# A tale of three diagonalizations

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**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 these notes, we carry out each of these diagonalization procedures for the most general $2 \times 2$ matrices for which the diagonalization is possible and provide explicit analytical results in each of the three cases.

In quantum physics, some problems can be reduced to two state systems. The solution to these problems involve the diagonalization of the $2 \times 2$ hermitian matrix Hamiltonian, in which the latter is related by a unitary similarity transformation to a diagonal matrix whose elements are the corresponding (real) eigenvalues. 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 $2 \times 2$ 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, in these notes, we will begin by providing the explicit diagonalization of a general $2 \times 2$ normal matrix.

Two additional diagonalization procedures are common in 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. The mass matrix that arises in a theory of charged fermions is a generic complex matrix. 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 decomposition also produces a diagonal matrix whose diagonal elements are real and nonnegative, corresponding to the physical masses of the neutral fermions.

In these notes, we will apply the three diagonalization procedures mentioned above to a complex normal matrix, a generic complex matrix and a complex symmetric matrix, respectively. In each case, we will diagonalize the corresponding $2 \times 2$ matrix explicitly and provide analytic results for the corresponding diagonalization matrix and the elements of the resulting diagonal matrix.

# 1 The diagonalization of a $2 \times 2$ normal matrix by a unitary similarity transformation

Consider a generic $2 \times 2$ 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]

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

It is then straightforward to verify that the matrix

$$A = e^{-i(\alpha+\beta)/2}(N - a\mathbb{1}_{2\times 2}) = \begin{pmatrix} 0 & |b|e^{i(\alpha-\beta)/2} \\ |b|e^{-i(\alpha-\beta)/2} & (d-a)e^{-i(\alpha+\beta)/2} \end{pmatrix} , \tag{4}$$

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

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

$$U^{-1} N U = \begin{pmatrix} \mu_1 & 0 \\ 0 & \mu_2 \end{pmatrix} , \tag{5}$$

where $\mu_1$ and $\mu_2$ are the eigenvalues of $N$,

$$\mu_{1,2} = \frac{1}{2}\left[a + d \mp \sqrt{(a-d)^2 + 4|b|^2 e^{i(\alpha+\beta)}}\right] . \tag{6}$$

Using eq. (4), it follows that

$$U^{-1} N U = e^{i(\alpha+\beta)/2} U^{-1} A U + a\mathbb{1}_{2\times 2} . \tag{7}$$

Hence, to diagonalize $N$, we must diagonalize the hermitian matrix $A$. We will carry out this procedure in Section 2, 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 $\lambda_1$ and $\lambda_2$, one easily obtains

$$\lambda_{1,2} = \frac{1}{2}\left[(d-a)e^{-i(\alpha+\beta)/2} \mp \sqrt{\big[(d-a)e^{-i(\alpha+\beta)/2}\big]^2 + 4|b|^2}\right] . \tag{8}$$

Note that in light of eq. (3), it follows that $\lambda_1$ and $\lambda_2$ are real numbers. Hence, eq. (7) yields,

$$\mu_{1,2} = e^{i(\alpha+\beta)}\lambda_{1,2} + a . \tag{9}$$

It is straightforward to check that eqs. (9) and (6) are equivalent.

[1] Eqs. (3) and (4) have been inspired by Problem 2.5.P29 of Ref. [1].

## 2 The diagonalization of a $2 \times 2$ hermitian matrix by a unitary similarity transformation

Consider a general $2 \times 2$ hermitian matrix

$$A = \begin{pmatrix} a & c \\ c^* & b \end{pmatrix}, \tag{10}$$

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

$$c = |c|e^{i\phi}, \qquad \text{where } 0 \leq \phi < 2\pi\,. \tag{11}$$

The eigenvalues are the roots of the characteristic equation:

$$\det \begin{pmatrix} a-\lambda & c \\ c^* & b-\lambda \end{pmatrix} = (a-\lambda)(b-\lambda) - |c|^2 = \lambda^2 - \lambda(a+b) + (ab - |c|^2) = 0\,. \tag{12}$$

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

$$\lambda_1 = \tfrac{1}{2}\left[a + b - \sqrt{(a-b)^2 + 4|c|^2}\right] \quad \text{and} \quad \lambda_2 = \tfrac{1}{2}\left[a + b + \sqrt{(a-b)^2 + 4|c|^2}\right], \tag{13}$$

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

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

$$U^{-1}AU = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}, \tag{14}$$

where $\lambda_1$ and $\lambda_2$ are the eigenvalues obtained in eq. (13). Note that one can always transform $U \to e^{i\zeta}U$ without modifying eq. (14), since the phase cancels out. Since $\det U$ is a pure phase, one can choose $\det U = 1$ in eq. (14) without loss of generality. The most general $2 \times 2$ 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 $\lambda_1$ and $\lambda_2$, respectively. But, we are always free to multiply any normalized eigenvector by an arbitrary complex phase. 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 $\chi$. Hence, we will take

$$U = \begin{pmatrix} \cos\theta & e^{i\chi}\sin\theta \\ -e^{-i\chi}\sin\theta & \cos\theta \end{pmatrix}, \tag{15}$$

where

$$0 \leq \theta \leq \tfrac{1}{2}\pi\,, \quad \text{and} \quad 0 \leq \chi < 2\pi\,. \tag{16}$$

We now plug in eq. (15) into eq. (14). Since the off-diagonal terms must vanish, one obtains constraints on the angles $\theta$ and $\chi$. 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

$$\lambda_1 = a\cos^2\theta - 2|c|\cos\theta\sin\theta\cos(\phi-\chi) + b\sin^2\theta\,, \tag{17}$$

$$\lambda_2 = a\sin^2\theta + 2|c|\cos\theta\sin\theta\cos(\phi-\chi) + b\cos^2\theta\,, \tag{18}$$

$$Z = e^{i\chi}\left\{(a-b)\cos\theta\sin\theta + |c|\left[e^{i(\phi-\chi)}\cos^2\theta - e^{-i(\phi-\chi)}\sin^2\theta\right]\right\}. \tag{19}$$

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,

$$\tfrac{1}{2}(a-b)\sin 2\theta + |c|\cos 2\theta\cos(\phi-\chi) = 0\,, \tag{20}$$

$$|c|\sin(\phi-\chi) = 0\,. \tag{21}$$

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 $\theta$ and $\chi$ are arbitrary and hence undefined, as indicated above.

