A tale of three diagonalizations

Howard E. Haber

Santa Cruz Institute for Particle Physics
University of California, Santa Cruz, CA 95064, USA

Abstract

In addition to the diagonalization of a normal matrix by a unitary similarity transformation, there are two other types of diagonalization procedures that sometimes arise in quantum theory applications—the singular value decomposition and the Autonne-Takagi factorization. In this pedagogical review, each of these diagonalization procedures is performed for the most general 2×2 matrices for which the corresponding diagonalization is possible, and explicit analytical results are provided in each of the three cases.

1 Introduction

In quantum physics, some problems can be reduced to two state systems. The solution to these problems involves the diagonalization of the 2×2 hermitian matrix Hamiltonian H, which consists of reducing H via a unitary similarity transformation to a diagonal matrix whose elements are the (real) eigenvalues of H. Instead of repeating the diagonalization every time a problem of this type arises, it is convenient to solve it once and for all by considering the diagonalization of a general 2×2 hermitian matrix. In fact, it is possible to be slightly more general. Recall that a matrix is normal (i.e. the matrix commutes with its hermitian adjoint) if and only if it is diagonalizable by a unitary similarity transformation (see, e.g., Theorem 2.5.3 of Ref. [1]). Hence, this pedagogical review will begin by providing the explicit diagonalization of a general 2×2 normal matrix.

Two additional diagonalization procedures often arise in the quantum field theories of fermions (see, e.g., Ref. [2]). The fermion mass eigenstates are identified by reducing the fermion mass matrix to diagonal form. But, in such problems, the relevant diagonalization procedure is not carried out by a unitary similarity transformation. In general, the mass matrix that arises in a theory of charged fermions is a complex matrix with no other special features. The relevant diagonalization procedure is called the singular value decomposition of a complex matrix (see, e.g., Refs. [1, 3]). This decomposition produces a diagonal matrix whose diagonal elements are real and nonnegative, corresponding to the physical masses of the charged fermions. In contrast, the mass matrix that arises in a theory of neutral (Majorana) fermions is a complex symmetric matrix. The relevant diagonalization procedure is called the Autonne-Takagi factorization of a complex symmetric matrix [4, 5]. This factorization also produces a diagonal matrix whose diagonal elements are real and nonnegative, corresponding to the physical masses of the neutral fermions.

In this review, we apply the three diagonalization procedures mentioned above to a complex normal matrix, an arbitrary complex matrix, and a complex symmetric matrix, respectively. In each case, we diagonalize the corresponding 2×2 matrix explicitly and provide analytic results for the corresponding diagonalizing matrix and for the elements of the resulting diagonal matrix.

2 The diagonalization of a 2×2 normal matrix by a unitary similarity transformation

Consider a general 2×2 complex matrix,

$$N = \begin{pmatrix} a & b \\ c & d \end{pmatrix} . \tag{1}$$

Then, N is normal if

$$N^\dagger N = N N^\dagger . \tag{2}$$

Inserting eq. (1) into eq. (2), it follows that[1]

$$|b| = |c| , \qquad \mathrm{Im}\big[(d-a)e^{-i(\alpha+\beta)/2}\big] = 0 , \tag{3}$$

where

$$\alpha \equiv \arg b , \qquad \beta \equiv \arg c . \tag{4}$$

It is then straightforward to verify that the matrix

$$A = e^{-i(\alpha+\beta)/2}(N - a\mathbb{1}_{2\times 2}) = \begin{pmatrix} 0 & |b|e^{i(\alpha-\beta)/2} \\ |b|e^{-i(\alpha-\beta)/2} & (d-a)e^{-i(\alpha+\beta)/2} \end{pmatrix} , \tag{5}$$

is hermitian, where $\mathbb{1}_{2\times 2}$ is the 2×2 identity matrix.

The diagonalization of N by a unitary similarity transformation is given by,

$$U^{-1} N U = \begin{pmatrix} \mu_1 & 0 \\ 0 & \mu_2 \end{pmatrix} , \tag{6}$$

where μ_1 and μ_2 are the complex eigenvalues of N,

$$\mu_{1,2} = \frac{1}{2}\left[a + d \mp \sqrt{(a-d)^2 + 4|b|^2 e^{i(\alpha+\beta)}}\right] . \tag{7}$$

Using eq. (5), it follows that

$$U^{-1} N U = e^{i(\alpha+\beta)/2} U^{-1} A U + a\mathbb{1}_{2\times 2} . \tag{8}$$

Hence, to diagonalize N, we must diagonalize the hermitian matrix A. We will carry out this procedure in Section 3, which will provide an explicit expression for the diagonalizing matrix U.

The eigenvalues of an hermitian matrix are real. Denoting the eigenvalues of A by λ_1 and λ_2, one easily obtains

$$\lambda_{1,2} = \frac{1}{2}\left[(d-a)e^{-i(\alpha+\beta)/2} \mp \sqrt{\big[(d-a)e^{-i(\alpha+\beta)/2}\big]^2 + 4|b|^2}\right] . \tag{9}$$

Note that in light of eq. (3), it follows that λ_1 and λ_2 are real numbers. Hence, eq. (8) yields,

$$\mu_{1,2} = e^{i(\alpha+\beta)/2}\lambda_{1,2} + a . \tag{10}$$

It is straightforward to check that eqs. (10) and (7) are equivalent.

[1] Eqs. (3) and (5) have been inspired by Problem 2.5.P29 of Ref. [1].

3 The diagonalization of a 2×2 hermitian matrix by a unitary similarity transformation

Consider a general 2×2 hermitian matrix

$$A = \begin{pmatrix} a & c \\ c^* & b \end{pmatrix} , \tag{11}$$

where a and b are real numbers and the complex number c expressed in polar exponential form is given by,

$$c = |c| e^{i\phi} , \qquad \text{where } 0 \leq \phi < 2\pi . \tag{12}$$

The eigenvalues are the roots of the characteristic equation:

$$\det \begin{pmatrix} a - \lambda & c \\ c^* & b - \lambda \end{pmatrix} = (a - \lambda)(b - \lambda) - |c|^2 = \lambda^2 - \lambda(a + b) + (ab - |c|^2) = 0 . \tag{13}$$

Noting that $(a+b)^2 - 4(ab - |c|^2) = (a-b)^2 + 4|c|^2$, the two roots can be written as:

$$\lambda_1 = \tfrac{1}{2}\left[a + b - \sqrt{(a-b)^2 + 4|c|^2}\right] \quad \text{and} \quad \lambda_2 = \tfrac{1}{2}\left[a + b + \sqrt{(a-b)^2 + 4|c|^2}\right] , \tag{14}$$

where by convention we take $\lambda_1 \leq \lambda_2$. As expected, the eigenvalues of the hermitian matrix A are real.

An hermitian matrix can be diagonalized by a unitary matrix U,

$$U^{-1} A U = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} , \tag{15}$$

where λ_1 and λ_2 are the eigenvalues obtained in eq. (14). Note that one can always transform $U \to e^{i\zeta} U$ without modifying eq. (15), since the phase factor cancels out. Since $\det U$ is a complex number of unit modulus, one can choose $\det U = 1$ in eq. (15) without loss of generality. The most general 2×2 unitary matrix of unit determinant can be written as,

$$U = \begin{pmatrix} e^{i\beta} \cos\theta & e^{i\chi} \sin\theta \\ -e^{-i\chi} \sin\theta & e^{-i\beta} \cos\theta \end{pmatrix} .$$

The columns of U are the normalized eigenvectors of A corresponding to the eigenvalues λ_1 and λ_2, respectively. But, we are always free to multiply any normalized eigenvector by an arbitrary complex phase factor. Thus, without loss of generality, we can choose $\beta = 0$ and $\cos\theta \geq 0$. Moreover, the sign of $\sin\theta$ can always be absorbed into the definition of χ. Hence, we will take

$$U = \begin{pmatrix} \cos\theta & e^{i\chi} \sin\theta \\ -e^{-i\chi} \sin\theta & \cos\theta \end{pmatrix} , \tag{16}$$

where

$$0 \leq \theta \leq \tfrac{1}{2}\pi , \quad \text{and} \quad 0 \leq \chi < 2\pi . \tag{17}$$

We now plug in eq. (16) into eq. (15). Since the off-diagonal terms must vanish, one obtains constraints on the angles θ and χ. In particular,

$$
\begin{aligned}
U^{-1}AU &= \begin{pmatrix} \cos\theta & -e^{i\chi}\sin\theta \\ e^{-i\chi}\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} a & |c|e^{i\phi} \\ |c|e^{-i\phi} & b \end{pmatrix} \begin{pmatrix} \cos\theta & e^{i\chi}\sin\theta \\ -e^{-i\chi}\sin\theta & \cos\theta \end{pmatrix} \\
&= \begin{pmatrix} \cos\theta & -e^{i\chi}\sin\theta \\ e^{-i\chi}\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} a\cos\theta - |c|e^{i(\phi-\chi)}\sin\theta & ae^{i\chi}\sin\theta + |c|e^{i\phi}\cos\theta \\ |c|e^{-i\phi}\cos\theta - be^{-i\chi}\sin\theta & |c|e^{-i(\phi-\chi)}\sin\theta + b\cos\theta \end{pmatrix} \\
&= \begin{pmatrix} \lambda_1 & Z \\ Z^* & \lambda_2 \end{pmatrix},
\end{aligned}
$$

where

$$\lambda_1 = a\cos^2\theta - 2|c|\cos\theta\sin\theta\cos(\phi-\chi) + b\sin^2\theta\,, \tag{18}$$

$$\lambda_2 = a\sin^2\theta + 2|c|\cos\theta\sin\theta\cos(\phi-\chi) + b\cos^2\theta\,, \tag{19}$$

$$Z = e^{i\chi}\left\{(a-b)\cos\theta\sin\theta + |c|\left[e^{i(\phi-\chi)}\cos^2\theta - e^{-i(\phi-\chi)}\sin^2\theta\right]\right\}. \tag{20}$$

The vanishing of the off-diagonal elements of $U^{-1}AU$ implies that:

$$(a-b)\cos\theta\sin\theta + |c|\left[e^{i(\phi-\chi)}\cos^2\theta - e^{-i(\phi-\chi)}\sin^2\theta\right] = 0\,.$$

This is a complex equation. Taking real and imaginary parts yields two real equations,

$$\tfrac{1}{2}(a-b)\sin 2\theta + |c|\cos 2\theta\cos(\phi-\chi) = 0\,, \tag{21}$$

$$|c|\sin(\phi-\chi) = 0\,. \tag{22}$$

Consider first the special case of $c=0$. Then, in light of our convention that $\lambda_1 \leq \lambda_2$,

$$
\begin{aligned}
&c=0 \quad \text{and} \quad a<b \quad \Longrightarrow \quad \theta = 0 \quad \text{and } \chi \text{ is undefined}\,, \\
&c=0 \quad \text{and} \quad a>b \quad \Longrightarrow \quad \theta = \tfrac{1}{2}\pi \;\; \text{and } \chi \text{ is undefined}\,, \\
&c=0 \quad \text{and} \quad a=b \quad \Longrightarrow \quad \theta \text{ and } \chi \text{ are undefined}\,.
\end{aligned}
$$

In particular, if $c=0$ and $a=b$, then $A = a\mathbb{1}_{2\times 2}$ and it follows that $U^{-1}AU = U^{-1}U = a\mathbb{1}_{2\times 2}$, which is satisfied for any unitary matrix U. Consequently, in this limit θ and χ are arbitrary and hence undefined, as indicated above.

