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Concrete minimal 3×3 Hermitian matrices and some general cases

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Abstract: Given a Hermitian matrix $M \in M_3(\mathbb{C})$ we describe explicitly the real diagonal matrices D_M such that

$$\|M + D_M\| \leqslant \|M + D\|$$

for all real diagonal matrices $D \in M_3(\mathbb{C})$, where $\|\cdot\|$ denotes the operator norm. Moreover, we generalize our techniques to some $n \times n$ cases.

Keywords: Minimal Hermitian matrix, diagonal matrix, quotient operator norm, best approximation

MSC: 15A12, 15A60, 15A83, 15B57, 41A35

1 Introduction

Let $M_3(\mathbb{C})$ and $D_3(\mathbb{R})$ be respectively the algebras of complex and real diagonal 3×3 matrices. Given a Hermitian matrix $M \in M_3(\mathbb{C})$ we study the diagonals D_M, that attain the quotient norm

$$\|M + D_M\| = |||\,[M]\,||| = \min_{D \in D_3(\mathbb{R})} \|M + D\| = \operatorname{dist}(M, D_3(\mathbb{R})),$$

or equivalently

$$\|M + D_M\| \leqslant \|M + D\|, \text{ for all } D \in D_3(\mathbb{R})$$

where $\|\cdot\|$ denotes the operator norm.

The matrices $M + D_M$ will be called minimal. These matrices appeared in the study of minimal length curves in the flag manifold $\mathcal{P}(n) = \mathcal{U}(M_n(\mathbb{C}))/\mathcal{U}(\mathcal{D}_n(\mathbb{C}))$, where $\mathcal{U}(\mathcal{A})$ denotes the unitary matrices of the algebra $\mathcal{A}$ when $\mathcal{P}(n)$ is endowed with the quotient Finsler metric of the operator norm [1]. The minimal length curves δ in $\mathcal{P}(n)$ are given by the left action of $\mathcal{U}(M_n(\mathbb{C}))$ on $\mathcal{P}(n)$. Namely

$$\delta(t) = \left[e^{itM}U\right],$$

where M is minimal and $[V]$ denotes the class of V in $\mathcal{P}(n)$. Some natural questions as well as particular examples that arise from the geometric description of these objects are related to problems that appear in other contexts: problems of minimization of operators related with optimization and control [2, 3], positivity and inequalities in matrix analysis [4, 5], Leibnitz seminorms [6, 7] and unitary stochastic matrices [8].

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Previous attempts to describe minimal matrices and their properties were made in [9] for 3×3 matrices. All 3×3 minimal matrices were parametrized [9]. We stress that there are no known results showing which is the minimizing diagonal for a given Hermitian matrix M (except on trivial cases).

Several attempts have been made recently to describe the closest diagonal matrix to a given Hermitian matrix (see for instance [6, 8] and [9]). These papers give qualitative properties of these matrices and even parametrize all the solutions. Nevertheless, the problem of finding the diagonal matrix or matrices closest to a concrete Hermitian matrix M remained open even for the first non-trivial case: 3×3.

Our goal in the present paper is to study this problem for 3×3 minimal matrices and some $n \times n$ cases where the 3×3 case techniques can be extended.

In Section 3 we describe all the minimal diagonal matrices for a given Hermitian 3×3 matrix M with some of its off-diagonal entries equal to zero. Some cases in this section give infinite solutions.

Section 4 is devoted to the case of Hermitian matrices with non-zero off-diagonal entries. In this section we study real matrices separately and propose a decomposition in the general case (see Theorems 6 and 7) that allows us to find the unique closest diagonal matrix to a given Hermitian matrix M (see Remark 9) in this case.

The last section studies specific types of $n \times n$ of Hermitian matrices for which the minimal diagonals can be computed explicitly, as well as some of their general properties. The continuity of the function that maps Hermitian matrices with zero diagonals into their unique minimizing diagonal (when this is the case) is studied. Theorem 9 generalizes Theorem 3 and provides many examples of minimal matrices for which the minimizing diagonals can be calculated. We also study some matrices that admit only one minimizing diagonal and others that do not.

2 Preliminaries and notation

Let $M_n(\mathbb{C})$ denote the algebra of square $n \times n$ complex matrices, $M_n^h(\mathbb{C})$ the real subspace of Hermitian complex matrices, and $D_n(\mathbb{R})$ the real subalgebra of the diagonal real matrices. The symbol $\sigma(A)$ denotes the spectrum of A, that is the (unordered) set of eigenvalues of A. We denote by $\|A\|$ the operator or spectral norm of $A \in M_n(\mathbb{C})$. In the case $A \in M_n^h(\mathbb{C})$ it can be calculated by $\|A\| = \max_{\lambda \in \sigma(A)} |\lambda|$. We write $\|C\|_2$ to represent the euclidean norm for $C \in \mathbb{C}^n$.

We denote by $\{e_i\}_{i=1}^n$ the canonical basis of $\mathbb{C}^n$. Given a matrix $A \in M_n(\mathbb{C})$, we denote by $A_{i,j}$ the (i, j) entry of A and we write $A = [A_{i,j}]$ for $i, j = 1, \ldots, n$.

For $M, N \in M_n(\mathbb{C})$ we denote by MN the usual matrix product, by $\operatorname{tr}(M)$ the usual (non-normalized) trace of M and by $C_i(M)$ the vector given by the i^{th} column of M.

For $(a_1, a_2, \ldots, a_n) \in \mathbb{R}^n$ we denote by $\operatorname{diag}(a_1, a_2, \ldots, a_n)$ the diagonal matrix of $M_n^h(\mathbb{R})$ with $(a_1, a_2, \ldots, a_n)$ in its diagonal. Nevertheless, if $M \in M_n(\mathbb{C})$, then $\operatorname{Diag}(M)$ denotes the diagonal matrix defined by the principal diagonal of M.

Observe that if $M \in M_n^h(\mathbb{C})$ and $D \in D_n(\mathbb{R})$, then $(M + D) \in M_n^h(\mathbb{C})$. Let us consider the quotient $M_n^h(\mathbb{C})/D_n(\mathbb{R})$ and the quotient norm

$$|| [M] || = \min_{D \in D_n(\mathbb{R})} \|M + D\| = \operatorname{dist}(M, D_n(\mathbb{R})) \tag{2.1}$$

for $[M] = \{M + D : D \in D_n(\mathbb{R})\} \in M_n^h(\mathbb{C})/D_n(\mathbb{R})$. Note that the candidates $D \in D_n(\mathbb{R})$ can be chosen to be in the closed ball $B_{\|M\|}(0) = \{D \in D_n(\mathbb{R}) : \|D\| \leqslant \|M\|\}$. This ball is compact and the function $n : B_{\|M\|}(0) \to \mathbb{R}$, $n(D) = \|M + D\|$ is continuous. Therefore, the minimum in (2.1) is clearly attained.

Definition 1. *A matrix $M \in M_n^h(\mathbb{C})$ is called* **minimal** *if*

$$\|M\| \leqslant \|M + D\|, \quad \text{for all } D \in D_n(\mathbb{R}),$$

or equivalently, if $\|M\| = ||| [M] ||| = \min_{D \in D_n(\mathbb{R})} \|M + D\| = \mathit{dist}\,(M, D_n(\mathbb{R}))$.

Definition 2. *Let $M \in M_n^h(\mathbb{C})$ and $D \in D_n(\mathbb{R})$ be such that $M+D$ is minimal. Then D is a* **minimizing diagonal** *of M.*

For a matrix $M \in M_3^h(\mathbb{C})$ with at least two non-zero off-diagonal entries this minimizing matrix D is unique (see [9, Theorem 3.14] for a proof).

Proposition 1. *If $M \in M_3^h(\mathbb{C})$ is a minimal matrix and at least two of $M_{1,2}$, $M_{1,3}$ and $M_{2,3}$ are non-zero, then the values of its minimizing diagonal are unique.*

Remark 1. *Observe that if $M \in M_n^h(\mathbb{C})$ is minimal, then $\pm\|M\| \in \sigma(M)$. Moreover, if $n = 3$, then $\sigma(M) = \{-\|M\|, tr(M), +\|M\|\}$ (see for example [9, Remark 3.1]).*

Throughout the paper, for a given non-zero minimal matrix $M \in M_3^h(\mathbb{C})$, we denote by $\sigma(M) = \{\lambda, \mu, -\lambda\}$ the spectrum of M, for $0 < \lambda = \|M\|$, $|\mu| \leqslant \lambda$ and $\mu = \operatorname{tr}(M)$.