If $c \neq 0$ then eq. (21) yields

$$\sin(\phi-\chi) = 0 \quad \text{and} \quad \cos(\phi-\chi) = \varepsilon\,, \quad \text{where } \varepsilon = \pm 1. \tag{22}$$

We can determine the sign $\varepsilon$ as follows. Since $\lambda_1 \leq \lambda_2$, we subtract eqs. (17) and (18) and make use of eq. (22) to obtain,

$$(a-b)\cos 2\theta - 2\varepsilon|c|\sin 2\theta \geq 0\,. \tag{23}$$

Likewise, we insert eq. (22) into eq. (20), which yields

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

Finally, we multiply eq. (23) by $\sin 2\theta$ and eq. (24) by $\cos 2\theta$ and subtract the two resulting equations. The end result is,

$$2\varepsilon|c| \geq 0\,. \tag{25}$$

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

$$\cos(\phi - \chi) = 1\,, \quad \text{for } c \neq 0. \tag{26}$$

By the conventions established in eqs. (16) and (11), we take $0 \leq \phi\,,\, \chi < 2\pi$. Hence, it follows that

$$\chi = \phi\,. \tag{27}$$

We can now determine $\theta$. Inserting eq. (26) into eq. (20) yields

$$\tan 2\theta = \frac{2|c|}{b-a}\,, \quad \text{for } c \neq 0 \text{ and } a \neq b\,. \tag{28}$$

Note that if $a = b$, then eq. (24) yields $\cos 2\theta = 0$. In light of our convention stated in eq. (16),

$$c \neq 0 \quad \text{and} \quad a = b \quad \Longrightarrow \quad \theta = \tfrac{1}{4}\pi\,. \tag{29}$$

If $c \neq 0$ and $a \neq b$, then we can use eq. (28) with the convention that $\sin 2\theta \geq 0$ [cf. eq. (16)] to conclude that

$$\sin 2\theta = \frac{2|c|}{\sqrt{(b-a)^2 + 4|c|^2}}\,. \tag{30}$$

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

Eq. (31) implies 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. (29).

To summarize, if $c \neq 0$, then eqs. (27), (30) and (31) uniquely specify the diagonalizing matrix $U$ [in the conventions stated in eqs. (16) and (11)]. When $c = 0$ and $a \neq b$, $\chi$ 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. (14), as required by the convention adopted below eq. (13).

# 3 The diagonalization of a $2 \times 2$ real symmetric matrix by an orthogonal similarity transformation

In this section, we consider a special case of the one treated in Section 2 in which the matrix $A$ given in eq. (10) 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. (13) 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. (11) implies that if $c \neq 0$ then $\phi = 0$ or $\phi = \pi$. Eq. (27) then yields

$$\chi = \begin{cases} 0\,, & \text{for } c \neq 0 \text{ and } \phi = 0\,, \\ \pi\,, & \text{for } c \neq 0 \text{ and } \phi = \pi\,, \end{cases} \tag{32}$$

which is equivalent to the statement that

$$e^{i\chi} = \operatorname{sgn} c\,, \quad \text{for real } c \neq 0. \tag{33}$$

It is convenient to redefine $\theta \to \theta \operatorname{sgn} c$ in eq. (15). With this modification, the range of $\theta$ can be taken as[3]

$$-\tfrac{1}{2}\pi < \theta \leq \tfrac{1}{2}\pi\,. \tag{34}$$

The diagonalizing matrix $U$ is now a real orthogonal $2 \times 2$ matrix,

$$U = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}, \qquad \text{where} \quad \begin{cases} c > 0 & \Longrightarrow \quad 0 < \theta < \frac{1}{2}\pi\,, \\ c < 0 & \Longrightarrow \quad -\frac{1}{2}\pi < \theta < 0\,. \end{cases} \tag{35}$$

Hence, for real $c \neq 0$ with the range of $\theta$ given by eq. (34), eqs. (28) and (30) are modified by replacing $|c|$ with $c$ in their numerators. That is,

$$\sin 2\theta = \frac{2c}{\sqrt{(b-a)^2 + 4c^2}}\,, \tag{36}$$

$$\cos 2\theta = \frac{b-a}{\sqrt{(b-a)^2 + 4c^2}}\,. \tag{37}$$

The sign of $c$ determines the quadrant in which $\theta$ lives. Moreover, eq. (37) provides additional information. 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.

# 4 The singular value decomposition of a complex $2 \times 2$ matrix

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

$$L^{\mathsf{T}} M R = M_D = \mathrm{diag}(m_1, m_2, \ldots, m_n), \tag{38}$$

where the $m_k$ are real and nonnegative. This is called the singular value decomposition of the matrix $M$. A proof of eq. (38) 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 $M^\dagger M$ (or equivalently of $MM^\dagger$).

An equivalent definition of the singular values can be established as follows. Since $M^\dagger M$ is an hermitian nonnegative 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 $MM^\dagger v_k^* = m_k^2 v_k^*$. The orthonormality of the $w_k$ implies the orthonormality of the $v_k^*$ (and hence the $v_k$):

$$\delta_{jk} = \langle w_j | w_k \rangle = \frac{1}{m_j m_k} \langle M^\dagger v_j^* | M^\dagger v_k^* \rangle = \frac{1}{m_j m_k} \langle v_j^* | M M^\dagger v_k^* \rangle = \frac{m_k}{m_j} \langle v_j^* | v_k^* \rangle \,, \tag{39}$$

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 $MM^\dagger$ 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 $MM^\dagger$ $[M^\dagger M]$ can be chosen orthonormal, the eigenvectors corresponding to the zero eigenvalues of $M$ $[M^{\mathsf{T}}]$ can be taken to be orthonormal.[5] Finally, these eigenvectors are also orthogonal to the eigenvectors corresponding to the non-zero eigenvalues of $MM^\dagger$ $[M^\dagger M]$. That is,

$$\langle w_j | w_i \rangle = \frac{1}{m_j} \langle M^\dagger v_j^* | w_i \rangle = \frac{1}{m_j} \langle v_j^* | M w_i \rangle = 0 \,, \tag{40}$$

and similarly $\langle v_j | v_i \rangle = 0$, where the index $i$ $[j]$ runs over the eigenvectors corresponding to the zero [non-zero] 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]

$$M w_k = m_k v_k^* \,, \qquad v_k^{\mathsf{T}} M = m_k w_k^\dagger \,. \tag{41}$$

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 $M^\dagger M$ $[MM^\dagger]$, which is equal to the number of linearly independent eigenvectors of $M^\dagger M$ $[MM^\dagger]$ with zero eigenvalue, coincides with the number of linearly independent eigenvectors of $M$ $[M^{\mathsf{T}}]$ 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. (41) 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 $\theta$.

