The Mathematics of Fermion Mass Diagonalization

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Abstract

A pedagogical review on the diagonalization of fermion mass in quantum field theory is given in a coherent and systematic way. This review is an abridged version of a longer review that is currently in preparation.

1 Introduction

In scalar field theory, the diagonalization of the scalar squared-mass matrix M^2 is straightforward. First, consider a collection of real spin-0 fields, $\widehat{\varphi}_i(x)$, where the flavor index i again labels the distinct scalar fields of the collection. The corresponding free-field Lagrangian is given by

$$\mathcal{L} = \tfrac{1}{2}\partial_\mu\widehat{\varphi}_i\,\partial^\mu\widehat{\varphi}_i - \tfrac{1}{2}M^2_{ij}\widehat{\varphi}_i\widehat{\varphi}_j\,, \tag{1}$$

where M^2_{ij} is a real symmetric matrix, and there is an implicit sum over repeated indices. We diagonalize the scalar squared-mass matrix by introducing mass-eigenstates φ_i and the orthogonal matrix Q such that $\widehat{\varphi}_i = Q_{ij}\varphi_j$, with $M^2_{ij}Q_{ik}Q_{j\ell} = m^2_k\delta_{k\ell}$ (no sum over k). In matrix form, the latter reads

$$Q^{\mathsf{T}}M^2Q = \boldsymbol{m}^2 = \mathrm{diag}(m_1^2, m_2^2, \ldots)\,. \tag{2}$$

This is the standard diagonalization problem for a real symmetric matrix. The eigenvalues m_k^2 are real.[1]

Second, consider a collection of complex spin-0 fields, $\widehat{\Phi}_i(x)$. The corresponding free-field Lagrangian is given by

$$\mathcal{L} = \partial_\mu\widehat{\Phi}^*_i\partial^\mu\widehat{\Phi}_i - (M^2)_{ij}\,\widehat{\Phi}_i\widehat{\Phi}^*_j\,, \tag{3}$$

[1]Negative eigenvalues of M^2 imply that the naive vacuum is unstable. One should shift the scalar fields by their vacuum expectation values and check that the resulting scalar squared-matrix possesses only non-negative eigenvalues.

where M^2 is an hermitian matrix. We diagonalize the scalar squared-mass matrix by introducing mass-eigenstates Φ_i and the unitary matrix W such that $\widehat{\Phi}_i = W_{ik}\Phi_k$, with $(M^2)_{ij}W^*_{ik}W_{j\ell} = m_k^2\delta_{k\ell}$ (no sum over k). In matrix form, the latter reads

$$W^\dagger M^2 W = \boldsymbol{M}^2 = \mathrm{diag}(m_1^2, m_2^2, \ldots)\,. \tag{4}$$

This is the standard diagonalization problem for an hermitian matrix. The eigenvalues m_k^2 are real.[1]

In spin-1/2 fermion field theory, the diagonalization of the fermion mass matrix does not take any of the above forms. In this paper, we review the linear algebra theory relevant for the matrix decompositions associated with the charged and neutral spin-1/2 fermion mass matrix diagonalizations, following Appendix D of Ref. [1]. The diagonalization of the charged Dirac fermion mass matrix employs the singular value decomposition[2] of a complex matrix, which is treated in Section 2. The diagonalization of the neutral Majorana fermion mass matrix employs Takagi diagonalization [4, 5] of a complex symmetric matrix, which is treated in Section 3. The relation between these two different diagonalization procedures is explored in Section 4. Sections 5 exhibits an explicit singular value decomposition of a complex 2×2 matrix, and Section 6 performs a Takagi diagonalization of a complex symmetric 2×2 matrix. Finally, in Appendix A, an alternative algorithm for Takagi diagonalization is given.

2 Singular value decomposition

The diagonalization of the charged Dirac fermion mass matrix requires the singular value decomposition of an arbitrary complex matrix M.

Theorem: For any complex [or real] $n\times n$ matrix M, unitary [or real orthogonal] matrices L and R exist such that

$$L^{\mathsf{T}} M R = M_D = \mathrm{diag}(m_1, m_2, \ldots, m_n), \tag{5}$$

where the m_k are real and non-negative. This is called the singular value decomposition of the matrix M (e.g., see refs. [2, 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 non-negative square roots of the eigenvalues of $M^\dagger M$ (or equivalently of $MM^\dagger$). An equivalent definition of the singular

[2]For a discussion of the singular value decomposition of a complex matrix, see e.g. Refs. [2, 3].

values can be established as follows. Since $M^\dagger M$ is an hermitian non-negative matrix, its eigenvalues are real and non-negative and its eigenvectors, v_k, defined by $M^\dagger M v_k = m_k^2 v_k$, can be chosen to be orthonormal.[3] Consider first the eigenvectors corresponding to the non-zero eigenvalues of $M^\dagger M$. Then, we define the vectors w_k such that $Mv_k = m_k w_k^*$. It follows that $m_k^2 v_k = M^\dagger M v_k = m_k M^\dagger w_k^*$, which yields: $M^\dagger w_k^* = m_k v_k$. Note that these equations also imply that $MM^\dagger w_k^* = m_k^2 w_k^*$. The orthonormality of the v_k implies the orthonormality of the w_k, and vice versa. For example,

$$\delta_{jk} = \langle v_j | v_k \rangle = \frac{1}{m_j m_k} \langle M^\dagger w_j^* | M^\dagger w_k^* \rangle = \frac{1}{m_j m_k} \langle w_j | M M^\dagger w_k^* \rangle = \frac{m_k}{m_j} \langle w_j^* | w_k^* \rangle \,, \tag{6}$$

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

If v_i is an eigenvector of $M^\dagger M$ with zero eigenvalue, then $0 = v_i^\dagger M^\dagger M v_i = \langle M v_i | M v_i \rangle$, which implies that $Mv_i = 0$. Likewise, if w_i^* is an eigenvector of $MM^\dagger$ with zero eigenvalue, then $0 = w_i^{\mathsf{T}} M M^\dagger w_i^* = \langle M^{\mathsf{T}} w_i | M^{\mathsf{T}} w_i \rangle^*$, which implies that $M^{\mathsf{T}} w_i = 0$. Because the eigenvectors of $M^\dagger M$ $[MM^\dagger]$ can be chosen orthonormal, the eigenvectors corresponding to the zero eigenvalues of M $[M^\dagger]$ can be taken to be orthonormal.[4] Finally, these eigenvectors are also orthogonal to the eigenvectors corresponding to the non-zero eigenvalues of $M^\dagger M$ $[MM^\dagger]$. That is, if the indices i and j run over the eigenvectors corresponding to the zero and non-zero eigenvalues of $M^\dagger M$ $[MM^\dagger]$, respectively, then

$$\langle v_j | v_i \rangle = \frac{1}{m_j} \langle M^\dagger w_j^* | v_i \rangle = \frac{1}{m_j} \langle w_j^* | M v_i \rangle = 0 \,, \tag{7}$$

