## 1. Properties of antisymmetric matrices

Let M be a complex  $d \times d$  antisymmetric matrix, i.e.  $M^{\mathsf{T}} = -M$ . Since

$$\det M = \det (-M^{\mathsf{T}}) = \det (-M) = (-1)^d \det M, \tag{1}$$

it follows that det M=0 if d is odd. Thus, the rank of M must be even. In these notes, the rank of M will be denoted by 2n. If  $d\equiv 2n$  then det  $M\neq 0$ , whereas if d>2n, then det M=0. All the results contained in these notes also apply to real antisymmetric matrices unless otherwise noted.

Two theorems concerning antisymmetric matrices are particularly useful.

**Theorem 1:** If M is an even-dimensional complex [or real] non-singular  $2n \times 2n$  antisymmetric matrix, then there exists a unitary [or real orthogonal]  $2n \times 2n$  matrix U such that:

$$U^{\mathsf{T}}MU = N \equiv \operatorname{diag}\left\{ \begin{pmatrix} 0 & m_1 \\ -m_1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & m_2 \\ -m_2 & 0 \end{pmatrix}, \cdots, \begin{pmatrix} 0 & m_n \\ -m_n & 0 \end{pmatrix} \right\},$$
 (2)

where N is written in block diagonal form with  $2 \times 2$  matrices appearing along the diagonal, and the  $m_j$  are real and positive. Moreover,  $\det U = e^{-i\theta}$ , where  $-\pi < \theta \le \pi$ , is uniquely determined. N is called the *real normal form* of a non-singular antisymmetric matrix [1-3].

If M is a complex [or real] singular antisymmetric  $d \times d$  matrix of rank 2n (where d is either even or odd and d > 2n), then there exists a unitary [or real orthogonal]  $d \times d$  matrix U such that

$$U^{\mathsf{T}}MU = N \equiv \operatorname{diag}\left\{ \begin{pmatrix} 0 & m_1 \\ -m_1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & m_2 \\ -m_2 & 0 \end{pmatrix}, \cdots, \begin{pmatrix} 0 & m_n \\ -m_n & 0 \end{pmatrix}, \mathbb{O}_{d-2n} \right\}, (3)$$

where N is written in block diagonal form with  $2 \times 2$  matrices appearing along the diagonal followed by an  $(d-2n) \times (d-2n)$  block of zeros (denoted by  $\mathbb{O}_{d-2n}$ ), and the  $m_j$  are real and positive. N is called the *real normal form* of an antisymmetric matrix [1–3]. Note that if d=2n, then eq. (3) reduces to eq. (2).

**Proof:** Details of the proof of this theorem are given in Appendices A and B.

**Theorem 2:** If M is an even-dimensional complex non-singular  $2n \times 2n$  antisymmetric matrix, then there exists a non-singular  $2n \times 2n$  matrix P such that:

$$M = P^{\mathsf{T}}JP\,, (4)$$

where the  $2n \times 2n$  matrix J written in  $2 \times 2$  block form is given by:

$$J \equiv \operatorname{diag} \left\{ \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \cdots, \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \right\}. \tag{5}$$

If M is a complex singular antisymmetric  $d \times d$  matrix of rank 2n (where d is either even or odd and d > 2n), then there exists a non-singular  $d \times d$  matrix P such that

$$M = P^{\mathsf{T}} \widetilde{J} P \,, \tag{6}$$

and  $\widetilde{J}$  is the  $d \times d$  matrix that is given in block form by

$$\widetilde{J} \equiv \begin{pmatrix} J & 0 \\ -- & -- \\ 0 & 0 \end{pmatrix},$$
(7)

where the  $2n \times 2n$  matrix J is defined in eq. (5) and O is a zero matrix of the appropriate number of rows and columns. Note that if d = 2n, then eq. (6) reduces to eq. (4).

**Proof:** The proof makes use of Theorem 1.<sup>1</sup> Simply note that for any non-singular matrix  $A_i$  with det  $A_i = m_i^{-1}$ , we have

$$A_i^{\mathsf{T}} \begin{pmatrix} 0 & m_i \\ -m_i & 0 \end{pmatrix} A_i = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} . \tag{8}$$

Define the  $d \times d$  matrix A (where d > 2n) such that

$$A = \operatorname{diag}\{A_1, A_2, \cdots, A_n, \mathbb{O}_{d-2n}\},$$
 (9)

where A is written in block diagonal form with  $2 \times 2$  matrices appearing along the diagonal followed by a  $(d-2n) \times (d-2n)$  block of zeros (denoted by  $\mathbb{O}_{d-2n}$ ). Then, in light of eqs. (3), (8) and (9), it follows that eq. (6) is established with P = UA. In the case of d = 2n, where  $\mathbb{O}_{d-2n}$  is absent in eq. (9), it follows that eq. (4) is established by the same analysis.

<u>REMARK:</u> Two matrices M and B are said to be congruent (e.g., see Refs. [4–6]) if there exists a non-singular matrix P such that

$$B = P^{\mathsf{T}} M P$$
.

Note that if M is an antisymmetric matrix, then so is B. A congruence class of M consists of the set of all matrices congruent to it. The structure of the congruence classes of antisymmetric matrices is completely determined by Theorem 2. Namely, eqs. (4) and (6) imply that all complex  $d \times d$  antisymmetric matrices of rank 2n (where  $n \leq \frac{1}{2}d$ ) belong to the same congruent class, which is uniquely specified by d and n.