If $c \neq 0$ then eq. (22) yields

$$\sin(\phi-\chi) = 0 \quad \text{and} \quad \cos(\phi-\chi) = \varepsilon\,, \quad \text{where } \varepsilon = \pm 1. \tag{23}$$

We can determine the sign ε as follows. Since $\lambda_1 \leq \lambda_2$, we subtract eqs. (18) and (19) and make use of eq. (23) to obtain,

$$(a-b)\cos 2\theta - 2\varepsilon|c|\sin 2\theta \geq 0\,. \tag{24}$$

Likewise, we insert eq. (23) into eq. (21), which yields

$$(a-b)\sin 2\theta + 2\varepsilon|c|\cos 2\theta = 0\,. \tag{25}$$

Finally, we multiply eq. (24) by $\sin 2\theta$ and eq. (25) by $\cos 2\theta$ and subtract the two resulting equations. The end result is,

$$2\varepsilon|c| \geq 0\,. \tag{26}$$

By assumption, $c \neq 0$. Thus, it follows that $\varepsilon \geq 0$. Since $\varepsilon = \pm 1$, we can conclude that $\varepsilon = 1$. Hence,

$$\cos(\phi - \chi) = 1\,, \quad \text{for } c \neq 0. \tag{27}$$

By the conventions established in eqs. (12) and (17), we take $0 \leq \phi\,,\ \chi < 2\pi$. Hence, it follows that

$$\chi = \phi\,. \tag{28}$$

We can now determine θ. Inserting eq. (27) into eq. (21) yields

$$\tan 2\theta = \frac{2|c|}{b-a}\,, \quad \text{for } c \neq 0 \text{ and } a \neq b\,. \tag{29}$$

Note that if $a = b$, then eq. (25) yields $\cos 2\theta = 0$. In light of eq. (17),

$$c \neq 0 \quad \text{and} \quad a = b \quad \Longrightarrow \quad \theta = \tfrac{1}{4}\pi\,. \tag{30}$$

If $c \neq 0$ and $a \neq b$, then we can use eq. (29) with the convention that $\sin 2\theta \geq 0$ [cf. eq. (17)] to conclude that

$$\sin 2\theta = \frac{2|c|}{\sqrt{(b-a)^2 + 4|c|^2}}\,. \tag{31}$$

$$\cos 2\theta = \frac{b-a}{\sqrt{(b-a)^2 + 4|c|^2}}\,. \tag{32}$$

Using the well known identity, $\tan\theta = (1 - \cos 2\theta)/\sin 2\theta$, it follows that

$$\tan\theta = \frac{a - b + \sqrt{(b-a)^2 + 4|c|^2}}{2|c|}\,, \tag{33}$$

which is manifestly positive. It then follows that,

$$\sin\theta = \left(\frac{a - b + \sqrt{(b-a)^2 + 4|c|^2}}{2\sqrt{(b-a)^2 + 4|c|^2}}\right)^{1/2}, \qquad \cos\theta = \left(\frac{b - a + \sqrt{(b-a)^2 + 4|c|^2}}{2\sqrt{(b-a)^2 + 4|c|^2}}\right)^{1/2}. \tag{34}$$

Indeed, the above results imply that the sign of $b - a$ determines whether $0 < \theta < \frac{1}{4}\pi$ or $\frac{1}{4}\pi < \theta < \frac{1}{2}\pi$. The former corresponds to $a < b$ while the latter corresponds to $a > b$. The borderline case of $a = b$ has already been treated in eq. (30).

To summarize, if $c \neq 0$, then eqs. (28), (31) and (32) uniquely specify the diagonalizing matrix U [in the conventions specified in eqs. (12) and (17)]. When $c = 0$ and $a \neq b$, it follows that χ is arbitrary and $\theta = 0$ or $\frac{1}{2}\pi$ for the two cases of $a < b$ or $a > b$, respectively.[2] Finally, if $c = 0$ and $a = b$, then $A = a\mathbb{1}_{2\times 2}$, in which case U is arbitrary.

[2]Note that in the case of $c = 0$ and $a > b$, the matrix A is diagonal. Nevertheless, the "diagonalizing" matrix, $U \neq \mathbb{1}_{2\times 2}$. Indeed, in this case $\theta = \frac{1}{2}\pi$, and $U^{-1}AU$ simply interchanges the two diagonal elements of A to ensure that $\lambda_1 \leq \lambda_2$ in eq. (15), as required by the convention adopted below eq. (14).

4 The diagonalization of a 2×2 real symmetric matrix by an orthogonal similarity transformation

In this section, we consider a special case of the one treated in Section 3 in which the matrix A given in eq. (11) is real. That is, $c = c^*$, in which case A is a real symmetric matrix that can be diagonalized by a real orthogonal matrix. The two eigenvalues are still given by eq. (14) in the convention that $\lambda_1 \leq \lambda_2$, although the absolute values signs are no longer needed since for real values of c, we have $|c|^2 = c^2$. Moreover, since c is real, eq. (12) implies that if $c \neq 0$ then $\phi = 0$ or $\phi = \pi$. Eq. (28) then yields

$$\chi = \begin{cases} 0\,, & \text{for } c \neq 0 \text{ and } \phi = 0\,, \\ \pi\,, & \text{for } c \neq 0 \text{ and } \phi = \pi\,, \end{cases} \tag{35}$$

which is equivalent to the statement that

$$e^{i\chi} = \operatorname{sgn} c\,, \quad \text{for real } c \neq 0. \tag{36}$$

It is convenient to redefine $\theta \to \theta \operatorname{sgn} c$ in eq. (16). With this modification, the range of θ can be taken as[3]

$$-\tfrac{1}{2}\pi < \theta \leq \tfrac{1}{2}\pi\,. \tag{37}$$

The diagonalizing matrix U is now a real orthogonal 2×2 matrix,

$$U = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}, \qquad \text{where} \quad \begin{cases} c > 0 & \Longrightarrow \quad 0 < \theta < \tfrac{1}{2}\pi\,, \\ c = 0 & \Longrightarrow \quad \theta = 0 \text{ or } \theta = \tfrac{1}{2}\pi\,, \\ c < 0 & \Longrightarrow \quad -\tfrac{1}{2}\pi < \theta < 0\,. \end{cases} \tag{38}$$

Hence, for real $c \neq 0$ with the range of θ specified in eq. (37), we see that eqs. (29) and (31)–(33) are modified by replacing $|c|$ with c. For example,

$$\sin 2\theta = \frac{2c}{\sqrt{(b-a)^2 + 4c^2}}\,, \qquad \cos 2\theta = \frac{b-a}{\sqrt{(b-a)^2 + 4c^2}}\,. \tag{39}$$

It then follows that

$$\sin\theta = \operatorname{sgn}(c) \left(\frac{a - b + \sqrt{(b-a)^2 + 4c^2}}{2\sqrt{(b-a)^2 + 4c^2}} \right)^{1/2}, \qquad \cos\theta = \left(\frac{b - a + \sqrt{(b-a)^2 + 4c^2}}{2\sqrt{(b-a)^2 + 4c^2}} \right)^{1/2}. \tag{40}$$

The sign of c determines the quadrant in which θ lives. Moreover, for $c > 0$, the sign of $b - a$ determines whether $0 < \theta < \frac{1}{4}\pi$ or $\frac{1}{4}\pi < \theta < \frac{1}{2}\pi$. The former corresponds to $a < b$ while the latter corresponds to $a > b$. Likewise, for $c < 0$, the sign of $b - a$ determines whether $-\frac{1}{2}\pi < \theta < -\frac{1}{4}\pi$ or $-\frac{1}{4}\pi < \theta < 0$. The former corresponds to $a > b$ while the latter corresponds to $a < b$. The borderline cases are likewise determined:

$$a = b \quad \text{and} \quad c \neq 0 \quad \Longrightarrow \quad \sin 2\theta = \operatorname{sgn}(c)\,,$$

$$a \neq b \quad \text{and} \quad c = 0 \quad \Longrightarrow \quad \cos 2\theta = \operatorname{sgn}(b-a)\,,$$

If $a = b$ and $c = 0$, then $A = a\mathbb{1}_{2\times 2}$, in which case U is arbitrary.

[3] Using $\cos(\theta + \pi) = -\cos\theta$ and $\sin(\theta + \pi) = -\sin\theta$, it follows that shifting $\theta \to \theta + \pi$ simply multiplies U by an overall factor of -1. In particular, $U^{-1}AU$ is unchanged. Hence, the convention $-\frac{1}{2}\pi < \theta \leq \frac{1}{2}\pi$ may be chosen without loss of generality.

5 The singular value decomposition of a complex 2×2 matrix

For any complex $n \times n$ matrix M, unitary $n \times n$ matrices L and R exist such that

$$L^{\mathsf{T}} M R = M_D = \mathrm{diag}(m_1, m_2, \ldots, m_n), \tag{41}$$

where the m_k are real and nonnegative. This is called the singular value decomposition of the matrix M. A proof of eq. (41) is given in Appendix D of Ref. [2] (see also Refs. [1, 3]). In general, the m_k are *not* the eigenvalues of M. Rather, the m_k are the *singular values* of the general complex matrix M, which are defined to be the nonnegative square roots of the eigenvalues of either $M^\dagger M$ or $M M^\dagger$ (both yield the same results).

An equivalent definition of the singular values can be established as follows. Since $M^\dagger M$ is a nonnegative hermitian matrix, its eigenvalues are real and nonnegative and its eigenvectors, w_k, defined by $M^\dagger M w_k = m_k^2 w_k$, can be chosen to be orthonormal.[4] Consider first the eigenvectors corresponding to the positive eigenvalues of $M^\dagger M$. Then, we define the vectors v_k such that $M w_k = m_k v_k^*$. It follows that $m_k^2 w_k = M^\dagger M w_k = m_k M^\dagger v_k^*$, which yields: $M^\dagger v_k^* = m_k w_k$. Note that these equations also imply that $M M^\dagger v_k^* = m_k^2 v_k^*$. The orthonormality of the w_k implies the orthonormality of the v_k^* (and hence the v_k):

$$\delta_{jk} = \langle w_j | w_k \rangle = \frac{1}{m_j m_k} \langle M^\dagger v_j^* | M^\dagger v_k^* \rangle = \frac{1}{m_j m_k} \langle v_j^* | M M^\dagger v_k^* \rangle = \frac{m_k}{m_j} \langle v_j^* | v_k^* \rangle \,, \tag{42}$$

which yields $\langle v_j^* | v_k^* \rangle = \delta_{jk}$.

If w_i is an eigenvector of $M^\dagger M$ with zero eigenvalue, then $0 = w_i^\dagger M^\dagger M w_i = \langle M w_i | M w_i \rangle$, which implies that $M w_i = 0$. Likewise, if v_i^* is an eigenvector of $M M^\dagger$ with zero eigenvalue, then $0 = v_i^{\mathsf{T}} M M^\dagger v_i^* = \langle M^{\mathsf{T}} v_i | M^{\mathsf{T}} v_i \rangle^*$, which implies that $M^{\mathsf{T}} v_i = 0$. Because the eigenvectors of $M M^\dagger$ [$M^\dagger M$] can be chosen orthonormal, the eigenvectors corresponding to the zero eigenvalues of M [M^{T}] can be taken to be orthonormal.[5] Finally, these eigenvectors are also orthogonal to the eigenvectors corresponding to the nonzero eigenvalues of $M M^\dagger$ [$M^\dagger M$]. That is,

$$\langle w_j | w_i \rangle = \frac{1}{m_j} \langle M^\dagger v_j^* | w_i \rangle = \frac{1}{m_j} \langle v_j^* | M w_i \rangle = 0 \,, \tag{43}$$

and similarly $\langle v_j | v_i \rangle = 0$, where the index i [j] runs over the eigenvectors corresponding to the zero [nonzero] eigenvalues. Thus, we can define the singular values of a general complex matrix M to be the simultaneous solutions (with real nonnegative m_k) of,[6]

$$M w_k = m_k v_k^* \,, \qquad v_k^{\mathsf{T}} M = m_k w_k^\dagger \,. \tag{44}$$

The corresponding v_k (w_k), normalized to have unit norm, are called the left (right) singular vectors of M.

[4] We define the inner product of two vectors to be $\langle v | w \rangle \equiv v^\dagger w$.

[5] The multiplicity of zero eigenvalues of $M^\dagger M$ [$M M^\dagger$], which is equal to the number of linearly independent eigenvectors of $M^\dagger M$ [$M M^\dagger$] with zero eigenvalue, coincides with the number of linearly independent eigenvectors of M [M^{T}] with zero eigenvalue. Moreover, the number of linearly independent w_i coincides with the number of linearly independent v_i.

[6] One can always find a solution to eq. (44) such that the m_k are real and nonnegative. Given a solution where m_k is complex, we simply write $m_k = |m_k| e^{i\theta}$ and redefine $v_k \to v_k e^{i\theta}$ to remove the phase θ.

The singular value decomposition of a general 2×2 complex matrix can be performed fully analytically. The result is more involved than the standard diagonalization of a 2×2 hermitian matrix by a unitary similarity transformation. Let us consider the non-diagonal complex matrix,

$$M = \begin{pmatrix} a & c \\ \tilde{c} & b \end{pmatrix}, \tag{45}$$

where at least one of the two quantities c or $\tilde{c}$ is nonzero. The singular value decomposition of the complex matrix M is

$$L^{\mathsf{T}} M R = \begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix}, \tag{46}$$

where L and R are unitary 2×2 matrices and m_1, m_2 are nonnegative. Following Ref. [6], one can parameterize the matrices L and R as follows,[7]

$$L = U_L P = \begin{pmatrix} \cos\theta_L & e^{i\phi_L}\sin\theta_L \\ -e^{-i\phi_L}\sin\theta_L & \cos\theta_L \end{pmatrix} \begin{pmatrix} e^{-i\alpha} & 0 \\ 0 & e^{-i\beta} \end{pmatrix}, \tag{47}$$

$$R = U_R P = \begin{pmatrix} \cos\theta_R & e^{i\phi_R}\sin\theta_R \\ -e^{-i\phi_R}\sin\theta_R & \cos\theta_R \end{pmatrix} \begin{pmatrix} e^{-i\alpha} & 0 \\ 0 & e^{-i\beta} \end{pmatrix}, \tag{48}$$

where $0 \leq \theta_{L,R} \leq \frac{1}{2}\pi$, $0 \leq \alpha, \beta < \pi$, and $0 \leq \phi_L, \phi_R < 2\pi$.