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

Thus, we can define the singular values of a general complex $n \times n$ matrix M to be the simultaneous solutions (with real non-negative m_k) of:[5]

$$M v_k = m_k w_k^* \,, \qquad\qquad w_k^{\mathsf{T}} M = m_k v_k^\dagger \,. \tag{8}$$

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

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

[4] This analysis shows that the number of linearly independent zero eigenvectors of $M^\dagger M$ $[MM^\dagger]$ with zero eigenvalue, coincides with the number of linearly independent eigenvectors of M $[M^\dagger]$ with zero eigenvalue.

[5] One can always find a solution to eq. (8) such that the m_k are real and non-negative. Given a solution where m_k is complex, we simply write $m_k = |m_k| e^{i\theta}$ and redefine $w_k \to w_k e^{i\theta}$ to remove the phase θ.

Proof of the singular value decomposition theorem: Eqs. (6) and (7) imply that the right [left] singular vectors can be chosen to be orthonormal. Consequently, the unitary matrix R [L] can be constructed such that its kth column is given by the right [left] singular vector v_k [w_k]. It then follows from eq. (8) that:

$$w_k^{\mathsf{T}} M v_\ell = m_k \delta_{k\ell} \,, \qquad\qquad \text{(no sum over } k\text{).} \tag{9}$$

In matrix form, eq. (9) coincides with eq. (5), and the singular value decomposition is established. If M is real, then the right and left singular vectors, v_k and w_k, can be chosen to be real, in which case eq. (5) holds for real orthogonal matrices L and R.

The singular values of a complex matrix M are unique (up to ordering), as they correspond to the eigenvalues of $M^\dagger M$ (or equivalently the eigenvalues of $MM^\dagger$). The unitary matrices L and R are not unique. The matrix R must satisfy

$$R^\dagger M^\dagger M R = M_D^2 \,, \tag{10}$$

which follows directly from eq. (5) by computing $M_D^\dagger M_D = M_D^2$. That is, R is a unitary matrix that diagonalizes the non-negative definite matrix $M^\dagger M$. Since the eigenvectors of $M^\dagger M$ are orthonormal, each v_k corresponding to a non-degenerate eigenvalue of $M^\dagger M$ can be multiplied by an arbitrary phase $e^{i\theta_k}$. For the case of degenerate eigenvalues, any orthonormal linear combination of the corresponding eigenvectors is also an eigenvector of $M^\dagger M$. It follows that within the subspace spanned by the eigenvectors corresponding to non-degenerate eigenvalues, R is uniquely determined up to multiplication on the right by an arbitrary diagonal unitary matrix. Within the subspace spanned by the eigenvectors of $M^\dagger M$ corresponding to a degenerate eigenvalue, R is determined up to multiplication on the right by an arbitrary unitary matrix.

Once R is fixed, L is obtained from eq. (5):

$$L = (M^{\mathsf{T}})^{-1} R^* M_D \,. \tag{11}$$

However, if some of the diagonal elements of M_D are zero, then L is not uniquely defined. Writing M_D in 2×2 block form such that the upper left block is a diagonal matrix with positive diagonal elements and the other three blocks are equal to the zero matrix of the appropriate dimensions, it follows that, $M_D = M_D W$, where

$$W = \left(\begin{array}{c:c} \mathbb{1} & \mathbb{O} \\ \hdashline \mathbb{O} & W_0 \end{array}\right) , \tag{12}$$

W_0 is an arbitrary unitary matrix whose dimension is equal to the number of zeros that appear in the diagonal elements of M_D, and $\mathbb{1}$ and $\mathbb{O}$ are respectively the identity matrix and zero matrix of the appropriate size. Hence, we can multiply both sides of eq. (11) on the right by W, which means that L is only determined up to multiplication on the right by an arbitrary unitary matrix whose form is given by eq. (12).[6]

3 Takagi Diagonalization

A neutral Majorana fermion mass matrix is complex and symmetric. To identify the physical eigenstates, this matrix must be diagonalized. However, the equation that governs the identification of the physical fermion states is *not* the standard unitary similarity transformation. Instead it is a different diagonalization equation that was discovered by Takagi [4], and rediscovered many times since [2].[7]

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

$$\Omega^{\mathsf{T}} M\,\Omega = M_D = \mathrm{diag}(m_1, m_2, \ldots, m_n)\,, \tag{13}$$

where the m_k are real and non–negative. This is the Takagi diagonalization[8] of the complex symmetric matrix M.

In general, the m_k are *not* the eigenvalues of M. Rather, the m_k are the singular values of the symmetric matrix M. From eq. (13) it follows that:

$$\Omega^\dagger M^\dagger M \Omega = M_D^2 = \mathrm{diag}(m_1^2, m_2^2, \ldots, m_n^2)\,. \tag{14}$$

[6]Of course, one can reverse the above procedure by first determining the unitary matrix L. Eq. (5) implies that $L^{\mathsf{T}} M M^\dagger L^* = M_D^2$, in which case L is determined up to multiplication on the right by an arbitrary [diagonal] unitary matrix within the subspace spanned by the eigenvectors corresponding to the degenerate [non-degenerate] eigenvalues of $MM^\dagger$. Having fixed L, one can obtain $R = M^{-1} L^* M_D$ from eq. (5). As above, R is only determined up to multiplication on the right by a unitary matrix whose form is given by eq. (12).

[7]Subsequently, it was recognized in Ref. [3] that the Takagi diagonalization was first established for nonsingular complex symmetric matrices by Autonne [5].

[8]In Ref. [2], eq. (13) is called the Takagi factorization of a complex symmetric matrix. We choose to refer to this as Takagi *diagonalization* to emphasize and contrast this with the more standard diagonalization of normal matrices by a unitary similarity transformation. In particular, not all *complex* symmetric matrices are diagonalizable by a similarity transformation, whereas complex symmetric matrices are *always* Takagi-diagonalizable.