Given $v = (v_1, v_2, v_3) \in \mathbb{C}^3$, $v \otimes v$ denotes the matrix, such that $(v \otimes v)_{i,j} = v_i \overline{v_j}$, for $i, j = 1, 2, 3$.

For $M \in M_3^h(\mathbb{C})$ and $v \in \mathbb{C}^n$ we write $\overline{M}$ and $\overline{v}$ to denote the matrix and vector obtained from M and v by conjugation of its coordinates.

If $M, N \in \mathbb{C}^{n\times m}$ we denote by $M \circ N$ the Schur or Hadamard product of these matrices, defined by $(M \circ N)_{i,j} = M_{i,j}N_{i,j}$, for $1 \leqslant i \leqslant n$, $1 \leqslant j \leqslant m$. Therefore, if $v \in \mathbb{C}^3$, with coordinates in the canonical basis given by $v = (v_1, v_2, v_3)$,

$$v \circ \overline{v} = (|v_1|^2, |v_2|^2, |v_3|^2) = \sum_{j=1}^{3} |v_j|^2 e_j \in \mathbb{R}_+^3.$$

If $A \in \mathbb{C}^{n\times m}$, we denote by $A^t \in \mathbb{C}^{m\times n}$ its transpose, by $\operatorname{ran}(A)$ the range of the linear transformation A and by $\ker(A)$ its kernel.

3 Minimal 3 × 3 matrices with zero entries

Proposition 2. *Let $x, y, z \in \mathbb{C}$. If $c \in \mathbb{R}$ with $|c| \leqslant |x|$, $b \in \mathbb{R}$ with $|b| \leqslant |y|$ and $a \in \mathbb{R}$ with $|a| \leqslant |z|$, then the matrices*

$$M_x = \begin{pmatrix} 0 & x & 0 \\ \overline{x} & 0 & 0 \\ 0 & 0 & c \end{pmatrix} \quad M_y = \begin{pmatrix} 0 & 0 & \overline{y} \\ 0 & b & 0 \\ y & 0 & 0 \end{pmatrix} \quad M_z = \begin{pmatrix} a & 0 & 0 \\ 0 & 0 & z \\ 0 & \overline{z} & 0 \end{pmatrix}$$

are minimal. Moreover, these are all the possible diagonals such that M_x, M_y and M_z are minimal matrices.

Proof. Let $v \in \mathbb{C}^3$ with $\|v\| = 1$. It is easy to prove that $\|M_x v\| \leqslant |x|$, for all $c \in \mathbb{R}$ such that $|c| \leqslant |x|$. Since $\|M_x e_2\| = |x|$, then $\|M_x\| = |x|$. Moreover, if we consider

$$M = \begin{pmatrix} \alpha & x & 0 \\ \overline{x} & \beta & 0 \\ 0 & 0 & \gamma \end{pmatrix}$$

with $\alpha \neq 0$, then $\|Me_1\| = \|(\alpha, \overline{x}, 0)\| > |x|$. Therefore, $\|M\| > \|M_x\|$. Similarly, if $\beta \neq 0$, then $\|Me_2\| > |x|$. If $\alpha = \beta = 0$ and $|\gamma| > |x|$, then $\|M\| = \max\{|x|, |\gamma|\} > \|M_x\|$. Therefore, M_x is minimal if and only if $|c| \leqslant |x|$.

The proof for the matrices M_y and M_z is similar. □

A generalization of the previous result to $n \times n$ Hermitian matrices is presented in Proposition 10 of Section 5.

The following theorem is proved in [9, Theorem 3.7]. We restate it for the sake of clarity.

Theorem 1. *Let $M_{3\times 3}^h(\mathbb{C})$ with $\|M\| = \lambda > 0$. Then M is minimal if and only if there exist two eigenvectors, v_+ corresponding to the eigenvalue λ, and v_- corresponding to the eigenvalue $-\lambda$, such that their coordinates have the same modules. That is, if for every e_i $|\langle v_+, e_i\rangle| = |\langle v_-, e_i\rangle|$, or equivalently $v_+ \circ \overline{v_+} = v_- \circ \overline{v_-}$.*

Remark 2. *This equivalence does not hold for $n \geqslant 3$. In general, for $M \in M^h_{n\times n}(\mathbb{C})$, if there exist two eigenvectors v_+ and v_- corresponding to the eigenvalues $\pm\lambda$ (respectively), such that $|\langle v_+, e_i\rangle| = |\langle v_-, e_i\rangle|$, then M is minimal (see Corollary 3).*

Nevertheless, there are examples in $M^h_{4\times 4}(\mathbb{C})$ where M is minimal and there is not pair corresponding to eigenvectors of $+\lambda$ and $-\lambda$ (respectively) such that their coordinates have the same modules (see Remark 4 in [8]).

The following result was proved in [9, Theorem 3.15].

Theorem 2. *Let x, y, z be non-zero complex numbers. Then the matrices*

$$M_{xy} = \begin{pmatrix} 0 & x & \overline{y} \\ \overline{x} & 0 & 0 \\ y & 0 & 0 \end{pmatrix} \quad M_{yz} = \begin{pmatrix} 0 & 0 & \overline{y} \\ 0 & 0 & z \\ y & \overline{z} & 0 \end{pmatrix} \quad M_{xz} = \begin{pmatrix} 0 & x & 0 \\ \overline{x} & 0 & z \\ 0 & \overline{z} & 0 \end{pmatrix}$$

are minimal. These are the only Hermitian minimal matrices with four non-zero entries outside the diagonal.

4 Minimal 3×3 matrices with non-zero entries

The following theorem describes minimizing diagonals for matrices M with real non-zero entries.

Theorem 3. ***Real (symmetric) minimal matrices***

Let $x, y, z \in \mathbb{R}$, $x, y, z \neq 0$.

- *Case 1: if*
$$x^2y^2 > z^2(x^2+y^2), \tag{4.1}$$
then $M = \begin{pmatrix} 0 & x & y \\ x & -\frac{yz}{x} & z \\ y & z & -\frac{xz}{y} \end{pmatrix}$ *is minimal.*
- *Case 2: if $x^2z^2 > y^2(x^2+z^2)$, then* $M = \begin{pmatrix} -\frac{yz}{x} & x & y \\ x & 0 & z \\ y & z & -\frac{xy}{z} \end{pmatrix}$ *is minimal.*
- *Case 3: if $y^2z^2 > x^2(y^2+z^2)$, then* $M = \begin{pmatrix} -\frac{xz}{y} & x & y \\ x & -\frac{xy}{z} & z \\ y & z & 0 \end{pmatrix}$ *is minimal.*
- *Case 4: if none of the previous cases hold, that is*
$$-x^2z^2 + y^2(x^2+z^2) \geqslant 0 \;\wedge\; -x^2y^2 + z^2(x^2+y^2) \geqslant 0 \;\wedge\; -y^2z^2 + x^2(y^2+z^2) \geqslant 0, \tag{4.2}$$
then
$$M = \begin{pmatrix} \frac{1}{2}\left(+\frac{xy}{z} - \frac{xz}{y} - \frac{zy}{x}\right) & x & y \\ x & \frac{1}{2}\left(-\frac{xy}{z} + \frac{xz}{y} - \frac{zy}{x}\right) & z \\ y & z & \frac{1}{2}\left(-\frac{xy}{z} - \frac{xz}{y} + \frac{zy}{x}\right) \end{pmatrix} \text{ is minimal.}$$

Note that in each case the minimizing diagonal is unique (see Proposition 1).