The singular values $m_{1,2}$ of the matrix M can be determined by taking the positive square root of the nonnegative eigenvalues, $m^2_{1,2}$, of the hermitian matrix $M^\dagger M$,

$$m^2_{1,2} = \tfrac{1}{2}\left[|a|^2 + |b|^2 + |c|^2 + |\tilde{c}|^2 \mp \Delta\right], \tag{49}$$

in a convention where $0 \leq m_1 \leq m_2$ (i.e., $\Delta \geq 0$), with

$$\begin{aligned} \Delta &\equiv \left[(|a|^2 - |b|^2 - |c|^2 + |\tilde{c}|^2)^2 + 4|a^* c + b\tilde{c}^*|^2\right]^{1/2} \\ &= \left[(|a|^2 + |b|^2 + |c|^2 + |\tilde{c}|^2)^2 - 4|ab - c\tilde{c}|^2\right]^{1/2}. \end{aligned} \tag{50}$$

It follows that

$$m_1^2 + m_2^2 = |a|^2 + |b|^2 + |c|^2 + |\tilde{c}|^2, \qquad \Delta = m_2^2 - m_1^2. \tag{51}$$

Moreover, by taking the determinant of eq. (46), it follows that

$$m_1 m_2 = (ab - c\tilde{c})e^{-2i(\alpha+\beta)}. \tag{52}$$

Note that $m_1 = m_2$ if and only if $|a| = |b|$, $|c| = |\tilde{c}|$ and $a^* c + b\tilde{c}^* = 0$ are satisfied.

We first assume that $m_1 \neq m_2$. Using the results of Section 3 enables us to compute the rotation angles, $\theta_{L,R}$, and the phases, $e^{i\phi_{L,R}}$, by diagonalizing $M^\dagger M$ and $M^* M^{\mathsf{T}}$ with a diagonalizing matrix R and L, respectively. Explicitly, we have

$$M^\dagger M = \begin{pmatrix} |a|^2 + |\tilde{c}|^2 & a^* c + b\tilde{c}^* \\ ac^* + b^*\tilde{c} & |b|^2 + |c|^2 \end{pmatrix}, \tag{53}$$

[7] Without loss of generality, we have employed the same diagonal phase matrix P in defining L and R. Had we written $L = U_L P_L$ and $R = U_R P_R$ in eqs. (47) and (48) with $P_{L,R} \equiv \mathrm{diag}(e^{-i\alpha_{L,R}}, e^{-i\beta_{L,R}})$, we would have discovered that only the sums $\alpha_L + \alpha_R$ and $\beta_L + \beta_R$ are fixed. Moreover, since eq. (46) is unchanged under $\alpha \to \alpha + \pi$ or $\beta \to \beta + \pi$, one can fix the range of α and β as specified below eq. (48).

and M^*M^T is obtained form $M^\dagger M$ by interchanging c and $\tilde{c}$. Applying eqs. (28) and (34) to the diagonalization of $M^\dagger M$ and M^*M^T then yields,

$$\cos\theta_{R,L} = \sqrt{\frac{\Delta+|b|^2-|a|^2\pm|c|^2\mp|\tilde{c}|^2}{2\Delta}}\,, \qquad \sin\theta_{R,L} = \sqrt{\frac{\Delta-|b|^2+|a|^2\mp|c|^2\pm|\tilde{c}|^2}{2\Delta}}\,, \tag{54}$$

and

$$e^{i\phi_R} = \frac{a^*c+b\tilde{c}^*}{|a^*c+b\tilde{c}^*|}\,, \qquad e^{i\phi_L} = \frac{a^*\tilde{c}+bc^*}{|a^*\tilde{c}+bc^*|}\,. \tag{55}$$

For completeness, we note that the denominators in eq. (55) can be written in another form by employing the following results [which are a consequence of eq. (50)],

$$|a^*c+b\tilde{c}^*| = \tfrac{1}{2}\sqrt{\Delta^2-(|b|^2-|a|^2+|c|^2-|\tilde{c}|^2)^2}\,, \tag{56}$$

$$|a^*\tilde{c}+bc^*| = \tfrac{1}{2}\sqrt{\Delta^2-(|b|^2-|a|^2-|c|^2+|\tilde{c}|^2)^2}\,. \tag{57}$$

The final step of the computation is to determine the angles α and β. To perform this task, we first rewrite eq. (46) as,

$$MU_R = U_L^* \begin{pmatrix} m_1 e^{2i\alpha} & 0 \\ 0 & m_2 e^{2i\beta}\end{pmatrix}\,, \tag{58}$$

where we have made use of eqs. (47) and (48). Setting the diagonal elements of the left hand side and the right hand side of eq. (58) equal, we end up with the following two equations,

$$m_1\cos\theta_L e^{2i\alpha} = a\cos\theta_R - c\,e^{-i\phi_R}\sin\theta_R\,, \tag{59}$$

$$m_2\cos\theta_L e^{2i\beta} = b\cos\theta_R + \tilde{c}\,e^{i\phi_R}\sin\theta_R\,. \tag{60}$$

Next, we multiply both eqs. (59) and (60) by $\Delta\cos\theta_R$. Employing eqs. (54)–(55) on the right hand sides of the two resulting equations then yields,

$$\begin{aligned}\Delta\, m_1\cos\theta_L\cos\theta_R e^{2i\alpha} &= \tfrac{1}{2}a\big(\Delta+|b|^2-|a|^2+|c|^2-|\tilde{c}|^2\big)\\ &\quad -\frac{c(ac^*+b^*\tilde{c})}{2|a^*c+b\tilde{c}^*|}\sqrt{\Delta^2-(|b|^2-|a|^2+|c|^2-|\tilde{c}|^2)^2}\,,\end{aligned} \tag{61}$$

$$\begin{aligned}\Delta\, m_2\cos\theta_L\cos\theta_R e^{2i\beta} &= \tfrac{1}{2}b\big(\Delta+|b|^2-|a|^2+|c|^2-|\tilde{c}|^2\big)\\ &\quad -\frac{\tilde{c}(a^*c+b\tilde{c}^*)}{2|a^*c+b\tilde{c}^*|}\sqrt{\Delta^2-(|b|^2-|a|^2+|c|^2-|\tilde{c}|^2)^2}\,.\end{aligned} \tag{62}$$

We can simplify eqs. (61) and (62) further by making use of eq. (56). The end result is,

$$\Delta\, m_1\cos\theta_L\cos\theta_R e^{2i\alpha} = \tfrac{1}{2}a\big(\Delta+|b|^2-|a|^2-|c|^2-|\tilde{c}|^2\big) - b^*c\tilde{c}\,, \tag{63}$$

$$\Delta\, m_2\cos\theta_L\cos\theta_R e^{2i\beta} = \tfrac{1}{2}b\big(\Delta+|b|^2-|a|^2+|c|^2+|\tilde{c}|^2\big) + a^*c\tilde{c}\,. \tag{64}$$

Using eq. (49), it is convenient to eliminate Δ in favor of m_1^2 and m_2^2 on the right hand side of eqs. (63) and (64). It then immediately follows that,

$$\alpha = \tfrac{1}{2}\arg\big\{a\big(|b|^2-m_1^2\big) - b^*c\tilde{c}\big\}\,, \tag{65}$$

$$\beta = \tfrac{1}{2}\arg\big\{b\big(m_2^2-|a|^2\big) + a^*c\tilde{c}\big\}\,. \tag{66}$$

A useful identity can now be derived that exhibits a simple relation between the angles θ_L and θ_R. First, we make use eq. (54) to obtain,

$$\cos 2\theta_L = \frac{|b|^2 - |a|^2 - |c|^2 + |\tilde{c}|^2}{\Delta}\,, \qquad \cos 2\theta_R = \frac{|b|^2 - |a|^2 + |c|^2 - |\tilde{c}|^2}{\Delta}\,, \tag{67}$$

$$\sin 2\theta_L = \frac{|a^*\tilde{c} + bc^*|}{\Delta}\,, \qquad \sin 2\theta_R = \frac{|a^*c + b\tilde{c}^*|}{\Delta}\,. \tag{68}$$

Next, we note two different trigonometric identities for the tangent function to obtain,

$$\tan\theta_L = \frac{1 - \cos 2\theta_L}{\sin 2\theta_L} = \frac{m_2^2 - m_1^2 - |b|^2 + |a|^2 + |c|^2 - |\tilde{c}|^2}{2|a^*\tilde{c} + bc^*|} = \frac{|a|^2 + |c|^2 - m_1^2}{|a^*\tilde{c} + bc^*|}\,, \tag{69}$$

$$\tan\theta_R = \frac{\sin 2\theta_R}{1 + \cos 2\theta_R} = \frac{2|a^*c + b\tilde{c}^*|}{m_2^2 - m_1^2 + |b|^2 - |a|^2 + |c|^2 - |\tilde{c}|^2} = \frac{|a^*c + b\tilde{c}^*|}{m_2^2 - |a|^2 - |\tilde{c}|^2}\,, \tag{70}$$

where we have made use of eqs. (51), (67) and (68). It then follows that

$$\frac{\tan\theta_L}{\tan\theta_R} = \frac{(|a|^2 + |c|^2 - m_1^2)(m_2^2 - |a|^2 - |\tilde{c}|^2)}{|(a^*\tilde{c} + bc^*)(a^*c + b\tilde{c}^*)|}\,. \tag{71}$$

The numerator of eq. (71) can be simplified with a little help from eqs. (51) and (52) as follows,

$$\begin{aligned}
(|a|^2 + |c|^2 - m_1^2)(m_2^2 - |a|^2 - |\tilde{c}|^2) &= |a|^2(m_1^2 + m_2^2) + |c|^2 m_2^2 - |\tilde{c}|^2 m_1^2 - m_1^2 m_2^2 \\
&\qquad -(|a|^2 + |c|^2)(|a|^2 + |\tilde{c}|^2) \\
&= |a|^2(|a|^2 + |b|^2 + |c|^2 + |\tilde{c}|^2) + |c|^2 m_2^2 + |\tilde{c}|^2 m_1^2 \\
&\qquad -|ab - c\tilde{c}|^2 - (|a|^2 + |c|^2)(|a|^2 + |\tilde{c}|^2) \\
&= |c|^2 m_2^2 + |\tilde{c}|^2 m_1^2 + (ab - c\tilde{c})c^*\tilde{c}^* + (a^*b^* - c^*\tilde{c}^*)c\tilde{c} \\
&= (cm_2 e^{-i(\alpha+\beta)} + \tilde{c}^* m_1 e^{i(\alpha+\beta)})(c^* m_2 e^{i(\alpha+\beta)} + \tilde{c} m_1 e^{-i(\alpha+\beta)})\,.
\end{aligned} \tag{72}$$

Likewise, the denominator of eq. (71) can be simplified as follows,

$$\begin{aligned}
|(a^*\tilde{c} + bc^*)(a^*c + b\tilde{c}^*)| &= |(a\tilde{c}^* + b^*c)(a^*c + b\tilde{c}^*)| = |c\tilde{c}^*(|a|^2 + |b|^2) + ab\tilde{c}^{*\,2} + a^*b^*c^2| \\
&= |c\tilde{c}^*(|a|^2 + |b|^2 + |c|^2 + |\tilde{c}|^2) + (ab - c\tilde{c})c^{*\,2} + (a^*b^* - c^*\tilde{c}^*)c^2| \\
&= |c\tilde{c}^*(m_1^2 + m_2^2) + m_1 m_2(c^{*\,2} e^{2i(\alpha+\beta)} + c^2 e^{-2i(\alpha+\beta)})| \\
&= |(cm_2 e^{-i(\alpha+\beta)} + \tilde{c}^* m_1 e^{i(\alpha+\beta)})(\tilde{c}^* m_2 e^{i(\alpha+\beta)} + cm_1 e^{-i(\alpha+\beta)})|\,.
\end{aligned} \tag{73}$$

Hence, we end up with a remarkably simple result,

$$\frac{\tan\theta_L}{\tan\theta_R} = \left|\frac{c^* m_2 e^{i(\alpha+\beta)} + \tilde{c} m_1 e^{-i(\alpha+\beta)}}{\tilde{c}^* m_2 e^{i(\alpha+\beta)} + cm_1 e^{-i(\alpha+\beta)}}\right|\,. \tag{74}$$

If $m_1 \neq 0$, then one can employ eq. (52) to obtain an alternate form for eq. (74),

$$\frac{\tan\theta_L}{\tan\theta_R} = \left|\frac{c^*(ab - c\tilde{c}) + \tilde{c} m_1^2}{\tilde{c}^*(ab - c\tilde{c}) + cm_1^2}\right|\,. \tag{75}$$

The case of $m_1 = 0$ is noteworthy. This special case arises when $\det M = ab - c\tilde{c} = 0$, which implies that there is one singular value that is equal to zero. In particular, it then follows that $\Delta = |a|^2 + |b|^2 + |c|^2 + |\tilde{c}|^2$ [cf. eq. (50)] and

$$m_2^2 = \mathrm{Tr}(M^\dagger M) = |a|^2 + |b|^2 + |c|^2 + |\tilde{c}|^2 \,. \tag{76}$$

Eqs. (69), (70) and (76) then yield,[8]

$$\tan\theta_L = \left|\frac{c}{b}\right| = \left|\frac{a}{\tilde{c}}\right| \,, \qquad\qquad \tan\theta_R = \left|\frac{a}{c}\right| = \left|\frac{\tilde{c}}{b}\right| \,, \tag{77}$$

after using $c\tilde{c} = ab$, and

$$\phi_L = \arg(b/c) = \arg(\tilde{c}/a) \,, \qquad \phi_R = \arg(c/a) = \arg(b/\tilde{c}) \,, \qquad \beta = \tfrac{1}{2}\arg b \,. \tag{78}$$

As expected the angle α is undefined when $m_1 = 0$ [cf. eqs. (63) and (65)].