If all of the singular values m_k are non-degenerate, then one can find a solution to eq. (13) for Ω from eq. (14). 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. (14) yields $\Omega^\dagger\Omega = \mathbb{1}_{2\times 2}$, which does not specify Ω. That is, in the degenerate case, the physical fermion states *cannot* be determined by the diagonalization of $M^\dagger M$. Instead, one must make direct use of eq. (13). Below, we shall present a constructive method for determining Ω that is applicable in both the non-degenerate and the degenerate cases.

Eq. (13) can be rewritten as $M\Omega = \Omega^* M_D$, where the columns of Ω are orthonormal. If we denote the kth column of Ω by v_k, then,

$$M v_k = m_k v_k^* \,, \tag{15}$$

where the m_k are the singular values and the vectors v_k are normalized to have unit norm. Following Ref. [8], the v_k are called the *Takagi vectors* of the complex symmetric $n \times n$ matrix M. The Takagi vectors corresponding to non–degenerate non–zero [zero] singular values are unique up to an overall sign [phase]. Any orthogonal [unitary] linear combination of Takagi vectors corresponding to a set of degenerate non–zero [zero] singular values is also a Takagi vector corresponding to the same singular value. Using these results, one can determine the degree of non–uniqueness of the matrix Ω. For definiteness, we fix an ordering of the diagonal elements of M_D.[9] If the singular values of M are distinct, then the matrix Ω is uniquely determined up to multiplication by a diagonal matrix whose entries are either ± 1 (i.e., a diagonal orthogonal matrix). If there are degeneracies corresponding to non–zero singular values, then within the degenerate subspace, Ω is unique up to multiplication on the right by an arbitrary orthogonal matrix. Finally, in the subspace corresponding to zero singular values, Ω is unique up to multiplication on the right by an arbitrary unitary matrix.

Proof of the Takagi diagonalization. To prove the existence of the Takagi diagonalization of a complex symmetric matrix, it is sufficient to provide an algorithm for constructing the orthonormal Takagi vectors v_k that make up the columns of Ω.[10] This is achieved by rewriting the $n \times n$ complex matrix equation $Mv = mv^*$ [with m real and non–negative] as a $2n \times 2n$ real matrix equation [6]:[11]

$$M_R \begin{pmatrix} \operatorname{Re} v \\ \operatorname{Im} v \end{pmatrix} \equiv \begin{pmatrix} \operatorname{Re} M & -\operatorname{Im} M \\ -\operatorname{Im} M & -\operatorname{Re} M \end{pmatrix} \begin{pmatrix} \operatorname{Re} v \\ \operatorname{Im} v \end{pmatrix} = m \begin{pmatrix} \operatorname{Re} v \\ \operatorname{Im} v \end{pmatrix} \,, \quad \text{where } m \geq 0 \,. \tag{16}$$

[9] Permuting the order of the singular values is equivalent to permuting the order of the columns of Ω.

[10] An alternative algorithm for performing the Takagi diagonaization is given in Appendix A.

[11] A similar method of proof is outlined in Ref. [2], section 4.4, problem 2 (on pp. 212–213) and section 4.6, problem 15 (on p. 254).

Since $M = M^{\mathsf{T}}$, the $2n \times 2n$ matrix $M_R \equiv \left(\begin{smallmatrix} \operatorname{Re} M & -\operatorname{Im} M \\ -\operatorname{Im} M & -\operatorname{Re} M \end{smallmatrix}\right)$ is a real symmetric matrix.[12] In particular, M_R is diagonalizable by a real orthogonal similarity transformation, and its eigenvalues are real. Moreover, if m is an eigenvalue of M_R with eigenvector $(\operatorname{Re} v\,,\ \operatorname{Im} v)$, then $-m$ is an eigenvalue of M_R with (orthogonal) eigenvector $(-\operatorname{Im} v\,,\ \operatorname{Re} v)$. Hence, M_R has an equal number of positive and negative eigenvalues and an even number of zero eigenvalues.[13] Thus, eq. (15) has been converted into an ordinary eigenvalue problem for a real symmetric matrix. Since $m \geq 0$, we solve the eigenvalue problem $M_R u = mu$ for the real eigenvectors $u \equiv (\operatorname{Re} v\,,\ \operatorname{Im} v)$ corresponding to the non–negative eigenvalues of M_R,[14] which then yields the complex Takagi vectors, v. It is straightforward to prove that the total number of linearly independent Takagi vectors is equal to n. Simply note that the orthogonality of $(\operatorname{Re} v_1\,,\ \operatorname{Im} v_1)$ and $(-\operatorname{Im} v_1\,,\ \operatorname{Re} v_1)$ with $(\operatorname{Re} v_2\,,\ \operatorname{Im} v_2)$ implies that $v_1^\dagger v_2 = 0$.

Thus, we have derived a constructive method for obtaining the Takagi vectors v_k. If there are degeneracies, one can always choose the v_k in the degenerate subspace to be orthonormal. The Takagi vectors then make up the columns of the matrix Ω in eq. (13). A numerical package for performing the Takagi diagonalization of a complex symmetric matrix is given in ref. [7] (see also ref. [8, 9] for previous numerical approaches to Takagi diagonalization).

4 Relation between Takagi diagonalization and the singular value decomposition

The Takagi diagonalization is a special case of the singular value decomposition. If the complex matrix M in eq. (5) is symmetric, $M = M^{\mathsf{T}}$, then the Takagi diagonalization corresponds to $\Omega = L = R$. In this case, the right and left singular vectors coincide ($v_k = w_k$) and are identified with the Takagi vectors defined in eq. (15). However as previously noted, the matrix Ω cannot be determined from eq. (14) in cases where there is a degeneracy among the singular values.[15]

[12] The $2n \times 2n$ matrix M_R is a real representation of the $n \times n$ complex matrix M.

[13] Note that $(-\operatorname{Im} v\,,\ \operatorname{Re} v)$ corresponds to replacing v_k in eq. (15) by iv_k. However, for $m < 0$ these solutions are not relevant for Takagi diagonalization (where the m_k are by definition non–negative). The case of $m = 0$ is considered in footnote 14.

[14] For $m = 0$, the corresponding vectors $(\operatorname{Re} v\,,\ \operatorname{Im} v)$ and $(-\operatorname{Im} v\,,\ \operatorname{Re} v)$ are two linearly independent eigenvectors of M_R; but these yield only one independent Takagi vector v (since v and iv are linearly dependent).

[15] This is in contrast to the singular value decomposition, where R can be determined from eq. (10) modulo right multiplication by a [diagonal] unitary matrix in the [non-]degenerate subspace and L is then determined by eq. (11) modulo multiplication on the right by eq. (12).