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

$$M = \begin{pmatrix} a & c \\ \tilde{c} & b \end{pmatrix} , \tag{42}$$

where either $c$ or $\tilde{c}$ is non-vanishing. The singular value decomposition of $M$ is

$$L^{\mathsf{T}} M R = \begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix} . \tag{43}$$

In general we can parameterize two $2\times 2$ unitary matrices $L$ and $R$ in eq. (38) by [7][7]

$$L = U_L P = \begin{pmatrix} \cos\theta_L & e^{i\phi_L}\sin\theta_L \\ -e^{-i\phi_L}\sin\theta_L & \cos\theta_L \end{pmatrix} \begin{pmatrix} e^{-i\alpha} & 0 \\ 0 & e^{-i\beta} \end{pmatrix} , \tag{44}$$

$$R = U_R P = \begin{pmatrix} \cos\theta_R & e^{i\phi_R}\sin\theta_R \\ -e^{-i\phi_R}\sin\theta_R & \cos\theta_R \end{pmatrix} \begin{pmatrix} e^{-i\alpha} & 0 \\ 0 & e^{-i\beta} \end{pmatrix} , \tag{45}$$

where $0 \le \theta_{L,R} \le \frac{1}{2}\pi$, and $0 \le \alpha, \beta, \phi_{L,R} < 2\pi$ and $0 \le \alpha,\ \beta < 2\pi$.

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

$$m_{1,2}^2 = \tfrac{1}{2}\big[|a|^2 + |b|^2 + |c|^2 + |\tilde{c}|^2 \mp \Delta\big] , \tag{46}$$

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

$$\begin{aligned} \Delta &\equiv \big[(|a|^2 - |b|^2 - |c|^2 + |\tilde{c}|^2)^2 + 4|a^*c + b\tilde{c}^*|^2\big]^{1/2} \\ &= \big[|a|^2 + |b|^2 + |c|^2 + |\tilde{c}|^2)^2 - 4|ab - c\tilde{c}|^2\big]^{1/2} . \end{aligned} \tag{47}$$

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 $m_1 \ne m_2$. Using the results of Section 2 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

$$M^\dagger M = \begin{pmatrix} |a|^2 + |\tilde{c}|^2 & a^*c + b\tilde{c}^* \\ ac^* + b^*\tilde{c} & |b|^2 + |c|^2 \end{pmatrix} , \tag{48}$$

and $M^* M^{\mathsf{T}}$ is obtained form $M^\dagger M$ by interchanging $c$ and $\tilde{c}$. Applying eqs. (27) and (31) to the diagonalization of $M^\dagger M$ and $M^* M^{\mathsf{T}}$ then yields,

$$\cos\theta_{R,L} = \sqrt{\frac{\Delta + |b|^2 - |a|^2 \pm |c|^2 \mp |\tilde{c}|^2}{2\Delta}} , \qquad \sin\theta_{R,L} = \sqrt{\frac{\Delta - |b|^2 + |a|^2 \mp |c|^2 \pm |\tilde{c}|^2}{2\Delta}} , \tag{49}$$

and

$$e^{i\phi_R} = \frac{a^*c + b\tilde{c}^*}{|a^*c + b\tilde{c}^*|} , \qquad e^{i\phi_L} = \frac{a^*\tilde{c} + bc^*}{|a^*\tilde{c} + bc^*|} . \tag{50}$$

[7]Without loss of generality, we can employ 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. (44) and (45) 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.

For completeness, we note the following expressions that can be derived from eq. (49),

$$\tan 2\theta_R = \frac{|a^*c + b\tilde{c}^*|}{|b|^2 - |a|^2 + |c|^2 - |\tilde{c}|^2}\,, \qquad \tan 2\theta_L = \frac{|a^*\tilde{c} + bc^*|}{|b|^2 - |a|^2 - |c|^2 + |\tilde{c}|^2}\,, \tag{51}$$

In obtaining eq. (51), we employed the following results [which are a consequence of eq. (47)],

$$|a^*c + b\tilde{c}^*| = \tfrac{1}{2}\sqrt{\Delta^2 - (|b|^2 - |a|^2 + |c|^2 - |\tilde{c}|^2)^2}\,, \tag{52}$$

$$|a^*\tilde{c} + bc^*| = \tfrac{1}{2}\sqrt{\Delta^2 - (|b|^2 - |a|^2 - |c|^2 + |\tilde{c}|^2)^2}\,. \tag{53}$$

The final step of the computation is to determine the angles $\alpha$ and $\beta$. To perform this task, we first rewrite eq. (43) as,

$$MU_R = U_L^* \begin{pmatrix} m_1 e^{2i\alpha} & 0 \\ 0 & m_2 e^{2i\beta} \end{pmatrix}\,, \tag{54}$$

where we have made use of eqs. (44) and (45). Setting the diagonal elements of the left hand side and the right hand side of eq. (54) equal, we end up with the following two equations,

$$m_1 \cos\theta_L e^{2i\alpha} = a\cos\theta_R - c\, e^{-i\phi_R}\sin\theta_R\,, \tag{55}$$

$$m_2 \cos\theta_L e^{2i\beta} = b\cos\theta_R + \tilde{c}\, e^{i\phi_R}\sin\theta_R\,. \tag{56}$$

Next, we multiply both eqs. (55) and (56) by $\Delta\cos\theta_R$. Employing eqs. (49)–(50) on the right hand sides of the two resulting equations then yields,

$$\begin{aligned}\Delta\, m_1 \cos\theta_L \cos\theta_R e^{2i\alpha} &= \tfrac{1}{2}a\big(\Delta + |b|^2 - |a|^2 + |c|^2 - |\tilde{c}|^2\big) \\ &\quad - \frac{c(ac^* + b^*\tilde{c})}{2|a^*c + b\tilde{c}^*|}\sqrt{\Delta^2 - (|b|^2 - |a|^2 + |c|^2 - |\tilde{c}|^2)^2}\,, \end{aligned} \tag{57}$$

$$\begin{aligned}\Delta\, m_2 \cos\theta_L \cos\theta_R e^{2i\beta} &= \tfrac{1}{2}b\big(\Delta + |b|^2 - |a|^2 + |c|^2 - |\tilde{c}|^2\big) \\ &\quad - \frac{\tilde{c}(a^*c + b\tilde{c}^*)}{2|a^*c + b\tilde{c}^*|}\sqrt{\Delta^2 - (|b|^2 - |a|^2 + |c|^2 - |\tilde{c}|^2)^2}\,. \end{aligned} \tag{58}$$

We can simplify eqs. (57) and (58) further by making use of eq. (52). The end result is,

$$\Delta\, m_1 \cos\theta_L \cos\theta_R e^{2i\alpha} = \tfrac{1}{2}a\big(\Delta + |b|^2 - |a|^2 - |c|^2 - |\tilde{c}|^2\big) - b^*c\tilde{c}\,, \tag{59}$$

$$\Delta\, m_2 \cos\theta_L \cos\theta_R e^{2i\beta} = \tfrac{1}{2}b\big(\Delta + |b|^2 - |a|^2 + |c|^2 + |\tilde{c}|^2\big) + a^*c\tilde{c}\,. \tag{60}$$

