$

Again, to obtain (3.14), the following equality was used:

$$(-J_{2\ell-1}(0)^2)^{\ell-2}((-1)^\ell ce_{2\ell-3} + (-1)^\ell de_{2\ell-2}) = ce_1 + de_2.$$

Thus,

$$\widehat{G}_{\gamma-1} = \begin{bmatrix} 0 & 0 \\ 0 & (-1)^\ell \end{bmatrix},$$

and $\varepsilon_1 = (-1)^\ell$. Next, the linear transformation G_γ with respect to the basis $\{e_1\}$ for Ψ_γ is represented by the 1×1 matrix $(-1)^{\ell-1}$, and therefore $\varepsilon_2 = (-1)^{\ell-1}$.

Theorem 3.3 is proved.

4. Quaternionic case, ϕ the quaternionic conjugation. In this section we assume that the fixed involutory antiautomorphism ϕ of $\mathbf{H}$ is the quaternionic conjugation. Then $A_\phi = A^*$, where $*$ stands for the conjugate transpose.

Let $H \in \mathbf{H}^{n \times n}$ be a *skewhermitian* ($H = -H^*$) invertible matrix. The matrix H will be fixed throughout this section.

A matrix $A \in \mathbf{H}^{n \times n}$ is said to be *H-symmetric* if the equality $HA = A^*H$, equivalently $(HA)^* = -HA$ holds. A matrix $A \in \mathbf{H}^{n \times n}$ is said to be *H-skewsymmetric* if the equality $(HA)^* = HA$ holds. It is easy to see that if A and B are commuting *H-skewsymmetric* matrices, then AB is *H-symmetric*.

Our main result on existence of *H-skewsymmetric* square roots of *H-symmetric* matrices is given in Theorem 4.1 below. Again, a criterion concerning existence of ϕ -Hamiltonian square roots of ϕ -skew Hamiltonian matrices is contained as a particular case, but will not be separately stated.

In the next theorem, it will be convenient to use the notation $\mathfrak{V}(\gamma) = a_1i + a_2j + a_3k$ and $\Re(\gamma) = a_0$, where $\gamma = a_0 + a_1i + a_2j + a_3k \in \mathbf{H}$, $a_0, a_1, a_2, a_3 \in \mathbf{R}$.

Theorem 4.1. *An H-symmetric matrix $A \in \mathbf{H}^{n \times n}$ admits an H-skewsymmetric square root if and only if the following two conditions are satisfied for the Jordan form*

$$J_{\ell_1}(\beta_1) \oplus \cdots \oplus J_{\ell_q}(\beta_q), \quad \beta_1, \dots, \beta_q \in \mathbf{H}, \quad (4.1)$$

of A :

- (a) *for every eigenvalue β_j of A which is not real nonpositive, the partial multiplicities corresponding to β_j are double; in other words, for every positive integer k and for every $\gamma \in \mathbf{H}$ such that either $\mathfrak{V}(\gamma) \neq 0$ or $\mathfrak{V}(\gamma) = 0$ and $\Re(\gamma) > 0$, the number of indices j in (4.1) that satisfy the equalities*

$$\ell_j = k, \quad \Re(\beta_j) = \Re(\gamma), \quad \text{and} \quad |\mathfrak{V}(\beta_j)| = |\mathfrak{V}(\gamma)|$$

is even;

- (b) *If zero is an eigenvalue of A , then the part of the Jordan form of A corresponding to the zero eigenvalue can be presented in the form*

$$B_0 \oplus B_1 \oplus \cdots \oplus B_p, \quad (4.2)$$

where

$$B_0 = 0_{m_0 \times m_0}, \quad (4.3)$$

and for each $i = 1, 2, \dots, p$, the matrix B_i has one of the following two forms:

$$B_i = \begin{bmatrix} J_{m_i}(0) & 0 \\ 0 & J_{m_i}(0) \end{bmatrix}, \quad m_i > 1, \quad (4.4)$$

or

$$B_i = \begin{bmatrix} J_{m_i}(0) & 0 \\ 0 & J_{m_i-1}(0) \end{bmatrix}, \quad m_i > 1. \quad (4.5)$$

The following corollary is evident from Theorem 4.1.