Finally, we treat the case of degenerate nonzero singular values, i.e. $m \equiv m_1 = m_2 \neq 0$. As previously noted below eq. (50), degenerate singular values exist if and only if

$$|a| = |b| \,, \; |c| = |\tilde{c}| \,, \text{ and } a^* c = -b\tilde{c}^* . \tag{79}$$

Note that eq. (79) also implies that $a^*\tilde{c} = -bc^*$. It then follows from eq. (53) that

$$M^\dagger M = m^2 \mathbb{1}_{2\times 2} \,, \tag{80}$$

where the degenerate singular value is

$$m = \sqrt{|a|^2 + |c|^2} \,. \tag{81}$$

Hence, the diagonalization equation, $R^{-1} M^\dagger M R = m^2 \mathbb{1}_{2\times 2}$, is satisfied for any unitary matrix R. However, this does not necessarily mean that an arbitrary unitary matrix R is a solution to eq. (46). In the analysis given below, we shall see that in the case of degenerate singular values, $\alpha + \beta$ is fixed by the matrix M, whereas the remaining parameters that define the matrix R exhibited in eq. (48) can be taken as arbitrary.

Given the unitary matrix R, one can use eq. (46) to determine the matrix elements of the unitary matrix L. Using eqs. (47) and (48), it follows that

$$U_L^{\mathsf{T}} = m \begin{pmatrix} e^{2i\alpha} & 0 \\ 0 & e^{2i\beta} \end{pmatrix} U_R^\dagger M^{-1} \,. \tag{82}$$

In light of eqs. (79) and (81),

$$\det M = ab - c\tilde{c} = -\frac{cm^2}{\tilde{c}^*} \,. \tag{83}$$

Evaluating the left and right hand sides of eq. (82) yields,

$$\cos\theta_L = -\frac{\tilde{c}^*}{mc} e^{2i\alpha}\big(b\cos\theta_R + \tilde{c}e^{i\phi_R}\sin\theta_R\big) = -\frac{\tilde{c}^*}{mc} e^{2i\beta}\big(a\cos\theta_R - ce^{-i\phi_R}\sin\theta_R\big) \,, \tag{84}$$

$$e^{i\phi_L}\sin\theta_L = \frac{\tilde{c}^*}{mc} e^{2i\beta}\big(\tilde{c}\cos\theta_R - be^{-i\phi_R}\sin\theta_R\big) = -\frac{\tilde{c}}{mc^*} e^{-2i\alpha}\big(c^*\cos\theta_R + a^* e^{-i\phi_R}\sin\theta_R\big) \,. \tag{85}$$

[8] If either $c = 0$ or $\tilde{c} = 0$ then $ab = 0$, in which case one should discard any fractions appearing in eqs. (77) and (78) that are of indeterminate form.

We can rewrite the first part of eq. (84) as follows,

$$\begin{aligned} m\cos\theta_L &= -e^{-2i\alpha}\left(\frac{b^*\tilde{c}}{c^*}b^*\cos\theta_R+\frac{|\tilde{c}|^2}{c^*}e^{-i\phi_R}\sin\theta_R\right) \\ &= e^{-2i\alpha}\big(a\cos\theta_R-ce^{-i\phi_R}\sin\theta_R\big)\,, \end{aligned} \tag{86}$$

after complex conjugating and making use of eq. (79). A similar manipulation (without the complex conjugation) can be performed on the last term of eq. (85). The end result is

$$m\cos\theta_L = e^{-2i\alpha}\big(a\cos\theta_R-ce^{-i\phi_R}\sin\theta_R\big) = -\frac{\tilde{c}^*}{c}e^{2i\beta}\big(a\cos\theta_R-ce^{-i\phi_R}\sin\theta_R\big)\,, \tag{87}$$

$$me^{i\phi_L}\sin\theta_L = \frac{\tilde{c}^*}{c}e^{2i\beta}\big(\tilde{c}\cos\theta_R-be^{-i\phi_R}\sin\theta_R\big) = -e^{-2i\alpha}\big(\tilde{c}\cos\theta_R-be^{-i\phi_R}\sin\theta_R\big)\,. \tag{88}$$

Since both eqs. (87) and (88) cannot simultaneously vanish, it follows that

$$e^{2i(\alpha+\beta)} = -\frac{c}{\tilde{c}^*}\,. \tag{89}$$

We conclude that if θ_R, ϕ_R and $\alpha-\beta$ are taken to be arbitrary parameters, then θ_L and ϕ_L are fixed by eqs. (87) and (88) and $\alpha+\beta$ is fixed by eq. (89). In Appendix A, we show how to employ eqs. (87) and (88) to construct explicit examples of the singular decomposition of a 2×2 complex matrix M that possesses degenerate singular values.

For a simple example of the degenerate case, consider the singular value decomposition of the matrix,

$$M = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\,. \tag{90}$$

Setting $a=b=0$ and $c=\tilde{c}=m=1$ in eqs. (87)–(89), it then follows that

$$\cos\theta_L = e^{i(2\beta-\phi_R)}\sin\theta_R\,, \qquad \sin\theta_L = e^{i(2\beta-\phi_L)}\cos\theta_R\,, \qquad e^{-2i\alpha} = -e^{2i\beta}\,. \tag{91}$$

Hence, we conclude that $\phi_L=\phi_R\equiv\phi$, $\theta_L=\frac{1}{2}\pi-\theta_R$, $\beta=\frac{1}{2}\phi$ and $\alpha=-\frac{1}{2}(\phi\pm\pi)$. Plugging these values into eqs. (47) and (48), we obtain

$$L = \begin{pmatrix} \pm ie^{i\phi/2}\sin\theta_R & e^{i\phi/2}\cos\theta_R \\ \mp ie^{-i\phi/2}\cos\theta_R & e^{-i\phi/2}\sin\theta_R \end{pmatrix}\,, \qquad R = \begin{pmatrix} \pm ie^{i\phi/2}\cos\theta_R & e^{i\phi/2}\sin\theta_R \\ \mp ie^{-i\phi/2}\sin\theta_R & e^{-i\phi/2}\cos\theta_R \end{pmatrix}\,. \tag{92}$$

One can check that $L^{\mathsf{T}}MR=\mathbb{1}_{2\times 2}$. Thus, we have found a family of singular value decompositions of M that depend on two parameters θ_R and ϕ. This does not exhaust all possible singular value decompositions of M, since one is always free to multiply R on the right by $Q\,\mathrm{diag}(e^{-i\chi_1}\,,\,e^{-i\chi_2})$ and multiply L on the right by $Q\,\mathrm{diag}(e^{i\chi_1}\,,\,e^{i\chi_2})$, where Q is an arbitrary real orthogonal 2×2 matrix and $0\leq\chi_i<2\pi$.

We shall now exhibit two different singular value decompositions of M. First, if we choose the lower signs in eq. (92), with $\theta_R=\phi=\frac{1}{2}\pi$, $Q=\mathbb{1}_{2\times 2}$ and $\chi_1=\chi_2=\frac{1}{4}\pi$, then it follows that

$$L = \mathbb{1}_{2\times 2}\,, \qquad R = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\,. \tag{93}$$

Second, choosing the upper signs in eq. (92) with $\theta_R = \frac{1}{4}\pi$, $\phi = \chi_1 = \chi_2 = 0$ and $Q = \mathbb{1}_{2\times 2}$ yields,

$$L = R = \frac{1}{\sqrt{2}}\begin{pmatrix} i & 1 \\ -i & 1 \end{pmatrix} . \tag{94}$$

A singular value decomposition with $L = R$ corresponds to an Autonne-Takagi factorization of a complex symmetric matrix M. This is the subject of the Section 7.

6 The singular value decomposition of a real 2×2 matrix over the space of real matrices

For any real $n \times n$ matrix M, real orthogonal $n \times n$ matrices L and R exist such that

$$L^{\mathsf{T}} M R = M_D = \mathrm{diag}(m_1, m_2, \ldots, m_n), \tag{95}$$

where the m_k are real and nonnegative. This corresponds to the *real* singular value decomposition of M, which is restricted to the space of real matrices. A separate treatment independent of the one presented in Section 5 is warranted. As in the complex case treated in Section 5, the m_k are *not* the eigenvalues of M. Rather, the m_k are the singular values of a real matrix M, which are defined to be the nonnegative square roots of the eigenvalues of either $M^{\mathsf{T}}M$ or MM^{T} (both yield the same results).

An equivalent definition of the singular values can be established as follows. Since $M^{\mathsf{T}}M$ is a nonnegative real symmetric matrix, its eigenvalues are real and nonnegative and its eigenvectors, w_k, defined by $M^{\mathsf{T}}Mw_k = m_k^2 w_k$, can be chosen to be real and orthonormal. First, consider the eigenvectors of $M^{\mathsf{T}}M$ corresponding to the positive eigenvalues, $m_k \neq 0$. We then define the vectors v_k such that $Mw_k = m_k v_k$. It follows that $m_k^2 w_k = M^{\mathsf{T}}Mw_k = m_k M^{\mathsf{T}} v_k$, which yields $M^{\mathsf{T}} v_k = m_k w_k$. Note that these equations also imply that $MM^{\mathsf{T}} v_k = m_k^2 v_k$. The orthonormality of the w_k implies the orthonormality of the v_k,

$$\delta_{jk} = \langle w_j | w_k\rangle = \frac{1}{m_j m_k}\langle M^{\mathsf{T}} v_j | M^{\mathsf{T}} v_k\rangle = \frac{1}{m_j m_k}\langle v_j | MM^{\mathsf{T}} v_k\rangle = \frac{m_k}{m_j}\langle v_j | v_k\rangle \,, \tag{96}$$

which yields $\langle v_j | v_k\rangle = \delta_{jk}$.

Second, if w_i is an eigenvector of $M^{\mathsf{T}}M$ with zero eigenvalue $m_i = 0$, then it follows that $0 = w_i M^{\mathsf{T}} M w_i = \langle M w_i | M w_i\rangle$, which implies that $Mw_i = 0$. Likewise, if v_i is an eigenvector of MM^{T} with zero eigenvalue, then $0 = v_i^{\mathsf{T}} MM^{\mathsf{T}} v_i = \langle M^{\mathsf{T}} v_i | M^{\mathsf{T}} v_i\rangle$, which implies that $M^{\mathsf{T}} v_i = 0$. Because the eigenvectors of MM^{T} [$M^{\mathsf{T}}M$] can be chosen orthonormal, the eigenvectors corresponding to the zero eigenvalues of M [M^{T}] can be taken to be orthonormal. Finally, these eigenvectors are also orthogonal to the eigenvectors corresponding to the nonzero eigenvalues of MM^{T} [$M^{\mathsf{T}}M$]. That is,

$$\langle w_j | w_i\rangle = \frac{1}{m_j}\langle M^{\mathsf{T}} v_j | w_i\rangle = \frac{1}{m_j}\langle v_j | M w_i\rangle = 0 \,, \tag{97}$$

and similarly $\langle v_j | v_i\rangle = 0$, where the index i [j] runs over the eigenvectors corresponding to the zero [nonzero] eigenvalues. Thus, we can define the singular values of a real matrix M to be the simultaneous solutions (with real nonnegative m_k) of,[9]

$$Mw_k = m_k v_k\,, \qquad\qquad v_k^{\mathsf T} M = m_k w_k^{\mathsf T}\,. \tag{98}$$

The corresponding v_k (w_k), normalized to have unit norm, are called the left (right) singular vectors of M.

The real singular value decomposition of a general 2×2 real matrix can be performed fully analytically. Let us consider the non-diagonal real matrix,

$$M = \begin{pmatrix} a & c \\ \tilde{c} & b \end{pmatrix}\,, \tag{99}$$

where at least one of the two quantities c or $\tilde{c}$ is nonzero. The real singular value decomposition of the real matrix M is

$$L^{\mathsf T} M R = \begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix}\,, \tag{100}$$

where L and R are real 2×2 orthogonal matrices and m_1, m_2 are nonnegative. In general, one can parameterize L and R in eq. (100) by

$$L = \begin{pmatrix} \cos\theta_L & \sin\theta_L \\ -\sin\theta_L & \cos\theta_L \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & \varepsilon_L \end{pmatrix}\,, \qquad\qquad R = \begin{pmatrix} \cos\theta_R & \sin\theta_R \\ -\sin\theta_R & \cos\theta_R \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & \varepsilon_R \end{pmatrix}\,, \tag{101}$$

where $-\tfrac{1}{2}\pi < \theta_{L,R} \leq \tfrac{1}{2}\pi$, and $\varepsilon_{L,R} = \pm 1$. Note that $\det L = \varepsilon_L$ and $\det R = \varepsilon_R$, which implies that $\varepsilon_L\varepsilon_R \det M = m_1 m_2$. Since m_1, $m_2 \geq 0$, it follows that $\operatorname{sgn}(\det M) = \varepsilon_L\varepsilon_R$. Thus, only the product of ε_L and ε_R is fixed by eq. (100).