For example, one possible singular value decomposition of the matrix $M = \left(\begin{smallmatrix} 0 & m \\ m & 0 \end{smallmatrix}\right)$ [with m assumed real and positive] can be obtained by choosing $R = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$ and $L = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$, in which case $L^{\mathsf{T}}MR = \left(\begin{smallmatrix} m & 0 \\ 0 & m \end{smallmatrix}\right) = M_D$. Of course, this is not a Takagi diagonalization because $L \neq R$. Since R is only defined modulo the multiplication on the right by an arbitrary 2×2 unitary matrix $\mathcal{O}$, then at least one singular value decomposition exists that is also a Takagi diagonalization. For the example under consideration, it is not difficult to deduce the Takagi diagonalization: $\Omega^{\mathsf{T}}M\Omega = M_D$, where

$$\Omega = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix} \mathcal{O}\,, \tag{17}$$

and $\mathcal{O}$ is any 2×2 orthogonal matrix.

Since the Takagi diagonalization is a special case of the singular value decomposition, it seems plausible that one can prove the former from the latter. This turns out to be correct; for completeness, we provide the proof below. Our second proof depends on the following lemma:

Lemma: For any symmetric unitary matrix V, there exists a unitary matrix U such that $V = U^{\mathsf{T}}U$.

Proof of the Lemma: For any $n \times n$ unitary matrix V, there exists an hermitian matrix H such that $V = \exp(iH)$ (this is the polar decomposition of V). If $V = V^{\mathsf{T}}$ then $H = H^{\mathsf{T}} = H^*$ (since H is hermitian); therefore H is real symmetric. But, any real symmetric matrix can be diagonalized by an orthogonal transformation. It follows that V can also be diagonalized by an orthogonal transformation. Since the eigenvalues of any unitary matrix are pure phases, there exists a real orthogonal matrix Q such that $Q^{\mathsf{T}}VQ = \text{diag}\,(\mathrm{e}^{\mathrm{i}\theta_1}\,,\, \mathrm{e}^{\mathrm{i}\theta_2}\,,\, \ldots\,,\, \mathrm{e}^{\mathrm{i}\theta_\mathrm{n}})$. Thus, the unitary matrix,

$$U = \text{diag}\,(e^{i\theta_1/2}\,,\, e^{i\theta_2/2}\,,\, \ldots\,,\, e^{i\theta_n/2})\, Q^{\mathsf{T}}\,, \tag{18}$$

satisfies $V = U^{\mathsf{T}}U$ and the lemma is proved. Note that U is unique modulo multiplication on the left by an arbitrary real orthogonal matrix.

Second Proof of the Takagi diagonalization. Starting from the singular value decomposition of M, there exist unitary matrices L and R such that $M = L^*M_DR^\dagger$, where M_D is the diagonal matrix of singular values. Since $M = M^{\mathsf{T}} = R^*M_DL^\dagger$, we have two different singular value decompositions for M. However, as noted below eq. (10), R is unique modulo multiplication on the right by an arbitrary [diagonal] unitary matrix, V, within the [non-]degenerate subspace. Thus, it follows that a [diagonal] unitary matrix V exists such that

$L = RV$. Moreover, $V = V^{\mathsf{T}}$. This is manifestly true within the non-degenerate subspace where V is diagonal. Within the degenerate subspace, M_D is proportional to the identity matrix so that $L^* R^\dagger = R^* L^\dagger$. Inserting $L = RV$ then yields $V^{\mathsf{T}} = V$. Using the Lemma proved above, there exists a unitary matrix U such that $V = U^{\mathsf{T}} U$. That is,

$$L = RU^{\mathsf{T}} U \,, \tag{19}$$

for some unitary matrix U. Moreover, it is now straightforward to show that

$$M_D U^* = U^* M_D \,. \tag{20}$$

To see this, note that within the degenerate subspace, eq. (20) is trivially true since M_D is proportional to the identity matrix. Within the non-degenerate subspace V is diagonal; hence we may choose $U = U^{\mathsf{T}} = V^{1/2}$, so that eq. (20) is true since diagonal matrices commute. Using eqs. (19) and (20), we can write the singular value decomposition of M as follows

$$M = L^* M_D R^\dagger = R^* U^\dagger U^* M_D R^\dagger = (RU^{\mathsf{T}})^* M_D U^* R^\dagger = \Omega^* M_D \Omega^\dagger \,, \tag{21}$$

where $\Omega \equiv RU^{\mathsf{T}}$ is a unitary matrix. Thus the existence of the Takagi diagonalization of an arbitrary complex symmetric matrix [eq. (13)] is once again proved.

5 Singular value decomposition of a 2×2 complex matrix

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 single unitary matrix. Let us consider the complex matrix:

$$M = \begin{pmatrix} a & c \\ \tilde{c} & b \end{pmatrix} , \tag{22}$$

where either c or $\tilde{c}$ is non-vanishing. In general we can parameterize two 2×2 unitary matrices L and R in Eq. (5) by

$$L = U_L P_L = \begin{pmatrix} \cos\theta_L & e^{i\phi_L}\sin\theta_L \\ -e^{-i\phi_L}\sin\theta_L & \cos\theta_L \end{pmatrix} \begin{pmatrix} e^{-i\alpha_L} & 0 \\ 0 & e^{-i\beta_L} \end{pmatrix} , \tag{23}$$

$$R = U_R P_R = \begin{pmatrix} \cos\theta_R & e^{i\phi_R}\sin\theta_R \\ -e^{-i\phi_R}\sin\theta_R & \cos\theta_R \end{pmatrix} \begin{pmatrix} e^{-i\alpha_R} & 0 \\ 0 & e^{-i\beta_R} \end{pmatrix} , \tag{24}$$

where $0 \le \theta_{L,R} \le \pi/2$, $0 \le \phi_{L,R} \le 2\pi$ and $0 \le \alpha_{L,R}, \beta_{L,R} \le 2\pi$. However, as only the sums $\alpha_L + \alpha_R$ and $\beta_L + \beta_R$ are fixed, there is a freedom to set $\alpha_L = \alpha_R = \alpha$ and $\beta_L = \beta_R = \beta$ without loss of generality.