Using eq. (46), it is convenient to eliminate $\Delta$ in favor of $m_1^2$ and $m_2^2$ on the right hand side of eqs. (59) and (60). It then immediately follows that,

$$\alpha = \tfrac{1}{2}\arg\big\{a\big(|b|^2 - m_1^2\big) - b^*c\tilde{c}\big\}\,, \tag{61}$$

$$\beta = \tfrac{1}{2}\arg\big\{b\big(m_2^2 - |a|^2\big) + a^*c\tilde{c}\big\}\,. \tag{62}$$

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. In particular, it then follows that $\Delta = |a|^2 + |b|^2 + |c|^2 + |\tilde{c}|^2$ [cf. eq. (47)] and

$$m_2^2 = \mathrm{Tr}(M^\dagger M) = |a|^2 + |b|^2 + |c|^2 + |\tilde{c}|^2\,. \tag{63}$$

Eqs. (49) and (50) then yield,[8]

$$\cos 2\theta_R = \frac{|c|^2 - |a|^2}{|c|^2 + |a|^2}\,, \qquad \cos 2\theta_L = \frac{|b|^2 - |c|^2}{|b|^2 + |c|^2}\,, \tag{64}$$

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

$$\phi_R = \phi_L = \arg(b/c)\,, \qquad \beta = \tfrac{1}{2}\arg b\,. \tag{65}$$

As expected the angle $\alpha$ is undefined when $m_1 = 0$ [cf. eqs. (59) and (61)].

Finally, we treat the case of degenerate non-zero singular values, i.e. $m \equiv m_1 = m_2 \neq 0$. As previously noted below eq. (47), degenerate singular values exist if and only if

$$|a| = |b|\,,\ |c| = |\tilde{c}|\,,\ \text{and}\ a^*c = -b\tilde{c}^*. \tag{66}$$

It follows from eq. (48) that

$$M^\dagger M = m^2 \mathbb{1}_{2\times 2}\,, \tag{67}$$

where the degenerate singular value is

$$m = \sqrt{|a|^2 + |c|^2}\,. \tag{68}$$

Hence, the diagonalization equation, $R^{-1}M^\dagger MR = m^2\mathbb{1}_{2\times 2}$ is satisfied for any unitary matrix $R$. However, this does not necessarily mean that an arbitrary unitary matrix $R$ is a solution to eq. (43). 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 $R$ given in eq. (45) can be taken as arbitrary.

Given the unitary matrix $R$, one can use eq. (43) to determine the matrix elements of the unitary matrix $L$. Using eqs. (44) and (45), it follows that

$$U_L^{\mathsf{T}} = m \begin{pmatrix} e^{2i\alpha} & 0 \\ 0 & e^{2i\beta} \end{pmatrix} U_R^\dagger M^{-1}\,. \tag{69}$$

In light of eqs. (66) and (68),

$$\det M = ab - c\tilde{c} = -\frac{cm^2}{\tilde{c}^*}\,. \tag{70}$$

Evaluating the left and right hand sides of eq. (69) yields,

$$\cos\theta_L = -\frac{\tilde{c}^*}{mc}e^{2i\alpha}\big(b\cos\theta_R + \tilde{c}e^{i\phi_R}\sin\theta_R\big) = -\frac{\tilde{c}^*}{mc}e^{2i\beta}\big(a\cos\theta_R - ce^{-i\phi_R}\sin\theta_R\big)\,, \tag{71}$$

$$e^{i\phi_L}\sin\theta_L = \frac{\tilde{c}^*}{mc}e^{2i\beta}\big(\tilde{c}\cos\theta_R - be^{-i\phi_R}\sin\theta_R\big) = -\frac{\tilde{c}}{mc^*}e^{-2i\alpha}\big(c^*\cos\theta_R + a^*e^{-i\phi_R}\sin\theta_R\big)\,. \tag{72}$$

We can rewrite the first part of eq. (71) as follows,

$$\begin{aligned} m\cos\theta_L &= -e^{-2i\alpha}\left(\frac{b^*\tilde{c}}{c^*}b^*\cos\theta_R + \frac{|\tilde{c}|^2}{c^*}e^{-i\phi_R}\sin\theta_R\right) \\ &= e^{-2i\alpha}\big(a\cos\theta_R - ce^{-i\phi_R}\sin\theta_R\big)\,, \end{aligned} \tag{73}$$

[8]Note that eq. (64) is equivalent to $\tan\theta_R = |a|/|c|$ and $\tan\theta_L = |c|/|b|$, which apply in the case of $m_1 = 0$.

after complex conjugating and making use of eq. (66). A similar manipulation (without the complex conjugation) can be performed on the last term of eq. (72). The end result is

$$m\cos\theta_L = e^{-2i\alpha}\big(a\cos\theta_R - ce^{-i\phi_R}\sin\theta_R\big) = -\frac{\tilde{c}^*}{c}e^{2i\beta}\big(a\cos\theta_R - ce^{-i\phi_R}\sin\theta_R\big)\,, \tag{74}$$

$$me^{i\phi_L}\sin\theta_L = \frac{\tilde{c}^*}{c}e^{2i\beta}\big(\tilde{c}\cos\theta_R - be^{-i\phi_R}\sin\theta_R\big) = -e^{-2i\alpha}\big(\tilde{c}\cos\theta_R - be^{-i\phi_R}\sin\theta_R\big)\,. \tag{75}$$

Since both eqs. (74) and (75) cannot simultaneously vanish, it follows that

$$e^{2i(\alpha+\beta)} = -\frac{c}{\tilde{c}^*}\,. \tag{76}$$

We conclude that if $\theta_R$, $\phi_R$ and $\alpha-\beta$ are taken to be arbitrary parameters, then $\theta_L$ and $\phi_L$ are fixed by eqs. (74) and (75) and $\alpha+\beta$ is fixed by eq. (76). In the Appendix, we show how to employ eqs. (74) and (75) to construct explicit examples of the singular decomposition of a $2\times 2$ complex matrix $M$ that possesses degenerate singular values.