The parameterization of L and R given in eq. (101) is related to that of eqs. (47) and (48) as follows. When M is a real matrix, the quantities $e^{i\phi_L} = \operatorname{sgn}(a\tilde{c} + bc)$ and $e^{i\phi_R} = \operatorname{sgn}(ac + b\tilde{c})$. Hence, we can set $\phi_L = \phi_R = 0$ and redefine $\theta_L \to \theta_L \operatorname{sgn}(a\tilde{c} + bc)$ and $\theta_R \to \theta_R \operatorname{sgn}(ac + b\tilde{c})$, thereby extending the range of these angular variables to $-\tfrac{1}{2}\pi < \theta_{L,R} \leq \tfrac{1}{2}\pi$ as indicated above. Finally, it is convenient to replace the phase matrix P in eqs. (47) and (48) with $\operatorname{diag}(1, \varepsilon_L)$ and $\operatorname{diag}(1, \varepsilon_R)$, respectively, so that the matrices L and R are real orthogonal matrices (rather than the more general unitary matrices).

The singular values $m_{1,2}$ of the matrix M can be determined by taking the positive square root of the nonnegative eigenvalues, $m^2_{1,2}$, of the real orthogonal matrix $M^{\mathsf T}M$,

$$m^2_{1,2} = \tfrac{1}{2}\left[a^2 + b^2 + c^2 + \tilde{c}^2 \mp \Delta\right]\,, \tag{102}$$

in a convention where $0 \leq m_1 \leq m_2$ (i.e., $\Delta \geq 0$), with

$$\begin{aligned} \Delta &\equiv \left[(a^2 - b^2 - c^2 + \tilde{c}^2)^2 + 4(ac + b\tilde{c})^2\right]^{1/2} \\ &= \left[(a^2 + b^2 + c^2 + \tilde{c}^2)^2 - 4(ab - c\tilde{c})^2\right]^{1/2}\,. \end{aligned} \tag{103}$$

Note that

$$m_1^2 + m_2^2 = a^2 + b^2 + c^2 + \tilde{c}^2\,, \qquad\qquad m_1 m_2 = \varepsilon_L\varepsilon_R(ab - c\tilde{c})\,. \tag{104}$$

[9]One can always find a solution to eq. (44) such that the m_k are real and nonnegative. Given a solution where m_k is complex, we simply write $m_k = |m_k|e^{i\theta}$ and redefine $v_k \to v_k e^{i\theta}$ to remove the phase θ.

Moreover, $m_1 = m_2$ if and only if $a = \pm b$ and $c = \mp\tilde{c}$ (where the signs are correlated as indicated), which imply that $ac + b\tilde{c} = 0$ and $\Delta = 0$.

We first assume that $m_1 \neq m_2$. Then, if we rewrite eq. (100) in the form $MR = LM_D$, where $M_D \equiv \text{diag}(m_1\,,\, m_2)$, then we immediately obtain,

$$m_1 \cos\theta_L = a\cos\theta_R - c\sin\theta_R\,, \qquad \varepsilon_L\varepsilon_R m_2 \sin\theta_L = a\sin\theta_R + c\cos\theta_R\,, \tag{105}$$

$$m_1 \sin\theta_L = b\sin\theta_R - \tilde{c}\cos\theta_R\,, \qquad \varepsilon_L\varepsilon_R m_2 \cos\theta_L = \tilde{c}\sin\theta_R + b\cos\theta_R\,. \tag{106}$$

It follows that

$$m_1^2\cos^2\theta_L + m_2^2\sin^2\theta_L = a^2 + c^2\,, \qquad m_1^2\sin^2\theta_L + m_2^2\cos^2\theta_L = b^2 + \tilde{c}^2\,. \tag{107}$$

Subtracting these two equations, and employing eq. (103) yields,

$$\cos 2\theta_L = \frac{b^2 - a^2 - c^2 + \tilde{c}^2}{\Delta}\,, \qquad \cos 2\theta_R = \frac{b^2 - a^2 + c^2 - \tilde{c}^2}{\Delta}\,. \tag{108}$$

In obtaining $\cos 2\theta_R$, it is sufficient to note that eqs. (105)–(107) are valid under the interchange of $c \leftrightarrow \tilde{c}$ and the interchange of the subscripts $L \leftrightarrow R$.[10]

We can also use eqs. (105) and (106) to obtain,

$$m_1^2\cos\theta_L\sin\theta_L = (a\cos\theta_R - c\sin\theta_R)(b\sin\theta_R - \tilde{c}\cos\theta_R)\,, \tag{109}$$

$$m_2^2\cos\theta_L\sin\theta_L = (a\sin\theta_R + c\cos\theta_R)(\tilde{c}\sin\theta_R + b\cos\theta_R)\,. \tag{110}$$

Subtracting these two equations yields

$$\sin 2\theta_L = \frac{2(a\tilde{c} + bc)}{\Delta}\,, \qquad \sin 2\theta_R = \frac{2(ac + b\tilde{c})}{\Delta}\,, \tag{111}$$

after again noting the symmetry under $c \to \tilde{c}$ and the interchange of the subscripts $L \leftrightarrow R$.

Thus, employing eqs. (108) and (111), we have succeeded in uniquely determining the angles θ_L and θ_R (where $-\frac{1}{2}\pi < \theta_{L,R} \leq \frac{1}{2}\pi$). As noted below eq. (101), the individual signs ε_L and ε_R are not separately fixed (implying that one is free to set one of these two signs to $+1$); only the product $\varepsilon_L\varepsilon_R = \text{sgn}(\det M)$ is determined by the singular value decomposition of M.

A useful identity can now be derived that exhibits a simple relation between the angles θ_L and θ_R. First, we note two different trigonometric identities for the tangent function,

$$\tan\theta_L = \frac{1 - \cos 2\theta_L}{\sin 2\theta_L} = \frac{m_2^2 - m_1^2 - b^2 + a^2 + c^2 - \tilde{c}^2}{2(a\tilde{c} + bc)} = \frac{a^2 + c^2 - m_1^2}{a\tilde{c} + bc}\,, \tag{112}$$

$$\tan\theta_R = \frac{\sin 2\theta_R}{1 + \cos 2\theta_R} = \frac{2(ac + b\tilde{c})}{m_2^2 - m_1^2 + b^2 - a^2 + c^2 - \tilde{c}^2} = \frac{ac + b\tilde{c}}{m_2^2 - a^2 - \tilde{c}^2}\,, \tag{113}$$

where we have made use of eqs. (104), (108) and (111). It then follows that

$$\frac{\tan\theta_L}{\tan\theta_R} = \frac{(a^2 + c^2 - m_1^2)(m_2^2 - a^2 - \tilde{c}^2)}{(a\tilde{c} + bc)(ac + b\tilde{c})}\,. \tag{114}$$

[10] One can verify this by rewriting eq. (100) in the form $L^{\mathsf{T}}M = M_D R^{\mathsf{T}}$, which yields equations of the form given by eqs. (105) and (106) with $c \leftrightarrow \tilde{c}$ and the interchange of the subscripts $L \leftrightarrow R$. Note that Δ and hence $m_{1,2}^2$ are unaffected by these interchanges.

The numerator of eq. (114) can be simplified with a little help from eq. (104) as follows,

$$\begin{aligned}(a^2+c^2-m_1^2)(m_2^2-a^2-\tilde{c}^2) &= a^2(m_1^2+m_2^2)+c^2m_2^2-\tilde{c}^2m_1^2-(a^2+c^2)(a^2+\tilde{c}^2)-m_1^2m_2^2 \\ &= a^2(a^2+b^2+c^2+\tilde{c}^2)-(a^2+c^2)(a^2+\tilde{c}^2) \\ &\qquad +c^2m_2^2+\tilde{c}^2m_1^2-(ab-c\tilde{c})^2 \\ &= c^2m_2^2+\tilde{c}^2m_1^2+2(ab-c\tilde{c})c\tilde{c} = (cm_2+\varepsilon_L\varepsilon_R\tilde{c}m_1)^2\,. \end{aligned} \tag{115}$$

Likewise, the denominator of eq. (114) can be simplified as follows,

$$\begin{aligned}(a\tilde{c}+bc)(ac+b\tilde{c}) &= (ab-c\tilde{c})(c^2+\tilde{c}^2)+c\tilde{c}(a^2+b^2+c^2+\tilde{c}^2) \\ &= \varepsilon_L\varepsilon_R m_1m_2(c^2+\tilde{c}^2)+c\tilde{c}(m_1^2+m_2^2) \\ &= (cm_2+\varepsilon_L\varepsilon_R\tilde{c}m_1)(\tilde{c}m_2+\varepsilon_L\varepsilon_R cm_1)\,. \end{aligned} \tag{116}$$

Hence, we end up with a remarkably simple result,

$$\frac{\tan\theta_L}{\tan\theta_R} = \frac{cm_2+\varepsilon_L\varepsilon_R\tilde{c}m_1}{\tilde{c}m_2+\varepsilon_L\varepsilon_R cm_1}\,. \tag{117}$$

The case of $m_1=0$ is noteworthy. This special case arises when $\det M = ab-c\tilde{c}=0$, in which case there is one singular value that is equal to zero. If $\tilde{c}\neq 0$ then inserting $c=ab/\tilde{c}$ into eq. (103) yields $\Delta=(a^2+\tilde{c}^2)(b^2+\tilde{c}^2)/\tilde{c}^2$. It then follows that,[11]

$$\tan\theta_L = \frac{a}{\tilde{c}}\,, \qquad\qquad \tan\theta_R = \frac{\tilde{c}}{b}\,. \tag{118}$$

In particular, after using $ab=c\tilde{c}$, eq. (118) yields

$$\frac{\tan\theta_L}{\tan\theta_R} = \frac{c}{\tilde{c}}\,, \qquad \text{for } m_1=0. \tag{119}$$

This is indeed the correct limit of eq. (117) when $m_1=0$, as expected. In this case, the signs ε_L and ε_R are arbitrary, and one can choose $\varepsilon_L=\varepsilon_R=1$ without loss of generality.

The case of $m\equiv m_1=m_2\neq 0$ must be treated separately. In this case, $a=\pm b$ and $c=\mp\tilde{c}$, which yields $m=(a^2+c^2)^{1/2}$. Since eq. (100) implies that $MR=mL$, one can take R to be an arbitrary 2×2 real orthogonal matrix. Using eq. (101), the matrix L is now determined,

$$\cos\theta_L = \frac{a\cos\theta_R - c\sin\theta_R}{\sqrt{a^2+c^2}}\,, \qquad\qquad \sin\theta_L = \pm\left(\frac{c\cos\theta_R + a\sin\theta_R}{\sqrt{a^2+c^2}}\right)\,, \tag{120}$$

subject to $\varepsilon_L\varepsilon_R=\pm 1$, which determines the sign factor appearing in the expression for $\sin\theta_L$.

Applying the above results to $M=\left(\begin{smallmatrix}0&1\\1&0\end{smallmatrix}\right)$, we have $a=b=0$, $c=\tilde{c}=1$, $m=1$ and $\varepsilon_L\varepsilon_R=-1$. Using eq. (120), it follows that $\cos\theta_L=-\sin\theta_R$ and $\sin\theta_L=-\cos\theta_R$. The corresponding singular value decomposition is given by,

$$\begin{pmatrix}-\sin\theta_R & \cos\theta_R \\ \varepsilon_R\cos\theta_R & \varepsilon_R\sin\theta_R\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\cos\theta_R & \varepsilon_R\sin\theta_R \\ -\sin\theta_R & \varepsilon_R\cos\theta_R\end{pmatrix} = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\,, \tag{121}$$

which is valid for an arbitrary choice of θ_R and an arbitrary choice of sign $\varepsilon_R=-\varepsilon_L=\pm 1$. Eq. (121) provides yet another possible form for the singular value decomposition of $M=\left(\begin{smallmatrix}0&1\\1&0\end{smallmatrix}\right)$, to be compared with the result of eq. (92).

[11]One can repeat this calculation by dividing the equation $ab-c\tilde{c}=0$ by a different nonzero parameter. For example, if $c\neq 0$ then inserting $\tilde{c}=ab/c$ into eq. (103) yields $\Delta=(a^2+c^2)(b^2+c^2)/c^2$, in which case it follows that $\tan\theta_L=c/b$ and $\tan\theta_R=a/c$, and we again recover eq. (119).

