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Schur-Like Forms for Matrix Lie Groups, Lie Algebras and Jordan Algebras

Gregory Ammar Christian Mehl Volker Mehrmann[1]

Dedicated to Ludwig Elsner on the occasion of his sixtieth birthday

Abstract

We describe canonical forms for elements of a classical Lie group of matrices under similarity transformations in the group. Matrices in the associated Lie algebra and Jordan algebra of matrices inherit related forms under these similarity transformations. In general, one cannot achieve diagonal or Schur form, but the form that can be achieved displays the eigenvalues of the matrix. We also discuss matrices in intersections of these classes and their Schur-like forms. Such multistructered matrices arise in applications from quantum physics and quantum chemistry.

1 Introduction

Many problems that arise in applications have structures that give rise to eigenvalue problems for matrices that are members of a classical Lie group, its Lie algebra, or an associated Jordan algebra of matrices.

Any nonsingular matrix $K \in \mathbb{C}^{m,m}$ defines a nondegenerate sesquilinear form $< \cdot, \cdot >$ on $\mathbb{C}^m$ by

$$< x, y >= x^H K y \qquad \text{for } x, y \in \mathbb{C}^m,$$

where x^H denotes the conjugate transpose of the column vector x. It is natural to restrict ourselves to the case that

$$< x, y >= 0 \quad \text{if and only if} \quad < y, x >= 0.$$

This condition implies that K is either Hermitian or skew-Hermitian [2].

If K is Hermitian, we can perform a change of basis on $\mathbb{C}^m$ so that the sesquilinear form is represented by the matrix

$$\Sigma_{p,q} = \begin{bmatrix} -I_p & 0 \\ 0 & I_q \end{bmatrix},$$

where $p + q = m$, $p \geq 0$, and $q \geq 0$. On the other hand, if K is skew Hermitian, then the only interesting case is that m is even, and that after a change of basis, the skew Hermitian form is represented by the matrix

$$J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix},$$

where $m = 2n$.

The classical Lie groups we consider here are the matrices that are unitary with respect to J or $\Sigma_{p,q}$ [15]. We will discuss only classes of complex matrices here, but analogous results also exist for the real case.

Definition 1

1) The Lie group $\mathcal{O}_{p,q}$ *of* $\Sigma_{p,q}$-unitary matrices *is defined by*

$$\mathcal{O}_{p,q} = \{G \in \mathbb{C}^{p+q,p+q} : G^H \Sigma_{p,q} G = \Sigma_{p,q}\}.$$

An important special case is the unitary group $\mathcal{O}_n = \mathcal{O}_{0,n}$.

2) The Lie group $\mathcal{S}p_{2n}$ *of* symplectic matrices *is defined by*

$$\mathcal{S}p_{2n} = \{G \in \mathbb{C}^{2n,2n} : G^H J G = J\}.$$

Developing structure-preserving numerical methods for solving eigenvalue problems for matrices in these groups remains an active area of recent research [7, 9, 10, 23], motivated by applications arising in signal processing [1] and optimal control for discrete-time or continuous-time linear systems, see [23] and the references therein.

Of equal importance are the Lie algebras $\mathcal{A}_{p,q}$ and $\mathcal{H}_{2n}$ corresponding to the Lie groups $\mathcal{O}_{p,q}$ and $\mathcal{S}p_{2n}$.

Definition 2

1') The Lie algebra of $\Sigma_{p,q}$-skew Hermitian matrices *is defined by*

$$\begin{aligned}\mathcal{A}_{p,q} &= \{A \in \mathbb{C}^{p+q,p+q} : \Sigma_{p,q} A + A^H \Sigma_{p,q} = 0\} \\ &= \left\{ \begin{bmatrix} F & G \\ G^H & H \end{bmatrix} : F = -F^H \in \mathbb{C}^{p,p}, H = -H^H \in \mathbb{C}^{q,q}, G \in \mathbb{C}^{p,q} \right\}.\end{aligned}$$

A special case is the Lie algebra of skew Hermitian *matrices* $\mathcal{A}_n = \mathcal{A}_{0,n}$.

2') The Lie algebra of J-Hermitian matrices *(also called* Hamiltonian matrices *or* infinitesimally symplectic matrices*) is defined by*

$$\begin{aligned}\mathcal{H}_{2n} &= \{A \in \mathbb{C}^{2n,2n} : JA + A^H J = 0\} \\ &= \left\{ \begin{bmatrix} F & G \\ H & -F^H \end{bmatrix} : F, G, H \in \mathbb{C}^{n,n}, G = G^H, H = H^H \right\}.\end{aligned}$$

These Lie algebras also have great importance in practical applications, see [4, 5, 25] for applications of $\Sigma_{p,q}$-skew symmetric matrices and [8, 23, 20] for applications of Hamiltonian matrices.

The third class of matrices we consider plays a role similar to that of the Lie algebras. These are the Jordan algebras [3, 16] associated with the two Lie groups.

Definition 3

1") $\mathcal{C}_{p,q}=\{C \in \mathbb{C}^{p+q,p+q} : \Sigma_{p,q}C - C^H\Sigma_{p,q} = 0\}$
$$=\left\{ \begin{bmatrix} F & G \\ -G^H & H \end{bmatrix} : F = F^H \in \mathbb{C}^{p,p}, H = H^H \in \mathbb{C}^{q,q}, G \in \mathbb{C}^{p,q} \right\},$$
is the Jordan algebra of $\Sigma_{p,q}$-Hermitian matrices. *A special case is the Jordan algebra of Hermitian matrices* $\mathcal{C}_n = \mathcal{C}_{0,n}$.

2") $\mathcal{SH}_{2n}=\{C \in \mathbb{C}^{2n,2n} : JC - C^H J = 0\}$
$$=\left\{ \begin{bmatrix} F & G \\ H & F^H \end{bmatrix} : F, G, H \in \mathbb{C}^{n,n}, G = -G^H, H = -H^H \right\},$$
is the Jordan algebra of J-skew Hermitian matrices *or* skew Hamiltonian matrices.

For applications of these classes see, for example, [5, 26, 27].

In this paper we discuss structure-preserving similarity transformations to condensed forms from which the eigenvalues of the matrices can be read off in a simple way. For general matrices these are the Jordan canonical form (under similarity transformations with nonsingular matrices), see e.g. [13], and the Schur form (under similarity with unitary matrices), see e.g. [14]. While both the Jordan form and Schur form display all the eigenvalues, the transformation to Jordan form gives the eigenvectors and principle vectors, and the transformation to Schur form displays one eigenvector and a nested set of invariant subspaces. However, the numerical computation of the Schur form is a well-conditioned problem, while the reduction to Jordan canonical from is in general an ill-conditioned problem, see e.g. [14].

The Jordan structure of a matrix can be computed, with considerably more effort than computing the Schur form, by computing the Wyer characteristics, which are invariants under unitary similarity transformations, see [17]. But if the matrix has an extra symmetry structure, for example if it is Hermitian, skew Hermitian or unitary, then the matrix is normal, and the Jordan form and the Schur form coincide. Consequently, complete eigenstructure information can be obtained via a numerically stable procedure [14, 26, 28] for matrices in these classes.

We may expect that between the general case and these special cases there are more refined condensed forms for matrices from the classes defined above. For the classes defined via the skew-symmetric matrix J such forms have been discussed in detail in the context of the solution of algebraic Riccati equations [8, 23]. We will review these results in Section 3. In Section 4 we will then discuss analogous condensed forms for the classes defined by the symmetric matrix $\Sigma_{p,q}$.

In Section 5 we then discuss condensed forms for matrices which lie in the intersection of two of the classes defined above. Our main motivation to work on this topic arose from a class of matrices that occur in quantum chemistry [11, 12, 24]. In linear response theory one needs to compute eigenvalues and eigenvectors of matrices of the form
$$\begin{bmatrix} A & B \\ -B & -A \end{bmatrix}, \ A, B \in \mathbb{C}^{n,n}, \ A = A^H, B = B^H. \tag{1}$$

Such matrices are clearly in $\mathcal{H}_{2n} \cap \mathcal{C}_{n,n}$. A difficulty in computing the eigenstructure of such matrices was observed in [11, 12], where the structure-preserving methods sometimes had convergence difficulties. As we will show, these difficulties arise from the fact that the reduction to a structured Schur form is not always possible, essentially because nonzero vectors may have zero "length" in the indefinite form defined by the matrix $\Sigma_{p,q}$. Moreover, we will see that the eigenvalues and invariant subspaces of the matrix are already available in this situation, even though the matrix has not yet been reduced to a triangular-like structure.

2 Preliminaries

In this section we give some preliminary results.