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

$$M = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\,. \tag{77}$$

Setting $a=b=0$ and $c=\tilde{c}=m=1$ in eqs. (74)–(76), it then follows that

$$\cos\theta_L = e^{i(2\beta-\phi_R)}\sin\theta_R\,, \qquad \sin\theta_L = e^{i(2\beta-\phi_L)}\cos\theta_R\,, \qquad e^{-2i\alpha} = -e^{2i\beta}\,. \tag{78}$$

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. (44) and (45), we obtain

$$L = \begin{pmatrix} \pm ie^{i\phi/2}\sin\theta_R & e^{i\phi/2}\cos\theta_R \\ \mp ie^{-i\phi/2}\cos\theta_R & e^{-i\phi/2}\sin\theta_R \end{pmatrix}\,, \qquad R = \begin{pmatrix} \pm ie^{i\phi/2}\cos\theta_R & e^{i\phi/2}\sin\theta_R \\ \mp ie^{-i\phi/2}\sin\theta_R & e^{-i\phi/2}\cos\theta_R \end{pmatrix}\,. \tag{79}$$

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 $\theta_R$ and $\phi$. 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 $0\leq\chi_i<2\pi$.

We shall now exhibit two different singular value decompositions of $M$. First, if we choose the lower signs in eq. (79), 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

$$L = \mathbb{1}_{2\times 2}\,, \qquad R = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\,. \tag{80}$$

Second, choosing the upper signs in eq. (79) with $\theta_R=\frac{1}{4}\pi$, $\phi=\chi_1=\chi_2=0$ and $Q=\mathbb{1}_{2\times 2}$ yields,

$$L = R = \frac{1}{\sqrt{2}}\begin{pmatrix} i & 1 \\ -i & 1 \end{pmatrix}\,. \tag{81}$$

The singular value decomposition with $L=R$ corresponds to the Autonne-Takagi factorization of a symmetric matrix $M$. This is the subject of the next section.

# 5 The Autonne-Takagi factorization of a complex $2 \times 2$ symmetric matrix

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

$$U^{\mathsf{T}} M\, U = M_D = \mathrm{diag}(m_1, m_2, \ldots, m_n)\,, \tag{82}$$

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 sometimes shortened to Takagi factorization. Henceforth, we shall refer to eq. (82) 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 1–3. A proof of eq. (82) 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. (82) it follows that:

$$U^{\dagger} M^{\dagger} M U = M_D^2 = \mathrm{diag}(m_1^2, m_2^2, \ldots, m_n^2)\,. \tag{83}$$

If all of the singular values $m_k$ are non-degenerate, then one can find a solution to eq. (82) for $U$ from eq. (83). 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. (83) 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. (82).

Eq. (82) can be rewritten as $MU = U^* M_D$, where the columns of $U$ are orthonormal. If we denote the $k$th column of $U$ by $v_k$, then,

$$M v_k = m_k v_k^*\,, \tag{84}$$

where the $m_k$ are the singular values and the vectors $v_k$ are normalized to have unit norm. Following Ref. [6], 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. (82)] 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 $Z$,

$$Z^{\mathsf{T}} M Z = \mathrm{diag}(\varepsilon_1 m_1\,,\, \varepsilon_2 m_2\,,\, \ldots\,,\, \varepsilon_n m_n)\,, \tag{85}$$

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 $i$).[9]

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

$$M = \begin{pmatrix} a & c \\ c & b \end{pmatrix}\,, \tag{86}$$

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

where $c \neq 0$. We parameterize the $2 \times 2$ unitary matrix $U$ in eq. (82) by [7],

$$U = VP = \begin{pmatrix} \cos\theta & e^{i\phi}\sin\theta \\ -e^{-i\phi}\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} e^{-i\alpha} & 0 \\ 0 & e^{-i\beta} \end{pmatrix}, \tag{87}$$

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

$$U^{\mathsf{T}} M U = D = \begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix}, \tag{88}$$

where the singular values, $m_1$ and $m_2$ are nonnegative.

One can derive expressions for the angles $\theta$, $\phi$, $\alpha$ and $\beta$ by setting $c = \tilde{c}$, $\theta_L = \theta_R = \theta$ and $\phi_L = \phi_R = \phi$ in all results obtained in Section 4. However, for pedagogical purposes, a separate derivation of the Takagi diagonalization will be presented in this section. Using eq. (87), one can rewrite eq. (88) as follows,

$$V^{\mathsf{T}} M V = P^* D P^*\,. \tag{89}$$

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

Using eq. (87), we can rewrite eq. (89) as follows:

$$MV = V^* \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix}, \tag{90}$$

where

$$\sigma_1 \equiv m_1\, e^{2i\alpha}\,, \qquad \text{and} \qquad \sigma_2 \equiv m_2\, e^{2i\beta}\,, \tag{91}$$

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 $M^\dagger M$,

$$m_{1,2}^2 = |\sigma_{1,2}|^2 = \tfrac{1}{2}\left[|a|^2 + |b|^2 + 2|c|^2 \mp \widetilde{\Delta}\right], \tag{92}$$

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

$$\begin{aligned} \widetilde{\Delta} &\equiv \left[(|a|^2 - |b|^2)^2 + 4|a^* c + b c^*|^2\right]^{1/2} \\ &= \left[|a|^2 + |b|^2 + 2|c|^2)^2 - 4|ab - c^2|\right]^{1/2}. \end{aligned} \tag{93}$$

To evaluate the angles $\phi$ and $\theta$ (which determine the matrix $V$), we multiply out the matrices in eq. (90). The end result is,

$$\sigma_1 = a - c\, e^{-i\phi}\tan\theta = b\, e^{-2i\phi} - c\, e^{-i\phi}\cot\theta\,, \tag{94}$$

$$\sigma_2 = b + c\, e^{i\phi}\tan\theta \quad = a\, e^{2i\phi} + c\, e^{i\phi}\cot\theta\,. \tag{95}$$

We first assume that $m_1 \neq m_2$, corresponding to the case of nondegenerate singular values of $M$. Using either eq. (94) or (95), and making use of the trigonometric identity,

$$\tan 2\theta = 2(\cot\theta - \tan\theta)^{-1}\,, \tag{96}$$

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

$$\tan 2\theta = \frac{2c}{b\, e^{-i\phi} - a\, e^{i\phi}}\,. \tag{97}$$

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

$$\mathrm{Im}(bc^*\, e^{-i\phi} - ac^*\, e^{i\phi}) = 0\,. \tag{98}$$

One can then use eq. (98) to obtain an expression for $e^{2i\phi}$,

$$e^{2i\phi} = \frac{a^*c + bc^*}{ac^* + b^*c}\,, \tag{99}$$

or equivalently,

$$e^{i\phi} = \frac{\varepsilon(a^*c + bc^*)}{|a^*c + bc^*|}\,, \quad \text{where } \varepsilon = \pm 1. \tag{100}$$