<sup>&</sup>lt;sup>1</sup>One can also prove Theorem 2 directly without resorting to Theorem 1. For completeness, I provide a second proof of Theorem 2 in Appendix C.

## 2. The pfaffian and its properties

For any even-dimensional complex  $2n \times 2n$  antisymmetric matrix M, we define the *pfaffian* of M, denoted by pf M, as

$$pf M = \frac{1}{2^n n!} \epsilon_{i_1 j_1 i_2 j_2 \cdots i_n j_n} M_{i_1 j_1} M_{i_2 j_2} \cdots M_{i_n j_n}, \qquad (10)$$

where  $\epsilon$  is the rank-2n Levi-Civita tensor, and the sum over repeated indices is implied. One can rewrite eq. (10) by restricting the sum over indices in such a way that removes the combinatoric factor  $2^n n!$  in the denominator. Let P be the set of permutations,  $\{i_1, i_2, \ldots, i_{2n}\}$  with respect to  $\{1, 2, \ldots, 2n\}$ , such that [7, 8]:

$$i_1 < j_1, i_2 < j_2, \dots, i_{2n} < j_{2n}, \text{ and } i_1 < i_2 < \dots < i_{2n}.$$
 (11)

Then,

$$pf M = \sum_{P}' (-1)^{P} M_{i_1 j_1} M_{i_2 j_2} \cdots M_{i_n j_n}, \qquad (12)$$

where  $(-1)^P = 1$  for even permutations and  $(-1)^P = -1$  for odd permutations. The prime on the sum in eq. (12) has been employed to remind the reader that the set of permutations P is restricted according to eq. (11). Note that if M can be written in block diagonal form as  $M \equiv M_1 \oplus M_2 = \operatorname{diag}(M_1, M_2)$ , then

$$Pf(M_1 \oplus M_2) = (Pf M_1)(Pf M_2).$$

Finally, if M is an odd-dimensional complex antisymmetric matrix, the corresponding pfaffian is defined to be zero.

The pfaffian and determinant of an antisymmetric matrix are closely related, as we shall demonstrate in Theorems 3 and 4 below. For more details on the properties of the pfaffian, see e.g. Ref. [7–9].

**Theorem 3:** Given an arbitrary  $2n \times 2n$  complex matrix B and complex antisymmetric  $2n \times 2n$  matrix M, the following identity is satisfied,

$$pf(BMB^{\mathsf{T}}) = pf M \det B. \tag{13}$$

**Proof:** Using eq. (10),

$$pf(BMB^{\mathsf{T}}) = \frac{1}{2^{n}n!} \epsilon_{i_{1}j_{1}i_{2}j_{2}\cdots i_{n}j_{n}} (B_{i_{1}k_{1}}M_{k_{1}\ell_{1}}B_{j_{1}\ell_{1}}) (B_{i_{2}k_{2}}M_{k_{2}\ell_{2}}B_{j_{2}\ell_{2}}) \cdots (B_{i_{n}k_{n}}M_{k_{n}\ell_{n}}B_{j_{n}\ell_{n}})$$

$$= \frac{1}{2^{n}n!} \epsilon_{i_{1}j_{1}i_{2}j_{2}\cdots i_{n}j_{n}} B_{i_{1}k_{1}}B_{j_{1}\ell_{1}}B_{i_{2}k_{2}}B_{j_{2}\ell_{2}} \cdots B_{i_{n}k_{n}}B_{j_{n}\ell_{n}}M_{k_{1}\ell_{1}}M_{k_{2}\ell_{2}} \cdots M_{k_{n}\ell_{n}},$$

after rearranging the order of the matrix elements of M and B. We recognize the definition of the determinant of a  $2n \times 2n$ -dimensional matrix,

$$\det B \, \epsilon_{k_1 \ell_1 k_2 \ell_2 \cdots k_n \ell_n} = \epsilon_{i_1 j_1 i_2 j_2 \cdots i_n j_n} B_{i_1 k_1} B_{j_1 \ell_1} B_{i_2 k_2} B_{j_2 \ell_2} \cdots B_{i_n k_n} B_{j_n \ell_n} \,. \tag{14}$$

Inserting eq. (14) into the expression for pf  $(BAB^{\mathsf{T}})$  yields

$$pf(BMB^{\mathsf{T}}) = \frac{1}{2^{n} n!} \det B \, \epsilon_{k_{1} \ell_{1} k_{2} \ell_{2} \cdots k_{n} \ell_{n}} M_{k_{1} \ell_{1}} M_{k_{2} \ell_{2}} \cdots M_{k_{n} \ell_{n}} = pf M \det B.$$

and Theorem 3 is proved. Note that the above proof applies to both the cases of singular and non-singular M and/or B.

Here is a nice application of Theorem 3. Consider the following  $2n \times 2n$  complex antisymmetric matrix written in block form,

$$M \equiv \begin{pmatrix} 0 & A \\ --- & --- \\ -A^{\mathsf{T}} & 0 \end{pmatrix}, \tag{15}$$

where A is an  $n \times n$  complex matrix and O is the  $n \times n$  zero matrix. Then,

Pf 
$$M = (-1)^{n(n-1)/2} \det A$$
. (16)

To prove eq. (16), we write M defined by eq. (15) as [9]

$$M \equiv \begin{pmatrix} 0 & A \\ -------- \\ -A^{\mathsf{T}} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ ------- \\ A^{\mathsf{T}} & 0 \end{pmatrix} \begin{pmatrix} 0 & -1 \\ ------ \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & A \\ ----- \\ 1 & 0 \end{pmatrix}, \quad (17)$$

where  $\mathbb{1}$  is the  $n \times n$  identity matrix. Using eq. (17), Pf M is easily evaluated by employing Theorem 3 and explicitly evaluating the corresponding determinant and pfaffian.