Corollary 4.2. *If an H -symmetric matrix has only real negative eigenvalues, then it admits H -skewsymmetric square roots.*

We conclude with an example showing that in case both H and A are complex, the existence of a quaternionic H -skewsymmetric square root of an H -symmetric matrix A does not imply existence of a complex H -skewsymmetric square root of A .

Example 4.3. Let

$$A = J_2(0) \oplus J_1(0), \quad H = iF_2 \oplus iF_1.$$

Then A is H -symmetric, and Theorem 2.7 together with Remarks 2.8 and 2.9 imply that A has no complex H -skewsymmetric square roots. In contrast, one verifies that all quaternionic H -skewsymmetric square roots X of A are given by the formula

$$X = \begin{bmatrix} 0 & ia & jb + kc \\ 0 & 0 & 0 \\ 0 & -jb - kc & 0 \end{bmatrix},$$

where a, b, c are real numbers such that $b^2 + c^2 = 1$.

Example 4.3 is an illustration of the following general statement:

Corollary 4.4. *Let $H \in \mathbb{C}^{n \times n}$ be a skewhermitian invertible matrix, and let $A \in \mathbb{C}^{n \times n}$ be H -symmetric. Assume that A either has a positive eigenvalue, or at least one partial multiplicity corresponding to the zero eigenvalue of A is larger than 1, or both. Assume also that A has quaternionic H -skewsymmetric square roots. Then there exists an invertible skewhermitian matrix $H' \in \mathbb{C}^{n \times n}$ such that A is H' -symmetric, but there do not exist complex H' -skewsymmetric square roots of A .*

Note that by Theorem 4.1 existence of quaternionic H' -skewsymmetric square roots of A is guaranteed under the hypotheses of Corollary 4.4. Note also that if the spectral conditions on A in Corollary 4.4 do not hold, i.e., if A has no positive eigenvalues and the partial multiplicities corresponding to the zero eigenvalue (if zero is an eigenvalue) of A are all equal to 1, then by Theorem 2.7 (see also Remark 2.9) A has complex H -skewsymmetric square roots.

Proof. We may assume that A is in the Jordan form, so let A be given by the right hand side of (2.2). Then take iH to be the right hand side of (2.1) with all signs η_j equal $+1$. By Theorem 2.7 A has no complex H' -skewsymmetric square roots. $\square$

4.1. Proof of Theorem 4.1.. We start by recalling the relevant canonical forms.

Let $H \in \mathbb{H}^{n \times n}$ be an invertible skewhermitian matrix.

Define

$$\Xi_m(\alpha) := \begin{bmatrix} 0 & 0 & \cdots & 0 & \alpha \\ 0 & 0 & \cdots & -\alpha & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & (-1)^{m-2}\alpha & \cdots & 0 & 0 \\ (-1)^{m-1}\alpha & 0 & \cdots & 0 & 0 \end{bmatrix} \in \mathbb{H}^{m \times m}, \quad \alpha \in \mathbb{H}. \quad (4.6)$$

Note that

$$\Xi_m(\alpha) = (-1)^{m-1}(\Xi_m(\alpha))^T, \quad \alpha \in \mathbb{H};$$

in particular $\Xi_m(\alpha) = (-1)^m(\Xi_m(\alpha))^*$ if the real part of α is zero.

Proposition 4.5. *Let $H \in \mathbb{H}^{n \times n}$ be an invertible skewhermitian matrix, and let $X \in \mathbb{H}^{n \times n}$ be H -skewsymmetric. Then for some invertible quaternionic matrix S , the matrices S^*HS and $S^{-1}XS$ have simultaneously the following form:*

$$S^*HS = \bigoplus_{j=1}^r \eta_j iF_{\ell_j} \oplus \bigoplus_{v=1}^s \begin{bmatrix} 0 & F_{p_v} \\ -F_{p_v} & 0 \end{bmatrix} \oplus \bigoplus_{u=1}^q \zeta_u \Xi_{m_u}(i^{m_u}), \quad (4.7)$$

$$S^{-1}XS = \bigoplus_{j=1}^r J_{\ell_j}(0) \oplus \bigoplus_{v=1}^s \begin{bmatrix} -J_{p_v}((\alpha_v)^*) & 0 \\ 0 & J_{p_v}(\alpha_v) \end{bmatrix} \oplus \bigoplus_{u=1}^q J_{m_u}(\gamma_u), \quad (4.8)$$

where η_j, ζ_u are signs ± 1 with the additional condition that $\eta_j = 1$ if ℓ_j is odd, the quaternions $\alpha_1, \dots, \alpha_s$ have positive real parts, the quaternions $\gamma_1, \dots, \gamma_q$ are nonzero with zero real parts, and in addition $i\gamma_j$ is real if m_j is odd.