The choice of sign in eq. (100) 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 $\varepsilon$, we make use of eqs. (94) and (95) to obtain two different expressions for $|\sigma_2|^2 - |\sigma_1|^2$,

$$\begin{aligned} |\sigma_2|^2 - |\sigma_1|^2 &= |b|^2 - |a|^2 + \left[(ac^* + b^*c)e^{i\phi} + (a^*c + bc^*)e^{-i\phi}\right]\tan\theta \\ &= |a|^2 - |b|^2 + \left[(ac^* + b^*c)e^{i\phi} + (a^*c + bc^*)e^{-i\phi}\right]\cot\theta\,. \end{aligned} \tag{101}$$

Using eq. (100) to eliminate $\phi$, it follows that

$$|\sigma_2|^2 - |\sigma_1|^2 = |b|^2 - |a|^2 + 2\varepsilon|a^*c + bc^*|\tan\theta = |a|^2 - |b|^2 + 2\varepsilon|a^*c + bc^*|\cot\theta\,. \tag{102}$$

Adding the two expressions given in eq. (102) for $|\sigma_2|^2 - |\sigma_1|^2$, we end up with

$$|\sigma_2|^2 - |\sigma_1|^2 = \varepsilon|a^*c + bc^*|(\tan\theta + \cot\theta)\,. \tag{103}$$

Since $|\sigma_2|^2 > |\sigma_1|^2$ and $0 \leq \theta \leq \frac{1}{2}\pi$, it follows that $\varepsilon = 1$. Moreover, eq. (103) 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. (97), (99) and (100) vanish.

We can now obtain an explicit form for $\tan 2\theta$ by either subtracting the two expressions given in eq. (102) for $|\sigma_2|^2 - |\sigma_1|^2$ or by inserting the result for $e^{i\phi}$ back into eq. (97). Taking into account that $\varepsilon = 1$, both methods yield the same final result,

$$\tan 2\theta = \frac{2|a^*c + bc^*|}{|b|^2 - |a|^2}\,. \tag{104}$$

Using eqs. (96) and (104), it follows that

$$\tan\theta = \frac{|a|^2 - |b|^2 + \widetilde{\Delta}}{2|a^*c + bc^*|}\,, \qquad \cot\theta = \frac{|b|^2 - |a|^2 + \widetilde{\Delta}}{2|a^*c + bc^*|}\,. \tag{105}$$

If we now insert the results of eq. (105) into eq. (103) with $\varepsilon = 1$, it then follows that,

$$|\sigma_2|^2 - |\sigma_1|^2 = \widetilde{\Delta}\,. \tag{106}$$

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

$$|\sigma_1|^2 + |\sigma_2|^2 = m_1^2 + m_2^2 = \mathrm{Tr}(M^\dagger M) = |a|^2 + |b|^2 + 2|c|^2\,. \tag{107}$$

Adding and subtracting eqs. (106) and (107) reproduces the expressions of $m_{1,2}^2 = |\sigma_{1,2}|^2$ obtained in eq. (92).

It is sometimes more convenient to rewrite eq. (105) in another form,

$$\tan^2\theta = \frac{\widetilde{\Delta} + |a|^2 - |b|^2}{\widetilde{\Delta} - |a|^2 + |b|^2}\,. \tag{108}$$

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,

$$\cos 2\theta = \frac{|b|^2 - |a|^2}{\widetilde{\Delta}}\,. \tag{109}$$

One can now use this result to derive,

$$\cos\theta = \sqrt{\frac{\widetilde{\Delta} - |a|^2 + |b|^2}{2\widetilde{\Delta}}}\,, \qquad \sin\theta = \sqrt{\frac{\widetilde{\Delta} + |a|^2 - |b|^2}{2\widetilde{\Delta}}}\,. \tag{110}$$

The final step of the computation is the determination of the angles $\alpha$ and $\beta$ from eq. (91). Employing eq. (105) together with eq. (100) with $\varepsilon = 1$ and eq. (92), one can establish the following useful results,

$$e^{-i\phi}\tan\theta = \frac{ac^* + b^*c}{|b|^2 + |c|^2 - |\sigma_1|^2}\,, \qquad e^{i\phi}\tan\theta = \frac{a^*c + bc^*}{|\sigma_2|^2 - |a|^2 - |c|^2}\,. \tag{111}$$

Inserting eq. (111) into eqs. (94) and (95) yields,

$$\sigma_1 = m_1 e^{2i\alpha} = a - c\,e^{-i\phi}\tan\theta = \frac{a\big(|b|^2 - |\sigma_1|^2\big) - b^*c^2}{|b|^2 + |c|^2 - |\sigma_1|^2}\,, \tag{112}$$

$$\sigma_2 = m_2 e^{2i\beta} = b + c\,e^{i\phi}\tan\theta = \frac{b\big(|\sigma_2|^2 - |a|^2\big) + a^*c^2}{|\sigma_2|^2 - |a|^2 - |c|^2}\,. \tag{113}$$

Hence, it immediately follows that,

$$\alpha = \tfrac{1}{2}\arg\big\{a\big(|b|^2 - m_1^2\big) - b^*c^2\big\}\,, \tag{114}$$

$$\beta = \tfrac{1}{2}\arg\big\{b\big(m_2^2 - |a|^2\big) + a^*c^2\big\}\,. \tag{115}$$

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. (93)] 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,

$$\tan\theta = |a/b|^{1/2}\,, \qquad \phi = \arg(b/c) = \arg(c/a)\,, \qquad \beta = \tfrac{1}{2}\arg b\,. \tag{116}$$

However, $\alpha$ is undefined, since the argument of eq. (114) 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.[10]

One can now check that all the results obtained above agree with the corresponding results of Section 4 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,

$$M = \begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix}\,. \tag{117}$$

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 [1]. 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 $\alpha$ is indeterminate. The resulting Takagi diagonalization is $U^{\mathsf{T}} M U = \mathrm{diag}(0\,,\,2)$ with:

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}\begin{pmatrix} e^{-i\alpha} & 0 \\ 0 & -i \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}\begin{pmatrix} e^{-i\alpha} & 0 \\ 0 & 1 \end{pmatrix}\,. \tag{118}$$

Thus, $U$ is unique up to an overall factor of $-1$ and an arbitrary phase. 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 non-zero singular values, i.e. $m \equiv m_1 = m_2 \neq 0$. As indicated below eq. (86), we shall continue to assume that $c \neq 0$. In light of eq. (103), the degenerate case arises when

$$a^* c + b c^* = 0\,. \tag{119}$$

If eq. (119) is satisfied, then $|a| = |b|$ and it follows from eq. (92) that

$$m = m_1 = m_2 = \sqrt{|b|^2 + |c|^2}\,. \tag{120}$$

Moreover, $\phi$ and $\theta$ are indeterminate in light of eqs. (99) and (104). Nevertheless, these two indeterminate angles are related if $a$, $b \neq 0$. Using eqs. (94), (95) and (119), it follows that,

$$\tan 2\theta = \left[\mathrm{Re}(b/c)c_\phi + \mathrm{Im}(b/c)s_\phi\right]^{-1}\,, \tag{121}$$

[10]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. (98), the reality of $\tan 2\theta$ imposes no constraint on $\phi$ in the case of degenerate singular values. Consequently, the angle $\phi$ is indeed indeterminate.[11] Since $\phi$ is indeterminate, eq. (121) implies that $\theta$ is indeterminate as well, except in the special case of $a = b = 0$. In this latter case, eq. (119) is satisfied and the singular values of $M$ are degenerate. However, eq. (121) does not relate $\theta$ to the indeterminate angle $\phi$. Indeed, eq. (94) yields $\theta = \frac{1}{4}\pi$, which is also consistent with the $b \to 0$ limit of eq. (121).