**Theorem 4:** If M is a complex antisymmetric matrix, then

$$\det M = [\operatorname{pf} M]^2. \tag{18}$$

**Proof:** First, we assume that M is a non-singular complex  $2n \times 2n$  antisymmetric matrix. Using Theorem 3, we square both sides of eq. (13) to obtain

$$[pf(BMB^{\mathsf{T}})]^2 = (pf M)^2 (\det B)^2.$$
 (19)

Using the well known properties of determinants, it follows that

$$\det(BMB^{\mathsf{T}}) = (\det M)(\det B)^{2}. \tag{20}$$

By assumption, M is non-singular, so that  $\det M \neq 0$ . If B is a non-singular matrix, then we may divide eqs. (19) and (20) to obtain

$$\frac{(\operatorname{pf} M)^2}{\det M} = \frac{\left[\operatorname{pf}(BMB^{\mathsf{T}})\right]^2}{\det(BMB^{\mathsf{T}})}.$$
 (21)

Since eq. (21) is true for any non-singular matrix B, the strategy that we shall employ is to choose a matrix B that allows us to trivially evaluate the right hand side of eq. (21).

Motivated by Theorem 2, we choose  $B = P^{\mathsf{T}}$ , where the matrix P is determined by eq. (4). It follows that

$$\frac{(\operatorname{pf} M)^2}{\det M} = \frac{\operatorname{pf} J}{\det J},\tag{22}$$

where J is given by eq. (5). Then, by direct computation using the definitions of the pfaffian [cf. eq. (12)] and the determinant,

$$pf J = \det J = 1$$

Hence, eq. (22) immediately yields eq. (18). In the case where M is singular, det M = 0. For d even, we note that Pf  $\widetilde{J} = 0$  by direct computation. Hence, eq. (13) yields

$$Pf M = Pf(P^{\mathsf{T}}\widetilde{J}P) = (\det P)^{2} Pf \widetilde{J} = 0.$$

For d odd, Pf M=0 by definition. Thus, eq. (18) holds for both non-singular and singular complex antisymmetric matrices M. The proof is complete.

# 3. An alternative proof of det $M = [\operatorname{pf} M]^2$

In Section 2, a proof of eq. (18) was obtained by employing a particularly convenient choice for B in eq. (21). Another useful choice for B is motivated by Theorem 1. In particular, we shall choose  $B = U^{\mathsf{T}}$ , where U is the unitary matrix that yields the real normal form of M [cf. eq. (2)], i.e.  $N = U^{\mathsf{T}}MU$ . Then, eq. (21) can be written as

$$\frac{(\operatorname{pf} M)^2}{\det M} = \frac{(\operatorname{pf} N)^2}{\det N} \,. \tag{23}$$

The right hand side of eq. (21) can now directly computed using the definitions of the pfaffian [cf. eq. (12)] and the determinant. We find

$$pf N = m_1 m_2 \cdots m_n, \qquad (24)$$

$$\det N = m_1^2 m_2^2 \cdots m_n^2 \,. \tag{25}$$

Inserting these results into eq. (23) yields

$$\det M = [\operatorname{pf} M]^2, \tag{26}$$

which completes this proof of Theorem 4 for non-singular antisymmetric matrices M.

If M is a singular complex antisymmetric  $2n \times 2n$  matrix, then  $\det M = 0$  and at least one of the  $m_i$  appearing in eq. (2) is zero [cf. eq. (3)]. Thus, eq. (24) implies that pf N = 0. We can then use eqs. (2) and (13) to conclude that

$$\operatorname{pf} M = \operatorname{pf}(U^*NU^{\dagger}) = \operatorname{pf} N \det U^* = 0.$$

Finally, if M is a  $d \times d$  matrix where d is odd, then  $\det M = 0$  [cf. eq. (1)] and pf M = 0 by definition. In both singular cases, we have  $\det M = [\operatorname{pf} M]^2 = 0$ , and eq. (26) is still satisfied. Thus, Theorem 4 is established for both non-singular and singular antisymmetric matrices.

Many textbooks use eq. (26) and then assert incorrectly that

$$pf M = \sqrt{\det M}. WRONG!$$

The correct statement is

$$pf M = \pm \sqrt{\det M}, \qquad (27)$$

where the sign is determined by establishing the correct branch of the square root. To accomplish this, we first note that the determinant of a unitary matrix is a pure phase. It is convenient to write

$$\det U \equiv e^{-i\theta}$$
, where  $-\pi < \theta \le \pi$ . (28)

In light of eqs. (24) and (25), we see that eqs. (2) and (13) yield

$$m_1 m_2 \cdots m_n = \operatorname{pf} N = \operatorname{pf}(U^\mathsf{T} M U) = \operatorname{pf} M \det U = e^{-i\theta} \operatorname{pf} M,$$
 (29)

$$m_1^2 m_2^2 \cdots m_n^2 = \det N = \det(U^{\mathsf{T}} M U) = (\det U)^2 \det M = e^{-2i\theta} \det M.$$
 (30)

Then, eqs. (29) and (30) yield eq. (26) as expected. In addition, since Theorem 1 states that the  $m_i$  are all real and non-negative, we also learn that

$$\det M = e^{2i\theta} |\det M|, \qquad \text{pf } M = e^{i\theta} |\det M|^{1/2}.$$
 (31)