7 The Autonne-Takagi factorization of a complex 2×2 symmetric matrix

For any complex symmetric $n \times n$ matrix M, there exists a unitary matrix U such that,[12]

$$U^{\mathsf{T}} M\, U = M_D = \mathrm{diag}(m_1, m_2, \ldots, m_n)\,, \tag{122}$$

where the m_k are real and non–negative. This is the Autonne-Takagi factorization of the complex symmetric matrix M [4, 5], although this nomenclature is sometimes shortened to Takagi factorization. Henceforth, we shall refer to eq. (122) as the Takagi *diagonalization* of a complex symmetric matrix to contrast this with the diagonalization of normal matrices by a unitary similarity transformation treated in Sections 2–4. A proof of eq. (122) is given in Appendix D of Ref. [2] (see also Ref. [1]).

In general, the m_k are *not* the eigenvalues of M. Rather, the m_k are the singular values of the complex symmetric matrix M. From eq. (122) it follows that,

$$U^\dagger M^\dagger M U = M_D^2 = \mathrm{diag}(m_1^2, m_2^2, \ldots, m_n^2)\,. \tag{123}$$

If all of the singular values m_k are non-degenerate, then one can find a solution to eq. (122) for U from eq. (123). This is no longer true if some of the singular values are degenerate. For example, if $M = \left(\begin{smallmatrix} 0 & m \\ m & 0 \end{smallmatrix}\right)$, then the singular value $|m|$ is doubly–degenerate, but eq. (123) yields $U^\dagger U = \mathbb{1}_{2\times 2}$, which does not specify U. That is, in the degenerate case, the Takagi diagonalization *cannot* be determined by the diagonalization of $M^\dagger M$. Instead, one must make direct use of eq. (122).

Eq. (122) can be rewritten as $MU = U^* M_D$, where the columns of U are orthonormal. If we denote the kth column of U by v_k, then,

$$M v_k = m_k v_k^*\,, \tag{124}$$

where the m_k are the singular values and the vectors v_k are normalized to have unit norm. Following Ref. [7], the v_k are called the *Takagi vectors* of the complex symmetric $n \times n$ matrix M.

For a real symmetric matrix M, the Takagi diagonalization [eq. (122)] still holds for a unitary matrix U, which is easily determined as follows. Any real symmetric matrix M can be diagonalized by a real orthogonal matrix Z,

$$Z^{\mathsf{T}} M Z = \mathrm{diag}(\varepsilon_1 m_1\,,\, \varepsilon_2 m_2\,,\, \ldots\,,\, \varepsilon_n m_n)\,, \tag{125}$$

where the m_k are real and nonnegative and the $\varepsilon_k m_k$ are the real eigenvalues of M with corresponding signs $\varepsilon_k = \pm 1$. Then, the Takagi diagonalization of M is achieved by taking $U_{ij} = \varepsilon_i^{1/2} Z_{ij}$ (no sum over i).[13]

[12] In this section, M can be either a real or complex symmetric matrix. In the case of a real symmetric matrix M, there exists a real orthogonal matrix Q such that $Q^{\mathsf{T}} M Q = \mathrm{diag}(m_1, m_2, \ldots m_2)$, where the m_i are the eigenvalues of M. The eigenvalues m_i must be real, but in general they can be either positive, negative or zero. Only in the case of a nonnegative definite real symmetric matrix M, where the eigenvalues m_i are nonnegative, does the decomposition $Q^{\mathsf{T}} M Q = \mathrm{diag}(m_1, m_2, \ldots m_2)$ constitute a Takagi diagonalization of M in the space of real $n \times n$ matrices.

[13] In the case of $m_k = 0$, we conventionally choose the corresponding $\varepsilon_k = +1$.

The Takagi diagonalization of a 2×2 complex symmetric matrix can be performed analytically. Consider the non-diagonal complex symmetric matrix,

$$M = \begin{pmatrix} a & c \\ c & b \end{pmatrix} , \tag{126}$$

where $c \neq 0$. Following Ref. [6], one can parameterize the unitary 2×2 matrix U in eq. (122) as follows,

$$U = VP = \begin{pmatrix} \cos\theta & e^{i\phi}\sin\theta \\ -e^{-i\phi}\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} e^{-i\alpha} & 0 \\ 0 & e^{-i\beta} \end{pmatrix} , \tag{127}$$

where $0 \leq \theta \leq \frac{1}{2}\pi$ and $0 \leq \alpha\,,\,\beta\,,\,\phi < 2\pi$. However, we may restrict the angular parameter space further. The Takagi diagonalization equation is

$$U^{\mathsf{T}} M U = D = \begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix} , \tag{128}$$

where the singular values, m_1 and m_2 are nonnegative. One can derive expressions for the angles θ, ϕ, α and β by setting $c = \tilde{c}$, $\theta_L = \theta_R = \theta$ and $\phi_L = \phi_R = \phi$ in all results obtained in Section 5. However, for pedagogical purposes, a separate derivation of the Takagi diagonalization will be presented in this section. Using eq. (127), one can rewrite eq. (128) as follows,

$$V^{\mathsf{T}} M V = P^* D P^* . \tag{129}$$

However, P^*DP^* is unchanged under the separate transformations, $\alpha \to \alpha + \pi$ and $\beta \to \beta + \pi$. Hence, without loss of generality, one may restrict α and β to the range $0 \leq \alpha\,,\,\beta < \pi$.

Using eq. (127), we can rewrite eq. (129) as follows:

$$MV = V^* \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix} , \tag{130}$$

where

$$\sigma_1 \equiv m_1\, e^{2i\alpha} , \qquad \text{and} \qquad \sigma_2 \equiv m_2\, e^{2i\beta} , \tag{131}$$

with real and nonnegative m_1 and m_2. The singular values of M can be derived by taking the nonnegative square roots of the eigenvalues of $M^\dagger M$,

$$m_{1,2}^2 = |\sigma_{1,2}|^2 = \tfrac{1}{2}\left[|a|^2 + |b|^2 + 2|c|^2 \mp \widetilde{\Delta}\right], \tag{132}$$

in a convention where $0 \leq m_1 \leq m_2$ (i.e., $\widetilde{\Delta} \geq 0$), with

$$\begin{aligned} \widetilde{\Delta} &\equiv \left[(|a|^2 - |b|^2)^2 + 4|a^* c + b c^*|^2\right]^{1/2} \\ &= \left[(|a|^2 + |b|^2 + 2|c|^2)^2 - 4|ab - c^2|^2\right]^{1/2} . \end{aligned} \tag{133}$$

To evaluate the angles ϕ and θ (which determine the matrix V), we multiply out the matrices in eq. (130). The end result is,

$$\sigma_1 = a - c\, e^{-i\phi}\tan\theta = b\, e^{-2i\phi} - c\, e^{-i\phi}\cot\theta , \tag{134}$$

$$\sigma_2 = b + c\, e^{i\phi}\tan\theta \quad = a\, e^{2i\phi} + c\, e^{i\phi}\cot\theta . \tag{135}$$

We first assume that $m_1 \neq m_2$, corresponding to the case of nondegenerate singular values of M. Using either eq. (134) or (135), and making use of the trigonometric identity,

$$\tan 2\theta = 2(\cot\theta - \tan\theta)^{-1}\,, \tag{136}$$

one obtains a simple equation for $\tan 2\theta$,

$$\tan 2\theta = \frac{2c}{b\,e^{-i\phi} - a\,e^{i\phi}}\,. \tag{137}$$

Since $\tan 2\theta$ is real, it follows that

$$\mathrm{Im}(bc^*\,e^{-i\phi} - ac^*\,e^{i\phi}) = 0\,. \tag{138}$$

One can then use eq. (138) to obtain an expression for $e^{2i\phi}$,

$$e^{2i\phi} = \frac{a^*c + bc^*}{ac^* + b^*c}\,, \tag{139}$$

or equivalently,

$$e^{i\phi} = \frac{\varepsilon(a^*c + bc^*)}{|a^*c + bc^*|}\,, \quad \text{where } \varepsilon = \pm 1. \tag{140}$$

The choice of sign in eq. (140) is determined by our convention that $m_1 < m_2$ (in the nondegenerate case) or equivalently, $|\sigma_1|^2 < |\sigma_2|^2$. Thus, to determine ε, we make use of eqs. (134) and (135) to obtain two different expressions for $|\sigma_2|^2 - |\sigma_1|^2$,

$$\begin{aligned} |\sigma_2|^2 - |\sigma_1|^2 &= |b|^2 - |a|^2 + \left[(ac^* + b^*c)e^{i\phi} + (a^*c + bc^*)e^{-i\phi}\right]\tan\theta \\ &= |a|^2 - |b|^2 + \left[(ac^* + b^*c)e^{i\phi} + (a^*c + bc^*)e^{-i\phi}\right]\cot\theta\,. \end{aligned} \tag{141}$$

Using eq. (140) to eliminate ϕ, it follows that

$$|\sigma_2|^2 - |\sigma_1|^2 = |b|^2 - |a|^2 + 2\varepsilon|a^*c + bc^*|\tan\theta = |a|^2 - |b|^2 + 2\varepsilon|a^*c + bc^*|\cot\theta\,. \tag{142}$$

Adding the two expressions given in eq. (142) for $|\sigma_2|^2 - |\sigma_1|^2$, we end up with

$$|\sigma_2|^2 - |\sigma_1|^2 = \varepsilon|a^*c + bc^*|(\tan\theta + \cot\theta)\,. \tag{143}$$

Since $|\sigma_2|^2 > |\sigma_1|^2$ and $0 \leq \theta \leq \frac{1}{2}\pi$, it follows that $\varepsilon = 1$. Moreover, eq. (143) implies that in the case of nondegenerate singular values, $a^*c + bc^* \neq 0$. This latter condition ensures that none of the denominators in eqs. (137), (139) and (140) vanish.

We can now obtain an explicit form for $\tan 2\theta$ by either subtracting the two expressions given in eq. (142) for $|\sigma_2|^2 - |\sigma_1|^2$ or by inserting the result for $e^{i\phi}$ back into eq. (137). Taking into account that $\varepsilon = 1$, both methods yield the same final result,

$$\tan 2\theta = \frac{2|a^*c + bc^*|}{|b|^2 - |a|^2}\,. \tag{144}$$

Using eqs. (136) and (144), it follows that

$$\tan\theta = \frac{|a|^2 - |b|^2 + \widetilde{\Delta}}{2|a^*c + bc^*|}\,, \qquad\qquad \cot\theta = \frac{|b|^2 - |a|^2 + \widetilde{\Delta}}{2|a^*c + bc^*|}\,. \tag{145}$$

If we now insert the results of eq. (145) into eq. (143) with $\varepsilon = 1$, it then follows that,

$$|\sigma_2|^2 - |\sigma_1|^2 = \widetilde{\Delta}\,. \tag{146}$$

One can quickly compute $|\sigma_1|^2 + |\sigma_2|^2$ by noting that,

$$|\sigma_1|^2 + |\sigma_2|^2 = m_1^2 + m_2^2 = \mathrm{Tr}(M^\dagger M) = |a|^2 + |b|^2 + 2|c|^2\,. \tag{147}$$

Adding and subtracting eqs. (146) and (147) reproduces the expressions of $m_{1,2}^2 = |\sigma_{1,2}|^2$ obtained in eq. (132).

It is sometimes more convenient to rewrite eq. (145) in another form,

$$\tan^2\theta = \frac{\widetilde{\Delta} + |a|^2 - |b|^2}{\widetilde{\Delta} - |a|^2 + |b|^2}\,. \tag{148}$$

If we now make use of the trigonometric identity, $\cos 2\theta = (1 - \tan^2\theta)/(1 + \tan^2\theta)$, we end up with a rather simple expression,

$$\cos 2\theta = \frac{|b|^2 - |a|^2}{\widetilde{\Delta}}\,. \tag{149}$$

One can now use this result to derive,

$$\cos\theta = \sqrt{\frac{\widetilde{\Delta} - |a|^2 + |b|^2}{2\widetilde{\Delta}}}\,, \qquad\qquad \sin\theta = \sqrt{\frac{\widetilde{\Delta} + |a|^2 - |b|^2}{2\widetilde{\Delta}}}\,. \tag{150}$$

The final step of the computation is the determination of the angles α and β from eq. (131). Employing eq. (145) together with eq. (140) with $\varepsilon = 1$ and eq. (132), one can establish the following useful results,

$$e^{-i\phi}\tan\theta = \frac{ac^* + b^*c}{|b|^2 + |c|^2 - |\sigma_1|^2}\,, \qquad\qquad e^{i\phi}\tan\theta = \frac{a^*c + bc^*}{|\sigma_2|^2 - |a|^2 - |c|^2}\,. \tag{151}$$

Inserting eq. (151) into eqs. (134) and (135) yields,

$$\sigma_1 = m_1 e^{2i\alpha} = a - c\,e^{-i\phi}\tan\theta = \frac{a\big(|b|^2 - |\sigma_1|^2\big) - b^*c^2}{|b|^2 + |c|^2 - |\sigma_1|^2}\,, \tag{152}$$

$$\sigma_2 = m_2 e^{2i\beta} = b + c\,e^{i\phi}\tan\theta = \frac{b\big(|\sigma_2|^2 - |a|^2\big) + a^*c^2}{|\sigma_2|^2 - |a|^2 - |c|^2}\,. \tag{153}$$

Hence, it immediately follows that,

$$\alpha = \tfrac{1}{2}\arg\big\{a\big(|b|^2 - m_1^2\big) - b^*c^2\big\}\,, \tag{154}$$

$$\beta = \tfrac{1}{2}\arg\big\{b\big(m_2^2 - |a|^2\big) + a^*c^2\big\}\,. \tag{155}$$

The case of $m_1 = 0$ is noteworthy. This special case arises when $\det M = ab - c^2 = 0$, in which case there is one singular value that is equal to zero. In particular, it then follows that $\widetilde{\Delta} = (|a| + |b|)^2$ [cf. eq. (133)] and $m_2^2 = \mathrm{Tr}(M^\dagger M) = |a|^2 + |b|^2 + 2|c|^2$. Inserting $c^2 = ab$ in the latter expression yields $m_2 = |a| + |b|$. In addition,

$$\tan\theta = |a/b|^{1/2}\,, \qquad \phi = \arg(b/c) = \arg(c/a)\,, \qquad \beta = \tfrac{1}{2}\arg b\,. \tag{156}$$

However, α is undefined, since the argument of eq. (154) vanishes. This corresponds to the fact that for a zero singular value, the corresponding (normalized) Takagi vector is only unique up to an overall arbitrary phase.[14] One can now check that all the results obtained above agree with the corresponding results of Section 5 after making the substitutions, $\tilde{c} = c$, $\theta_{L,R} = \theta$ and $\phi_{L,R} = \phi$, as previously noted.