Proof. Let us consider the first case. Observe that $\|M\| \geqslant \|C_1(M)\|_2 = \sqrt{x^2+y^2}$. Moreover, direct calculations show that $\lambda = \sqrt{x^2+y^2}$ is an eigenvalue with corresponding eigenvector v_+, and $-\lambda$ is an eigenvalue with corresponding eigenvector v_-, where

$$v_+ = \left\{\frac{1}{\sqrt{2}}, \frac{x}{\sqrt{2}\sqrt{x^2+y^2}}, \frac{y}{\sqrt{2}\sqrt{x^2+y^2}}\right\},$$

$$\text{and } v_- = \left\{ \frac{1}{\sqrt{2}}, -\frac{x}{\sqrt{2}\sqrt{x^2+y^2}}, -\frac{y}{\sqrt{2}\sqrt{x^2+y^2}} \right\}.$$

If we consider $v_\mu = \left\{0, -\frac{y}{\sqrt{x^2+y^2}}, \frac{x}{\sqrt{x^2+y^2}}\right\}$ it is clear that v_μ is the corresponding eigenvector of $\mu = -\frac{(x^2+y^2)z}{xy}$. Then, using (4.1)

$$\mu^2 = \frac{\left(x^2+y^2\right)^2 z^2}{x^2y^2} < \left(x^2+y^2\right) = \lambda^2.$$

Therefore, v_+ and v_- satisfy the conditions of Theorem 1 and M is minimal.

Cases 2 and 3 are proved in a similar way.

Let us now consider case 4. Note that in this case the spectrum $\sigma(M)$ can be computed: $\sigma(M) = \left\{\pm\frac{x^2y^2+x^2z^2+y^2z^2}{2xyz}\right\}$. The eigenvalue $\frac{x^2y^2+x^2z^2+y^2z^2}{2xyz}$ has multiplicity one and its eigenspace is generated by $v = (xy, xz, yz)$. The eigenvector $\frac{1}{\|v\|}v$ is triangular in the sense of [9, Definition 3.2] because it satisfies inequalities (4.2). That is, the coordinates of $v \circ \overline{v}$ can form the sides of a triangle (any coordinate is greater than the sum of the two others). Under these hypotheses there is another triangular vector w orthogonal to v such that $v \circ \overline{v} = w \circ \overline{w}$ (see [9, Proposition 3.4]). Therefore, w belongs to the dimension two eigenspace of $-\frac{x^2y^2+x^2z^2+y^2z^2}{2xyz}$. Then M is minimal by Theorem 1. □

Remark 3. *From the previous Theorem it follows that in the first three cases the column (or row) of M with a zero entry is perpendicular to the other two columns (or rows, respectively). In the fourth case all the columns (and rows) are perpendicular to each other.*

In the first three cases the norm of the matrix M is the norm of its column (or row) vector that has a zero entry (being this the column with greatest norm). For example, using (4.1) in the first case:

$$\begin{aligned}\|C_2(M)\|_2^2 &= x^2 + \frac{y^2z^2}{x^2} + z^2 = x^2 + \frac{y^2z^2 + x^2z^2}{x^2} = x^2 + \frac{z^2(x^2+y^2)}{x^2} \\ &< x^2 + y^2 = \|C_1(M)\|_2^2 = \|M\|^2\end{aligned}$$

(and similarly with $\|C_3(M)\|_2^2$). The first three cases are generalized to $n \times n$ Hermitian matrices in Theorem 9.

In Case 4 the equality $\|C_i(M)\|_2 = \|M\|$ holds for $i = 1, 2, 3$.

The first three cases satisfy that $|\mu| < \lambda$ and the fourth that $|\mu| = \lambda$.

Remark 4. *Under the assumptions of Theorem 3 we can write all cases with a unifying formula for each element of the minimizing diagonal (a, b, c):*

$$a = \frac{D - 2|A|}{4xyz} \quad b = \frac{D - 2|B|}{4xyz} \quad c = \frac{D - 2|C|}{4xyz},$$

where

$$A = +x^2y^2 - y^2z^2 - z^2x^2 \quad B = -x^2y^2 - y^2z^2 + z^2x^2 \quad C = -x^2y^2 + y^2z^2 - z^2x^2$$

$$\text{and } D = A + |A| + B + |B| + C + |C|$$

The proof of this statement follows from direct computations (in each of the 4 different cases of Theorem 3).

Theorem 4. *If $x, y, z \in \mathbb{R}$, $x, y, z \neq 0$, then*

$$M = \begin{pmatrix} 0 & x\,i & -y\,i \\ -x\,i & 0 & z\,i \\ y\,i & -z\,i & 0 \end{pmatrix}$$

is minimal with norm equal to $\sqrt{x^2+y^2+z^2}$.

Proof. The eigenvalues of M are: $\pm\sqrt{x^2+y^2+z^2}$ and $\mu = 0$. Then

$$v_+ = \left(-\frac{x\sqrt{x^2+y^2+z^2}+iyz}{\sqrt{2}\left(z\sqrt{x^2+y^2+z^2}-ixy\right)}, -\frac{x^2+z^2}{\sqrt{2}\left(xy+iz\sqrt{x^2+y^2+z^2}\right)}, \frac{1}{\sqrt{2}}\right)$$

is an eigenvector associated to $\sqrt{x^2+y^2+z^2}$, and

$$v_- = \left(-\frac{x\sqrt{x^2+y^2+z^2}-iyz}{\sqrt{2}\left(z\sqrt{x^2+y^2+z^2}+ixy\right)}, -\frac{x^2+z^2}{\sqrt{2}\left(xy-iz\sqrt{x^2+y^2+z^2}\right)}, \frac{1}{\sqrt{2}}\right)$$

an eigenvector associated to $-\sqrt{x^2+y^2+z^2}$. Clearly, v_+ and v_- satisfy the conditions of Theorem 1 and therefore M is minimal. □

Remark 5. *Let $x, y, z \in \mathbb{R}_{\geqslant 0}$ and $\alpha, \beta, \gamma \in \mathbb{R}$. Then the characteristic polynomial of the matrix*

$$M = \begin{pmatrix} a & x\,e^{i\alpha} & y\,e^{-i\beta} \\ x\,e^{-i\alpha} & b & z\,e^{i\gamma} \\ y\,e^{i\beta} & z\,e^{-i\gamma} & c \end{pmatrix} \tag{4.3}$$

is

$$\begin{aligned} P_M[t] = -t^3 + t^2(a+b+c) + t\left(-ab-ac-bc+x^2+y^2+z^2\right) + \\ + abc - az^2 - by^2 - cx^2 + 2xyz\cos(\alpha+\beta+\gamma). \end{aligned} \tag{4.4}$$

Moreover, if $\cos(\theta) = \cos(\alpha+\beta+\gamma)$ *(where we can choose $0 \leqslant \theta \leqslant \pi$), then the following matrix*

$$M_\theta = \begin{pmatrix} a & x\,e^{i\theta} & y \\ x\,e^{-i\theta} & b & z \\ y & z & c \end{pmatrix} \tag{4.5}$$

has the same characteristic polynomial as M, and M is a minimal matrix if and only if M_θ is minimal. Note that $M_\theta = UMU^*$ for U the unitary diagonal matrix

$$U = \begin{pmatrix} e^{i\alpha} & 0 & 0 \\ 0 & e^{i(\alpha-\beta-\gamma)} & 0 \\ 0 & 0 & e^{i(\alpha-\beta)} \end{pmatrix}. \tag{4.6}$$

Proposition 3. *Let $x, y, z \in \mathbb{R}_{>0}$ and $\theta \in [0, \pi]$ such that $M_\theta = \begin{pmatrix} a & x\,e^{i\theta} & y \\ x\,e^{-i\theta} & b & z \\ y & z & c \end{pmatrix}$ is minimal. Then the matrices obtained by permuting any pair of rows of M_θ and the corresponding columns are also minimal.*

Proof. The proof follows from similar arguments as the ones done for the characteristic polynomials of the matrices in Remark 5 or using conjugation of M_θ by permutation matrices or unitary diagonals. □

Remark 6. *Observe that if we are looking for a minimizing diagonal for M as in (4.3), we can suppose that $M = M_\theta$ as in (4.5), since any other matrix has has its minimizing diagonal equal to one of this type or at least a permutation of its diagonal (see Remark 5 and the Proposition 3). Moreover, since minimizing diagonals have been described in the cases when an off-diagonal entry of the matrix is zero (see Proposition 2 and Theorem 2) and when the matrix is real (see Theorem 3) we can also suppose that*

- *$0 < \theta < \pi$ (because the cases $\theta = 0$ and $\theta = \pi$ have the same minimizing diagonals as the real symmetric matrices and for other $\theta \notin (0, \pi)$ it is enough to consider the case of $\theta_1 \in (0, \pi)$, such that $\cos(\theta_1) = \cos(\theta)$) and that*
- *$x \geqslant y \geqslant z > 0$ (in view of Proposition 3).*

Note that Proposition 3 above and Remark 5 prove that if two matrices have their off-diagonal entries with equal modules (even if their positions are permuted) and if $\cos(\theta) = \cos(\alpha+\beta+\gamma)$ (with α, β, γ as in (4.3) and θ as in (4.5)), then their minimizing diagonals coincide (with the corresponding permutations if necessary).