We shall employ a convention in which the principal value of the argument of a complex number z, denoted by  $\operatorname{Arg} z$ , lies in the range  $-\pi < \operatorname{Arg} z \le \pi$ . Since the range of  $\theta$  is specified in eq. (28), it follows that  $\theta = \operatorname{Arg}(\operatorname{pf} M)$  and

$$\operatorname{Arg}(\det M) = \begin{cases} 2\theta , & \text{if } -\frac{1}{2}\pi < \theta \le \frac{1}{2}\pi ,\\ 2\theta - \pi , & \text{if } \frac{1}{2}\pi < \theta \le \pi ,\\ 2\theta + \pi , & \text{if } -\pi < \theta \le -\frac{1}{2}\pi . \end{cases}$$

Likewise, given a complex number z, we define the principal value of the complex square root by  $\sqrt{z} \equiv |z|^{1/2} \exp\left(\frac{1}{2}i \operatorname{Arg} z\right)$ . This means that the principal value of the complex square root of det M is given by

$$\sqrt{\det M} = \begin{cases} e^{i\theta} |\det M|^{1/2} & \text{if } -\frac{1}{2}\pi < \theta \le \frac{1}{2}\pi, \\ -e^{i\theta} |\det M|^{1/2} & \text{if } -\frac{1}{2}\pi < \theta \le \pi \text{ or } -\pi < \theta \le -\frac{1}{2}\pi, \end{cases}$$

corresponding to the two branches of the complex square root function. Using this result in eq. (31) yields

$$\operatorname{pf} M = \begin{cases} \sqrt{\det M}, & \text{if } -\frac{1}{2}\pi < \theta \leq \frac{1}{2}\pi, \\ -\sqrt{\det M}, & \text{if } -\pi \leq \theta \leq -\frac{1}{2}\pi & \text{or } \frac{1}{2}\pi < \theta \leq \pi, \end{cases}$$
(32)

which is the more precise version of eq. (27).

As a very simple example, consider a complex antisymmetric  $2 \times 2$  matrix M with nonzero matrix elements  $M_{12} = -M_{21}$ . Hence, pf  $M = M_{12}$  and det  $M = (M_{12})^2$ . Thus if  $M_{12} = |M_{12}|e^{i\theta}$  where  $-\pi < \theta \le \pi$ , then one must choose the plus sign in eq. (27) if  $-\frac{1}{2}\pi < \theta \le \frac{1}{2}\pi$ ; otherwise, one must choose the minus sign. This conforms with the result of eq. (32). Note that if  $M_{12} = -1$  then pf M = -1 and det M = 1, corresponding to the negative sign in eq. (27). More generally, to determine the proper choice of sign in eq. (27), we can employ eq. (32), where  $\theta = \text{Arg}(\text{pf }M)$ . In particular,  $\theta$  can be determined either by an explicit calculation of pf M as illustrated in our simple example above, or by determining the real normal form of M and then extracting  $\theta$  from the phase of det U according to eq. (28).

## 4. The group of symplectic matrices

Consider the following set of matrices [4],

$$L_{2n}(M) = \left\{ S \mid S^{\mathsf{T}} M S = M \right\}, \tag{33}$$

where M is a fixed complex [or real] non-singular  $2n \times 2n$  antisymmetric matrix. It is easy to check that  $L_{2n}(M)$  satisfies the axioms of a group. First, taking the determinant of  $S^TMS = M$  yields det  $S = \pm 1$ , which implies that S is non-singular. Next, we note that  $S^TMS = M$  implies that  $(S^{-1})^TMS^{-1} = M$ , so that  $S^{-1} \in L_{2n}(M)$ . The  $2n \times 2n$  identity matrix  $\mathbb{1}_{2n} \in L_{2n}(M)$ . Finally,  $S_1^TMS_1 = M$  and  $(S_2^{-1})^TMS_2^{-1} = M$  yield

$$S_1^T M S_1 = (S_2^{-1})^T M S_2^{-1} \implies (S_1 S_2)^T M S_1 S_2 = M,$$

which means that  $S_1, S_2 \in L_{2n}(M)$  imply that  $S_1S_2 \in L_{2n}(M)$ .

We now make use of eq. (4) to write  $M = P^{\mathsf{T}}JP$ , where J is the antisymmetric  $2n \times 2n$  matrix given by eq. (5). It then follows that

$$L_{2n}(P^{\mathsf{T}}JP) = \{ S \mid (PSP^{-1})^{\mathsf{T}}J(PSP^{-1}) = J \}.$$
 (34)

Let us compare that with  $L_{2n}(J)$ , obtained by choosing M = J in eq. (33). To avoid confusion, we relabel S as T and write:

$$L_{2n}(J) = \left\{ T \mid T^{\mathsf{T}}JT = J \right\}.$$

Multiplying all the matrices that appear in  $L_{2n}(J)$  on the left by  $P^{-1}$  and on the right by P yields

$$P^{-1}L_{2n}(J)P = \{P^{-1}TP \mid T^{\mathsf{T}}JT = J\}.$$

If we now define  $T = PSP^{-1}$ , then it follows that

$$P^{-1}L_{2n}(J)P = \{ S \mid (PSP^{-1})^{\mathsf{T}}J(PSP^{-1}) = J \}.$$

Comparing with eq. (34), we conclude that

$$P^{-1}L_{2n}(J)P = L_{2n}(P^{\mathsf{T}}JP) = L_{2n}(M). \tag{35}$$

The meaning of eq. (35) is as follows. The matrix groups  $L_{2n}(M)$  and  $L_{2n}(J)$  are isomorphic, in light of the one-to-one and onto mapping,  $S \to PSP^{-1}$ . Equivalently, given the matrix group  $L_{2n}(J)$ , we can regard the set of matrices defined by  $L_{2n}(J)$  as the defining representation of this group. Then, the set of matrices defined by  $L_{2n}(M)$  provide an equivalent representation of this matrix group, for any non-singular antisymmetric matrix M.