Proposition 4

1. *Let $M \in \mathcal{O}_{p,q}$ and $Mx = \lambda x$ with $x \neq 0$. Then $\overline{\lambda}^{-1}$ is also an eigenvalue of M, and $M^H(\Sigma_{p,q}x) = \lambda^{-1}(\Sigma_{p,q}x)$. If $x^H\Sigma_{p,q}x \neq 0$ then $|\lambda| = 1$.*

2. *Let $M \in \mathcal{A}_{p,q}$ and $Mx = \lambda x$ with $x \neq 0$. Then $-\overline{\lambda}$ is also an eigenvalue of M, and $M^H(\Sigma_{p,q}x) = -\lambda(\Sigma_{p,q}x)$. If $x^H\Sigma_{p,q}x \neq 0$ then $\lambda = -\overline{\lambda}$.*

3. *Let $M \in \mathcal{C}_{p,q}$ and $Mx = \lambda x$ with $x \neq 0$. Then $\overline{\lambda}$ is also an eigenvalue of M, and $M^H(\Sigma_{p,q}x) = \lambda(\Sigma_{p,q}x)$. If $x^H\Sigma_{p,q}x \neq 0$ then $\lambda = \overline{\lambda}$.*

Proof. The proof follows directly from the definitions of the Lie group, Lie algebra, and Jordan algebra. □

Similar results are also known for the Lie group of symplectic matrices and the corresponding Lie algebra and Jordan algebra, see e.g. [23, 20].

There exist a vector space isomorphism between the Lie algebras and the associated Jordan algebras:

Proposition 5 *The map $A \mapsto iA$ is a vector space isomorphism between the Lie algebra $\mathcal{A}_{p,q}$ (or $\mathcal{H}_{2n}$) and the associated Jordan algebra $\mathcal{C}_{p,q}$ (or $\mathcal{SH}_{2n}$, respectively).*

Proof. The proof follows directly from the definitions. □

We will use similarity transformations that retain the structure to transform the matrices from the Lie groups, Lie algebras and Jordan algebras to a condensed form from which the eigenvalues can be read off in a simple way. These are symplectic similarity transformations for $\mathcal{S}p_{2n}$, $\mathcal{H}_{2n}$ and $\mathcal{SH}_{2n}$ and the $\Sigma_{p,q}$-unitary matrices for $\mathcal{O}_{p,q}$, $\mathcal{A}_{p,q}$ and $\mathcal{C}_{p,q}$. In order to use such transformations for numerical computation, we would prefer that these transformation matrices also be unitary, since then the methods can be implemented as numerically backwards stable procedures. These classes are characterized as follows.

Proposition 6

1. *Unitary symplectic matrices, i.e., matrices in* $\mathcal{S}p_{2n} \cap \mathcal{O}_{2n}$, *are of the form*

$$\begin{bmatrix} U_1 & U_2 \\ -U_2 & U_1 \end{bmatrix},$$

with $U_1U_1^H + U_2U_2^H = I_n$ *and* $U_1U_2^H - U_2U_1^H = 0$.

2. *Matrices in* $\mathcal{O}_{p,q} \cap \mathcal{O}_n$ $(n = p + q)$ *have the form*

$$\begin{bmatrix} Q_{11} & 0 \\ 0 & Q_{22} \end{bmatrix},$$

where $Q_{11} \in \mathcal{O}_p$ *and* $Q_{22} \in \mathcal{O}_q$.

Matrices in all the Lie groups and their intersections can be generated as products of elementary matrices in these classes, see e.g. [2, 5, 23]. Unfortunately, the class of matrices $\mathcal{O}_{p,q} \cap \mathcal{O}_n$ is not big enough to perform the reduction to the condensed forms. As an extra class of elementary $\Sigma_{p,q}$-unitary transformations, the hyperbolic rotations $H_p(c, s)$ are needed. These matrices are equal to the identity matrix except for the 2×2 submatrix in rows and columns 1 and $p + 1$, given by $\begin{bmatrix} \overline{c} & \overline{s} \\ s & c \end{bmatrix}$, with $|c|^2 - |s|^2 = 1$.

3 J-Schur-like forms

In this section we recall some of the known results concerning Schur-like forms for matrices in the classes defined by J. We will call these *J-Schur-like forms*.

Theorem 7

i) Let $M \in \mathcal{H}_{2n}$. *Then there exists a symplectic matrix* $Q \in \mathcal{S}p_{2n}$ *such that*

$$Q^{-1}MQ = \begin{bmatrix} T_1 & T_2 \\ 0 & -T_1^H \end{bmatrix}, \tag{2}$$

where $T_1, T_2 \in \mathbb{C}^{n,n}$, T_1 *is upper triangular and* T_2 *is Hermitian, if and only if every purely imaginary eigenvalue* λ *of* M *has even algebraic multiplicity, say* $2k$, *and any basis* $X_k \in \mathbb{C}^{2n,2k}$ *of the maximal invariant subspace for* M *corresponding to* λ *satisfies*

$$X_k^H J X_k \sim^c \begin{bmatrix} 0 & I_k \\ -I_k & 0 \end{bmatrix}. \tag{3}$$

Here '$\sim^c$*' denotes congruence.*

ii) Let $M \in \mathcal{SH}_{2n}$. *Then there exists a symplectic matrix* $Q \in \mathcal{S}p_{2n}$ *such that*

$$Q^{-1}MQ = \begin{bmatrix} T_1 & T_2 \\ 0 & T_1^H \end{bmatrix}, \tag{4}$$

where $T_1, T_2 \in \mathbb{C}^{n,n}$, T_1 is upper triangular and T_2 is skew Hermitian, if and only if every real eigenvalue λ of M has even algebraic multiplicity, say $2k$, and any basis $X_k \in \mathbb{C}^{2n,2k}$ of the maximal invariant subspace for M corresponding to λ satisfies (3).

iii) Let $M \in \mathcal{S}p_{2n}$. Then there exists a symplectic matrix $Q \in \mathcal{S}p_{2n}$ such that

$$Q^{-1}MQ = \begin{bmatrix} T_1 & T_2 \\ 0 & T_1^{-H} \end{bmatrix}, \tag{5}$$

where $T_1, T_2 \in \mathbb{C}^{n,n}$, T_1 is upper triangular and T_2 is Hermitian, if and only if every unimodular eigenvalue λ of M has even algebraic multiplicity, say $2k$, and any basis $X_k \in \mathbb{C}^{2n,2k}$ of the maximal invariant subspace for M corresponding to λ satisfies (3).

Proof. This result was first stated and proved in [22]. □

Note that there are also more refined Jordan-like forms for matrices in $\mathcal{H}_{2n}, \mathcal{SH}_{2n}$ and $\mathcal{S}p_{2n}$, which do not have a triangular structure, see [21].

It follows from a result in [6] that the matrices Q in each part of Theorem 7 can be chosen to be unitary symplectic. However, matrices in the J classes exist for which the forms (2)–(5) can be achieved only via non-symplectic transformations or not at all. For example, for the matrix $\begin{bmatrix} 0 & I_2 \\ -I_2 & 0 \end{bmatrix}$ a J-Schur-like form can only be achieved with non-symplectic matrices, while for the matrix $\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$ no J-Schur-like form exists.

4 $\Sigma_{p,q}$-Schur-like forms

In this section we present results analogous to Theorem 7 concerning Schur-like forms for matrices in the classes defined by $\Sigma_{p,q}$ under similarity transformations from the group $\mathcal{O}_{p,q}$. We will call these forms $\Sigma_{p,q}$-*Schur-like forms.*

Of course, if $p = 0$ or $q = 0$, then the matrices in question (unitary, Skew-Hermitian, and Hermitian matrices) are all normal, and their Schur forms under unitary similarity transformations are diagonal. So, unless explicitly mentioned, we will assume that p and q are both positive (and $m = p + q \geq 2$).

We describe the $\Sigma_{p,q}$-Schur-like forms in terms of a block 2×2 matrix

$$Q^{-1}MQ = \begin{array}{c} \\ p \\ q \end{array} \begin{array}{c} \begin{array}{cc} p & q \end{array} \\ \begin{bmatrix} A & C \\ D & B \end{bmatrix} \end{array}, \tag{6}$$

with the partitioning

$$\begin{array}{c} \\ p_1 \\ p_2 \\ p_3 \\ p_4 \\ \vdots \\ p_s \\ \\ q_1 \\ q_2 \\ q_3 \\ q_4 \\ \vdots \\ q_l \end{array} \begin{array}{c} \begin{array}{cccccccccccc} p_1 & p_2 & p_3 & p_4 & \cdots & p_s & q_1 & q_2 & q_3 & q_4 & \cdots & q_l \end{array} \\ \left[\begin{array}{cccccccccccc} A_{11} & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & A_{22} & A_{23} & A_{24} & \cdots & A_{2s} & 0 & C_{22} & C_{23} & C_{24} & \cdots & C_{2l} \\ 0 & A_{32} & A_{33} & 0 & \cdots & 0 & 0 & C_{32} & 0 & 0 & \cdots & 0 \\ 0 & A_{42} & 0 & A_{44} & \cdots & A_{4s} & 0 & C_{42} & 0 & C_{44} & \cdots & C_{4l} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & A_{s2} & 0 & A_{s4} & \cdots & A_{ss} & 0 & C_{s2} & 0 & C_{s4} & \cdots & C_{sl} \\ & & & & & & & & & & & \\ 0 & 0 & 0 & 0 & \cdots & 0 & B_{11} & 0 & 0 & 0 & \cdots & 0 \\ 0 & D_{22} & D_{23} & D_{24} & \cdots & D_{2s} & 0 & B_{22} & B_{23} & B_{24} & \cdots & B_{2l} \\ 0 & D_{32} & 0 & 0 & \cdots & 0 & & B_{32} & B_{33} & 0 & \cdots & 0 \\ 0 & D_{42} & 0 & D_{44} & \cdots & D_{4s} & 0 & B_{42} & 0 & B_{44} & \cdots & B_{4l} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & D_{l2} & 0 & D_{l4} & \cdots & D_{ls} & 0 & B_{l2} & 0 & B_{l4} & \cdots & B_{ll} \end{array}\right] \end{array}, \tag{7}$$

where $\sum_{j=1}^{s} p_j = p$, $\sum_{k=1}^{l} q_k = q$, and such that

1. For odd i, $p_i \geq 0$, $q_i \geq 0$, and the blocks A_{ii} and B_{ii} are each either diagonal or void;
2. for even i, $p_i = q_i \in \{0, 1\}$.

