Diagonalization of a general $2 \times 2$ hermitian matrix

Consider a general $2 \times 2$ hermitian matrix

\[ A = \begin{pmatrix} a & c \\ c^* & b \end{pmatrix}, \]

where $a$ and $b$ are real numbers and $c$ is a complex number. The eigenvalues are the roots of the characteristic equation:

\[ \begin{vmatrix} a - \lambda & c \\ c^* & b - \lambda \end{vmatrix} = (a - \lambda)(b - \lambda) - |c|^2 = \lambda^2 - \lambda(a + b) + (ab - |c|^2) = 0. \]

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

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

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

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

\[ U^{-1}AU = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}, \]

where $\lambda_1$ and $\lambda_2$ are the eigenvalues obtained in eq. (1). Note that one can always transform $U \to e^{i\xi}U$ without modifying eq. (2), since the phase cancels out. Since $\det U$ is a pure phase, one can choose $\det U = 1$ in eq. (2) 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

\[ U = \begin{pmatrix} \cos \theta & -e^{-i\chi} \sin \theta \\ e^{i\chi} \sin \theta & \cos \theta \end{pmatrix}, \]

where

\[ 0 \leq \theta \leq \frac{1}{2} \pi, \quad \text{and} \quad 0 \leq \chi < 2\pi. \]

We now plug in eq. (3) into eq. (2). Since the off-diagonal terms must vanish, one obtains constraints on the angles $\theta$ and $\chi$. It is convenient to define,

\[ c = |c|e^{i\psi}, \] \quad where \( 0 \leq \psi < 2\pi. \]
Then,

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

where

\[
\lambda_1 = a \cos^2 \theta + 2|c| \cos \theta \sin \theta \cos(\psi + \chi) + b \sin^2 \theta, \\
\lambda_2 = a \sin^2 \theta - 2|c| \cos \theta \sin \theta \cos(\psi + \chi) + b \cos^2 \theta, \\
Z = e^{-i\chi}\left\{ (b - a) \cos \theta \sin \theta + |c| \left[ e^{i(\psi + \chi)} \cos^2 \theta - e^{-i(\psi + \chi)} \sin^2 \theta \right] \right\}.
\]

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

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

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

\[
\frac{1}{2}(b - a) \sin 2\theta + |c| \cos 2\theta \cos(\psi + \chi) = 0, \\
|c| \sin(\psi + \chi) = 0.
\]

Consider first the special case of \(c = 0\). Then, eqs. (9) and (10) imply that:

\[
c = 0 \quad \text{and} \quad a > b \quad \Rightarrow \quad \theta = 0 \quad \text{and} \quad \chi \text{ is undefined}, \\
c = 0 \quad \text{and} \quad a < b \quad \Rightarrow \quad \theta = \frac{1}{2}\pi \quad \text{and} \quad \chi \text{ is undefined}, \\
c = 0 \quad \text{and} \quad a = b \quad \Rightarrow \quad \theta \text{ and } \chi \text{ are undefined}.
\]

In particular, if \(c = 0\) and \(a = b\), then \(A = I\) and it follows that \(U^{-1}AU = U^{-1}U = I\), which is satisfied for any unitary matrix \(U\). Consequently, in this limit \(\theta\) and \(\chi\) are undefined, as indicated above.

If \(c \neq 0\) then eq. (10) yields

\[
\sin(\psi + \chi) = 0 \quad \text{and} \quad \cos(\psi + \chi) = \pm 1.
\]

For the moment, we allow for the possibility of both signs in eq. (11).\(^*\) Hence, eq. (9) yields

\[
\tan 2\theta = \pm \frac{2|c|}{a - b}, \quad \text{for } c \neq 0 \text{ and } a \neq b.
\]

\(^*\)Below eq. (16), we shall verify that to be consistent with our convention that \(0 \leq \theta \leq \frac{1}{2}\pi\) [cf. eq. (4)], we must choose the positive sign.
Finally, in the case of $c \neq 0$ and $a = b$, eqs. (9) and (10) yield $\cos 2\theta = 0$, and $\chi$ is given by eq. (17). In light of our convention stated in eq. (4),

$$c \neq 0 \quad \text{and} \quad a = b \quad \implies \quad \theta = \frac{1}{4} \pi.$$  

However, we have not yet used all the available information. In particular, eqs. (6) and (7) also provide some information on the possible values of $\theta$, $\chi$ and $\beta$. Since $\lambda_1 + \lambda_2 = a + b = \text{Tr} \, A$ (as expected), we focus on the difference of the two diagonal elements,

$$\lambda_1 - \lambda_2 = (a - b) \cos 2\theta \pm 2|c| \sin 2\theta,$$

where we have used eqs. (6) and (7) with $\cos(\psi + \chi) = \pm 1$. Combining eqs. (1) and (13), we obtain

$$\lambda_1 - \lambda_2 = \sqrt{(a - b)^2 + 4|c|^2} = (a - b) \cos 2\theta \pm 2|c| \sin 2\theta. \quad (14)$$

Using eq. (12) to write:

$$a - b = \frac{2|c|}{\tan 2\theta} = \pm \frac{2|c| \cos 2\theta}{\sin 2\theta},$$

and inserting this on the left hand side of eq. (14), the latter reduces to:

$$(a - b) \cos 2\theta \pm 2|c| \sin 2\theta = \pm \left[2|c| \frac{\cos^2 2\theta}{\sin 2\theta} + 2|c| \sin 2\theta\right] = \pm \frac{2|c|}{\sin 2\theta}. \quad (15)$$