A complex  $2n \times 2n$  matrix S is called *symplectic* if  $S^T \mathcal{J} S = \mathcal{J}$ , where  $S^T$  is the transpose of S and

$$\mathcal{J} \equiv \begin{pmatrix} \mathbb{O}_n & \mathbb{1}_n \\ -\mathbb{1}_n & \mathbb{O}_n \end{pmatrix}, \tag{36}$$

where  $\mathbb{1}_n$  is the  $n \times n$  identity matrix and  $\mathbb{O}_n$  is the  $n \times n$  zero matrix. That is,

$$\operatorname{Sp}(n,\mathbb{C}) = \{ S \in \operatorname{GL}(2n,\mathbb{C}) \mid S^{\mathsf{T}} \mathcal{J} S = \mathcal{J} \}.$$

We see that  $\operatorname{Sp}(n,\mathbb{C}) = L_{2n}(\mathcal{J})$ . From the analysis above, it follows that for any non-singular, antisymmetric  $2n \times 2n$  matrix M, the matrix group  $L_{2n}(M)$  is isomorphic to  $\operatorname{Sp}(n,\mathbb{C})$  [4].

As previously noted, taking the determinant of  $S^TMS = M$  implies that det  $S = \pm 1$ . However, we can prove that det S = 1 by making use of the pfaffian. Using eq. (13),

$$\operatorname{pf}(S^{\mathsf{T}}MS) = \operatorname{pf} M \det S$$
,

for any non-singular antisymmetric matrix M. Using the fact that the elements of  $L_{2n}(M)$  satisfy  $S^{\mathsf{T}}MS = M$ , it follows that

$$pf M = pf M \det S, (37)$$

By assumption, M is non-singular so that  $\det M \neq 0$ . It follows from eq. (18) that pf  $M \neq 0$ . Thus, we can divide both sides of eq. (37) by pf M to conclude that [10]

$$\det S = 1. (38)$$

Thus, we have proven that all the elements of  $L_{2n}(M)$  are matrices of unit determinant, for any non-singular antisymmetric matrix M. In particular, the determinant of any complex [or real] symplectic matrix is equal to 1.

#### APPENDIX A: Singular values and singular vectors of a complex matrix

The material in this appendix is taken from Ref. [11] and provides some background for the proof of Theorem 1 presented in Appendix B. The presentation is inspired by the treatment of the singular value decomposition of a complex matrix in Refs. [12,13].

The singular values of the general complex  $n \times n$  matrix M are defined to be the real non-negative square roots of the eigenvalues of  $M^{\dagger}M$  (or equivalently of  $MM^{\dagger}$ ). An equivalent definition of the singular values can be established as follows. Since  $M^{\dagger}M$  is an hermitian non-negative matrix, its eigenvalues are real and non-negative

and its eigenvectors,  $v_k$ , defined by  $M^{\dagger}Mv_k = m_k^2 v_k$ , can be chosen to be orthonormal.<sup>2</sup> Consider first the eigenvectors corresponding to the non-zero eigenvalues of  $M^{\dagger}M$ . Then, we define the vectors  $w_k$  such that  $Mv_k = m_k w_k^*$ . It follows that

$$m_k^2 v_k = M^{\dagger} M v_k = m_k M^{\dagger} w_k^* \implies M^{\dagger} w_k^* = m_k v_k .$$
 (39)

Note that eq. (39) also implies that  $MM^{\dagger}w_k^* = m_k^2w_k^*$ . The orthonormality of the  $v_k$  implies the orthonormality of the  $w_k$ , and vice versa. For example,

$$\delta_{jk} = \langle v_j | v_k \rangle = \frac{1}{m_j m_k} \langle M^{\dagger} w_j^* | M^{\dagger} w_k^* \rangle = \frac{1}{m_j m_k} \langle w_j | M M^{\dagger} w_k^* \rangle = \frac{m_k}{m_j} \langle w_j^* | w_k^* \rangle , \qquad (40)$$

which yields  $\langle w_k | w_j \rangle = \delta_{jk}$ . If M is a real matrix, then the eigenvectors  $v_k$  can be chosen to be real, in which case the corresponding  $w_k$  are also real.

If  $v_i$  is an eigenvector of  $M^{\dagger}M$  with zero eigenvalue, then

$$0 = v_i^{\dagger} M^{\dagger} M v_i = \langle M v_i | M v_i \rangle,$$

which implies that  $Mv_i=0$ . Likewise, if  $w_i^*$  is an eigenvector of  $MM^{\dagger}$  with zero eigenvalue, then

$$0 = w_i^\mathsf{T} M M^\dagger w_i^* = \langle M^\mathsf{T} w_i | M^\mathsf{T} w_i \rangle^*,$$

which implies that  $M^{\mathsf{T}}w_i = 0$ .