If two singular values $m_{1,2}$ of the matrix M is non-degenerate, then one can determine them by taking the positive square root of the non-negative eigenvalues, $m_{1,2}^2$, of the hermitian matrix $M^\dagger M$:

$$\begin{aligned} m_{1,2}^2 &= \frac{1}{2}\left[|a|^2+|b|^2+|c|^2+|\tilde{c}|^2 \mp \sqrt{(|a|^2-|b|^2+|\tilde{c}|^2-|c|^2)^2+4|ac^*+b^*\tilde{c}|^2}\right] \\ &= \frac{1}{2}\left[|a|^2+|b|^2+|c|^2+|\tilde{c}|^2 \mp \sqrt{(|a|^2+|b|^2+|c|^2+|\tilde{c}|^2)^2-4|ab-c\tilde{c}|^2}\right] \end{aligned} \tag{25}$$

with $0 \le m_1 \le m_2$ by definition. Two eigenvalues become identical only when $|a| = |b|$, $|c| = |\tilde{c}|$ and $ac^* + b^*\tilde{c} = 0$ are satisfied, and the smaller one is vanishing when $\det M = ab - c\tilde{c} = 0$.

Explicitly performing the diagonalization of $M^\dagger M$ by R and $M^* M^T$ by L enables us to compute the rotation angles, $\theta_{L,R}$, and the phases, $e^{i\phi_{L,R}}$:

$$\cos\theta_{L,R} = \sqrt{\frac{\Delta+|b|^2-|a|^2 \pm |\tilde{c}|^2 \mp |c|^2}{2\Delta}} \quad \text{and} \quad \sin\theta_{L,R} = \sqrt{\frac{\Delta-|b|^2+|a|^2 \mp |\tilde{c}|^2 \pm |c|^2}{2\Delta}}, \tag{26}$$

with $\Delta = \left[(|a|^2+|b|^2+|c|^2+|\tilde{c}|^2)^2 - 4|ab-c\tilde{c}|^2\right]^{1/2}$, which is identical to the difference $m_2 - m_1$, and

$$e^{i\phi_L} = \frac{a^*\tilde{c}+bc^*}{|a^*\tilde{c}+bc^*|} \qquad \text{and} \qquad e^{i\phi_R} = \frac{a^*c+b\tilde{c}^*}{|a^*c+b\tilde{c}^*|}\,. \tag{27}$$

The final step of the computation is to determine the angles α and β, inserting Eqs. (26) and (27) into Eq. (5), we end up with:

$$\begin{aligned} \alpha &= \frac{1}{2}\arg\left[a(\Delta+|b|^2-|a|^2) - a(|c|^2+|\tilde{c}|^2) - 2b^*c\tilde{c}\right]\,, \\ \beta &= \frac{1}{2}\arg\left[b(\Delta+|b|^2-|a|^2) + b(|c|^2+|\tilde{c}|^2) + 2a^*c\tilde{c}\right]\,. \end{aligned} \tag{28}$$

As pointed out before, the smaller singular value m_1 is vanishing for $\det M = 0$. In this case, the angle α is undefined while all the other angles are uniquely determined.

We end this subsection by treating the case of degenerate (non-zero) singular values, which arises when $|a| = |b|$, $|c| = |\tilde{c}|$ and $ac^* = -b^*\tilde{c}$. Reexpressing b in terms of a, c and $\tilde{c}$, one can cast the mass matrix in the form:

$$\begin{aligned} M &= \begin{pmatrix} |a|\,e^{i\phi_a} & |c|\,e^{i\phi_c} \\ |c|\;e^{i\phi_{\tilde{c}}} & -|a|\,e^{i(\phi_c+\phi_{\tilde{c}}-\phi_a)} \end{pmatrix} \\ &\equiv \begin{pmatrix} e^{i\phi_a/2} & 0 \\ 0 & e^{i(\phi_{\tilde{c}}-\phi_a/2)} \end{pmatrix} \begin{pmatrix} |a| & |c| \\ |c| & -|a| \end{pmatrix} \begin{pmatrix} e^{i\phi_a/2} & 0 \\ 0 & e^{i(\phi_c-\phi_a/2)} \end{pmatrix}\,. \end{aligned} \tag{29}$$

The two 2×2 diagonal phase matrices in Eq. (29) can be absorbed by redefining the unitary matrices $U_L = \mathrm{diag}(e^{-i\phi_a/2},\, e^{-i(\phi_{\tilde{c}}-\phi_a/2)})\,O$ and $U_R = \mathrm{diag}(e^{-i\phi_a/2},\, e^{-i(\phi_c-\phi_a/2)})\,O$ in terms of an orthogonal matrix O. This orthogonal matrix O, along with a diagonal phase matrix $P_L = P_R = P = \mathrm{diag}(i, 1)$, leads to the diagonalization of the remaining real and symmetric matrix as

$$\begin{aligned} m\,\mathbb{I}_{2\times 2} &= P^T O^T \begin{pmatrix} |a| & |c| \\ |c| & -|a| \end{pmatrix} OP \\ &= \begin{pmatrix} i & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} |a| & |c| \\ |c| & -|a| \end{pmatrix} \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} i & 0 \\ 0 & 1 \end{pmatrix} \end{aligned} \tag{30}$$

with the degenerate singular value $m = \sqrt{|a|^2 + |c|^2}$ and the rotation angle θ of the orthogonal matrix O satisfying

$$\cos\theta = \frac{\sqrt{1 - |a|/m}}{\sqrt{2}} \qquad \text{and} \qquad \sin\theta = \frac{\sqrt{1 + |a|/m}}{\sqrt{2}} \tag{31}$$

We note that in this degenerate case the unitary matrices L and R can be multiplied by any orthogonal matrix to the right while preserving the relation (30).

6 Takagi diagonalization of a 2×2 complex symmetric matrix

The Takagi diagonalization of a 2×2 complex symmetric matrix can be performed analytically.[16] The result is somewhat more complicated than the standard diagonalization of a 2×2 hermitian matrix by a unitary similarity transformation. Nevertheless, the corresponding analytic formulae for the Takagi diagonalization will prove useful in Appendix C in the treatment of nearly degenerate states. Consider the complex symmetric matrix:

$$M = \begin{pmatrix} a & c \\ c & b \end{pmatrix}, \tag{32}$$

where $c \neq 0$ and, without loss of generality, $|a| \leq |b|$. We parameterize the 2×2 unitary matrix U in Eq. (13) by [10]:

$$U = VP = \begin{pmatrix} \cos\theta & e^{i\phi}\sin\theta \\ -e^{-i\phi}\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} e^{-i\alpha} & 0 \\ 0 & e^{-i\beta} \end{pmatrix}, \tag{33}$$

where $0 \leq \theta \leq \pi/2$ and $0 \leq \alpha\,, \beta\,, \phi < 2\pi$. However, we may restrict the angular parameter space further. Since the normalized Takagi vectors are unique up to an overall sign if the

[16] The main results of this subsection have been obtained, e.g., in Ref. [7]. Nevertheless, we provide some of the details here, which include minor improvements over the results previously obtained.

corresponding singular values are non–degenerate and non–zero,[17] one may restrict α and β to the range $0 \leq \alpha\,,\, \beta < \pi$ without loss of generality. Finally, we may restrict θ to the range $0 \leq \theta \leq \pi/4$. This range corresponds to one of two possible orderings of the singular values in the diagonal matrix M_D.