Theorem 8

i) Let $M \in \mathcal{O}_{p,q}$, then there exists $Q \in \mathcal{O}_{p,q}$ such that

$$Q^{-1}MQ = \begin{array}{c} \\ p \\ q \end{array} \begin{array}{c} \begin{array}{cc} p & q \end{array} \\ \left[\begin{array}{cc} A & C \\ D & B \end{array}\right] \end{array}$$

is in the form (7). For odd indicies i, the blocks $A_{ii} \in \mathcal{O}_{p_i}$ and $B_{ii} \in \mathcal{O}_{q_i}$ are either void or diagonal (with eigenvalues of modulus 1). For the even indicies i, the blocks A_{ii}, B_{ii} are either both void or both 1×1. Furthermore, if these blocks are not void, then

$$\begin{array}{rcccl} A_{2i,2i} + C_{2i,2i} & = & D_{2i,2i} + B_{2i,2i} & = & \lambda, \\ A_{2i,2i} - D_{2i,2i} & = & B_{2i,2i} - C_{2i,2i} & = & \overline{\lambda}^{-1}, \end{array} \tag{8}$$

and

$$\begin{gathered} \left[\begin{array}{c} A_{2i+1,2i} \\ \vdots \\ A_{s,2i} \end{array}\right] = -\left[\begin{array}{c} C_{2i+1,2i} \\ \vdots \\ C_{s,2i} \end{array}\right], \quad \left[\begin{array}{c} B_{2i+1,2i} \\ \vdots \\ B_{l,2i} \end{array}\right] = -\left[\begin{array}{c} D_{2i+1,2i} \\ \vdots \\ D_{l,2i} \end{array}\right], \\ \left[\begin{array}{ccc} A_{2i,2i+1} & \cdots & A_{2i,s} \end{array}\right] = \left[\begin{array}{ccc} D_{2i,2i+1} & \cdots & D_{2i,s} \end{array}\right], \\ \left[\begin{array}{ccc} B_{2i,2i+1} & \cdots & B_{2i,l} \end{array}\right] = \left[\begin{array}{ccc} C_{2i,2i+1} & \cdots & C_{2i,l} \end{array}\right]. \end{gathered} \tag{9}$$

Moreover the eigenvalues of M are the eigenvalues of the matrix obtained by deleting all the off-diagonal blocks in A, B, C, D.

ii) Let $M \in \mathcal{A}_{p,q}$. Then there exists $Q \in \mathcal{O}_{p,q}$ such that

$$Q^{-1}MQ = \begin{bmatrix} A & C \\ C^H & B \end{bmatrix}, \tag{10}$$

with $B = -B^H$, $A = -A^H$, and A, B, C structured as in (7), where for the blocks with odd numbered indices, $A_{ii} \in \mathcal{A}_{p_i}$ and $B_{ii} \in \mathcal{A}_{q_i}$ are diagonal with purely imaginary eigenvalues or void and the even numbered blocks A_{ii}, B_{ii} are either both 1×1 or are both void. Furthermore, if these blocks are not void, then

$$A_{2i,2i} + C_{2i,2i} = \overline{C}_{2i,2i} + B_{2i,2i} = \lambda. \tag{11}$$

Again the eigenvalues of M are the eigenvalues of the matrix obtained by deleting all the off-diagonal blocks in A, B, and C.

iii) Let $M \in \mathcal{C}_{p,q}$. Then there exists $Q \in \mathcal{O}_{p,q}$ such that

$$Q^{-1}MQ = \begin{bmatrix} A & C \\ -C^H & B \end{bmatrix}, \tag{12}$$

with $B = B^H$, $A = A^H$, and A, B, C structured as in (7), where for the blocks with odd numbered indices, $A_{ii} \in \mathcal{C}_{p_i}, B_{ii} \in \mathcal{C}_{q_i}$ are diagonal with real eigenvalues or void and the even numbered blocks A_{ii}, B_{ii} are either both 1×1 or are both void. Furthermore, if these blocks are not void, then

$$A_{2i,2i} + C_{2i,2i} = -\overline{C}_{2i,2i} + B_{2i,2i} = \lambda. \tag{13}$$

Again the eigenvalues of M are the eigenvalues of the matrix obtained by deleting all the off-diagonal blocks in A, B and C.

Proof. i) The proof proceeds via induction on the dimension $m = p + q$. The case $m = 1$ is trivial, since in this case $p = 0$ or $q = 0$. Assume that p and q are both positive. Let λ be an eigenvalue of M, and let $x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \neq 0$ be an associated eigenvector, with $x_1 \in \mathbb{C}^p$ and $x_2 \in \mathbb{C}^q$, and let $Q_{11} \in \mathcal{O}_p$, $Q_{22} \in \mathcal{O}_q$ be such that

$$Q_{11}^H x_1 = \alpha_1 e_1, \; Q_{22}^H x_2 = \alpha_2 e_{p+1},$$

where $\alpha_1 = \|x_1\|$, $\alpha_2 = \|x_2\|$ are real and nonnegative and e_i denotes the i-th unit vector, e.g. [14].

If α_1 and α_2 are both nonzero, then we cannot eliminate another element using a matrix in $\mathcal{O}_{p,q} \cap \mathcal{O}_m$. So if we wish to retain that the matrix remains in the group, we have to use hyperbolic rotations.

If $\alpha_1 \neq \alpha_2$, then a hyperbolic transformation can be applied to further reduce the transformed vector. We then have to consider the three cases $\alpha_1 > \alpha_2$, $\alpha_1 = \alpha_2 \neq 0$ and $\alpha_1 < \alpha_2$. The case that both parameters are 0 cannot happen, since $x \neq 0$.

If $\alpha_1 > \alpha_2$, then there exists a hyperbolic rotation $\begin{bmatrix} \overline{c} & \overline{s} \\ s & c \end{bmatrix} \in \mathcal{O}_{1,1}$ such that

$$\begin{bmatrix} \overline{c} & \overline{s} \\ s & c \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} = \begin{bmatrix} \beta_1 \\ 0 \end{bmatrix},$$

with $\beta_1 = (\alpha_1^2 - \alpha_2^2)^{1/2} > 0$.

If $\alpha_1 < \alpha_2$, then there exists a hyperbolic rotation such that

$$\begin{bmatrix} \overline{c} & \overline{s} \\ s & c \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} = \begin{bmatrix} 0 \\ \beta_2 \end{bmatrix},$$

with $\beta_2 = (\alpha_2^2 - \alpha_1^2)^{1/2} > 0$.

In the third case, $\alpha_1 = \alpha_2$, no hyperbolic rotation exists that eliminates either of the two elements. Then we set $c = 1,\ s = 0$.

Having chosen c and s, set

$$Q_1^{-1} := H_p(c,s) \begin{bmatrix} Q_{11}^H & 0 \\ 0 & Q_{22}^H \end{bmatrix} \in \mathcal{O}_{p,q}.$$

It follows that

$$Q_1^{-1}x = \begin{cases} \begin{bmatrix} \beta_1 & 0 & \dots & 0 & 0 & 0 & \dots & 0 \end{bmatrix}^T; & \alpha_1 > \alpha_2, \\ \begin{bmatrix} 0 & 0 & \dots & 0 & \beta_2 & 0 & \dots & 0 \end{bmatrix}^T; & \alpha_1 < \alpha_2, \\ \begin{bmatrix} \alpha_1 & 0 & \dots & 0 & \alpha_2 & 0 & \dots & 0 \end{bmatrix}^T; & \alpha_1 = \alpha_2 \neq 0. \end{cases}$$

In the first case, we see that

$$Q_1^{-1} M Q_1 e_1 = \lambda e_1,$$

so that

$$\tilde{M} := Q_1^{-1} M Q_1 = \begin{bmatrix} \lambda & w^H \\ 0 & M' \end{bmatrix} \tag{14}$$

and since $\tilde{M} \in \mathcal{O}_{p,q}$, we obtain $|\lambda| = 1$, $w = 0$, $p_1 = 1$, $q_1 = 0$, and $M' \in \mathcal{O}_{p-1,q}$.