Corollary 1. *Let $x \in \mathbb{R}_{>0}$ and $0 < \theta < \pi$, then $M = \begin{pmatrix} a & x\,e^{i\theta} & x \\ x\,e^{-i\theta} & b & x \\ x & x & c \end{pmatrix}$ is minimal if and only if $a = b = c = -x\cos\left(\frac{\theta+\pi}{3}\right)$.*

Proof. The equality $a = b = c$ follows as a special case of Theorem 3, Case 4. If we set $a = b = c = -x\cos\left(\frac{\theta+\pi}{3}\right)$, the eigenvalues and eigenvectors of M can be explicitly computed. Then using Theorem 1 it can be proved that M is a minimal matrix with respect to that choice of a, b and c. This is the only possible choice because the minimizing diagonal is unique (see Proposition 1). □

Proposition 4. *Let M be a matrix as in (4.3) with $x, y, z \in \mathbb{R}_{>0}$, $\alpha, \beta, \gamma, a, b, c \in \mathbb{R}$. Then the following statements are equivalent:*

(i) $\alpha+\beta+\gamma = k\pi + \frac{\pi}{2}$, with $k \in \mathbb{Z}$ and $a = b = c = 0$,
(ii) M is minimal and $\sigma(M) = \{\lambda, -\lambda, 0\}$, for $\lambda = \|M\|$.

Proof. (i)⇒ (ii). If $\alpha+\beta+\gamma = k\pi + \frac{\pi}{2}$ and $a = b = c = 0$ it can be checked that the eigenvalues of M are $\pm\lambda = \pm\sqrt{x^2+y^2+z^2}$ and 0. Moreover, there are corresponding eigenvectors of $\pm\lambda$ that satisfy the conditions of Theorem 1. Therefore (ii) holds.

(ii)⇒(i). If M is minimal, there exist v_+ and v_- eigenvectors of unit norm λ and $-\lambda$ respectively, such that $v_+ \circ v_+ = v_- \circ v_-$ (see Theorem 1). We can factorize $M = U\cdot \operatorname{diag}(\lambda, -\lambda, 0)\cdot U^*$ with v_+ and v_- in the first and second column of the unitary matrix U. A direct calculation then shows that the diagonal of M has entries $\lambda|(v_+)_i|^2 - \lambda|(v_-)_i|^2$, for $i = 1, 2, 3$. Then the condition $v_+ \circ v_+ = v_- \circ v_-$ implies that the diagonal of M must be zero. Then $a = b = c = 0$.

Then $\det(M) = (-\lambda)\lambda\, 0 = 0 = 2xyz\cos(\alpha+\beta+\gamma)$ (see 4.4). Therefore, since $x, y, z \in \mathbb{R}_{>0}$, then $\alpha+\beta+\gamma = k\pi + \frac{\pi}{2}$, with $k \in \mathbb{Z}$. □

Corollary 2. *Let M be a minimal matrix as in (4.3), with $x, y, z \in \mathbb{R}_{>0}$, $\alpha, \beta, \gamma, a, b, c \in \mathbb{R}$.*
Then the following statements are equivalent:

(a) $\alpha+\beta+\gamma = k\pi + \frac{\pi}{2}$, for $k \in \mathbb{Z}$,
(b) $a = b = c = 0$,
(c) $\sigma(M) = \{\lambda, -\lambda, 0\}$, for $\lambda = \|M\|$.

Proof. The proof of (c)⇒(a) and (c)⇒(b) follows directly from (ii)⇒(i) of Proposition 4.

(b)⇒(c) can be proved using that for M is minimal, then $\sigma(M) = \{\lambda, \mu, \lambda\}$, for $\lambda = \|M\|$ and $|\mu| \leqslant \lambda$. This implies that $\operatorname{tr}(M) = a + b + c = 0 = \mu$.

For (a)⇒(b): As seen in Remark 5 the minimizing diagonal of M is the same as that of M_θ as in (4.5) with $\theta = k\pi + \frac{\pi}{2}$ and $e^\theta = \pm i$. It can be verified that if M_θ has zeros on its diagonal, it has eigenvalues $\{\pm\sqrt{x^2+y^2+z^2}, 0\}$. Then, calculating the corresponding eigenvectors of such M_θ and using Theorem 1, it can be proved that M_θ is minimal. Proposition 1 implies the uniqueness of the minimizing diagonal and therefore $a = b = c = 0$. □

Proposition 5. *Let $M_\theta = \begin{pmatrix} a & xe^{i\theta} & y \\ xe^{-i\theta} & b & z \\ y & z & c \end{pmatrix} \in M_3^h(\mathbb{C})$ be as in (4.5), and M_θ a minimal non-zero matrix such that $\sigma(M) = \{\lambda, \mu, -\lambda\}$, with $|\mu| = \lambda$. Then x, y, z must be non-zero and $\theta = k\pi$, with $k \in \mathbb{Z}$.*

Proof. Denote by v_δ a corresponding unit norm eigenvector of the eigenvalue δ of M_θ. Then $M_\theta = \lambda\, v_\lambda \otimes v_\lambda - \lambda\, v_{-\lambda} \otimes v_{-\lambda} + \mu\, v_\mu \otimes v_\mu$ (with $|\mu| = \lambda$) and $M_\theta^2 = \lambda^2 I$. Then the columns of M_θ are orthogonal vectors of norm

λ. Then direct calculations prove that if one of the off-diagonal entries of M_θ is zero, then all the others must be zero. Then it must be $x \neq 0$, $y \neq 0$ and $z \neq 0$.

Using the perpendicularity of the columns of M_θ it is clear that $axe^{i\theta}+bxe^{i\theta}+yz = 0$ and then $ia\sin(\theta)x + ib\sin(\theta)x = 0$. Let us suppose $\sin(\theta) \neq 0$. This implies that $a = -b$. In the same way we can prove that $aye^{-i\theta} + cye^{-i\theta} + xz = 0$, hence $a = -c$; and that $bze^{i\theta} + cze^{i\theta} + xy = 0$, which implies that $b = -c$. Therefore, $a = -b = -(-c) = -a$ and then $a = b = c = 0$. Nevertheless, $a + b + c = \mu \neq 0$, and then it must be $\sin(\theta) = 0$, which proves that $\theta = k\pi$, for $k \in \mathbb{Z}$. □

Theorem 5. *If $M \in M_3^h(\mathbb{C})$ is a minimal matrix with non-zero off-diagonal entries and spectrum $\{\lambda, \mu, -\lambda\}$ ($\|M\| = \lambda \geqslant |\mu|$), then there exist corresponding orthogonal unit norm eigenvectors v_λ, $v_{-\lambda}$ and v_μ such that*

$$M = \lambda\ (v_\lambda \otimes v_\lambda) - \lambda\ \left(v_{-\lambda} \otimes v_{-\lambda}\right) + \mu\ (v_\mu \otimes v_\mu),$$

where $N = \lambda\ (v_\lambda \otimes v_\lambda) - \lambda\ \left(v_{-\lambda} \otimes v_{-\lambda}\right)$ is minimal and $\mathrm{Diag}(\mu\ (v_\mu \otimes v_\mu)) = \mathrm{Diag}(M)$.

Proof. Let us suppose first that $|\mu| < \lambda$. Then all eigenspaces have dimension one and any choice of unit norm eigenvectors v_λ, $v_{-\lambda}$ corresponding to λ and $-\lambda$ satisfy Theorem 1. Then, using the same theorem, N is minimal, and Proposition 4 implies that $\mathrm{Diag}(N) = 0$. Therefore, $\mathrm{Diag}(\mu\ (v_\mu \otimes v_\mu)) = \mathrm{Diag}(M)$.