Using the transformation (33), we can rewrite eq. (13) as follows:

$$\begin{pmatrix} a & c \\ c & b \end{pmatrix} V = V^* \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix}\,, \tag{34}$$

where

$$\sigma_1 \equiv m_1\, e^{2i\alpha}\,, \qquad \text{and} \qquad \sigma_2 \equiv m_2\, e^{2i\beta}\,, \tag{35}$$

with real and non–negative m_k. Multiplying out the matrices in Eq. (34) yields:

$$\sigma_1 \;=\; a - c\, e^{-i\phi} t_\theta = b\, e^{-2i\phi} - c\, e^{-i\phi} t_\theta^{-1}\,, \tag{36}$$

$$\sigma_2 \;=\; b + c\, e^{i\phi} t_\theta \;= a\, e^{2i\phi} + c\, e^{i\phi} t_\theta^{-1}\,, \tag{37}$$

where $t_\theta \equiv \tan\theta$. Using either Eq. (36) or (37), one immediately obtains a simple equation for $\tan 2\theta = 2(t_\theta^{-1} - t_\theta)^{-1}$:

$$\tan 2\theta = \frac{2c}{b\, e^{-i\phi} - a\, e^{i\phi}}\,. \tag{38}$$

Since $\tan 2\theta$ is real, it follows that $bc^*\, e^{-i\phi} - ac^*\, e^{i\phi}$ is real and must be equal to its complex conjugate. The resulting equation can be solved for $e^{2i\phi}$:

$$e^{2i\phi} = \frac{bc^* + a^*c}{b^*c + ac^*}\,, \tag{39}$$

or equivalently

$$e^{i\phi} = \frac{bc^* + a^*c}{|bc^* + a^*c|}\,. \tag{40}$$

The (positive) choice of sign in Eq. (40) follows from the fact that $\tan 2\theta \geq 0$ (since by assumption, $0 \leq \theta \leq \pi/4$), which implies $0 \leq c^*(b\, e^{-i\phi} - a\, e^{i\phi}) = |c|^2(|b|^2 - |a|^2)$ after inserting the results of Eq. (40). Since $|b| \geq |a|$ by assumption, the asserted inequality holds as required.

[17] 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 as discussed below Eq. (15). These cases will be treated separately at the end of this subsection.

Inserting the result for $e^{i\phi}$ back into Eq. (38) yields:

$$\tan 2\theta = \frac{2|bc^* + a^*c|}{|b|^2 - |a|^2}\,. \tag{41}$$

One can compute $\tan\theta$ in terms of $\tan 2\theta$ for $0 \leq \theta \leq \pi/4$:

$$\begin{aligned}
\tan\theta &= \frac{1}{\tan 2\theta}\left[\sqrt{1+\tan^2 2\theta} - 1\right] \\
&= \frac{|a|^2 - |b|^2 + \sqrt{(|b|^2 - |a|^2)^2 + 4|bc^* + a^*c|^2}}{2|bc^* + a^*c|}\,, \qquad (42) \\
&= \frac{2|bc^* + a^*c|}{|b|^2 - |a|^2 + \sqrt{(|b|^2 - |a|^2)^2 + 4|bc^* + a^*c|^2}}\,. \qquad (43)
\end{aligned}$$

Starting from Eqs. (36) and (37), it is now straightforward, using Eqs. (40) and (42), to compute the squared magnitudes of σ_k:

$$m_k^2 = |\sigma_k|^2 = \frac{1}{2}\left[|a|^2 + |b|^2 + 2|c|^2 \mp \sqrt{(|b|^2 - |a|^2)^2 + 4|bc^* + a^*c|^2}\right]\,, \tag{44}$$

with $|\sigma_1| \leq |\sigma_2|$. This ordering of the $|\sigma_k|$ is governed by the convention that $0 \leq \theta \leq \pi/4$ (the opposite ordering would occur for $\pi/4 \leq \theta \leq \pi/2$). Indeed, one can check explicitly that the $|\sigma_k|^2$ are the eigenvalues of $M^\dagger M$, which provides the more direct way of computing the singular values.

The final step of the computation is the determination of the angles α and β from Eq. (35). Inserting Eqs. (40) and (43) into Eqs. (36) and (37), we end up with:

$$\begin{aligned}
\alpha &= \tfrac{1}{2}\arg\left\{a(|b|^2 - |\sigma_1|^2) - b^*c^2\right\}\,, \qquad (45) \\
\beta &= \tfrac{1}{2}\arg\left\{b(|\sigma_2|^2 - |a|^2) + a^*c^2\right\}\,. \qquad (46)
\end{aligned}$$

If $\det M = ab - c^2 = 0$ (with $M \neq \mathbf{0}$) , then there is one singular value which is equal to zero. In this case, it is easy to verify that $\sigma_1 = 0$ and $|\sigma_2|^2 = \mathrm{Tr}\,(M^\dagger M) = |a|^2 + |b|^2 + 2|c|^2$. All the results obtained above remain valid, except that α is undefined [since in this case, the argument of arg in Eq. (45) 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 [cf. footnote 17].