Substituting this result back into eq. (14) and solving for $\sin 2\theta$, we find:

$$\sin 2\theta = \pm \frac{2|c|}{\sqrt{(a - b)^2 + 4|c|^2}}. \quad (16)$$

In order to be consistent with our convention that $0 \leq \theta \leq \frac{1}{2} \pi$ [cf. eq. (4)], we must have $\sin 2\theta \geq 0$, which implies that one must choose the positive sign in eq. (16). This means that in eqs. (11)–(15), we must also choose the positive sign. In particular, $\cos(\psi + \chi) = 1$, so that $\psi + \chi = 2\pi n$ for some integer $n$. By the conventions established in eqs. (4) and (5), we assume that $0 \leq \psi, \chi < 2\pi$. Hence, it follows that

$$\chi = \begin{cases} 2\pi - \psi, & \text{for } c \neq 0 \text{ and } \psi \neq 0, \\ 0, & \text{for } c \neq 0 \text{ and } \psi = 0. \end{cases} \quad (17)$$

We therefore conclude that

$$\sin 2\theta = \frac{2|c|}{\sqrt{(a - b)^2 + 4|c|^2}}. \quad (18)$$

We can also obtain $\cos 2\theta$ using eqs. (12) and (18):

$$\cos 2\theta = \frac{a - b}{\sqrt{(a - b)^2 + 4|c|^2}}. \quad (19)$$

Eq. (19) implies that the sign of $a - b$ determines whether $0 < \theta < \frac{1}{4} \pi$ or $\frac{1}{4} \pi < \theta < \frac{1}{2} \pi$. The former corresponds to $a - b > 0$ while the latter corresponds to $a - b < 0$. The borderline case of $a = b$ has already been treated above.

To summarize, if $c \neq 0$, then eqs. (17), (18) and (19) uniquely specify the diagonalizing matrix $U$ [in the convention specified in eq. (4)]. 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. Finally, if $c = 0$ and $a = b$, then $A = I$, in which case $U$ is arbitrary.
Diagonalization of a real symmetric $2 \times 2$ matrix

Finally, we can easily treat the special case in which the matrix $A$ is real. In this case, we can diagonalize a real symmetric $2 \times 2$ matrix by a real orthogonal matrix. The two eigenvalues are still given by eq. (1), 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. (5) implies that if $c \neq 0$ then $\psi = 0$ or $\psi = \pi$. Eq. (17) then yields

$$
\chi = \begin{cases} 
0, & \text{for } c \neq 0 \text{ and } \psi = 0, \\
\pi, & \text{for } c \neq 0 \text{ and } \psi = \pi.
\end{cases} \quad (20)
$$

It is therefore simpler to modify the convention established in eq. (4) by choosing

$$
0 \leq \theta < \pi, \quad \text{and} \quad 0 \leq \chi < \pi. \quad (21)
$$

In this convention, eq. (20) is replaced by $\chi = 0$, and we must allow for both signs in eqs. (11)–(16). It is easy to check that for real values of $c$, the proper choice of sign corresponds to the sign of $c$, i.e., $c = \pm |c|$. The diagonalizing matrix $U$ is now a real orthogonal $2 \times 2$ matrix,†

$$
U = \begin{pmatrix} 
\cos \theta & -\sin \theta \\
\sin \theta & \cos \theta
\end{pmatrix}, \quad \text{where } 0 \leq \theta < \pi.
$$

Consequently in the case of $c$ real, we can replace $\pm |c|$ with $c$ in the numerator of eq. (16) in the convention where $0 \leq \theta < \pi$. Hence,

$$
\sin 2\theta = \frac{2c}{\sqrt{(a-b)^2 + 4c^2}}, \quad (22)
$$

$$
\cos 2\theta = \frac{a-b}{\sqrt{(a-b)^2 + 4c^2}}. \quad (23)
$$

Eq. (22) tells us in which quadrant $\theta$ lives. If $0 < \theta < \frac{1}{2} \pi$, then $\sin 2\theta > 0$, which implies that $c > 0$. If $\frac{1}{2} \pi < \theta < \pi$, then $\sin 2\theta < 0$, which implies that $c < 0$. Thus, the sign of $c$ determines the quadrant of $\theta$. Eq. (23) provides additional information. For $c > 0$, the sign of $a - b$ determines whether $0 < \theta < \frac{1}{4} \pi$ or $\frac{1}{4} \pi < \theta < \frac{1}{2} \pi$. The former corresponds to $a - b > 0$ while the latter corresponds to $a - b < 0$. Likewise, if $c < 0$, the sign of $a - b$ determines whether $\frac{1}{2} \pi < \theta < \frac{3}{4} \pi$ or $\frac{3}{4} \pi < \theta < \pi$. The former corresponds to $a - b < 0$ while the latter corresponds to $a - b > 0$. The borderline cases are likewise determined:

- $c = 0$ and $a > b \implies \theta = 0$,
- $c = 0$ and $a < b \implies \theta = \frac{1}{2} \pi$,
- $a = b$ and $c > 0 \implies \theta = \frac{1}{4} \pi$,
- $a = b$ and $c < 0 \implies \theta = \frac{3}{4} \pi$.

If $c = 0$ and $a = b$, then $A = I$ and it follows that $U^{-1}AU = U^{-1}U = I$, which is satisfied for any invertible matrix $U$. Consequently, in this limit $\theta$ is undefined.

†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 $0 \leq \theta < \pi$ may be chosen without loss of generality.