The form (4.7), (4.8) is uniquely determined by the pair (X, H) , up to a permutation of primitive blocks, up to replacements of some α_k with similar quaternions, and up to replacements of some γ_j with similar quaternions, subject to the additional condition that $i\gamma_j$ is real if m_j is odd.

Proposition 4.6. *Let $A \in \mathbb{H}^{n \times n}$ be H -symmetric. Then there exists an invertible matrix $S \in \mathbb{H}^{n \times n}$ such that*

$$S^{-1}AS = J_{\ell_1}(\beta_1) \oplus \cdots \oplus J_{\ell_q}(\beta_q), \quad S^*HS = iF_{\ell_1} \oplus \cdots \oplus iF_{\ell_q}, \quad (4.9)$$

where $\beta_1, \dots, \beta_q$ are quaternions such that $i\beta_j$ ($j = 1, 2, \dots, q$) have zero real parts.

The form (4.9) is uniquely determined by the pair (A, H) up to a simultaneous permutation of blocks in $S^{-1}AS$ and S^*HS , and up to replacement of each β_j by a similar quaternion β'_j subject to the condition that $i\beta'_j$ has zero real part.

Thus, the quaternions β_p in (4.9) are of the form $\beta_p = a_p + c_pj + d_pk$, where $a_p, c_p, d_p \in \mathbb{R}$.

Again, the canonical forms of H -skewsymmetric and H -symmetric matrices Z under the transformations $Z \rightarrow S^{-1}ZS$, $H \rightarrow S^*HS$, $S \in \mathbb{H}^{n \times n}$ is invertible, are well known; see, e.g., [3, 4, 22]. Complete proofs of Propositions 4.5 and 4.6 using matrix techniques are given in [19].

It follows from Proposition 4.6 that two H -symmetric matrices are $\mathbb{H}$ -similar if and only if they are H -symplectically similar. Also, every $n \times n$ quaternionic matrix is $\mathbb{H}$ -similar to an H -symmetric matrix.

For the proof of Theorem 4.1, we first of all note that by Proposition 4.6, without loss of generality we may (and do) assume that A and H are given by

$$A = J_{\ell_1}(\beta_1) \oplus \cdots \oplus J_{\ell_q}(\beta_q), \quad H = iF_{\ell_1} \oplus \cdots \oplus iF_{\ell_q}, \quad (4.10)$$

where $\beta_1, \dots, \beta_q$ are quaternions such that $i\beta_j$ ($j = 1, 2, \dots, q$) have zero real parts. Furthermore, by Lemma (3.6), we may assume that one of the three cases holds:

- (1) $\sigma(A) = \{0\}$;
- (2) $\sigma(A) = \{\mu\}$, where μ is real and negative;
- (3) $\sigma(A) = \{\nu^{-1}\mu\nu : \nu \in \mathbb{H} \setminus \{0\}\}$, where either μ is nonreal, or μ is real and positive (in the latter case $\sigma(A) = \{\mu\}$).