In the case of degenerate singular values, eqs. (114) and (115) are no longer valid, as their derivation relies on the results of eqs. (100) and (105), which are indeterminate expressions when $a^*c + bc^* = 0$. Hence, we need another technique to determine the angles $\alpha$ and $\beta$. Employing eqs. (94), (95) and (119) we can derive the following results after some manipulations,

$$\sigma_1 = me^{2i\alpha} = -c\, e^{-i\phi}\big[(1+A^2)^{1/2} + iB\big] \tag{122}$$

$$\sigma_2 = me^{2i\beta} = c\, e^{i\phi}\big[(1+A^2)^{1/2} - iB\big]\,, \tag{123}$$

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

$$A \equiv \mathrm{Re}(b/c)c_\phi + \mathrm{Im}(b/c)s_\phi\,, \qquad B \equiv \mathrm{Re}(b/c)s_\phi - \mathrm{Im}(b/c)c_\phi\,. \tag{124}$$

Thus, the angles $\alpha$ and $\beta$ are separately determined by eqs. (122) and (123) in terms of the indeterminate angle $\phi$. Nevertheless, the sum $\alpha + \beta$ is independent of $\phi$. This is most easily seen by employing eqs. (122) and (123) to obtain,

$$c\sigma_1^* + c^*\sigma_2 = 0\,. \tag{125}$$

Hence, it follows that,

$$e^{2i(\alpha+\beta)} = -\frac{c}{c^*}\,. \tag{126}$$

Thus, the matrix $U$ in eq. (88) is now fixed in terms of the quantity $\alpha+\beta$ and the indeterminate angle $\phi$.

We illustrate the above results with the example of $M = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$. 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. (87) yields,

$$\begin{aligned} U &= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & e^{i\phi} \\ -e^{-i\phi} & 1 \end{pmatrix}\begin{pmatrix} \pm ie^{i\phi/2} & 0 \\ 0 & e^{-i\phi/2} \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} \pm ie^{i\phi/2} & e^{i\phi/2} \\ \mp ie^{-i\phi/2} & e^{-i\phi/2} \end{pmatrix} \\ &= \frac{1}{\sqrt{2}}\begin{pmatrix} i & 1 \\ -i & 1 \end{pmatrix}\begin{pmatrix} \pm\cos(\phi/2) & \sin(\phi/2) \\ \mp\sin(\phi/2) & \cos(\phi/2) \end{pmatrix}\,, \end{aligned} \tag{127}$$

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

[11] The same conclusion also follows from eq. (88). 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, $\phi$ simply represents the freedom to choose $\mathcal{O}$ [cf. eq. (127)].

# Appendix: Singular value decomposition with degenerate singular values revisited

Recall that the singular value decomposition of the $2\times 2$ 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,

$$L^{\mathsf{T}} M R = m \mathbb{1}_{2\times 2}\,. \tag{128}$$

In general we can parameterize two $2 \times 2$ unitary matrices $L$ and $R$ in eq. (38) by

$$L = U_L P_L = \begin{pmatrix} \cos\theta_L & e^{i\phi_L}\sin\theta_L \\ -e^{-i\phi_L}\sin\theta_L & \cos\theta_L \end{pmatrix} \begin{pmatrix} e^{-i\alpha_L} & 0 \\ 0 & e^{-i\beta_L} \end{pmatrix}, \tag{129}$$

$$R = U_R P_R = \begin{pmatrix} \cos\theta_R & e^{i\phi_R}\sin\theta_R \\ -e^{-i\phi_R}\sin\theta_R & \cos\theta_R \end{pmatrix} \begin{pmatrix} e^{-i\alpha_R} & 0 \\ 0 & e^{-i\beta_R} \end{pmatrix}, \tag{130}$$

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. (128)

Consider the case of degenerate singular values treated in Section 4. If $P_L \neq P_R$, then eqs. (74)–(76) are slightly modified,

$$m\cos\theta_L = e^{-i(\alpha_L+\alpha_R)}\big(a\cos\theta_R - ce^{-i\phi_R}\sin\theta_R\big) = -\frac{\tilde{c}^*}{c}e^{i(\beta_L+\beta_R)}\big(a\cos\theta_R - ce^{-i\phi_R}\sin\theta_R\big), \tag{131}$$

$$me^{i\phi_L}\sin\theta_L = \frac{\tilde{c}^*}{c}e^{i(\beta_L+\beta_R)}\big(\tilde{c}\cos\theta_R - be^{-i\phi_R}\sin\theta_R\big) = -e^{-i(\alpha_L+\alpha_R)}\big(\tilde{c}\cos\theta_R - be^{-i\phi_R}\sin\theta_R\big). \tag{132}$$

Since both eqs. (74) and (75) cannot simultaneously vanish, it follows that

$$e^{i(\alpha_L+\alpha_R+\beta_L+\beta_R)} = -\frac{c}{\tilde{c}^*}\,. \tag{133}$$

As previously noted, degenerate singular values exist if and only if

$$|a| = |b|\,,\ |c| = |\tilde{c}|\,,\ \text{and}\ a^*c = -b\tilde{c}^*. \tag{134}$$