In the second case, we have

$$Q_1^{-1} M Q_1 e_{p+1} = \lambda e_{p+1},$$

so the transformed matrix takes the form

$$\tilde{M} = Q_1^{-1} M Q_1 = \begin{bmatrix} M_{11} & 0 & M_{13} \\ w_1^H & \lambda & w_3^H \\ M_{31} & 0 & M_{33} \end{bmatrix}, \tag{15}$$

and since $\tilde{M} \in \mathcal{O}_{p,q}$, we obtain $|\lambda| = 1$, $w_1 = 0$, $w_3 = 0$, $p_1 = 0$, $q_1 = 1$, and $M' = \begin{bmatrix} M_{11} & M_{13} \\ M_{31} & M_{33} \end{bmatrix} \in \mathcal{O}_{p,q-1}$.

In the third case no further reduction of the vector $Q_1^{-1}x = \alpha_1 e_1 + \alpha_2 e_{p+1}$ is possible with a hyperbolic rotation. In this case we have

$$\tilde{M} = Q_1^{-1} M Q_1 = \begin{bmatrix} m_{11} & w_{12}^H & m_{1,p+1} & w_{14}^H \\ y_{21} & M_{22} & y_{23} & M_{24} \\ m_{p+1,1} & w_{32}^H & m_{p+1,p+1} & w_{34}^H \\ y_{41} & M_{42} & y_{43} & M_{44} \end{bmatrix} \tag{16}$$

and $\tilde{M}(\alpha_1 e_1 + \alpha_2 e_{p+1}) = (\alpha_1 e_1 + \alpha_2 e_{p+1})\lambda$. From $\alpha_1 = \alpha_2$ we obtain that

$$m_{11} + m_{1,p+1} = \lambda,\ m_{p+1,1} + m_{p+1,p+1} = \lambda \tag{17}$$

and

$$y_{41} + y_{43} = 0,\ y_{21} + y_{23} = 0. \tag{18}$$

By Proposition 4 we have that $\Sigma_{p,q}(e_1 + e_{p+1}) = e_1 - e_{p+1}$ is a left eigenvector associated with the eigenvalue $\overline{\lambda}^{-1}$. Hence we obtain

$$m_{11} - m_{p+1,1} = \overline{\lambda}^{-1},\ m_{1,p+1} + m_{p+1,p+1} = \overline{\lambda}^{-1} \tag{19}$$

and

$$w_{12} - w_{32} = 0,\ w_{14} - w_{34} = 0. \tag{20}$$

We immediately obtain that the submatrix $\begin{bmatrix} m_{11} & m_{1,p+1} \\ m_{p+1,1} & m_{p+1,p+1} \end{bmatrix}$ has the eigenvalues $\lambda, \overline{\lambda}^{-1}$.

If we consider the unitary matrix

$$U = \begin{bmatrix} \sqrt{2}^{-1} & & & \sqrt{2}^{-1} & & \\ & 1 & & & & \\ & & \ddots & & & \\ & & & 1 & & \\ -\sqrt{2}^{-1} & & & \sqrt{2}^{-1} & & \\ & & & & 1 & \\ & & & & & \ddots \\ & & & & & & 1 \end{bmatrix}, \tag{21}$$

then we obtain from the identities (17) through (20) that

$$U\tilde{M}U^H = \begin{bmatrix} \lambda & w_{12}^H & 0 & w_{14}^H \\ 0 & M_{22} & y_{23} & M_{24} \\ 0 & 0 & \overline{\lambda}^{-1} & 0 \\ 0 & M_{42} & y_{43} & M_{44} \end{bmatrix}. \tag{22}$$

As a consequence we obtain that the spectrum of M is equal to the union of the spectra of $\begin{bmatrix} m_{11} & m_{1,p+1} \\ m_{p+1,1} & m_{p+1,p+1} \end{bmatrix}$ and $M' = \begin{bmatrix} M_{22} & M_{24} \\ M_{42} & M_{44} \end{bmatrix}$. Furthermore, from (18) and (20) it is easy to see that $M' \in \mathcal{O}_{p-1,q-1}$. In this case, $p_1 = q_1 = 0$ and $p_2 = q_2 = 1$.

The proof now follows by induction. In each of the above three cases, we perform a similarity transformation based on the given eigenvector, and produce a matrix in a smaller group whose eigenvalues are the remaining eigenvalues of the original matrix. By induction, there is a $\Sigma_{p',q'}$-unitary matrix V such that $V^{-1}M'V$ is in the form of (7)–(9). Partitioning V compatibly with (14), (15) or (16), and embedding the partitioned matrix into a $\Sigma_{p,q}$-unitary matrix Q_2 in the obvious fashion, we see that $Q^{-1}MQ$ has the desired form, where $Q = Q_1Q_2$.

The proof for ii) is analogous while iii) follows from ii) using Proposition 5. □

Remark 9 We see from the fact that we have to use a unitary transformation $U \notin \mathcal{O}_{p,q}$ to obtain appropriate 0-blocks that the class of transformation matrices $\mathcal{O}_{p,q}$ is too small to bring every matrix in $\mathcal{O}_{p,q}$, (in $\mathcal{A}_{p,q}$ or $\mathcal{C}_{p,q}$) to upper triangular form via similarity. On the other hand, the form (7) displays all the eigenvalue information. The columns of the part of the matrix that cannot be eliminated have length 0 in the indefinite scalar product defined as $< u, v >_{p,q} = u^H \Sigma_{p,q} v$.

We also see that, in contrast with the symplectic case, we cannot obtain the condensed form using transformations in $\mathcal{O}_{p,q} \cap \mathcal{O}_m$, again since this class is too small to perform the necessary reductions.

Remark 10 In some cases we can reduce the form (7) further if subparts in the off-diagonal blocks of the top and bottom part do not have equal length. But since we can never eliminate in these blocks completely and since the eigenvalues are displayed, we may as well avoid further reduction.

Analogous results can also be obtained in the case of real matrices in all three classes. To obtain these results, we always combine complex conjugate pairs of eigenvalues and the associated eigenvectors.

We have presented structured condensed forms from which the eigenvalues can be read off in a simple way. These results simplify considerably in the case that the matrices have multiple structures. We will discuss Schur forms for such matrices in the next section.

5 Schur-like forms for multi-structured matrices.

In some applications one needs the computation of eigenvalues of matrices that have more than one structure. In this section we present Schur-like forms for matrices from intersections of two of the classes introduced in Section 1.

5.1 Intersections of two $\Sigma_{p,q}$ classes.

Let us first consider the intersections of classes defined by $\Sigma_{p,q}$ and $\Sigma_{\tilde{p},\tilde{q}}$, where $p+q = \tilde{p}+\tilde{q} = m$ and, w.l.o.g., $p > \tilde{p}$. Directly from the definitions we obtain the following structures.

Proposition 11

i) Matrices in $\mathcal{A}_{p,q} \cap \mathcal{A}_{\tilde{p},\tilde{q}}$ *have the form*

$$\begin{bmatrix} A_1 & A_2 & 0 & C_1 \\ -A_2^H & A_3 & 0 & C_2 \\ 0 & 0 & B_1 & 0 \\ C_1^H & C_2^H & 0 & B_2 \end{bmatrix} \tag{23}$$

with $\begin{bmatrix} A_1 & A_2 & C_1 \\ -A_2^H & A_3 & C_2 \\ C_1^H & C_2^H & B_2 \end{bmatrix} \in \mathcal{A}_{\tilde{p},q}$ *and* $B_1 \in \mathcal{A}_{\tilde{q}-q}$.

ii) Matrices in $\mathcal{C}_{p,q} \cap \mathcal{C}_{\tilde{p},\tilde{q}}$ *have the form*

$$\begin{bmatrix} A_1 & A_2 & 0 & C_1 \\ A_2^H & A_3 & 0 & C_2 \\ 0 & 0 & B_1 & 0 \\ -C_1^H & -C_2^H & 0 & B_2 \end{bmatrix} \tag{24}$$

with $\begin{bmatrix} A_1 & A_2 & C_1 \\ A_2^H & A_3 & C_2 \\ -C_1^H & -C_2^H & B_2 \end{bmatrix} \in \mathcal{C}_{\tilde{p},q}$ *and* $B_1 \in \mathcal{C}_{\tilde{q}-q}$.

iii) Matrices in $\mathcal{O}_{p,q} \cap \mathcal{O}_{\tilde{p},\tilde{q}}$ *have the form*

$$\begin{bmatrix} A_{11} & A_{12} & 0 & C_1 \\ A_{21} & A_{22} & 0 & C_2 \\ 0 & 0 & B_1 & 0 \\ D_1 & D_2 & 0 & B_2 \end{bmatrix} \tag{25}$$

with $\begin{bmatrix} A_{11} & A_{12} & C_1 \\ A_{21} & A_{22} & C_2 \\ D_1 & D_2 & B_2 \end{bmatrix} \in \mathcal{O}_{\tilde{p},q}$ *and* $B_1 \in \mathcal{O}_{\tilde{q}-q}$.