We prove first the “only if” part. Thus, assume that there exists a square root X of A that is H -skewsymmetric. Clearly, $(\sigma(X))^2 = \sigma(A)$ (as easily follows, for example, from the Jordan form of X). In case (2) the conditions (a) and (b) of Theorem 4.1 are vacuous. Notice that in case (1), the condition (b) of Theorem 4.1 represents a criterion for existence of a quaternionic square root (irrespective of H -skewsymmetry) of A , and therefore (b) is obviously satisfied; cf. [5], for example. Finally, suppose (3) holds. Since the square of any nonzero quaternion with zero real part is real negative number, a comparison with the Jordan form of X given by (4.8) shows that A is $\mathbb{H}$ -similar to

$$\bigoplus_{v=1}^s \begin{bmatrix} (J_{p_v}((\alpha_v)^*))^2 & 0 \\ 0 & (J_{p_v}(\alpha_v))^2 \end{bmatrix},$$

where the quaternions $\alpha_1, \dots, \alpha_v$ have positive real parts and are such that $\alpha_1^2, \dots, \alpha_v^2$ are similar to μ . However, the matrix $(J_{p_v}(\alpha_v))^2$ is $\mathbb{H}$ -similar to $J_{p_v}(\mu)$, and (since $((\alpha_v)^*)^2 = ((\alpha_v)^2)^*$) the matrix $(J_{p_v}((\alpha_v)^*))^2$ is $\mathbb{H}$ -similar to $J_{p_v}((\mu)^*)$, which in turn is $\mathbb{H}$ -similar to $J_{p_v}(\mu)$. The condition (a) of Theorem 4.1 follows.

We now turn to the “if” part of Theorem 4.1. Thus, assume that (a) and (b) of Theorem 4.1 hold. Consider first the case when $\sigma(A) = \{0\}$. In view of the condition (b), and leaving aside the trivial case of $B = 0$, we only need to prove the following two claims:

Claim 4.7. *Let $H = iF_m \oplus iF_{m-1}$, where $m > 1$. Then there exists an H -skewsymmetric matrix X such that*

$$X^2 = J_m(0) \oplus J_{m-1}(0).$$

Claim 4.8. *Let $H = iF_m \oplus iF_m$, where $m > 1$. Then there exists an H -skewsymmetric matrix X such that*

$$X^2 = J_m(0) \oplus J_m(0).$$

To satisfy the statement of Claim 4.7, take

$$X = \begin{bmatrix} 0_m & \begin{bmatrix} jI_{m-1} \\ 0 \\ 0_{m-1} \end{bmatrix} \\ \begin{bmatrix} 0 & -jI_{m-1} \end{bmatrix} & \end{bmatrix}.$$

For Claim 4.8, it will be convenient to do a preliminary transformation. First, note that there exists an invertible $T \in \mathbb{H}^{2m \times 2m}$ such that

$$T^{-1}(J_m(0) \oplus J_m(0))T = (-J_m(0)) \oplus (-J_m(0)), \quad T^*(iF_m \oplus iF_m)T = \hat{H},$$

where

$$\hat{H} = iF_m \oplus (-iF_m).$$

Indeed, the following equalities

$$(\text{diag}(1, -1, 1, \dots, (-1)^{m-1}))^{-1} J_m(0) (\text{diag}(1, -1, 1, \dots, (-1)^{m-1})) = -J_m(0),$$

$$(\text{diag}(1, -1, 1, \dots, (-1)^{m-1}))^* (iF_m) (\text{diag}(1, -1, 1, \dots, (-1)^{m-1})) = (-1)^{m-1} (iF_m),$$

and

$$(\text{diag}(j, -j, j, \dots, (-1)^{m-1}j))^{-1} J_m(0) (\text{diag}(j, -j, j, \dots, (-1)^{m-1}j)) = -J_m(0),$$

$$(\text{diag}(j, -j, j, \dots, (-1)^{m-1}j))^* (iF_m) (\text{diag}(j, -j, j, \dots, (-1)^{m-1}j)) = (-1)^m (iF_m),$$

easily yield existence of T with the required properties. Thus, it will suffice to find an $\hat{H}$ -skewsymmetric matrix Y such that

$$Y^2 = (-J_m(0)) \oplus (-J_m(0)). \quad (4.11)$$

Let $S \in \mathbb{R}^{2m \times 2m}$ be defined as follows (a construction borrowed from the proof of [2, Theorem 4.4]): The columns of S from left to right are

$$\frac{1}{\sqrt{2}}(e_1 + e_{m+1}), \frac{1}{\sqrt{2}}(e_1 - e_{m+1}), \frac{1}{\sqrt{2}}(e_2 + e_{m+2}), \frac{1}{\sqrt{2}}(e_2 - e_{m+2}), \dots, \\ \frac{1}{\sqrt{2}}(e_{m-1} + e_{2m-1}), \frac{1}{\sqrt{2}}(e_{m-1} - e_{2m-1}), \frac{1}{\sqrt{2}}(e_m + e_{2m}), \frac{1}{\sqrt{2}}(e_m - e_{2m}),$$