Because the eigenvectors of  $M^{\dagger}M$   $[MM^{\dagger}]$  can be chosen orthonormal, the eigenvectors corresponding to the zero eigenvalues of M  $[M^{\dagger}]$  can be taken to be orthonormal.<sup>3</sup> Finally, these eigenvectors are also orthogonal to the eigenvectors corresponding to the non-zero eigenvalues of  $M^{\dagger}M$   $[MM^{\dagger}]$ . That is, if the indices i and j run over the eigenvectors corresponding to the zero and non-zero eigenvalues of  $M^{\dagger}M$   $[MM^{\dagger}]$ , respectively, then

$$\langle v_j | v_i \rangle = \frac{1}{m_j} \langle M^{\dagger} w_j^* | v_i \rangle = \frac{1}{m_j} \langle w_j^* | M v_i \rangle = 0, \qquad (41)$$

and similarly  $\langle w_j | w_i \rangle = 0$ .

Thus, we can define the singular values of a general complex  $n \times n$  matrix M to be the simultaneous solutions (with real non-negative  $m_k$ ) of:<sup>4</sup>

$$Mv_k = m_k w_k^*, w_k^{\mathsf{T}} M = m_k v_k^{\dagger}. (42)$$

The corresponding  $v_k$  ( $w_k$ ), normalized to have unit norm, are called the right (left) singular vectors of M. In particular, the number of linearly independent  $v_k$  coincides with the number of linearly independent  $w_k$  and is equal to n.

<sup>&</sup>lt;sup>2</sup>We define the inner product of two vectors to be  $\langle v|w\rangle \equiv v^{\dagger}w$ . Then, v and w are orthonormal if  $\langle v|w\rangle = 0$ . The norm of a vector is defined by  $||v|| = \langle v|v\rangle^{1/2}$ .

<sup>&</sup>lt;sup>3</sup>This analysis shows that the number of linearly independent zero eigenvectors of  $M^{\dagger}M$  [ $MM^{\dagger}$ ] with zero eigenvalue, coincides with the number of linearly independent eigenvectors of M [ $M^{\dagger}$ ] with zero eigenvalue.

<sup>&</sup>lt;sup>4</sup>One can always find a solution to eq. (42) such that the  $m_k$  are real and non-negative. Given a solution where  $m_k$  is complex, we simply write  $m_k = |m_k|e^{i\theta}$  and redefine  $w_k \to w_k e^{i\theta}$  to remove the phase  $\theta$ .

#### APPENDIX B: Proof of Theorem 1

In this appendix, we provide a proof of Theorem 1.

**Theorem 1:** If M is an even-dimensional complex [or real] non-singular  $2n \times 2n$  antisymmetric matrix, then there exists a unitary [or real orthogonal]  $2n \times 2n$  matrix U such that:

$$U^{\mathsf{T}}MU = N \equiv \operatorname{diag}\left\{ \begin{pmatrix} 0 & m_1 \\ -m_1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & m_2 \\ -m_2 & 0 \end{pmatrix}, \cdots, \begin{pmatrix} 0 & m_n \\ -m_n & 0 \end{pmatrix} \right\}, \tag{43}$$

where N is written in block diagonal form with  $2 \times 2$  matrices appearing along the diagonal, and the  $m_j$  are real and positive. Moreover,  $\det U = e^{-i\theta}$ , where  $-\pi < \theta \le \pi$ , is uniquely determined.

If M is a complex [or real] singular antisymmetric  $d \times d$  matrix of rank 2n (where d is either even or odd and d > 2n), then there exists a unitary [or real orthogonal]  $d \times d$  matrix U such that

$$U^{\mathsf{T}}MU = N \equiv \operatorname{diag} \left\{ \begin{pmatrix} 0 & m_1 \\ -m_1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & m_2 \\ -m_2 & 0 \end{pmatrix}, \cdots, \begin{pmatrix} 0 & m_n \\ -m_n & 0 \end{pmatrix}, \mathbb{O}_{d-2n} \right\},$$
(44)

where N is written in block diagonal form with  $2 \times 2$  matrices appearing along the diagonal followed by a  $(d-2n) \times (d-2n)$  block of zeros (denoted by  $\mathbb{O}_{d-2n}$ ), and the  $m_j$  are real and positive. Note that if d=2n, then eq. (44) reduces to eq. (43).

**Proof:** A number of proofs can be found in the literature [1-3, 12, 14, 15]. Perhaps the simplest proof is the one given in Ref. [3]. The proof that is provided here was inspired by Ref. [2] and is given in Appendix D.4 of Ref. [11]. The advantage of this proof is that it provides a constructive algorithm for obtaining the unitary matrix U.

Following Appendix A, we first consider the eigenvalue equation for  $M^{\dagger}M$ :

$$M^{\dagger}Mv_k = m_k^2 v_k$$
,  $m_k > 0$ , and  $M^{\dagger}Mu_k = 0$ , (45)

where we have distinguished between the two classes of eigenvectors corresponding to positive eigenvalues and zero eigenvalues, respectively. The quantities  $m_k$  are the singular values of M. Noting that  $u_k^{\dagger}M^{\dagger}Mu_k = \langle Mu_k | Mu_k \rangle = 0$ , it follows that

$$Mu_k = 0, (46)$$

so that the  $u_k$  are the eigenvectors corresponding to the zero eigenvalues of M. For each eigenvector of  $M^{\dagger}M$  with  $m_k \neq 0$ , we define a new vector

$$w_k \equiv \frac{1}{m_k} M^* v_k^* \,. \tag{47}$$

It follows that  $m_k^2 v_k = M^{\dagger} M v_k = m_k M^{\dagger} w_k^*$ , which yields  $M^{\dagger} w_k^* = m_k v_k$ . Comparing with eq. (42), we identify  $v_k$  and  $w_k$  as the right and left singular vectors, respectively,

corresponding to the non-zero singular values of M. For any antisymmetric matrix,  $M^{\dagger} = -M^*$ . Hence,

$$Mv_k = m_k w_k^*, \qquad Mw_k = -m_k v_k^*, \tag{48}$$

and

$$M^{\dagger} M w_k = -m_k M^{\dagger} v_k^* = m_k M^* v_k^* = m_k^2 w_k , \qquad m_k > 0 .$$
 (49)

That is, the  $w_k$  are also eigenvectors of  $M^{\dagger}M$ .