iv) Matrices in $\mathcal{A}_{p,q} \cap \mathcal{C}_{\tilde{p},\tilde{q}}$ *have the form*

$$\begin{bmatrix} 0 & 0 & C_1 & 0 \\ 0 & 0 & C_2 & 0 \\ C_1^H & C_2^H & 0 & B \\ 0 & 0 & -B^H & 0 \end{bmatrix}. \tag{26}$$

The intersection of a group with one of the algebras does not show any obvious structure. In cases i)–iii), the problem reduces to two smaller problems, each having a single structure for which the results of Section 4 apply. For case iv) the computation of the eigenvalues reduces to the computation of the singular values of the matrix $\left[\begin{array}{ccc} C_1^H & C_2^H & B \end{array}\right]$. An important special case that arises in particle physics [18, 19], is the case $p = q$ and $\tilde{p} = 0$. In this case the matrices have the form

$$\left[\begin{array}{cc} 0 & C \\ -C^H & 0 \end{array}\right], \tag{27}$$

where $C \in \mathbb{C}^{p\times p}$. Again, the eigenvalues can be determined via the singular values of C.

5.2 Intersections of a J class and a $\Sigma_{p,q}$ class, $p \neq n$.

In this subsection we consider matrices with a multiple structure related to both J and $\Sigma_{p,q}$, with $p+q = 2n$ and w.l.o.g. $p > n$. We obtain the following obvious structures which follow directly from the definitions.

Proposition 12

i) Matrices in $\mathcal{H}_{2n} \cap \mathcal{A}_{p,q}$ *have the form*

$$\left[\begin{array}{cccc} A_1 & 0 & C_1 & 0 \\ 0 & A_2 & 0 & C_2 \\ -C_1 & 0 & A_1 & 0 \\ 0 & C_2 & 0 & A_2 \end{array}\right], \tag{28}$$

with $\left[\begin{array}{cc} A_1 & C_1 \\ -C_1 & A_1 \end{array}\right] \in \mathcal{H}_{2(n-q)} \cap \mathcal{A}_{2(n-q)}$ *and* $\left[\begin{array}{cc} A_2 & C_2 \\ C_2 & A_2 \end{array}\right] \in \mathcal{H}_{2q} \cap \mathcal{A}_{q,q}$.

ii) Matrices in $\mathcal{H}_{2n} \cap \mathcal{C}_{p,q}$ *have the form*

$$\left[\begin{array}{cccc} A_1 & 0 & C_1 & 0 \\ 0 & A_2 & 0 & C_2 \\ C_1 & 0 & -A_1 & 0 \\ 0 & -C_2 & 0 & -A_2 \end{array}\right], \tag{29}$$

with $\left[\begin{array}{cc} A_1 & C_1 \\ C_1 & -A_1 \end{array}\right] \in \mathcal{H}_{2(n-q)} \cap \mathcal{C}_{2(n-q)}$ *and* $\left[\begin{array}{cc} A_2 & C_2 \\ -C_2 & -A_2 \end{array}\right] \in \mathcal{H}_{2q} \cap \mathcal{C}_{q,q}$.

iii) Matrices in $\mathcal{SH}_{2n} \cap \mathcal{A}_{p,q}$ *have the form*

$$\left[\begin{array}{cccc} A_1 & 0 & C_1 & 0 \\ 0 & A_2 & 0 & C_2 \\ C_1 & 0 & -A_1 & 0 \\ 0 & -C_2 & 0 & -A_2 \end{array}\right], \tag{30}$$

with $\left[\begin{array}{cc} A_1 & C_1 \\ C_1 & -A_1 \end{array}\right] \in \mathcal{SH}_{2(n-q)} \cap \mathcal{A}_{2(n-q)}$ *and* $\left[\begin{array}{cc} A_2 & C_2 \\ -C_2 & -A_2 \end{array}\right] \in \mathcal{SH}_{2q} \cap \mathcal{A}_{q,q}$.

iv) Matrices in $\mathcal{SH}_{2n} \cap \mathcal{C}_{p,q}$ *have the form*

$$\begin{bmatrix} A_1 & 0 & C_1 & 0 \\ 0 & A_2 & 0 & C_2 \\ -C_1 & 0 & A_1 & 0 \\ 0 & C_2 & 0 & A_2 \end{bmatrix}, \tag{31}$$

with $\begin{bmatrix} A_1 & C_1 \\ -C_1 & A_1 \end{bmatrix} \in \mathcal{SH}_{2(n-q)} \cap \mathcal{C}_{2(n-q)}$ *and* $\begin{bmatrix} A_2 & C_2 \\ C_2 & A_2 \end{bmatrix} \in \mathcal{SH}_{2q} \cap \mathcal{C}_{q,q}$.

No obvious simplified structure occurs in intersections of $\mathcal{A}_{p,q}$ or $\mathcal{C}_{p,q}$ with $\mathcal{S}p_{2n}$ or of $\mathcal{H}_{2n}$ or $\mathcal{SH}_{2n}$ with $\mathcal{O}_{p,q}$. In all four cases of Proposition 12 the treatment of the smaller matrices is relatively easy. The first submatrices in each of the cases are discussed in detail in [8] while the second submatrices will be discussed in the next section.

5.3 Intersections of a J class and a $\Sigma_{p,q}$ class, $p = q = n$.

In this section we discuss the most important multi-structured case in applications, $p = q = n$.

Theorem 13

i) Let

$$M \in \mathcal{O}_{n,n} \cap Sp_{2n} = \left\{ \begin{bmatrix} U & V \\ V & U \end{bmatrix} : UU^H - VV^H = I_n,\ UV^H = VU^H \right\}$$

Then there exists $\hat{Q} \in \mathcal{O}_{n,n} \cap Sp_{2n}$, *such that the eigenvalues of*

$$\hat{Q}^{-1} M \hat{Q} = \begin{bmatrix} \hat{U} & \hat{V} \\ \hat{V} & \hat{U} \end{bmatrix}. \tag{32}$$

are given by $u_{ii} \pm v_{ii}$, *where* u_{ii} *and* v_{ii} *denote the* i*-th diagonal element of* $\hat{U}$ *and* $\hat{V}$, *respectively. Furthermore we have* $(u_{ii} + v_{ii})\overline{(u_{ii} - v_{ii})} = 1$.

ii) Let

$$M \in \mathcal{A}_{n,n} \cap \mathcal{H}_{2n} = \left\{ \begin{bmatrix} A & B \\ B & A \end{bmatrix} : A = -A^H, B = B^H \right\}.$$

Then there exists $Q \in \mathcal{O}_{n,n} \cap \mathcal{S}p_{2n}$, *such that the eigenvalues of*

$$Q^{-1} M Q = \begin{bmatrix} A & B \\ B & A \end{bmatrix}. \tag{33}$$

are given by $a_{ii} \pm b_{ii}$, *where* a_{ii} *and* b_{ii} *denote the* i*-th diagonal element of* A *and* B, *respectively, Furthermore* $\pm b_{ii}$ *is the real part and* $-i \cdot a_{ii}$ *the imaginary part of the eigenvalue* $a_{ii} \pm b_{ii}$.

iii) Let

$$M \in \mathcal{C}_{n,n} \cap \mathcal{SH}_{2n} = \left\{ \begin{bmatrix} A & B \\ B & A \end{bmatrix} : A = A^H, B = -B^H \right\}.$$

Then there exists $Q \in \mathcal{O}_{n,n} \cap \mathcal{S}p_{2n}$, *such that the eigenvalues of*

$$Q^{-1}MQ = \begin{bmatrix} A & B \\ B & A \end{bmatrix}. \tag{34}$$

are given by $a_{ii} \pm b_{ii}$, *where* a_{ii} *and* b_{ii} *denote the* i*-th diagonal element of* A *and* B, *respectively. Furthermore* a_{ii} *is the real part and* $\mp i \cdot b_{ii}$ *the imaginary part of the eigenvalue* $a_{ii} \pm b_{ii}$.