where e_k stands for the k th unit coordinate vector in $\mathbb{R}^{2m \times 1}$ (1 in the k th position and zeros in all other positions). One verifies that S is invertible, and (cf. the proof of [2, Theorem 4.4])

$$S^{-1}((-J_m(0)) \oplus (-J_m(0)))S = -J_{2m}(0)^2, \quad S^* \hat{H} S = iF_{2m}. \quad (4.12)$$

Now take $Y = S(iJ_{2m}(0))S^{-1}$. Using equalities (4.12), a straightforward calculation shows that Y is $\hat{H}$ -skewsymmetric and equality (4.11) is satisfied.

Next, consider the case (3). Since we suppose that condition (a) of Theorem 4.1 holds, we may (and do) assume that

$$A = J_m(\mu_1) \oplus J_m(\mu_2), \quad H = iF_m \oplus iF_m,$$

where $\mu_1, \mu_2 \in \mathbb{H}$ are not real nonpositive, and have the properties that $i\mu_1$ and $i\mu_2$ have zero real parts, and μ_1 and μ_2 are similar to each other. First, we show that without loss of generality we may take $\mu_1 = \mu_2$. Indeed, this is obvious if μ_1 is real positive. If μ_1 and μ_2 are nonreal and similar, and if $i\mu_1$ and $i\mu_2$ have zero real parts, then a straightforward computation shows that we have $\mu_1 = \alpha^{-1}\mu_2\alpha$ for some $\alpha \in \text{Span}_{\mathbb{R}}\{1, i\}$ with $|\alpha| = 1$. Obviously, $\alpha^*i\alpha = i$. Now

$$J_m(\mu_1) = (\alpha I)^{-1}J_m(\mu_2)(\alpha I), \quad iF_m = (\alpha I)^*(iF_m)(\alpha I),$$

and the replacement of μ_2 with μ_1 is justified. Thus, assume $\mu_1 = \mu_2 = \mu$. We seek a matrix X such that $X^2 = A$ and HX is hermitian in the form

$$X = \begin{bmatrix} 0 & X_1 \\ -X_1 & 0 \end{bmatrix},$$

where

$$X_1 = \begin{bmatrix} a_1 & a_2 & a_3 & \cdots & a_m \\ 0 & a_1 & a_2 & \cdots & a_{m-1} \\ 0 & 0 & a_1 & \cdots & a_{m-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & a_1 \end{bmatrix}$$

is an upper triangular Toeplitz matrix with entries $a_j \in \text{Span}_{\mathbb{R}} \{1, j, k\}$. Then HX is hermitian (use the equality $iX_1 = \overline{X_1}i$ to verify that), and the condition that $X^2 = A$ amounts to

$$X_1^2 = -J_m(\mu). \quad (4.13)$$

Clearly, there exists X_1 that satisfies (4.13) and has entries in $\text{Span}_{\mathbb{R}} \{1, j, k\}$ (if μ is non real, there is such an X_1 already in $\text{Span}_{\mathbb{R}} \{1, \mu\}$).

Finally, we consider the case (2): $\sigma(A) = \{\mu\}$, where μ is real and negative. In this case, the conditions (a) and (b) are vacuous. Therefore, we need to prove that there exists an iF_m -skewsymmetric matrix X such that $X^2 = J_m(\mu)$. It is easy to see that there is a square root of $J_m(\mu)$ of the form

$$X = i \begin{bmatrix} x_1 & x_2 & x_3 & \cdots & x_m \\ 0 & x_1 & x_2 & \cdots & x_{m-1} \\ 0 & 0 & x_1 & \cdots & x_{m-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & x_1 \end{bmatrix}, \quad x_1, \dots, x_m \in \mathbb{R}.$$

(For example, $x_1 = \sqrt{-\mu}$.) Then $iF_m X$ is hermitian, and we are done.

This completes the proof of Theorem 4.1.

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