We provide one illuminating example of the above results. Consider the complex symmetric matrix,

$$M = \begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix}. \tag{157}$$

The eigenvalues of M are degenerate and equal to zero. However, there is only one linearly independent eigenvector, which is proportional to $(1\,,\,i)$. Thus, M cannot be diagonalized by a similarity transformation. In contrast, all complex symmetric matrices are Takagi-diagonalizable. The singular values of M are 0 and 2 (since these are the non–negative square roots of the eigenvalues of $M^\dagger M$), which are *not* degenerate. Thus, all the formulae derived above apply in this case. One quickly determines that $\theta = \frac{1}{4}\pi$, $\phi = \frac{1}{2}\pi$, $\beta = \frac{1}{2}\pi$ and α is indeterminate. The resulting Takagi diagonalization is $U^{\mathsf{T}} M U = \mathrm{diag}(0\,,\,2)$ with:

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}\begin{pmatrix} e^{-i\alpha} & 0 \\ 0 & -i \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\alpha} & 1 \\ ie^{-i\alpha} & -i \end{pmatrix}. \tag{158}$$

Thus, U is unique up to an overall factor of -1 and an arbitrary phase α. The latter is a consequence of the presence of a zero singular value. This example illustrates the distinction between the (absolute values of the) eigenvalues of M and its singular values. It also exhibits the fact that one cannot always perform a Takagi diagonalization by computing the eigenvalues and eigenvectors of $M^\dagger M$.

Finally, we treat the case of degenerate nonzero singular values, i.e. $m \equiv m_1 = m_2 \neq 0$. As indicated below eq. (126), we shall continue to assume that $c \neq 0$. In light of eq. (143), the degenerate case arises when

$$a^* c + bc^* = 0\,. \tag{159}$$

If eq. (159) is satisfied, then it follows from eq. (132) that

$$m = m_1 = m_2 = \sqrt{|b|^2 + |c|^2}\,. \tag{160}$$

Moreover, ϕ and θ are indeterminate in light of eqs. (139) and (144). Nevertheless, these two indeterminate angles are related if a, $b \neq 0$. Using eqs. (134), (135) and (159), it follows that,

$$\tan 2\theta = \left[\mathrm{Re}(b/c)c_\phi + \mathrm{Im}(b/c)s_\phi\right]^{-1}, \tag{161}$$

[14] The normalized Takagi vectors are unique up to an overall sign if the corresponding singular values are non–degenerate and non–zero. However, in the case of a zero singular value or a pair of degenerate of singular values, there is more freedom in defining the Takagi vectors. For further details, see Appendix D of Ref. [2].

where $c_\phi \equiv \cos\phi$ and $s_\phi \equiv \sin\phi$. In contrast to eq. (138), the reality of $\tan 2\theta$ imposes no constraint on ϕ in the case of degenerate singular values. Consequently, the angle ϕ is indeed indeterminate.[15] Since ϕ is indeterminate, eq. (161) implies that θ is indeterminate as well, except in the special case of $a = b = 0$. In this latter case, eq. (159) is satisfied and the singular values of M are degenerate. However, eq. (161) does not relate θ to the indeterminate angle ϕ. Indeed, eq. (134) yields $\theta = \frac{1}{4}\pi$, which is also consistent with the $b \to 0$ limit of eq. (161).

In the case of degenerate singular values, eqs. (154) and (155) are no longer valid, as their derivation relies on the results of eqs. (140) and (145), which are indeterminate expressions when $a^*c + bc^* = 0$. Hence, we need another technique to determine the angles α and β. Employing eqs. (134), (135) and (159) we can derive the following results after some manipulations,

$$\sigma_1 = me^{2i\alpha} = -c\,e^{-i\phi}\big[(1+A^2)^{1/2} + iB\big] \tag{162}$$

$$\sigma_2 = me^{2i\beta} = c\,e^{i\phi}\big[(1+A^2)^{1/2} - iB\big]\,, \tag{163}$$

where $m = (|b|^2 + |c|^2)^{1/2}$ and

$$A \equiv \mathrm{Re}(b/c)c_\phi + \mathrm{Im}(b/c)s_\phi\,, \qquad B \equiv \mathrm{Re}(b/c)s_\phi - \mathrm{Im}(b/c)c_\phi\,. \tag{164}$$

Thus, the angles α and β are separately determined by eqs. (162) and (163) in terms of the indeterminate angle ϕ. Nevertheless, the sum $\alpha + \beta$ is independent of ϕ. This is most easily seen by employing eqs. (162) and (163) to obtain,

$$c\sigma_1^* + c^*\sigma_2 = 0\,. \tag{165}$$

Hence, it follows that,

$$e^{2i(\alpha+\beta)} = -\frac{c}{c^*}\,. \tag{166}$$

Thus, the matrix U in eq. (128) is now fixed in terms of the quantity $\alpha+\beta$ and the indeterminate angle ϕ.

We illustrate the above results with the example of $M = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0\end{smallmatrix}\right)$.[16] In this case $M^\dagger M = \mathbb{1}_{2\times 2}$, so U cannot be deduced by diagonalizing $M^\dagger M$. Setting $a = b = 0$ and $c = 1$ in the above formulae, it follows that $m = 1$, $\theta = \frac{1}{4}\pi$, $\sigma_1 = -e^{-i\phi}$ and $\sigma_2 = e^{i\phi}$, which yields $\alpha = -\frac{1}{2}(\phi \pm \pi)$ and $\beta = \frac{1}{2}\phi$. Thus, eq. (127) yields,

$$\begin{aligned} U &= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & e^{i\phi} \\ -e^{-i\phi} & 1\end{pmatrix}\begin{pmatrix} \pm i e^{i\phi/2} & 0 \\ 0 & e^{-i\phi/2}\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} \pm i e^{i\phi/2} & e^{i\phi/2} \\ \mp i e^{-i\phi/2} & e^{-i\phi/2}\end{pmatrix} \\ &= \frac{1}{\sqrt{2}}\begin{pmatrix} i & 1 \\ -i & 1\end{pmatrix}\begin{pmatrix} \pm\cos(\phi/2) & \sin(\phi/2) \\ \mp\sin(\phi/2) & \cos(\phi/2)\end{pmatrix}\,, \end{aligned} \tag{167}$$

which shows that in the case of degenerate singular values, U is unique only up to multiplication on the right by an arbitrary orthogonal matrix.

[15] The same conclusion also follows from eq. (128). If $D = m\mathbb{1}_{2\times 2}$ then $(U\mathcal{O})^{\mathsf{T}} M (U\mathcal{O}) = \mathcal{O}^{\mathsf{T}} D \mathcal{O} = D$ for any real orthogonal matrix $\mathcal{O}$. In particular, ϕ simply represents the freedom to choose $\mathcal{O}$ [cf. eq. (167)].

[16] This example is of particular interest to physicists, since the matrix mM (for positive number m) corresponds to the mass matrix of a Dirac fermion of mass m that arises when expressed in a basis of two-component spinors. The Takagi diagonalization of mM demonstrates that a Dirac fermion of mass m is physically equivalent to two mass-degenerate Majorana fermions of mass m. Further details can be found in Ref. [2].

For completeness, it is instructive to examine the special case of the Takagi diagonalization of a non-diagonal *real* symmetric matrix $M = \left(\begin{smallmatrix} a & c \\ c & b\end{smallmatrix}\right)$, where $c \neq 0$. In this case, the singular values, m_1 and m_2 are the nonnegative square roots of

$$m^2_{1,2} = \tfrac{1}{2}\left[a^2 + b^2 + 2c^2 \mp \widetilde{\Delta}\right], \tag{168}$$

where

$$\widetilde{\Delta} \equiv |a+b|\big[(a-b)^2 + 4c^2\big]^{1/2} = \big[(a^2+b^2+2c^2)^2 - 4(ab-c^2)^2\big]^{1/2}. \tag{169}$$

in a convention where $0 \leq m_1 \leq m_2$. Assuming that $m_1 \neq m_2$, the latter implies that one must take $\varepsilon = 1$ in eq. (140), which yields

$$\phi = \begin{cases} 0\,, & \text{if } \operatorname{sgn}\big(c(a+b)\big) = +1\,, \\ \pi\,, & \text{if } \operatorname{sgn}\big(c(a+b)\big) = -1\,. \end{cases} \tag{170}$$

It is therefore convenient to redefine $\theta \to \theta \operatorname{sgn}\big(c(a+b)\big)$, in which case $-\tfrac{1}{2}\pi < \theta \leq \tfrac{1}{2}\pi$. Then, the Takagi diagonalization of M is given by eq. (128), where

$$U = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} e^{-i\alpha} & 0 \\ 0 & e^{-i\beta} \end{pmatrix}, \tag{171}$$

and the redefined angle θ is given by,

$$\tan\theta = \frac{\widetilde{\Delta} + a^2 - b^2}{2c(a+b)}\,. \tag{172}$$

It then follows that

$$\cos\theta = \sqrt{\frac{\widetilde{\Delta} - a^2 + b^2}{2\widetilde{\Delta}}}\,, \qquad\qquad \sin\theta = \operatorname{sgn}\big(c(a+b)\big)\sqrt{\frac{\widetilde{\Delta} + a^2 - b^2}{2\widetilde{\Delta}}}\,. \tag{173}$$

Finally, one can obtain compact expressions for the angles α and β using eqs. (154) and (155),

$$\alpha = \begin{cases} 0\,, & \text{if } \operatorname{sgn}\big(b\det M - am_1^2\big) = +1, \\ \tfrac{1}{2}\pi\,, & \text{if } \operatorname{sgn}\big(b\det M - am_1^2\big) = -1, \end{cases} \qquad \beta = \begin{cases} 0\,, & \text{if } \operatorname{sgn}\big(bm_2^2 - a\det M\big) = +1, \\ \tfrac{1}{2}\pi\,, & \text{if } \operatorname{sgn}\big(bm_2^2 - a\det M\big) = -1. \end{cases} \tag{174}$$

In the special case of $m_1 = 0$, we have $ab = c^2 \neq 0$, in which case the angle α is indeterminate and $\beta = 0$ $[\tfrac{1}{2}\pi]$ for $b > 0$ $[b < 0]$. Henceforth, we shall assume that $m_1 > 0$.

Considering that $\det M = ab - c^2 = \xi m_1 m_2$, where $\xi \equiv \operatorname{sgn}(ab - c^2)$, it then follows that

$$\alpha = \begin{cases} 0\,, & \text{if } \operatorname{sgn}\big(\xi bm_2 - am_1\big) = +1, \\ \tfrac{1}{2}\pi\,, & \text{if } \operatorname{sgn}\big(\xi bm_2 - am_1\big) = -1, \end{cases} \qquad \beta = \begin{cases} 0\,, & \text{if } \operatorname{sgn}\big(\xi bm_2 - am_1\big) = +\xi, \\ \tfrac{1}{2}\pi\,, & \text{if } \operatorname{sgn}\big(\xi bm_2 - am_1\big) = -\xi. \end{cases} \tag{175}$$

That is, the matrix U is real and orthogonal (corresponding to $\alpha = \beta = 0$) if and only if $ab \geq c^2$ and $bm_2 > am_1$. In Appendix B, we show that $ab \geq c^2$ and $bm_2 > am_1$ are both satisfied if and only if $\det M \geq 0$ and $\operatorname{Tr} M > 0$. In particular, we can identify m_1 and m_2 as the two eigenvalues of M. Hence, in this case the diagonalization of M by a real orthogonal matrix given in Section 4 constitutes a Takagi diagonalization of M [cf. footnote 12].