The key observation is that for fixed k the vectors  $v_k$  and  $w_k$  are orthogonal, since eq. (48) implies that:

$$\langle w_k | v_k \rangle = \langle v_k | w_k \rangle^* = -\frac{1}{m_k^2} \langle M w_k | M v_k \rangle = -\frac{1}{m_k^2} \langle w_k | M^{\dagger} M v_k \rangle = -\langle w_k | v_k \rangle , \qquad (50)$$

which yields  $\langle w_k | v_k \rangle = 0$ . Thus, if all the  $m_k$  are distinct, it follows that  $m_k^2$  is a doubly degenerate eigenvalue of  $M^{\dagger}M$ , with corresponding linearly independent eigenvectors  $v_k$  and  $w_k$ , where k = 1, 2, ..., n (and  $n \leq \frac{1}{2}d$ ). The remaining zero eigenvalues are (d-2n)-fold degenerate, with corresponding eigenvectors  $u_k$  (for k = 1, 2, ..., d - 2n). If some of the  $m_k$  are degenerate, these conclusions still apply. For example, suppose that  $m_j = m_k$  for  $j \neq k$ , which means that  $m_k^2$  is at least a three-fold degenerate eigenvalue of  $M^{\dagger}M$ . Then, there must exist an eigenvector  $v_j$  that is orthogonal to  $v_k$  and  $w_k$  such that  $M^{\dagger}Mv_j = m_k^2v_j$ . We now construct  $w_j \equiv M^*v_j^*/m_k$  according to eq. (47). According to eq. (50),  $w_j$  is orthogonal to  $v_j$ . But, we still must show that  $w_j$  is also orthogonal to  $v_k$  and  $w_k$ . But this is straightforward:

$$\langle w_j | w_k \rangle = \langle w_k | w_j \rangle^* = \frac{1}{m_k^2} \langle M v_k | M v_j \rangle = \frac{1}{m_k^2} \langle v_k | M^{\dagger} M v_j \rangle = \langle v_k | v_j \rangle = 0, \qquad (51)$$

$$\langle w_j | v_k \rangle = \langle v_k | w_j \rangle^* = -\frac{1}{m_k^2} \langle M w_k | M v_j \rangle = -\frac{1}{m_k^2} \langle w_k | M^{\dagger} M v_j \rangle = -\langle w_k | v_j \rangle = 0, (52)$$

where we have used the assumed orthogonality of  $v_j$  with  $v_k$  and  $w_k$ , respectively. It follows that  $v_j$ ,  $w_j$ ,  $v_k$  and  $w_k$  are linearly independent eigenvectors corresponding to a four-fold degenerate eigenvalue  $m_k^2$  of  $M^{\dagger}M$ . Additional degeneracies are treated in the same way.

Thus, the number of non-zero eigenvalues of  $M^{\dagger}M$  must be an even number, denoted by 2n above. Moreover, one can always choose the complete set of eigenvectors  $\{u_k, v_k, w_k\}$  of  $M^{\dagger}M$  to be orthonormal. These orthonormal vectors can be used to construct a unitary matrix U with matrix elements:

$$U_{\ell,2k-1} = (w_k)_{\ell}, \qquad U_{\ell,2k} = (v_k)_{\ell}, \qquad k = 1, 2, \dots, n,$$
  
 $U_{\ell,k+2p} = (u_k)_{\ell}, \qquad k = 1, 2, \dots, d-2n,$  (53)

for  $\ell = 1, 2, \ldots, d$ , where e.g.,  $(v_k)_\ell$  is the  $\ell$ th component of the vector  $v_k$  with respect to the standard orthonormal basis. The orthonormality of  $\{u_k, v_k, w_k\}$  implies that  $(U^{\dagger}U)_{\ell k} = \delta_{\ell k}$  as required. Eqs. (46) and (48) are thus equivalent to the matrix equation

 $MU = U^*N$ , which immediately yields eq. (44), and the theorem is proven. If M is a real antisymmetric matrix, then all the eigenvectors of  $M^{\dagger}M$  can be chosen to be real, in which case U is a real orthogonal matrix.

Finally, we address the non-uniqueness of the matrix U. For definiteness, we fix an ordering of the  $2 \times 2$  blocks containing the  $m_k$  in the matrix N. In the subspace corresponding to a non-zero singular value of degeneracy d, the matrix U is unique up to multiplication on the right by a  $2d \times 2d$  unitary matrix S that satisfies:

$$S^{\mathsf{T}}JS = J\,, (54)$$

where the  $2r \times 2r$  matrix J, defined by

$$J = \operatorname{diag}\left\{ \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \cdots, \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \right\}, \tag{55}$$

is a block diagonal matrix with r blocks of  $2 \times 2$  matrices. A unitary matrix S that satisfies eq. (54) is an element of the unitary symplectic group,  $\operatorname{Sp}(d)$ . Since the determinant of a symplectic matrix is unity [cf. eq. (38)], it follows that  $\det U = e^{-i\theta}$  is uniquely determined in eq. (43). In particular, the principal value of  $\theta = \arg \det U$  (typically chosen such that  $-\frac{1}{2}\pi < \theta \le \pi$ ) is uniquely determined in eq. (43).