If $|\mu| = \lambda$, then one of the eigenspaces corresponding to λ or $-\lambda$ has dimension two. Since M is minimal there exist eigenvectors v_λ and $v_{-\lambda}$ corresponding to the eigenvalues λ and $-\lambda$ such that $v_\lambda \circ \overline{v_\lambda} = v_{-\lambda} \circ \overline{v_{-\lambda}}$ (Theorem 1). Pick these eigenvectors and any v_μ orthogonal to both of them. Then it can be proved similarly to above that they satisfy the identities of the theorem. □

Proposition 6. *Let $M_0, M_1 \in M_3^h(\mathbb{C})$ be two minimal matrices with the same diagonal and eigenvalues $\{\lambda, \mu, -\lambda\}$, with $0 \neq |\mu| \leqslant \lambda$, given by*

$$M_0 = \begin{pmatrix} a & x_0\, e^{\alpha_0 i} & y_0\, e^{-\beta_0 i} \\ x_0\, e^{-\alpha_0 i} & b & z_0\, e^{\gamma_0 i} \\ y_0\, e^{\beta_0 i} & z_0\, e^{-\gamma_0 i} & c \end{pmatrix} \text{ and } M_1 = \begin{pmatrix} a & x_1\, e^{\alpha_1 i} & y_1\, e^{-\beta_1 i} \\ x_1\, e^{-\alpha_1 i} & b & z_1\, e^{\gamma_1 i} \\ y_1\, e^{\beta_1 i} & z_1\, e^{-\gamma_1 i} & c \end{pmatrix},$$

with $x_0, y_0, z_0, x_1, y_1, z_1, \in \mathbb{R}_{>0}$.

Then $x_0 = x_1$, $y_0 = y_1$, $z_0 = z_1$ and $\cos(\alpha_0 + \beta_0 + \gamma_0) = \cos(\alpha_1 + \beta_1 + \gamma_1)$.

Proof. M_0 and M_1 are matrices of *non-extremal* type in the sense of Definition 3.5 of [9]. Note that $\mu = a + b + c \neq 0$. With the same notations of (3.9) and (3.10) in [9] for α, β, χ, $(n_{12})_0$, $(m_{12})_0$ (for M_0) and $(n_{12})_1$, $(m_{12})_1$ (for M_1), then it must be $\alpha = \frac{a}{2(a+b+c)}$, $\beta = \frac{b}{2(a+b+c)}$ and $\chi = \frac{c}{2(a+b+c)}$. Considering all the cases, it can be proved that $x_0 = |x_0| = |\mu\,(n_{12})_0 + \lambda\,(m_{12})_0\,| = |\mu\,(n_{12})_1 + \lambda\,(m_{12})_1\,| = |x_1| = x_1$. The same reasoning could be used to prove $y_0 = y_1$ and $z_0 = z_1$.

Finally, $\cos(\alpha_0 + \beta_0 + \gamma_0) = \cos(\alpha_1 + \beta_1 + \gamma_1)$ because the coefficients of the characteristic polynomial of each matrix are determined by $\{\lambda, \mu, -\lambda\}$. Using (4.4) we obtain that $-\lambda^2\mu = abc - az^2 - by^2 - cx^2 + 2xyz\cos(\alpha_0 + \beta_0 + \gamma_0) = abc - az^2 - by^2 - cx^2 + 2xyz\cos(\alpha_1 + \beta_1 + \gamma_1)$. □

We state the following result that was already mentioned in Remark 6.

Proposition 7. *Let M_0 and M_1 be matrices with the structure of those of Proposition 6. If their off-diagonal entries have equal modulus $x_0 = x_1$, $y_0 = y_1$, $z_0 = z_1$, and $\cos(\alpha_0 + \beta_0 + \gamma_0) = \cos(\alpha_1 + \beta_1 + \gamma_1)$, then both matrices have the same minimizing diagonal.*

Proof. The proof follows from reducing each matrix to one like M_θ as in Remark 5 and then applying Proposition 3. □

Theorem 6. *Let $x, y, z \in \mathbb{R}_{>0}$, $\theta \in \mathbb{R}$ and $M = \begin{pmatrix} a & x\, e^{i\theta} & y \\ x\, e^{-i\theta} & b & z \\ y & z & c \end{pmatrix}$ be a minimal matrix.*

Then there exist $\alpha, \beta, \gamma \in [0, \pi]$ such that:

(i) $\cos(\alpha+\beta+\gamma)=\cos(\theta)$,

(ii) *the matrices N, S defined by*

$$N=\begin{pmatrix} 0 & i\,x\,\sin\alpha & -i\,y\,\sin\beta \\ -i\,x\,\sin\alpha & 0 & i\,z\,\sin\gamma \\ i\,y\,\sin\beta & -i\,z\,\sin\gamma & 0 \end{pmatrix} \text{ and } S=\begin{pmatrix} a & x\,\cos\alpha & y\,\cos\beta \\ x\,\cos\alpha & b & z\,\cos\gamma \\ y\,\cos\beta & z\,\cos\gamma & c \end{pmatrix} \tag{4.7}$$

satisfy:

a) $Diag(N+S)=Diag(M)$,

b) *if* $v\in\ker(N)$ *with* $\|v\|=1$, then $S=(a+b+c)\,(v\otimes v)$,

c) $M_0=N+S$ *is minimal,*

d) M_0 *is unitarily equivalent to* M *or to* M^t *by means of unitary diagonals.*

(iii) *If* $\theta\neq k\pi/2$ *with* $k\in\mathbb{Z}$, *then* α, β *and* γ *satisfy*

1) $\cos\alpha\neq 0$, $\cos\beta\neq 0$ *and* $\cos\gamma\neq 0$,

2) $x^2\sin(2\alpha)=y^2\sin(2\beta)=z^2\sin(2\gamma)$,

3) $\|M\|^2=\|M_0\|^2=(x\sin\alpha)^2+(y\sin\beta)^2+(z\sin\gamma)^2$,

4) $Diag(M_0)$=$Diag(S)$=$Diag(M)$=$\left(\frac{xy\cos(\alpha)\cos(\beta)}{z\cos(\gamma)},\frac{xz\cos(\alpha)\cos(\gamma)}{y\cos(\beta)},\frac{yz\cos(\beta)\cos(\gamma)}{x\cos(\alpha)}\right)$,

5) $(x\sin\alpha)^2+(y\sin\beta)^2+(z\sin\gamma)^2\geqslant\left(\frac{xy\cos(\alpha)\cos(\beta)}{z\cos(\gamma)}+\frac{xz\cos(\alpha)\cos(\gamma)}{y\cos(\beta)}+\frac{yz\cos(\beta)\cos(\gamma)}{x\cos(\alpha)}\right)^2$.

Proof. Let us suppose that $\sigma(M)=\{\lambda,\mu,-\lambda\}$ with $|\mu|\leqslant\lambda=\|M\|$. Then, using Theorem 5, it can be proved that there exist v_λ, $v_{-\lambda}$ and v_μ orthonormal eigenvectors of λ, $-\lambda$ and μ respectively, such that $M=N+S$, with $N=\lambda(v_\lambda\otimes v_\lambda)-\lambda(v_{-\lambda}\otimes v_{-\lambda})$ a minimal matrix with $\mathrm{Diag}(N)=0$ and $S=\mu(v_\mu\otimes v_\mu)$, satisfying $\mathrm{Diag}(S)=\mathrm{Diag}(M)$ (even in the case $|\mu|=\lambda$). Let $v_\mu=(r,s,t)$, then it is clear that $a=\mu\,|r|^2$, $b=\mu\,|s|^2$, $c=\mu\,|t|^2$. Furthermore, defining $\xi=|r|$, $\psi=|s|$ and $\zeta=|t|$, the matrix $N_1=\lambda\begin{pmatrix} 0 & i\,\zeta & -i\,\psi \\ -i\,\zeta & 0 & i\,\xi \\ i\,\psi & -i\,\xi & 0 \end{pmatrix}$ is a minimal matrix and $\|N_1\|=\lambda$ (see Theorem 4 and Propositions 2 and 3). Moreover, $v=(\xi,\psi,\zeta)$ is a unit norm eigenvector corresponding to the eigenvalue 0 of N_1.