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

$$M = \begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix}\,. \tag{47}$$

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 [2]. 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 $\theta = \pi/4$, $\phi = \pi/2$, $\beta = \pi/2$ and α is indeterminate (so one is free to choose $\alpha = 0$). The resulting Takagi diagonalization is $U^T M U = \mathrm{diag}(0\,,\,2)$ with:

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}. \tag{48}$$

This example clearly indicates 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 using the standard techniques for computing eigenvalues and eigenvectors.[18]

We end this subsection by treating the case of degenerate (non–zero) singular values, which arises when $bc^* = -a^*c$. Special considerations are required since not all the formulae derived above are applicable to this case [cf. footnote 17]. The condition $bc^* = -a^*c$ implies that $|a| = |b|$, so that $|\sigma_1|^2 = |\sigma_2|^2 = |b|^2 + |c|^2$. After noting that $a/c = -b^*/c^*$, Eq. (38) then yields:

$$\tan 2\theta = \left[\,\mathrm{Re}\,(b/c)\, c_\phi + \,\mathrm{Im}\,(b/c)\, s_\phi\right]^{-1}\,, \tag{49}$$

where $c_\phi \equiv \cos\phi$ and $s_\phi \equiv \sin\phi$. The reality of $\tan 2\theta$ imposes no constraint on ϕ; hence, ϕ is indeterminate [a fact that is suggested by Eq. (40)]. The same conclusion also follows immediately from Eq. (13). Namely, if $M_D = m\mathbb{1}_{2\times 2}$, then $(U\mathcal{O})^T M (U\mathcal{O}) = \mathcal{O}^T M_D \mathcal{O} = M_D$ for any real orthogonal matrix $\mathcal{O}$. In particular, ϕ simply represents the freedom to choose $\mathcal{O}$ [see, e.g., Eq. (54)]. Since ϕ is indeterminate, Eq. (49) implies that θ is indeterminate as well. In practice, it is often simplest to choose a convenient value, say $\phi = 0$, which would then fix θ such that $\tan 2\theta = [\,\mathrm{Re}\,(b/c)]^{-1}$. For pedagogical reasons, we shall keep ϕ as a free parameter below.

Naively, it appears that α and β are also indeterminates. After all, the arguments of arg in both Eqs. (45) and (46) vanish in the degenerate limit. However, this is not a correct

[18] For *real* symmetric matrices M, one can always find a real orthogonal V such that $V^T M V$ is diagonal. In this case the Takagi diagonalization is achieved by $U = VP$, where P is a diagonal matrix whose kk element is 1 [i] if the corresponding *eigenvalue* m_k is positive (negative). Of course, this procedure fails for complex symmetric matrices [such as M in Eq. (47)] that are not diagonalizable.

conclusion, as the derivation of Eqs. (45) and (46) involves a division by $|bc^* + a^*c|$, which vanishes in the degenerate limit. Thus, to determine α and β in the degenerate case, one must return to Eqs. (36) and (37). A straightforward calculation [which uses Eq. (49)] yields:

$$\frac{\sigma_2}{c} = -\frac{\sigma_1^*}{c^*}\,, \tag{50}$$

which implies

$$\alpha + \beta = \arg c \pm \frac{\pi}{2}\,. \tag{51}$$

Note that separately, α and β depend on the choice of ϕ (although ϕ drops out in the sum).

Explicitly, we have

$$\sigma_1 = -c\,e^{-i\phi}\left\{\sqrt{1+\left[c_\phi\,\mathrm{Re}\,(b/c)+s_\phi\,\mathrm{Im}\,(b/c)\right]^2}+i\left[s_\phi\,\mathrm{Re}\,(b/c)-c_\phi\,\mathrm{Im}\,(b/c)\right]\right\}\,, \tag{52}$$

$$\sigma_2 = \quad c\,e^{i\phi}\left\{\sqrt{1+\left[c_\phi\,\mathrm{Re}\,(b/c)+s_\phi\,\mathrm{Im}\,(b/c)\right]^2}-i\left[s_\phi\,\mathrm{Re}\,(b/c)-c_\phi\,\mathrm{Im}\,(b/c)\right]\right\}\,. \tag{53}$$

One easily verifies that Eq. (50) is satisfied. Moreover, using Eq. (35), α and β are now separately determined.

We illustrate the above results with the classic case 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 $\theta = \pi/4$, $\sigma_1 = -e^{-i\phi}$ and $\sigma_2 = e^{i\phi}$, which yields $\alpha = -(\phi\pm\pi)/2$ and $\beta = \phi/2$. Thus, Eq. (33) yields:

$$\begin{aligned} U &= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & e^{i\phi} \\ -e^{-i\phi} & 1\end{pmatrix}\begin{pmatrix} \pm i e^{i\phi/2} & 0 \\ 0 & e^{-i\phi/2}\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} \pm i e^{i\phi/2} & e^{i\phi/2} \\ \mp i e^{-i\phi/2} & e^{-i\phi/2}\end{pmatrix} \\ &= \frac{1}{\sqrt{2}}\begin{pmatrix} i & 1 \\ -i & 1\end{pmatrix}\begin{pmatrix} \pm\cos(\phi/2) & \sin(\phi/2) \\ \mp\sin(\phi/2) & \cos(\phi/2)\end{pmatrix}\,, \end{aligned} \tag{54}$$

which illustrates explicitly that in the degenerate case, U is unique only up to multiplication on the right by an arbitrary orthogonal matrix.

Appendix A: Takagi diagonalization revisited

In order to perform the Takagi diagonalization of a complex symmetric matrix M, one must construct the unitary matrix Ω such that:

$$\Omega^{\mathsf{T}} M\, \Omega = M_D = \mathrm{diag}(m_1, m_2, \ldots, m_n)\,, \tag{A.1}$$

where the m_k are real and non-negative. In this appendix, we provide an alternate algorithm for constructing Ω. Equivalently, we seek a method for determining the orthonormal singular vectors v_k [eq. (15)] that make up the columns of Ω. The algorithm depends on the following lemma:

Lemma 1: Consider the eigenvalue problem $M^\dagger M y = m^2 y$, where y is an eigenvector normalized to unity corresponding to the eigenvalue m^2. Let m be the positive square root of m^2. Then, the vector

$$u = M^* y^* + m y \tag{A.2}$$

satisfies:

$$Mu = m u^*\,. \tag{A.3}$$

Proof of Lemma 1: Noting that a symmetric matrix satisfies $M^\dagger = M^*$, and

$$M^\dagger M y = M^* M y = m^2 y\,, \tag{A.4}$$

eq. (A.3) follows after multiplying eq. (A.2) on the left by M.