Re-expressing $b$ in terms of $a, c$ and $\tilde{c}$, one can cast the matrix $M$ in the form,

$$M = \begin{pmatrix} |a|\,e^{i\phi_a} & |c|\,e^{i\phi_c} \\ |c|\,e^{i\phi_{\tilde{c}}} & -|a|\,e^{i(\phi_c+\phi_{\tilde{c}}-\phi_a)} \end{pmatrix} = \begin{pmatrix} e^{i\phi_a/2} & 0 \\ 0 & e^{i(\phi_{\tilde{c}}-\phi_a/2)} \end{pmatrix} \begin{pmatrix} |a| & |c| \\ |c| & -|a| \end{pmatrix} \begin{pmatrix} e^{i\phi_a/2} & 0 \\ 0 & e^{i(\phi_c-\phi_a/2)} \end{pmatrix}, \tag{135}$$

where $a \equiv |a|\phi_a$, $c \equiv |c|e^{i\phi_c}$ 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. (128)] is to employ the unitary matrices

$$L = \begin{pmatrix} e^{-i\phi_a/2} & 0 \\ 0 & e^{-i(\phi_{\tilde{c}}-\phi_a/2)} \end{pmatrix} QP\,, \qquad R = \begin{pmatrix} e^{-i\phi_a/2} & 0 \\ 0 & e^{-i(\phi_c-\phi_a/2)} \end{pmatrix} QP\,, \tag{136}$$

where $Q$ is a real orthogonal matrix and $P$ is a $2\times 2$ diagonal phase matrix $P = \mathrm{diag}(i\,,1)$. Then, eq. (43) yields

$$Q^{\mathsf{T}}\begin{pmatrix} |a| & |c| \\ |c| & -|a| \end{pmatrix} Q = P^{*}\begin{pmatrix} m & 0 \\ 0 & m \end{pmatrix} P^{*} = \begin{pmatrix} -m & 0 \\ 0 & m \end{pmatrix}\,, \tag{137}$$

where

$$m = \sqrt{|a|^2 + |c|^2}\,. \tag{138}$$

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 3.

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

$$\begin{aligned} m\mathbb{1}_{2\times 2} = L^{\mathsf{T}}MR &= P^{\mathsf{T}}Q^{\mathsf{T}}\begin{pmatrix} |a| & |c| \\ |c| & -|a| \end{pmatrix} QP \\ &= \begin{pmatrix} i & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} |a| & |c| \\ |c| & -|a| \end{pmatrix}\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} i & 0 \\ 0 & 1 \end{pmatrix}\,, \end{aligned} \tag{139}$$

where the rotation angle $\theta$ of the orthogonal matrix $Q$ is given by [cf. eqs. (35)–(37)],

$$\cos\theta = \sqrt{\frac{1-|a|/m}{2}}\,, \qquad \sin\theta = \sqrt{\frac{1+|a|/m}{2}}\,. \tag{140}$$

It is instructive to check that eqs. (139) and (140) are consistent with the general form of the singular value decomposition in the degenerate case obtained in eqs. (131)–(133). If we compare eq. (136) with the forms for $L$ and $R$ given in eqs. (129) and (130), we can identify,

$$\begin{aligned} &\theta_L = \theta_R\,, \qquad \alpha_L = \alpha_R = \tfrac{1}{2}(\phi_a - \pi)\,, \qquad \beta_L = \phi_{\tilde{c}} - \tfrac{1}{2}\phi_a\,, \qquad \beta_R = \phi_c - \tfrac{1}{2}\phi_a\,, \\ &\phi_L = \phi_{\tilde{c}} - \phi_a\,, \qquad \phi_R = \phi_c - \phi_a\,. \end{aligned} \tag{141}$$

Note that by inserting $c = |c|e^{i\phi_c}$ and $\tilde{c} = |c|e^{i\phi_{\tilde{c}}}$ into eq. (133), it follows that

$$\alpha_L + \alpha_R + \beta_L + \beta_R = \phi_c + \phi_{\tilde{c}} - \pi\,, \tag{142}$$

which is consistent with eq. (141).

Finally, we insert eq. (141) into eqs. (131) and (132) to obtain,

$$m\cos\theta = |c|\sin\theta - |a|\cos\theta\,, \tag{143}$$

$$m\sin\theta = |a|\sin\theta + |c|\cos\theta\,, \tag{144}$$

where $\theta \equiv \theta_L = \theta_R$. Both equations above are consistent, in light of eq. (138), and yield

$$\tan\theta = \frac{|c|}{m-|a|} = \frac{\sqrt{m^2-|a|^2}}{m-|a|} = \sqrt{\frac{m+|a|}{m-|a|}}\,, \tag{145}$$

which coincides with the result of eq. (140).

Of course, eq. (139) is not the most general singular value decomposition of $M$, since we are free to choose a more general form for $R$ that would yield $\theta_L \neq \theta_R$ via eqs. (131) and (75). Indeed, it is possible to choose $L = \mathbb{1}_{2\times 2}$ by employing the following parameters:

$$\theta_L = \phi_L = \alpha_L = \beta_L = 0\,, \qquad \alpha_R = \phi_a\,, \qquad \beta_R = \phi_c + \phi_{\tilde{c}} - \phi_a - \pi\,, \qquad \phi_R = \phi_c - \phi_a - \pi\,. \tag{146}$$

One can check that eq. (146) is consistent with eqs. (131) and (132). Hence, it follows that,

$$R = \begin{pmatrix} e^{-i\phi_a}\cos\theta_R & e^{-i\phi_{\tilde{c}}}\sin\theta_R \\ e^{-i\phi_c}\sin\theta_R & -e^{-i(\phi_c+\phi_{\tilde{c}})-\phi_a}\cos\theta_R \end{pmatrix}. \tag{147}$$

It then follows that

$$L^{\mathsf{T}} M R = M R = \begin{pmatrix} |a|\cos\theta_R + |c|\sin\theta_R & -(|c|\cos\theta_R - |a|\sin\theta_R)e^{i(\phi_a-\phi_{\tilde{c}})} \\ (|c|\cos\theta_R - |a|\sin\theta_R)e^{-i(\phi_a-\phi_{\tilde{c}})} & |a|\cos\theta_R + |c|\sin\theta_R \end{pmatrix}, \tag{148}$$

where we have used eq. (134) to write

$$b e^{-i(\phi_c+\phi_{\tilde{c}}-\phi_a)} = -|a|\,. \tag{149}$$

Thus, eq. (128) is satisfied if

$$m = \sqrt{|a|^2 + |c|^2} = |a|\cos\theta_R + |c|\sin\theta_R\,, \qquad |c|\cos\theta_R - |a|\sin\theta_R = 0\,. \tag{150}$$

These equations have the unique solution,

$$\sin\theta_R = \frac{|c|}{m}\,, \qquad \cos\theta_R = \frac{|a|}{|m|}\,. \tag{151}$$

Plugging these results back into eq. (147) yields,

$$R = \frac{1}{m} M^\dagger\,. \tag{152}$$

Indeed, in the case of degenerate singular values, the matrix $M^\dagger/m$ is unitary in light of,

$$L^{\mathsf{T}} M R = \frac{1}{m} M M^\dagger = m\mathbb{1}_{2\times 2}\,. \tag{153}$$

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