Let $S_1=\mu(v\otimes v)=\mu\begin{pmatrix} \xi^2 & \xi\psi & \xi\zeta \\ \psi\xi & \psi^2 & \psi\zeta \\ \zeta\xi & \zeta\psi & \zeta^2 \end{pmatrix}$.

By construction N_1 is minimal with $\sigma(N_1)=\{\lambda,0,-\lambda\}$ and $\sigma(S_1)=\{\mu,0\}$. Then,

$$M_1=N_1+S_1=\begin{pmatrix} \mu\xi^2 & \mu\xi\psi+i\,\lambda\zeta & \mu\xi\,\zeta-i\,\lambda\psi \\ \mu\psi\xi-\,i\,\lambda\zeta & \mu\psi^2 & \mu\psi\zeta+i\,\lambda\xi \\ \mu\zeta\xi+i\,\lambda\psi & \mu\zeta\psi-i\,\lambda\xi & \mu\zeta^2 \end{pmatrix}$$

has the same diagonal as M and $\sigma(M_1)=\sigma(M)$. Now we will consider the cases $\mu=0$ and $\mu\neq 0$.

- In the case $\mu=0$ the diagonal of M must be zero and, using Proposition 4, $\theta=k\pi+\frac{\pi}{2}$ for $k\in\mathbb{Z}$ and $\lambda=\sqrt{x^2+y^2+z^2}$. Moreover, it easy to check in this case that $v_\mu\circ v_\mu=1/\lambda^2(z^2,y^2,x^2)=(|r|^2,|s|^2,|t|^2)$ (because (z,y,x) is an eigenvector of M of eigenvalue $\mu=0$). Then $\zeta=x/\sqrt{x^2+y^2+z^2}$, $\psi=y/\sqrt{x^2+y^2+z^2}$, $\xi=z/\sqrt{x^2+y^2+z^2}$. If $\theta=(2k+1)\pi+\pi/2$, with $k\in\mathbb{Z}$. Then $\alpha=\beta=\gamma=\pi/2$ satisfy the conditions of the theorem and follows easily that N_1 is unitarily equivalent to M by means of diagonal matrices: $M=UN_1U^*$ for $U=\mathrm{Diag}(i,-i,1)$. In the case $\theta=(2k+1)\pi+\pi/2$, with $k\in\mathbb{Z}$, the matrix M is the transpose of the one considered in the case of $\theta=2k\pi+\pi/2$, with $k\in\mathbb{Z}$. Therefore, the theorem is proved in this case taking $\alpha=\beta=\gamma=\pi/2$, $N=N_1$ and $S=0$.
- If $\mu\neq 0$, then $M_1=N_1+S_1$ is minimal because N_1 is, and $S_1=\mu(v_\mu\otimes v_\mu)$ with v_μ orthogonal to the non-zero eigenvector of N_1 and $|\mu|\leqslant\lambda=\|N_1\|$. Moreover, none of the entries of M_1 can be null. Suppose for example that $(M_1)_{1,3}=0$ which implies that $\xi=\psi=0$ or $\zeta=\psi=0$. If we consider the case $\xi=\psi=0$, then M has $(0,0,1)$ as an eigenvector of μ (because $v_\mu=(r,s,t)$ is an eigenvector of the eigenvalue μ and $\xi=|r|$, $\psi=|s|$). But this implies that the entries $(M)_{1,3}=y=0$ and $(M)_{2,3}=z=0$, which

contradicts the assumptions of the theorem. If we consider the case $\zeta = \psi = 0$ we obtain $x = y = 0$, also a contradiction. With similar arguments we can prove that, in any case considered, assuming that one of the entries of M_1 is null leads to a contradiction.
We can use Proposition 6 to prove that $x = |\mu\xi\psi + i\,\lambda\zeta|$, $y = |\mu\xi\zeta - i\,\lambda\psi|$ and $z = |\mu\psi\zeta + i\,\lambda\xi|$. If we consider $0 \leqslant \arg(z) < 2\pi$ and define

$$\alpha = \arg(\mu\xi\psi + i\,\lambda\zeta)\ ,\ \beta = 2\pi - \arg(\mu\xi\zeta - i\,\lambda\psi)\ ,\ \gamma = \arg(\mu\psi\zeta + i\,\lambda\xi), \tag{4.8}$$

and $\theta_1 = \alpha + \beta + \gamma$, then $\alpha, \beta, \gamma \in [0, \pi]$. From Proposition 6 it follows that $\cos(\theta) = \cos(\theta_1)$.
Moreover, M_1 is unitarily equivalent by means of unitary diagonals to M_{θ_1} (see (4.5) and (4.6)). Since $M_{\theta_1} = M_\theta$, or $M_{\theta_1} = M_{-\theta} = (M_\theta)^t$, it follows that M_1 is unitary equivalent (by means of unitary diagonals) to M_θ or to its transpose. Choosing α, β and γ as defined before and putting $N = N_1$ and $S = S_1$ points (i) and (ii) of the theorem follow.

Proof of (iii).
If $\theta \neq k\pi/2$, for $k \in \mathbb{Z}$, then ζ, ξ and ψ are non-zero. The claim follows after considering the following cases.

- As seen in the proof of (ii) above, two of the numbers ζ, ξ, ψ cannot be zero simultaneously if $x, y, z \in \mathbb{R}_{>0}$.
- If only one of ζ, ξ, ψ is zero, M_0 is equivalent to a real matrix by means of diagonal unitary matrices (see (4.8) and Remark 5) and therefore $\theta = k\pi$, $k \in \mathbb{Z}$, a contradiction.

If ζ, ξ and ψ are not all zero and $\mu \neq 0$ ($\theta \neq k\pi + \pi/2$, $k \in \mathbb{Z}$), since we supposed $\lambda = \|M\| = \|M_0\|$, it follows that $\operatorname{Im}((M_0)_{1,2}) = x \sin\alpha = \lambda\zeta \neq 0$, $\operatorname{Im}((M_0)_{1,3}) = y \sin\beta = \lambda\psi \neq 0$ and $\operatorname{Im}((M_0)_{2,3}) = z \sin\gamma = \lambda\xi \neq 0$. Therefore, in this case (since $x, y, z \in \mathbb{R}_{>0}$) $\sin\alpha \neq 0$, $\sin\beta \neq 0$ and $\sin\gamma \neq 0$ and also (since $\mu \neq 0$) $\cos\alpha \neq 0$, $\cos\beta \neq 0$ and $\cos\gamma \neq 0$ which proves 1).
Then it can be verified that

$$v_\mu = \frac{1}{\sqrt{(x\sin\alpha)^2 + (y\sin\beta)^2 + (z\sin\gamma)^2}}\,(z\sin\gamma, y\sin\beta, x\sin\alpha) \tag{4.9}$$

is an eigenvector of M_0. Therefore, by construction

$$a = \frac{(a+b+c)(z\sin\gamma)^2}{\lambda^2}\ ,\ b = \frac{(a+b+c)(y\sin\beta)^2}{\lambda^2}\ ,\ c = \frac{(a+b+c)(x\sin\alpha)^2}{\lambda^2}$$

and $\lambda^2 = (x\sin\alpha)^2 + (y\sin\beta)^2 + (z\sin\gamma)^2$.
Pick v_μ as in (4.9). Then $S_{1,2} = x\cos\alpha = ((a+b+c)\,(v_\mu \otimes v_\mu))_{1,2} = \frac{\mu z y \sin\gamma \sin\beta}{\lambda^2}$. Thus $\frac{\mu}{\lambda^2} = \frac{x\cos\alpha}{zy\sin\gamma\sin\beta}$. Similarly, considering $S_{1,3}$ we obtain $\frac{\mu}{\lambda^2} = \frac{y\cos\beta}{zx\sin\gamma\sin\alpha}$ and therefore $\frac{x\cos\alpha}{zy\sin\gamma\sin\beta} = \frac{y\cos\beta}{zx\sin\gamma\sin\alpha}$. Reordering we obtain

$$x^2 \sin 2\alpha = y^2 \sin 2\beta.$$

Using $S_{1,3}$ we obtain $\frac{\mu}{\lambda^2} = \frac{z\cos\gamma}{xy\sin\alpha\sin\beta}$ and reasoning as before we can prove 2).
From (ii) d) of Theorem 6, is clear that M_0 and M have the same norm (that of N) and diagonal (that of S). The norm of N is $\sqrt{(x\sin\alpha)^2 + (y\sin\beta)^2 + (z\sin\gamma)^2}$ which proves 3).
Using the same v_μ as in (4.9) we obtain

$$\begin{aligned} S_{1,1} &= \mu(z\sin\gamma)^2/\lambda^2 \\ &= \frac{\left(\mu(\frac{z\sin\gamma}{\lambda})(\frac{y\sin\beta}{\lambda})\right)\left(\mu(\frac{x\sin\alpha}{\lambda})(\frac{z\sin\gamma}{\lambda})\right)}{(\mu(\frac{x\sin\alpha}{\lambda})(\frac{y\sin\beta}{\lambda}))} = \frac{S_{1,2}\,S_{1,3}}{S_{2,3}} \\ &= \frac{(x\cos\alpha)(y\cos\beta)}{(z\cos\gamma)} = \frac{xy\cos\alpha\cos\beta}{z\cos\gamma}. \end{aligned}$$