Proof. i) Let $M = \begin{bmatrix} U & V \\ V & U \end{bmatrix} \in \mathcal{O}_{n,n} \cap Sp_{2n}$, and let $\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \neq 0$, with $x_1, x_2 \in \mathbb{C}^n$, be an eigenvector associated with the eigenvalue λ of M. It follows immediately that $\begin{bmatrix} x_1 + x_2 \\ x_1 + x_2 \end{bmatrix}$ is also an eigenvector of M associated with the eigenvalue λ. Let $Q \in \mathcal{O}_n$ be such that $Q^H(x_1 + x_2) = \alpha e_1^{(n)}$, where $\alpha \neq 0$. If we form

$$\tilde{M} = \begin{bmatrix} Q^H & 0 \\ 0 & Q^H \end{bmatrix} M \begin{bmatrix} Q & 0 \\ 0 & Q \end{bmatrix} = \begin{bmatrix} u_{11} & z_u^H & v_{11} & z_v^H \\ y_u & M_u & y_v & M_v \\ v_{11} & z_v^H & u_{11} & z_u^H \\ y_v & M_v & y_u & M_u \end{bmatrix},$$

where $u_{11}, v_{11} \in \mathbb{C}$ and $M_u, M_v \in \mathbb{C}^{(n-1)\times(n-1)}$, then we see that $e_1^{(2n)} + e_{n+1}^{(2n)}$ is an eigenvector of $\tilde{M}$ associated with the eigenvalue λ, i.e., we have

$$\begin{bmatrix} u_{11} & v_{11} \\ v_{11} & u_{11} \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \lambda \begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

The eigenvalues of $\begin{bmatrix} u_{11} & v_{11} \\ v_{11} & u_{11} \end{bmatrix}$ are $u_{11} \pm v_{11}$. Furthermore we have $y_u + y_v = 0$. Similarly, by Proposition 4 the vector $e_1^{(2n)} - e_{n+1}^{(2n)}$ is a left eigenvector of $\tilde{M}$ associated with the eigenvalue $\overline{\lambda}^{-1}$, so that $z_u^H - z_v^H = 0$ as well. Hence we obtain $\begin{bmatrix} M_u & M_v \\ M_v & M_u \end{bmatrix} \in \mathcal{O}_{n-1,n-1} \cap \mathcal{S}p_{2(n-1)}$ and $\begin{bmatrix} u_{11} & v_{11} \\ v_{11} & u_{11} \end{bmatrix} \in \mathcal{O}_{1,1} \cap \mathcal{S}p_2$. Since the latter matrix is symplectic, we have

$$(u_{ii} + v_{ii})\overline{(u_{ii} - v_{ii})} = 1.$$

If we consider

$$S := \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & I_{n-1} & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & I_{n-1} \end{bmatrix},$$

then we obtain

$$S^{-1}\tilde{M}S = \begin{bmatrix} 0 & z_u^H & v_{11} & z_v^H \\ 0 & M_u & y_v & M_v \\ 0 & 0 & 0 & 0 \\ 0 & M_v & y_u & M_u \end{bmatrix},$$

i.e., the spectrum of $\tilde{M}$ is equal to the union of the spectra of $\begin{bmatrix} u_{11} & v_{11} \\ v_{11} & u_{11} \end{bmatrix}$ and $\begin{bmatrix} M_u & M_v \\ M_v & M_v \end{bmatrix}$. The rest of the proof follows by induction.

The proof of ii) is analogous to the proof of i) noting that A is skew-Hermitian and that B is Hermitian. The proof of iii) follows from ii) and Proposition 5. □

The intersections of algebras with groups again does not give any particular structure, so it remains to discuss the final class which motivated our interest in analyzing multi-structured matrices. Matrices from the set

$$\mathcal{H}_{2n} \cap \mathcal{C}_{n,n} = \left\{ \begin{bmatrix} A & B \\ -B & -A \end{bmatrix} : A = A^H, B = B^H \right\} \tag{35}$$

arise in linear response theory in quantum chemistry [11, 12, 24]. By definition, similarity transformations with matrices from $\mathcal{O}_{n,n} \cap \mathcal{S}p_{2n}$ will preserve the structure. The elements of $\mathcal{H}_{2n}$ have the eigenvalue-symmetry '$\lambda, -\overline{\lambda}$' while we find the eigenvalue-symmetry '$\lambda, \overline{\lambda}$' for the matrices from $\mathcal{C}_{n,n}$. Therefore the eigenvalues of $M \in \mathcal{H}_{2n} \cap \mathcal{C}_{n,n}$ will occur in quadruples '$\lambda, -\lambda, \overline{\lambda}, -\overline{\lambda}$' unless λ is real or purely imaginary. So we expect 4×4-blocks to occur in Schur-like forms for these matrices. Before we formulate the main result let us state some properties of the matrices under consideration.

Proposition 14 *Let* $M = \begin{bmatrix} A & B \\ -B & -A \end{bmatrix} \in \mathcal{H}_{2n} \cap \mathcal{C}_{n,n}$, *let* $x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \neq 0$, *with* $x_1, x_2 \in \mathbb{C}^n$, *be an eigenvector of* M *associated with the eigenvalue* λ *of* M *and let* $y := \begin{bmatrix} x_2 \\ x_1 \end{bmatrix}$. *Then*

1. y *is an eigenvector of* M *associated with the eigenvalue* $-\lambda$.
2. $\begin{bmatrix} x_2^H & -x_1^H \end{bmatrix}$ *is a left eigenvector of* M *associated with the eigenvalue* $-\overline{\lambda}$.
3. *If* λ *is not purely imaginary, then* $x_2^H x_1 - x_1^H x_2 = 0$.
4. $M(x+y) = \lambda(x-y)$ *and* $M(x-y) = \lambda(x+y)$.
5. $\begin{bmatrix} ix_1 + x_2 \\ ix_2 + x_1 \end{bmatrix}$ *is an eigenvector of* $\begin{bmatrix} B & A \\ -A & -B \end{bmatrix}$ *associated with the eigenvalue* $i\lambda$.

Proof. 1., 2., 4. and *5.* are easy to verify. Furthermore we have by *2.* that

$$\lambda(x_2^H x_1 - x_1^H x_2) \;=\; \lambda \begin{bmatrix} x_2^H & -x_1^H \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$
\begin{aligned}
&= \begin{bmatrix} x_2^H & -x_1^H \end{bmatrix} \begin{bmatrix} A & B \\ -B & -A \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \\
&= -\overline{\lambda} \begin{bmatrix} x_2^H & -x_1^H \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \\
&= -\overline{\lambda}(x_2^H x_1 - x_1^H x_2),
\end{aligned}
$$

i.e., $(\lambda + \overline{\lambda})(x_2^H x_1 - x_1^H x_2) = 0$. □

Theorem 15

i) For each $M \in \mathcal{H}_{2n} \cap \mathcal{C}_{n,n}$, there exists $\hat{Q} \in \mathcal{S}p_{2n} \cap \mathcal{O}_{n,n}$ such that the matrix

$$
\hat{Q}^{-1} M \hat{Q} = \begin{bmatrix}
A_{11} & A_{12} & \cdots & A_{1k} & B_{11} & B_{12} & \cdots & B_{1k} \\
A_{21} & A_{22} & \cdots & A_{2k} & B_{21} & B_{22} & \cdots & B_{2k} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
A_{k1} & A_{k2} & \cdots & A_{kk} & B_{k1} & B_{k2} & \cdots & B_{kk} \\
-B_{11} & -B_{12} & \cdots & -B_{1k} & -A_{11} & -A_{12} & \cdots & -A_{1k} \\
-B_{21} & -B_{22} & \cdots & -B_{2k} & -A_{21} & -A_{22} & \cdots & -A_{2k} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
-B_{k1} & -B_{k2} & \cdots & -B_{kk} & -A_{k1} & -A_{k2} & \cdots & -A_{kk}
\end{bmatrix},
$$

with $A_{ij}, B_{ij} \in \mathbb{C}^{n_i \times n_j}$ and $n_i, n_j \in \{1, 2\}$, has the following properties:

1. *The eigenvalues of M are the eigenvalues of the matrix obtained by deleting all the off-diagonal blocks in $A = [A_{ij}]$ and $B = [B_{ij}]$.*
2. *If $n_i = 1$, then the eigenvalues of $\begin{bmatrix} A_{ii} & B_{ii} \\ -B_{ii} & -A_{ii} \end{bmatrix}$ are $\pm\sqrt{A_{ii}^2 - B_{ii}^2}$. In particular these eigenvalues are both real or both purely imaginary.*
3. *If $n_i = 2$, let m_a denote the $(1,2)$ element of A_{ii} and m_b denote the $(1,2)$ element of B_{ii}. Then the eigenvalues of $\begin{bmatrix} A_{ii} & B_{ii} \\ -B_{ii} & -A_{ii} \end{bmatrix}$ are either $m_a \pm m_b$ and $-m_a \pm m_b$, where m_a is real and m_b is purely imaginary, or $\pm i m_b$, where m_b is real.*

ii) Let $M \in \mathcal{SH}_{2n} \cap \mathcal{A}_{n,n} = \{\begin{bmatrix} A & B \\ -B & -A \end{bmatrix} : A = -A^H, B = -B^H\}$. Then there exists $\hat{Q} \in \mathcal{S}p_{2n} \cap \mathcal{O}_{n,n}$, such that the matrix

$$
\hat{Q}^{-1} M \hat{Q} = \begin{bmatrix}
A_{11} & A_{12} & \cdots & A_{1k} & B_{11} & B_{12} & \cdots & B_{1k} \\
A_{21} & A_{22} & \cdots & A_{2k} & B_{21} & B_{22} & \cdots & B_{2k} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
A_{k1} & A_{k2} & \cdots & A_{kk} & B_{k1} & B_{k2} & \cdots & B_{kk} \\
-B_{11} & -B_{12} & \cdots & -B_{1k} & -A_{11} & -A_{12} & \cdots & -A_{1k} \\
-B_{21} & -B_{22} & \cdots & -B_{2k} & -A_{21} & -A_{22} & \cdots & -A_{2k} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
-B_{k1} & -B_{k2} & \cdots & -B_{kk} & -A_{k1} & -A_{k2} & \cdots & -A_{kk}
\end{bmatrix},
$$

with $A_{ij}, B_{ij} \in \mathbb{C}^{n_i \times n_j}$ *and* $n_i, n_j \in \{1, 2\}$, *has the following properties:*

1. *The eigenvalues of* M *are the eigenvalues of the matrix obtained by deleting all the off-diagonal blocks in* $A = [A_{ij}]$ *and* $B = [B_{ij}]$.