In the case of $m_1 = m_2$, it follows that $a = -b$, so that $\det M < 0$. Indeed, eq. (166) yields $\alpha + \beta = \tfrac{1}{2}\pi$, which implies that the Takagi diagonalization matrix U is not real, as expected.

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Appendix A Singular value decomposition of a matrix with degenerate singular values revisited

Recall that the singular value decomposition of the 2×2 matrix $M=\left(\begin{smallmatrix} a & c\\ \tilde{c} & b\end{smallmatrix}\right)$ with two degenerate singular values given by $m=\sqrt{|a|^2+|c|^2}$ is,

$$L^{\mathsf{T}} M R = m\mathbb{1}_{2\times 2}\,. \tag{A.1}$$

In general we can parameterize two 2×2 unitary matrices L and R in eq. (41) by

$$L = U_L P_L = \begin{pmatrix} \cos\theta_L & e^{i\phi_L}\sin\theta_L \\ -e^{-i\phi_L}\sin\theta_L & \cos\theta_L \end{pmatrix}\begin{pmatrix} e^{-i\alpha_L} & 0 \\ 0 & e^{-i\beta_L}\end{pmatrix}, \tag{A.2}$$

$$R = U_R P_R = \begin{pmatrix} \cos\theta_R & e^{i\phi_R}\sin\theta_R \\ -e^{-i\phi_R}\sin\theta_R & \cos\theta_R \end{pmatrix}\begin{pmatrix} e^{-i\alpha_R} & 0 \\ 0 & e^{-i\beta_R}\end{pmatrix}, \tag{A.3}$$

Here, we will allow the phase matrices P_L and P_R to be different, although in the end only $\alpha_L+\alpha_R$ and $\beta_L+\beta_R$ are fixed by eq. (A.1).

Consider the case of degenerate singular values treated in Section 5. If $P_L\neq P_R$, then eqs. (87)–(89) are slightly modified,

$$m\cos\theta_L = e^{-i(\alpha_L+\alpha_R)}\big(a\cos\theta_R - ce^{-i\phi_R}\sin\theta_R\big) = -\frac{\tilde{c}^*}{c}e^{i(\beta_L+\beta_R)}\big(a\cos\theta_R - ce^{-i\phi_R}\sin\theta_R\big), \tag{A.4}$$

$$me^{i\phi_L}\sin\theta_L = \frac{\tilde{c}^*}{c}e^{i(\beta_L+\beta_R)}\big(\tilde{c}\cos\theta_R - be^{-i\phi_R}\sin\theta_R\big) = -e^{-i(\alpha_L+\alpha_R)}\big(\tilde{c}\cos\theta_R - be^{-i\phi_R}\sin\theta_R\big). \tag{A.5}$$

Since both eqs. (87) and (88) cannot simultaneously vanish, it follows that

$$e^{i(\alpha_L+\alpha_R+\beta_L+\beta_R)} = -\frac{c}{\tilde{c}^*}\,. \tag{A.6}$$

As previously noted in eq. (79), degenerate singular values exist if and only if

$$|a|=|b|\,,\ |c|=|\tilde{c}|\,,\ \text{and } a^*c=-b\tilde{c}^*. \tag{A.7}$$

Eq. (A.7) also implies that $a^*\tilde{c}=-bc^*$. By re-expressing b in terms of a, c and $\tilde{c}$, one can cast the matrix M in the form,

$$M = \begin{pmatrix} |a|\,e^{i\phi_a} & |c|\,e^{i\phi_c} \\ |c|\,e^{i\phi_{\tilde{c}}} & -|a|\,e^{i(\phi_c+\phi_{\tilde{c}}-\phi_a)}\end{pmatrix} = \begin{pmatrix} e^{i\phi_a/2} & 0 \\ 0 & e^{i(\phi_{\tilde{c}}-\phi_a/2)}\end{pmatrix}\begin{pmatrix} |a| & |c| \\ |c| & -|a|\end{pmatrix}\begin{pmatrix} e^{i\phi_a/2} & 0 \\ 0 & e^{i(\phi_c-\phi_a/2)}\end{pmatrix}, \tag{A.8}$$

where $a \equiv |a|e^{i\phi_a}$, $c \equiv |c|e^{i\phi_c}$ and $\tilde{c} \equiv |c|e^{i\phi_{\tilde{c}}}$ (after making use of $|c| = |\tilde{c}|$).

One possible choice for the singular value decomposition of M [eq. (A.1)] is to employ the unitary matrices

$$L = \begin{pmatrix} e^{-i\phi_a/2} & 0 \\ 0 & e^{-i(\phi_{\tilde{c}}-\phi_a/2)} \end{pmatrix} QP\,, \qquad R = \begin{pmatrix} e^{-i\phi_a/2} & 0 \\ 0 & e^{-i(\phi_c-\phi_a/2)} \end{pmatrix} QP\,, \tag{A.9}$$

where Q is a real orthogonal matrix and P is a 2×2 diagonal phase matrix $P = \mathrm{diag}(i\,,\,1)$. Then, eq. (46) yields

$$Q^{\mathsf{T}} \begin{pmatrix} |a| & |c| \\ |c| & -|a| \end{pmatrix} Q = P^* \begin{pmatrix} m & 0 \\ 0 & m \end{pmatrix} P^* = \begin{pmatrix} -m & 0 \\ 0 & m \end{pmatrix}\,, \tag{A.10}$$

where

$$m = \sqrt{|a|^2 + |c|^2}\,. \tag{A.11}$$

That is, Q is the real orthogonal matrix that diagonalizes the real symmetric matrix, $\left(\begin{smallmatrix} |a| & |c| \\ |c| & -|a| \end{smallmatrix}\right)$, whose eigenvalues are $\lambda_{1,2} = -m,\ m$ (whereas its singular values are degenerate and equal to m). The explicit form for Q can be determined using the results of Section 4.

Hence, one possible choice for the singular value decomposition of M takes the following form in the case degenerate singular values,

$$\begin{aligned} m\mathbb{1}_{2\times 2} = L^{\mathsf{T}} M R &= P^{\mathsf{T}} Q^{\mathsf{T}} \begin{pmatrix} |a| & |c| \\ |c| & -|a| \end{pmatrix} QP \\ &= \begin{pmatrix} i & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} |a| & |c| \\ |c| & -|a| \end{pmatrix} \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} i & 0 \\ 0 & 1 \end{pmatrix}\,, \end{aligned} \tag{A.12}$$

where the rotation angle θ of the orthogonal matrix Q is given by [cf. eqs. (38)–(39)],

$$\cos\theta = \sqrt{\frac{1 - |a|/m}{2}}\,, \qquad \sin\theta = \sqrt{\frac{1 + |a|/m}{2}}\,. \tag{A.13}$$

It is instructive to check that eqs. (A.12) and (A.13) are consistent with the general form of the singular value decomposition in the degenerate case obtained in eqs. (A.4)–(A.6). If we compare eq. (A.9) with the forms for L and R given in eqs. (A.2) and (A.3), we can identify,

$$\begin{aligned} &\theta_L = \theta_R\,, \qquad \alpha_L = \alpha_R = \tfrac{1}{2}(\phi_a - \pi)\,, \qquad \beta_L = \phi_{\tilde{c}} - \tfrac{1}{2}\phi_a\,, \qquad \beta_R = \phi_c - \tfrac{1}{2}\phi_a\,, \\ &\phi_L = \phi_{\tilde{c}} - \phi_a\,, \qquad \phi_R = \phi_c - \phi_a\,. \end{aligned} \tag{A.14}$$

Note that by inserting $c = |c|e^{i\phi_c}$ and $\tilde{c} = |c|e^{i\phi_{\tilde{c}}}$ into eq. (A.6), it follows that

$$\alpha_L + \alpha_R + \beta_L + \beta_R = \phi_c + \phi_{\tilde{c}} - \pi\,, \tag{A.15}$$

which is consistent with eq. (A.14).

Finally, we insert eq. (A.14) into eqs. (A.4) and (A.5) to obtain,

$$m\cos\theta = |c|\sin\theta - |a|\cos\theta\,, \tag{A.16}$$
$$m\sin\theta = |a|\sin\theta + |c|\cos\theta\,, \tag{A.17}$$

where $\theta \equiv \theta_L = \theta_R$. Both equations above are consistent, in light of eq. (A.11), and yield

$$\tan\theta = \frac{|c|}{m-|a|} = \frac{\sqrt{m^2-|a|^2}}{m-|a|} = \sqrt{\frac{m+|a|}{m-|a|}}\,, \tag{A.18}$$

which coincides with the result of eq. (A.13).

Of course, eq. (A.12) is not the most general singular value decomposition of M in the case of degenerate singular values, since we are free to choose a more general form for R that would yield $\theta_L \neq \theta_R$. For example, it is possible to choose $L = \mathbb{1}_{2\times 2}$. To see that this is a consistent choice, we plug this result back into eq. (A.1) to obtain

$$MR = m\mathbb{1}_{2\times 2}\,. \tag{A.19}$$

Multiplying this equation by its adjoint yields,

$$MM^\dagger = M^\dagger M = m^2\mathbb{1}_{2\times 2}\,. \tag{A.20}$$

By explicit computation with $M = \left(\begin{smallmatrix} a & c \\ \tilde{c} & b\end{smallmatrix}\right)$,

$$MM^\dagger = M^\dagger M = (|a|^2+|c|^2)\mathbb{1}_{2\times 2}\,, \tag{A.21}$$

after making use of eq. (A.7). Indeed, eqs. (A.20) and (A.21) are equivalent in light of eq. (A.11). Therefore, it follows that $M^\dagger = m^2 M^{-1}$. Inserting this last result into eq. (A.19), we conclude that one of the singular value decompositions of M in the case of degenerate singular values is given by

$$L^{\mathsf{T}}MR = m\mathbb{1}_{2\times 2}\,, \qquad \text{where } L = \mathbb{1}_{2\times 2} \text{ and } R = \frac{1}{m}M^\dagger. \tag{A.22}$$

By a similar argument, one can obtain another singular value decompositions of M in the case of degenerate singular values by taking $R = \mathbb{1}_{2\times 2}$, which yields

$$L^{\mathsf{T}}MR = m\mathbb{1}_{2\times 2}\,, \qquad \text{where } L = \frac{1}{m}M^* \text{ and } R = \mathbb{1}_{2\times 2}. \tag{A.23}$$

Appendix B On the Takagi diagonalization of a real 2×2 symmetric matrix

At the end of Section 7, we considered the Takagi diagonalization of a real symmetric matrix, $U^T MU = \mathrm{diag}(m_1, m_2)$, where m_1 and m_2 are the singular values of M (which are nonnegative quantities). Thus the Takagi diagonalization of $M = \left(\begin{smallmatrix} a & c \\ c & b\end{smallmatrix}\right)$ differs from the diagonalization of M treated in Section 4 unless the eigenvalues of M are nonnegative. One consequence of eq. (175) is that the Takagi diagonalization matrix U is a real orthogonal matrix if and only if $ab \geq c^2 \neq 0$ and $bm_2 > am_1$. In this Appendix, we shall verify this last assertion.

Since $ab \geq c^2 \neq 0$, then a and b are either both positive or both negative. First, assume that $a, b > 0$. Then, the condition $bm_2 > am_1$ is equivalent to the condition that $(m_2/m_1)^2 > (a/b)^2$. Employing eq. (168), it follows that

$$b^2\big[a^2+b^2+2c^2+\widetilde{\Delta}\big] > a^2\big[a^2+b^2+2c^2-\widetilde{\Delta}\big]\,, \tag{B.1}$$

which yields

$$(a^2+b^2)\widetilde{\Delta} > (a^2-b^2)(a^2+b^2+2c^2)\,. \tag{B.2}$$

This equality is trivially satisfied if $a \leq b$, so let us assume that $a > b$. Then, one can square both sides of the inequality above to obtain,

$$(a^2+b^2)^2\big[(a^2+b^2+2c^2)^2-4(ab-c^2)^2\big]-(a^2-b^2)^2(a^2+b^2+2c^2)^2 > 0\,. \tag{B.3}$$

After some algebraic manipulations, the end result is

$$4c^2(a+b)^2\big[ab(a+b)^2+(ab-c^2)(a-b)^2\big] > 0\,, \tag{B.4}$$

which is manifestly true given that a, $b > 0$ and $ab \geq c^2$.

Second, assume that a, $b < 0$. Then, the condition $bm_2 > am_1$ is equivalent to the condition that $(m_2/m_1)^2 < (a/b)^2$. Following the same steps as above, one obtains inequalities that are never satisfied. Hence, one can conclude that if $ab \geq c^2$, then $bm_2 > am_1$ is satisfied if and only if a, $b > 0$. Finally, the conditions $ab \geq c^2$ and a, $b > 0$ are equivalent to the conditions that $\det M \geq 0$ and $\operatorname{Tr} M > 0$. Thus, when these two conditions are satisfied, then the matrix U can be chosen to be real and orthogonal, in which case the Takagi diagonalization of M reduces to the standard diagonalization of a real symmetric matrix M by a real orthogonal similarity transformation.

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