The formulas for $S_{2,2}$ and $S_{3,3}$ are obtained similarly. This proves 4).
Points 3) and 4) imply 5): since M is minimal, then $\operatorname{tr}(M)$ is an eigenvalue of M and therefore $\operatorname{tr}(M)^2 \leqslant \|M\|^2$. □

Proposition 8. *If $\alpha, \beta, \gamma \in \mathbb{R}$, $\alpha, \beta, \gamma \neq k\pi/2$ with $k \in \mathbb{Z}$, and $x, y, z \in \mathbb{R}_{>0}$, $M_0 = N + S$, with*

$$N = \begin{pmatrix} 0 & i\,x\,\sin\alpha & -i\,y\,\sin\beta \\ -i\,x\,\sin\alpha & 0 & i\,z\,\sin\gamma \\ i\,y\,\sin\beta & -i\,z\,\sin\gamma & 0 \end{pmatrix} \quad \textit{and}$$

$$S = \begin{pmatrix} \frac{xy\cos(\alpha)\cos(\beta)}{z\cos(\gamma)} & x\,\cos\alpha & y\,\cos\beta \\ x\,\cos\alpha & \frac{xz\cos(\alpha)\cos(\gamma)}{y\cos(\beta)} & z\,\cos\gamma \\ y\,\cos\beta & z\,\cos\gamma & \frac{yz\cos(\beta)\cos(\gamma)}{x\cos(\alpha)} \end{pmatrix},$$

then $\alpha, \beta, \gamma, x, y, z$ satisfy:

1) $x^2\sin(2\alpha) = y^2\sin(2\beta) = z^2\sin(2\gamma)$,
2) $(x\sin\alpha)^2 + (y\sin\beta)^2 + (z\sin\gamma)^2 \geqslant \left(\frac{xy\cos(\alpha)\cos(\beta)}{z\cos(\gamma)} + \frac{xz\cos(\alpha)\cos(\gamma)}{y\cos(\beta)} + \frac{yz\cos(\beta)\cos(\gamma)}{x\cos(\alpha)}\right)^2$.

Then, $NS = SN = 0$ and $M_0 = N + S$ is minimal.

Proof. Using 1) it follows that $NS = 0$ and $SN = 0$. Furthermore, S has rank one and N rank two. Then $\operatorname{ran}(S) = \ker(N)$ and $\ker(S) = \operatorname{ran}(N)$ and $\sigma(S) = \{0, \operatorname{tr}(S)\}$. Therefore, if we set

$$\lambda = \sqrt{x^2\sin^2(\alpha) + y^2\sin^2(\beta) + z^2\sin^2(\gamma)},$$

it follows that $\sigma(N) = \{0, \lambda, -\lambda\}$. Then $\sigma(N + S) = \{\operatorname{tr}(S), \lambda, -\lambda\}$, and by 2) $M_0 = N + S$ satisfies $\|M_0\| = \|N\| = \lambda = \sqrt{x^2\sin^2(\alpha) + y^2\sin^2(\beta) + z^2\sin^2(\gamma)}$. Furthermore, the eigenvectors of M_0 corresponding to the eigenvalues $\pm\lambda$ are the same as that of N (that is a minimal matrix as seen in the proof of Theorem 6) and therefore they satisfy the conditions of Theorem 1. Therefore, M_0 is minimal. ☐

Theorem 7. *Given a minimal matrix of the form*

$$M = \begin{pmatrix} a & x\,e^{i\theta} & y \\ x\,e^{-i\theta} & b & z \\ y & z & c \end{pmatrix} \textit{ with } x \geqslant y \geqslant z > 0 \textit{ and } \theta \in \left(\frac{3}{2}\pi, 2\pi\right) \tag{4.10}$$

there exist unique $\alpha \in (\pi/2, \frac{3}{4}\pi]$, $\beta \in (\pi/2, \frac{3}{4}\pi]$, $\gamma \in (\pi/2, \pi)$, which are continuous functions of θ, x, y, z such that:

1) $\alpha + \beta + \gamma = \theta$,
2) *The matrices N, S defined by*

$$N = \begin{pmatrix} 0 & i\,x\,\sin\alpha & -i\,y\,\sin\beta \\ -i\,x\,\sin\alpha & 0 & i\,z\,\sin\gamma \\ i\,y\,\sin\beta & -i\,z\,\sin\gamma & 0 \end{pmatrix} \tag{4.11}$$

and

$$S = \begin{pmatrix} a & x\,\cos\alpha & y\,\cos\beta \\ x\,\cos\alpha & b & z\,\cos\gamma \\ y\,\cos\beta & z\,\cos\gamma & c \end{pmatrix} \tag{4.12}$$

satisfy

a) $\mathit{Diag}(N + S) = \mathit{Diag}(M)$,
b) *if $v \in \ker(N)$ with $v \in \mathbb{R}^3$ and $\|v\| = 1$,* then $S = (a + b + c)\,(v \otimes v)$,
c) *$M_0 = N + S$ is minimal,*
d) *M_0 is unitarily equivalent to M or to M^t by means of diagonal unitaries;*

and

1’) $x^2\sin(2\alpha) = y^2\sin(2\beta) = z^2\sin(2\gamma)$,

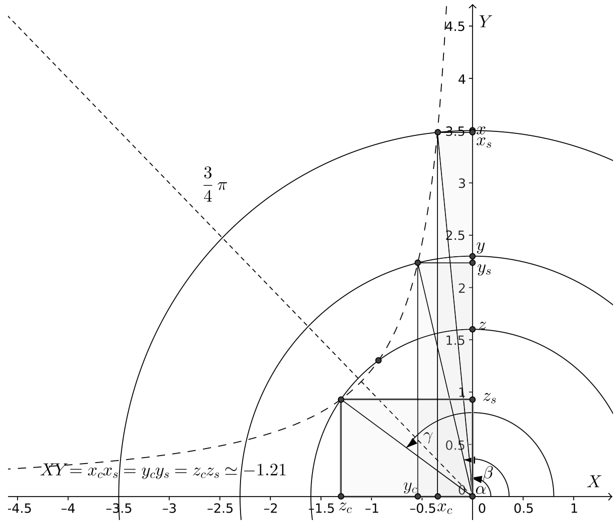

Figure 1: The corresponding α, β and γ for $\theta = 6.$, $x = 3.5$, $y = 2.3$ and $z = 1.6$.

2') $\|M\|^2 = \|M_0\|^2 = (x\sin\alpha)^2 + (y\sin\beta)^2 + (z\sin\gamma)^2$,

3') $Diag(M_0) = Diag(M) = \left(\frac{xy\cos(\alpha)\cos(\beta)}{z\cos(\gamma)}, \frac{xz\cos(\alpha)\cos(\gamma)}{y\cos(\beta)}, \frac{yz\cos(\beta)\cos(\gamma)}{x\cos(\alpha)}\right)$,

4') $(x\sin\alpha)^2 + (y\sin\beta)^2 + (z\sin\gamma)^2 \geqslant \left(\frac{xy\cos(\alpha)\cos(\beta)}{z\cos(\gamma)} + \frac{xz\cos(\alpha)\cos(\gamma)}{y\cos(\beta)} + \frac{yz\cos(\beta)\cos(\gamma)}{x\cos(\alpha)}\right)^2$.