If there are no degeneracies among the  $m_k$ , then r = 1. Since  $\operatorname{Sp}(1) \cong \operatorname{SU}(2)$ , it follows that within the subspace corresponding to a non-degenerate singular value, U is unique up to multiplication on the right by an arbitrary  $\operatorname{SU}(2)$  matrix. Finally, in the subspace corresponding to the zero eigenvalues of M, the matrix U is unique up to multiplication on the right by an arbitrary unitary matrix.

#### APPENDIX C: Alternative Proof of Theorem 2

In this appendix, we provide an alternative proof [4–6] of Theorem 2 that does not employ the results of Theorem 1.

**Theorem 2:** If M is an even-dimensional complex non-singular  $2n \times 2n$  antisymmetric matrix, then there exists a non-singular  $2n \times 2n$  matrix P such that:

$$M = P^{\mathsf{T}}JP\,, (56)$$

where the  $2n \times 2n$  matrix J written in  $2 \times 2$  block form is given by:

$$J \equiv \operatorname{diag}\left\{ \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \cdots, \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \right\}. \tag{57}$$

If M is a complex singular antisymmetric  $d \times d$  matrix of rank 2n (where d is either even or odd and d > 2n), then there exists a non-singular  $d \times d$  matrix P such that

$$M = P^{\mathsf{T}} \widetilde{J} P \,, \tag{58}$$

and  $\widetilde{J}$  is the  $d \times d$  matrix that is given in block form by

$$\widetilde{J} \equiv \begin{pmatrix} J & 0 \\ ---- & 0 \\ 0 & 0 \end{pmatrix},$$
(59)

where the  $2n \times 2n$  matrix J is defined in eq. (57) and  $\mathbb{O}$  is a zero matrix of the appropriate number of rows and columns. Note that if d = 2n, then eq. (58) reduces to eq. (56).

**Proof:** Recall that an elementary row operation consists of one of the following three operations:

- 1. Interchange two rows  $(R_i \leftrightarrow R_j \text{ for } i \neq j)$ ;
- 2. Multiply a given row  $R_i$  by a non-zero constant scalar  $(R_i \to cR_i \text{ for } c \neq 0)$ ;
- 3. Replace a given row  $R_i$  as follows:  $R_i \to R_i + cR_j$  for  $i \neq j$  and  $c \neq 0$ .

Each elementary row operation can be carried out by the multiplication of an appropriate non-singular matrix (called the elementary row transformation matrix) from the left.<sup>5</sup> Likewise, one can define elementary column operations by replacing "row" with "column" in the above. Each elementary column operation can be carried out by the multiplication of an appropriate non-singular matrix (called the elementary column transformation matrix) from the right.<sup>5</sup> Finally, an elementary cogredient operation<sup>6</sup> is an elementary row operation applied to a square matrix followed by the same elementary column operation (i.e., one performs the identical operation on the columns that was performed on the rows) or vice versa.

The key observation is the following. If M and B are square matrices, then M is congruent to B if and only if B is obtainable from M by a sequence of elementary cogredient operations.<sup>7</sup> That is, a non-singular matrix R exists such that  $B = R^{\mathsf{T}}MR$ , where  $R^{\mathsf{T}}$  is the non-singular matrix given by the product of the elementary row operations that are employed in the sequence of elementary cogredient operations.

With this observation, it is easy to check that starting from a complex  $d \times d$  anti-symmetric matrix, one can apply a simple sequence of elementary cogredient operations to convert M into the form given by

$$\begin{pmatrix}
0 & 1 & 0^{\mathsf{T}} \\
-1 & 0 & 0^{\mathsf{T}} \\
0 & 0 & B
\end{pmatrix},$$
(60)

where B is a  $(d-2)\times(d-2)$  complex antisymmetric matrix, and O is (d-2)-dimensional column vector made up entirely of zeros. (Try it!) If B=0, then we are done. Otherwise,

<sup>&</sup>lt;sup>5</sup> Note that elementary row and column transformation matrices are always non-singular.

<sup>&</sup>lt;sup>6</sup>The term *cogredient operation* employed by Refs. [4,5], is not commonly used in the modern literature. Nevertheless, I have introduced this term here as it is a convenient way to describe the sequential application of identical row and column operations.

<sup>&</sup>lt;sup>7</sup>This is Theorem of 5.3.4 of Ref. [5].

we repeat the process starting with B. Using induction, we see that the process continues until M has been converted by a sequence of elementary cogredient operations into J or  $\widetilde{J}$ . In particular, if the rank of M is equal to 2n, then A will be converted into  $\widetilde{J}$  after n steps. Hence, in light of the above discussion, it follows that  $M = P^{\mathsf{T}}JP$ , where  $[P^{\mathsf{T}}]^{-1}$  is the product of all the elementary row operation matrices employed in the sequence of elementary cogredient operations used to reduce M to its canonical form given by J if d = 2n or  $\widetilde{J}$  if d > 2n. That is, Theorem 2 is proven.

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