2. *If* $n_i = 1$, *then the eigenvalues of* $\begin{bmatrix} A_{ii} & B_{ii} \\ -B_{ii} & -A_{ii} \end{bmatrix}$ *are* $A_{ii} \pm B_{ii}$. *In particular these eigenvalues are both purely imaginary or both real.*

3. *If* $n_i = 2$, *let* m_a *and* m_b *denote the* $(1, 2)$*-element of* A_{ii} *and* B_{ii}, *respectively. Then the eigenvalues of* $\begin{bmatrix} A_{ii} & B_{ii} \\ -B_{ii} & -A_{ii} \end{bmatrix}$ *are either* $m_a \pm m_b$ *and* $-m_a \pm m_b$, *where* m_a *is purely imaginary and* m_b *is real, or* $\pm m_b$, *where* m_b *is real.*

Proof. i) Let $M = \begin{bmatrix} A & B \\ -B & -A \end{bmatrix}$ with $A^H = A, B^H = B \in \mathbb{C}^{n \times n}$ and let $\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \neq 0$, with $x_1, x_2 \in \mathbb{C}^n$, be an eigenvector of M associated with the eigenvalue λ. We will use transformation matrices that are either of the form $\begin{bmatrix} Q & 0 \\ 0 & Q \end{bmatrix}$ with $Q \in \mathcal{O}_n$ or hyperbolic rotations $H_n(c, s)$ with $c, s \in \mathbb{R}$. We have to distinguish two cases:

1. x_1 and x_2 are linearly dependent. If we assume w.l.o.g. that $x_1 \neq 0$, then there exists $\gamma \in \mathbb{C}$ such that $x_2 = \gamma x_1$. (In the case $x_1 = 0$ we consider $\begin{bmatrix} x_2 \\ x_1 \end{bmatrix}$ and $-\lambda$, according to Proposition 14.1.)

   Let $e_i^{(n)}$ denote the i-th unit vector in $\mathbb{C}^n$, and choose a unitary matrix $Q \in \mathcal{O}_n$ such that $Q^H x_1 = \alpha e_1^{(n)}$, where $\alpha \neq 0$. Then we obtain

   $$Q^H x_2 = \gamma \alpha e_1^{(n)},$$

   and hence we have

   $$\tilde{M} = \begin{bmatrix} Q & 0 \\ 0 & Q \end{bmatrix}^H M \begin{bmatrix} Q & 0 \\ 0 & Q \end{bmatrix} = \begin{bmatrix} m_a & y_a^H & m_b & y_b^H \\ y_a & M_a & y_b & M_b \\ -m_b & -y_b^H & -m_a & -y_a^H \\ -y_b & -M_b & -y_a & -M_a \end{bmatrix}$$

   where $m_a, m_b \in \mathbb{C}$ and $M_a, M_b \in \mathbb{C}^{(n-1)\times(n-1)}$. Since $e_1^{(2n)} + \gamma e_{n+1}^{(2n)}$ is an eigenvector of $\tilde{M}$ associated with the eigenvalue λ, we have

   $$m_a(1 - \gamma^2) = (1 + \gamma^2)\lambda \quad \text{and} \quad (1 - \gamma^2) y_a = 0.$$

   (a) If $\gamma^2 = 1$, i.e., $\gamma = \pm 1$, then $\lambda = 0$ and

   $$m_a + \gamma m_b = 0 \ \text{ and } \ y_a + \gamma y_b = 0.$$

Hence, using

$$S := \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & I_{n-1} & 0 & 0 \\ \gamma & 0 & 1 & 0 \\ 0 & 0 & 0 & I_{n-1} \end{bmatrix}$$

we obtain

$$S^{-1}\tilde{M}S = \begin{bmatrix} 0 & y_a^H & m_b & y_b^H \\ 0 & M_a & y_b & M_b \\ 0 & 0 & 0 & 0 \\ 0 & -M_b & -y_a & -M_a \end{bmatrix},$$

i.e., the spectrum of $\tilde{M}$ is the union of the spectra of $\begin{bmatrix} m_a & m_b \\ -m_b & -m_a \end{bmatrix}$ and $\begin{bmatrix} M_a & M_b \\ -M_b & -M_a \end{bmatrix}$.

(b) If $\gamma^2 \neq 1$, then $\begin{bmatrix} 1 \\ \gamma \end{bmatrix}$ and $\begin{bmatrix} \gamma \\ 1 \end{bmatrix}$ are linearly independent and by Proposition 14.1 they are eigenvectors of $\begin{bmatrix} m_a & m_b \\ -m_b & -m_a \end{bmatrix}$ associated with the eigenvalues λ and $-\lambda$. Forming

$$S := \begin{bmatrix} 1 & 0 & \gamma & 0 \\ 0 & I_{n-1} & 0 & 0 \\ \gamma & 0 & 1 & 0 \\ 0 & 0 & 0 & I_{n-1} \end{bmatrix},$$

we obtain

$$S^{-1}\tilde{M}S = \begin{bmatrix} \lambda & * & 0 & * \\ 0 & M_a & 0 & M_b \\ 0 & * & -\lambda & * \\ 0 & -M_b & 0 & -M_a \end{bmatrix},$$

i.e., the spectrum of $\tilde{M}$ is the union of the spectra of $\begin{bmatrix} m_a & m_b \\ -m_b & -m_a \end{bmatrix}$ and $\begin{bmatrix} M_a & M_b \\ -M_b & -M_a \end{bmatrix}$. Since $\begin{bmatrix} m_a & m_b \\ -m_b & -m_a \end{bmatrix} \in \mathcal{H}_2 \cap \mathcal{C}_{1,1}$, we find by symmetry that λ must be real or purely imaginary.

2. If x_1 and x_2 are linearly independent, (i.e., in particular $n \geq 2$), then this also holds for $x_1 + \beta x_2$ and $x_1 - \beta x_2$, where $\beta \neq 0$.

(a) If λ is not purely imaginary then we have by Proposition 14.3. that $x_2^H x_1 - x_1^H x_2 = 0$. Therefore, $\beta = \sqrt{\frac{x_1^H x_1}{x_2^H x_2}} \in \mathbb{R}$ yields

$$(x_1 + \beta x_2)^H (x_1 - \beta x_2) = x_1^H x_1 - \beta^2 x_2^H x_2 + \beta(x_2^H x_1 - x_1^H x_2) = 0.$$

Consequently there exists $Q \in \mathcal{O}_n$ such that

$$Q^H(x_1 + \beta x_2) = \alpha_1 e_1^{(n)} \text{ and } Q^H(x_1 - \beta x_2) = \alpha_2 e_2^{(n)},$$

where α_1 and α_2 are positive and w.l.o.g. $\alpha_1 \geq \alpha_2$ (otherwise we exchange the first two columns of Q). Considering

$$\tilde{M} = \begin{bmatrix} Q & 0 \\ 0 & Q \end{bmatrix}^H M \begin{bmatrix} Q & 0 \\ 0 & Q \end{bmatrix} = \begin{bmatrix} m_a & * & m_b & * \\ * & M_a & * & M_b \\ -m_b & * & -m_a & * \\ * & -M_b & * & -M_a \end{bmatrix},$$

with $m_a, m_b \in \mathbb{C}^{2\times 2}$ and $M_a, M_b \in \mathbb{C}^{(n-2)\times(n-2)}$, we see that $\alpha_1 e_1 + \alpha_2 e_2 + \frac{\alpha_1}{\beta} e_{n+1} - \frac{\alpha_2}{\beta} e_{n+2}$ is an eigenvector of $\tilde{M}$ associated with the eigenvalue λ:

$$\begin{aligned} & \tilde{M}(\alpha_1 e_1 + \alpha_2 e_2 + \frac{\alpha_1}{\beta} e_{n+1} - \frac{\alpha_2}{\beta} e_{n+2}) \\ = & \begin{bmatrix} Q & 0 \\ 0 & Q \end{bmatrix}^H M \begin{bmatrix} x_1 + \beta x_2 + x_1 - \beta x_2 \\ \frac{1}{\beta} x_1 + x_2 - \frac{1}{\beta} x_1 + x_2 \end{bmatrix} \\ = & \begin{bmatrix} Q & 0 \\ 0 & Q \end{bmatrix}^H M \begin{bmatrix} 2x_1 \\ 2x_2 \end{bmatrix} \\ = & \lambda \begin{bmatrix} Q & 0 \\ 0 & Q \end{bmatrix}^H \begin{bmatrix} 2x_1 \\ 2x_2 \end{bmatrix} \\ = & \lambda(\alpha_1 e_1 + \alpha_2 e_2 + \frac{\alpha_1}{\beta} e_{n+1} - \frac{\alpha_2}{\beta} e_{n+2}). \end{aligned}$$

i. If $\beta \neq 1$, there are hyperbolic rotations $\begin{bmatrix} c_i & s_i \\ s_i & c_i \end{bmatrix}$, $i = 1, 2$, such that

$$\begin{bmatrix} c_1 & s_1 \\ s_1 & c_1 \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \frac{\alpha_1}{\beta} \end{bmatrix} = \begin{bmatrix} \tilde{\alpha}_1 \\ 0 \end{bmatrix} \text{ and } \begin{bmatrix} c_2 & s_2 \\ s_2 & c_2 \end{bmatrix} \begin{bmatrix} \alpha_2 \\ -\frac{\alpha_2}{\beta} \end{bmatrix} = \begin{bmatrix} \tilde{\alpha}_2 \\ 0 \end{bmatrix}.$$

Since $\alpha_1, \alpha_2, \beta \in \mathbb{R}$, we can choose c_i and s_i to be real. Transforming $\tilde{M}$ and the eigenvector associated with λ analogously, we have reduced the problem to the case 1.(b). In particular it follows that λ is real or purely imaginary.

ii. If $\beta = 1$, there exist no hyperbolic rotation as before. Then let $m_a := \begin{bmatrix} m_{a1} & m_{a2} \\ \overline{m}_{a2} & m_{a3} \end{bmatrix}$ and $m_b := \begin{bmatrix} m_{b1} & m_{b2} \\ \overline{m}_{b2} & m_{b3} \end{bmatrix}$. The relevant eigenvector is $e_1 + e_2 + e_{n+1} - e_{n+2}$, because $\beta = 1$ yields $\alpha_1 = \alpha_2$. Thus, using Proposition 14.4 we obtain:

$$\begin{bmatrix} m_{a1} & m_{a2} & m_{b1} & m_{b2} \\ \overline{m}_{a2} & m_{a3} & \overline{m}_{b2} & m_{b3} \\ -m_{b1} & -m_{b2} & -m_{a1} & -m_{a2} \\ -\overline{m}_{b2} & -m_{b3} & -\overline{m}_{a2} & -m_{a3} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \end{bmatrix} = \lambda \begin{bmatrix} 0 \\ 1 \\ 0 \\ -1 \end{bmatrix}$$

and

$$\begin{bmatrix} m_{a1} & m_{a2} & m_{b1} & m_{b2} \\ \overline{m}_{a2} & m_{a3} & \overline{m}_{b2} & m_{b3} \\ -m_{b1} & -m_{b2} & -m_{a1} & -m_{a2} \\ -\overline{m}_{b2} & -m_{b3} & -\overline{m}_{a2} & -m_{a3} \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \\ -1 \end{bmatrix} = \lambda \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \end{bmatrix}.$$

In particular we have $\overline{m_{a2} + m_{b2}} = \lambda$ and $m_{a2} - m_{b2} = \lambda$, i.e., m_{a2} is real and m_{b2} is purely imaginary. If $m_{a2}m_{b2} \neq 0$ it follows that λ is neither real nor purely imaginary, so the eigenvalues of $\begin{bmatrix} m_a & -m_b \\ m_b & -m_a \end{bmatrix}$ are $\lambda, -\lambda, \overline{\lambda}$ and $-\overline{\lambda}$. This also holds in the case that $m_{a2}m_{b2} = 0$, since the eigenvalues depend continuously on the entries of a matrix and, and replacing m_{a2} by $m_{a2} + \varepsilon_a$ and m_{b2} by $m_{b2} + i \cdot \varepsilon_b$, respectively, where $\varepsilon_a, \varepsilon_b \in \mathbb{R}$, does not change the eigenvector $\begin{bmatrix} 1 & 1 & 1 & -1 \end{bmatrix}^H$. Forming the unitary matrix

$$S := [s_1 \ \cdots \ s_{2_n}] = \frac{1}{2} \begin{bmatrix} 1 & 1 & 0 & 1 & -1 & 0 \\ 1 & 1 & 0 & -1 & 1 & 0 \\ 0 & 0 & I_{n-2} & 0 & 0 & 0 \\ 1 & -1 & 0 & 1 & 1 & 0 \\ -1 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & I_{n-2} \end{bmatrix}$$

and noting that according to Proposition 14 1. the columns s_1 and s_{n+1} are right eigenvectors of $\tilde{M}$ associated with the eigenvalues λ resp. $-\lambda$ and according to Proposition 14 2. the columns s_2 and s_{n+2} are left eigenvectors of $\tilde{M}$ associated with the eigenvalues $-\overline{\lambda}$ and $\overline{\lambda}$, we obtain

$$S^{-1}\tilde{M}S = \begin{bmatrix} \lambda & * & * & * & 0 & * & * & * \\ 0 & -\overline{\lambda} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & * & \multicolumn{2}{c}{\multirow{2}{*}{M_a}} & 0 & * & \multicolumn{2}{c}{\multirow{2}{*}{M_b}} \\ 0 & * & \multicolumn{2}{c}{} & 0 & * & \multicolumn{2}{c}{} \\ 0 & * & * & * & -\lambda & * & * & * \\ 0 & 0 & 0 & 0 & 0 & \overline{\lambda} & 0 & 0 \\ 0 & * & \multicolumn{2}{c}{\multirow{2}{*}{$-M_b$}} & 0 & * & \multicolumn{2}{c}{\multirow{2}{*}{$-M_a$}} \\ 0 & * & \multicolumn{2}{c}{} & 0 & * & \multicolumn{2}{c}{} \end{bmatrix},$$

i.e., the spectrum of $\tilde{M}$ is the union of the spectra of the 4×4 matrix $\begin{bmatrix} m_a & m_b \\ -m_b & m_a \end{bmatrix}$ and $\begin{bmatrix} M_a & M_b \\ -M_a & -M_b \end{bmatrix}$.

(b) If $\lambda = -i\mu$ is purely imaginary, then it follows from Proposition 14 5. that $\begin{bmatrix} ix_1 + x_2 \\ ix_2 + x_1 \end{bmatrix}$ is an eigenvector of $\begin{bmatrix} B & A \\ -A & -B \end{bmatrix}$ associated with the eigenvalue μ. Transforming this matrix as in the case 2.(a), yields analogous results for M,

since we have for all transformations $\begin{bmatrix} U & V \\ V & U \end{bmatrix} \in \mathcal{O}_{n,n} \cap \mathcal{S}p_{2n}$ that

$$\begin{bmatrix} U & V \\ V & U \end{bmatrix} \begin{bmatrix} A & B \\ -B & -A \end{bmatrix} \begin{bmatrix} U^H & -V^H \\ -V^H & U^H \end{bmatrix} = \begin{bmatrix} S & -T \\ T & S \end{bmatrix}$$
$$\Leftrightarrow \begin{bmatrix} U & V \\ V & U \end{bmatrix} \begin{bmatrix} B & A \\ -A & -B \end{bmatrix} \begin{bmatrix} U^H & -V^H \\ -V^H & U^H \end{bmatrix} = \begin{bmatrix} T & -S \\ S & T \end{bmatrix}.$$

Note that the element m_b in the case 2.(a) is now real.

In all cases we have $\begin{bmatrix} M_a & M_b \\ -M_b & -M_a \end{bmatrix} \in \mathcal{H}_{2k} \cap \mathcal{C}_{k,k}$ with $k = n-1$ or $k = n-2$. So the proof follows by induction.

The proof for ii) follows directly from Proposition 5. □

Remark 16 In general the remaining 4×4-blocks in Theorem 15 cannot be divided further into two 2×2-blocks. This is possible only if the eigenvalues are real or purely imaginary.

Remark 17 As we see from the proof of Theorem 15, the only time we need hyperbolic rotations is when we want to split certain 4×4-blocks into two 2×2-blocks. That means that we are able to achieve a Schur-like form whose eigenvalues are displayed by at most 4×4-blocks by using only unitary transformations. This result does not hold in the real case.

6 Conclusions

We have discussed Schur-like forms for matrices with one or more algebraic structures arising from a classical Lie group, Lie algebra or Jordan algebra. In all cases we obtain a structured Schur-like form that displays all the eigenvalues. In particular, we have obtained such Schur-like forms for multi-structured matrices which arise in quantum chemistry.

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