Algorithm for Takagi diagonalization: Consider one of the solutions to the eigenvalue problem $M^\dagger M y_1 = m_1^2 y_1$, where y_1 is normalized to unity. Using Lemma 1, is is easy to construct the corresponding solution to

$$M v_1 = m_1 v_1^*\,, \tag{A.5}$$

where m_1 is the positive square root of m_1^2 and v_1 is normalized to unity.[19] One can then construct $n-1$ orthonormal vectors $s_1\,,\, s_2\,,\, \ldots\,,\, s_{n-1}$, each of which is orthogonal to v_1. Define the unitary matrix V_1 whose columns are given by:

$$V_1 = (v_1\,,\, s_1\,,\, s_2\,,\, \ldots\,,\, s_{n-1})\;. \tag{A.6}$$

Using eq. (A.5) and the fact that M is symmetric, it is straightforward to compute:

$$V_1^{\mathsf{T}} M V_1 = \left(\begin{array}{c:c} m_1 & \mathbf{0} \\ \hdashline \mathbf{0} & M_2 \end{array}\right)\,, \tag{A.7}$$

[19]If $u_1 = 0$, then $M y_1 = -m y^*$, and we choose $v_1 = i y_1$. If $u_1 \neq 0$, then we choose $v_1 = u_1/\|u_1\|$.

where the boldface zero above (below) the horizontal dashed line represents $n-1$ columns (rows) of zeros and M_2 is a *symmetric* $(n-1)\times(n-1)$ matrix whose matrix elements are given by

$$(M_2)_{ij} = s_i^{\mathsf{T}} M s_j \,. \tag{A.8}$$

Thus, we next consider one of the solutions to the eigenvalue problem $M_2^\dagger M_2 z_2 = m_2^2 z_2$, where z_2 is normalized to unity. Using Lemma 1, we again construct the corresponding solution to

$$M_2 w_2 = m_2 w_2^* \,, \tag{A.9}$$

where m_2 is the positive square root of m_2^2 and w_2 is normalized to unity. One can then construct $n-2$ orthonormal vectors $t_1\,,\, t_2\,,\,\ldots\,,\, t_{n-2}$, each of which is orthogonal to w_2. Define the $n\times n$ unitary matrix V_2 by:

$$V_2 = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & (w_2)_1 & (t_1)_1 & \cdots & (t_{n-2})_1 \\ 0 & (w_2)_2 & (t_1)_2 & \cdots & (t_{n-2})_2 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & (w_2)_{n-1} & (t_1)_{n-1} & \cdots & (t_{n-2})_{n-1} \end{pmatrix} . \tag{A.10}$$

The columns of the matrix product V_1V_2 are given by:

$$V_1V_2 = \left(v_1\,,\, v_2\,,\, \sum_{k=1}^{n-1} (t_1)_k s_k\,,\,\ldots\,,\, \sum_{k=1}^{n-1} (t_{n-2})_k s_k \right) , \tag{A.11}$$

where

$$v_2 = \sum_{k=1}^{n-1} (w_2)_k s_k \,. \tag{A.12}$$

Using eq. (A.9) and the fact that M_2 is symmetric, it is straightforward to compute:

$$(V_1V_2)^{\mathsf{T}} M (V_1V_2) = \left(\begin{array}{cc:c} m_1 & 0 & \mathbf{0} \\ 0 & m_2 & \mathbf{0} \\ \hdashline \mathbf{0} & \mathbf{0} & M_3 \end{array} \right) , \tag{A.13}$$

where the boldface zeros above (below) the horizontal dashed line represent $n-2$ columns (rows) of zeros and M_3 is a symmetric $(n-2)\times(n-2)$ matrix whose matrix elements are given by

$$(M_3)_{ij} = t_i^{\mathsf{T}} M_2 t_j \,. \tag{A.14}$$

Indeed, eq. (A.13) implies that:

$$M v_2 = m_2 v_2^* \,. \tag{A.15}$$

Iterating the above procedure produces n unitary matrices V_1 , V_2 , . . . , V_n, such that

$$V^{\mathsf{T}} M V = \operatorname{diag}(m_1\,,\, m_2\,,\,\ldots\,,\, m_n)\,, \tag{A.16}$$

where $V \equiv V_1 V_2 \cdots V_n$ and the m_i are the singular values of M. Thus, we have established the Takagi diagonalization of an arbitrary complex symmetric matrix M. Indeed, the above procedure succeeds even if some of the singular values are zero and/or degenerate.

Note that singular vectors corresponding to two unequal singular values are orthogonal, since any symmetric matrix M satisfies:

$$\langle M^* v_j^* | v_k \rangle = \langle v_j^* | M v_k \rangle\,. \tag{A.17}$$

Using eq. (15), it follows that $\langle v_j | v_k \rangle = 0$ for $m_j \neq m_k$. The singular vectors corresponding to non-degenerate singular values are unique up to multiplication by an overall sign. This corresponds precisely to the multiplication of Ω on the right by an arbitrary diagonal orthogonal matrix (within the non-degenerate subspace).

Application: As a simple example, consider $M = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$. If we apply the above procedure to compute the Takagi factorization of M, we may choose $y_1 = \left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)$. Computing u_1 using eq. (A.2) and normalizing it yields $v_1 = \frac{1}{\sqrt{2}}\left(\begin{smallmatrix} 1 \\ 1 \end{smallmatrix}\right)$. Choosing the vector orthogonal to v_1 to be $s_1 = \left(\begin{smallmatrix} 1 \\ -1 \end{smallmatrix}\right)$ determines the matrix V_1, and the final step of the iteration yields V_2:

$$V_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\,, \qquad\qquad V_2 = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}\,. \tag{A.18}$$

Hence, $V = V_1 V_2$, which is unique up to multiplication on the right by an arbitrary 2×2 orthogonal matrix $\mathcal{O}$. We conclude that $\Omega^{\mathsf{T}} M \Omega = I_2$, where $\Omega = V\mathcal{O}$, which reproduces the result of eq. (17).

If the singular values of M are non-degenerate, then the Takagi factorization of M is particularly simple. In particular, if $M^\dagger M y = m^2 y$, where m^2 is a non-degenerate eigenvalue of $M^\dagger M$, then

$$My = \alpha y^*\,, \tag{A.19}$$

for some complex number α. That is, My and y^* are linearly dependent. To prove this, we examine u defined in eq. (A.2). If $u = 0$, then $My = -my^*$ ($i.e$, $\alpha = -m$). If $u \neq 0$, then multiplying eq. (A.3) on the left by $M^\dagger$ yields $M^\dagger M u = m^2 u$. It then follows that $u = \beta y$ for some non-zero complex number β. Inserting this result back into eq. (A.2), one obtains eq. (A.19) with $\alpha = \beta^* - m$. From eq. (A.19), it follows that:

$$m^2 y = M^\dagger M y = M^* M y = |\alpha|^2 y\,. \tag{A.20}$$

Hence, we can write: $\alpha = me^{i\theta}$ with m real and non-negative, which implies that $v = e^{-i\theta/2}y$ is a singular vector (normalized to unity) that satisfies eq. (15). Thus, in the non-degenerate case, the columns of Ω consist of the eigenvectors of $M^\dagger M$, normalized to unity with overall phases chosen such that the singular values are non-negative.

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