Proof. Most of the statements of this theorem were proved in Theorem 6. It only remains to prove that for fixed θ, x, y, z the angles α, β and γ that fulfil the conditions of the Theorem are unique, that they can be chosen in the specified intervals and that they are continuous functions of θ.

Analysing the signs of the real and imaginary parts of the complexes such that their arguments define the angles α, β and γ that appear in the proof of the Theorem 6 we can conclude that in this case, (since we can prove that $\mu \leqslant 0 \Leftrightarrow \theta \in [\frac{3}{2}\pi, 2\pi]$) we can choose $\alpha,\beta,\gamma \in [\pi/2, 2\pi]$. If we consider $\mu < 0$ ($\mu = 0$ corresponds to $\theta = 3\pi/2$ since by Corollary 2 it has the same minimizing diagonals as those considered in Theorem 4), then we can suppose that (for α, β, γ from Theorem 6) $x_c = x\cos\alpha$, $x_s = x\sin\alpha$, $y_c = y\cos\beta$, $y_s = y\sin\beta$, $z_c = z\cos\gamma$ and $z_s = z\sin\gamma$ are all non-zero (as it analysed in the proof of Theorem 6 (iii)). Then using the inequality 4') we obtain

$$z_c^2y_c^2x_c^2\left(x_s^2 + y_s^2 + z_s^2\right) \geqslant \left(x_c^2y_c^2 + x_c^2z_c^2 + y_c^2z_c^2\right)^2$$

and together with 1'), denoting $k = x_cx_s = y_cy_s = z_cz_s$ we can prove that

$$k^2 \geqslant \left(x_c^2y_c^2 + x_c^2z_c^2 + y_c^2z_c^2\right) \tag{4.13}$$

We will prove first that $\alpha \notin (\frac{3}{4}\pi, \pi)$. Suppose that $\alpha \in (\frac{3}{4}\pi, \pi)$ and consider two cases:

a) $\beta \in (\alpha, \pi)$: in this case since $x_cx_s = y_cy_s \wedge y \leqslant x$, then $\sin(\beta) < \sin(\alpha)$, $y_s < x_s$ and $x_s \leqslant |x_c| < |y_c|$. Hence,

$$k^2 = x_s^2x_c^2 < y_c^2x_c^2 < \left(x_c^2y_c^2 + x_c^2z_c^2 + y_c^2z_c^2\right),$$

which contradicts (4.13).

b) $\beta \in (\pi/2, \alpha]$:

– (i) if $\beta \in [3/4\pi, \alpha]$, then $|y_s| \leqslant |y_c| \leqslant |x_c|$ and so

$$k^2 = y_s^2y_c^2 \leqslant x_c^2y_c^2 < \left(x_c^2y_c^2 + x_c^2z_c^2 + y_c^2z_c^2\right),$$

which contradicts (4.13).

– (ii) if $\beta \in (\pi/2, 3/4\pi)$ we will compare $|x_c|$ with y_s

– (ii$_1$) If $|x_c| \geqslant y_s$, then
$$k^2 = y_s^2 y_c^2 \leqslant x_c^2 y_c^2 < \left(x_c^2 y_c^2 + x_c^2 z_c^2 + y_c^2 z_c^2 \right),$$
which contradicts (4.13).

– (ii$_2$) If $|x_c| < y_s$, then (recall that $x_c, y_c < 0$) $y_s + x_c > 0$. Moreover, $x_s^2 + x_c^2 = x^2 \geqslant y^2 = y_s^2 + y_c^2$, then $(x_s + x_c)^2 = x_s^2 + 2x_s x_c + x_c^2 \geqslant y_s^2 + 2y_s y_c + y_c^2 = (y_s + y_c)^2$, and so $|x_s + x_c| \geqslant |y_s + y_c|$, . But $0 < x_s < |x_c|$ and $0 < |y_c| < y_s$, which proves that $-x_s - x_c \geqslant y_s + y_c$. Then $-x_s - y_c \geqslant y_s + x_c > 0$ and hence $-y_c > x_s$ holds and
$$k^2 = x_s^2 x_c^2 < y_c^2 x_c^2 < \left(x_c^2 y_c^2 + x_c^2 z_c^2 + y_c^2 z_c^2 \right),$$
which contradicts (4.13).

Thus, $\alpha \notin (\frac{3}{4}\pi, \pi)$ holds and if $\theta \in (\frac{3}{2}\pi, 2\pi)$ then $\alpha \in (\pi/2, \frac{3}{4}\pi]$.

Similarly, comparing $|y_c|$ with $|z_c|$ it can be proved that $\beta \notin (\frac{3}{4}\pi, \pi)$. Therefore, $\beta \in (\pi/2, \frac{3}{4}\pi]$ and $\gamma \in [\beta, \frac{3}{2}\pi - \beta] \subset [\pi/2, \pi]$ (see Figure 1).

Uniqueness:

The angles α and β are unique in these intervals since they must satisfy the conditions $x_c x_s = y_c y_s = k$, $\pi/2 \leqslant \alpha \leqslant \frac{3}{4}\pi$ and $\pi/2 \leqslant \beta \leqslant \frac{3}{4}\pi$. If there are two different angles γ and γ' in $(\pi/2, \pi)$ that satisfy the conditions of Theorem 6, then the only possible case is that one belongs to $(\beta, \frac{3}{4}\pi)$ and the other one to $(\frac{3}{4}\pi, \frac{3}{2}\pi - \beta)$. Suppose that $\beta < \gamma \leqslant \frac{3}{4}\pi$ and $\frac{3}{4}\pi < \gamma' \leqslant \frac{3}{2}\pi - \beta$. Then only γ' satisfies the conditions of Theorem 6 (iii). This is because, if both satisfy the minimality conditions there, then $\lambda^2 = \|M\| = (x \sin\alpha)^2 + (y \sin\beta)^2 + (z \sin\gamma)^2 = (x \sin\alpha)^2 + (y \sin\beta)^2 + (z \sin\gamma')^2$, which is a contradiction because $\sin\gamma' < \sin\gamma$.

If x, y, z are fixed, we denote with $\alpha = \alpha(\theta)$, $\beta = \beta(\theta)$ and $\gamma = \gamma(\theta)$ the angles that are uniquely determined by θ in the corresponding intervals. If we look at the definition of these angles given in 4.8 of Theorem 6, it can be seen that it is a continuous function with respect to θ (and also with respect to x,y,z).

The sum of α, β, and γ gives θ:

Since $\theta \in (\frac{3}{2}\pi, 2\pi)$, $\alpha(\theta), \beta(\theta) \in (\pi/2, \frac{3}{4}\pi)$, $\gamma(\theta) \in \left(\beta(\theta), \frac{3}{2}\pi - \beta(\theta)\right)$, then $3/2\,\pi \leqslant \alpha(\theta) + \beta(\theta) + \gamma(\theta) \leqslant 9/4\,\pi$. Using that $\cos(\alpha(\theta) + \beta(\theta) + \gamma(\theta)) = \cos(\theta)$ the continuity and uniqueness arguments imply that $\alpha(\theta) + \beta(\theta) + \gamma(\theta) = \theta$ holds for every $\theta \in (\frac{3}{2}\pi, 2\pi)$.

□

Remark 7. *Given a minimal matrix M_θ as in 4.10 with $\theta = \frac{3}{2}\pi$, $x \geqslant y \geqslant z > 0$ we have $\sigma(M_{3\pi/2}) = \{\lambda, 0, -\lambda\}$ (see Corollary 2). $M_{3\pi/2}$ has the same null minimizing diagonals as those matrices considered in Theorem 4 (see Remark 5). Then we can define $\alpha(3\pi/2) = \beta(3\pi/2) = \gamma(3\pi/2) = \pi/2$ and they satisfy 1), 2) and 1') through 4') of Theorem 7. As we will see this definition makes α, β and γ continuous in terms of $\theta \in (\pi, 2\pi)$.*

In the case $\theta \in (\pi, \frac{3}{2}\pi)$ let us consider $\theta' = 3\pi - \theta$. Then $\theta' \in (\frac{3}{2}\pi, 2\pi)$ and if we denote by α', β' and γ' the solutions whose existence was proved in Theorem 7, then it is enough to take $\alpha = \pi - \alpha'$, $\beta = \pi - \beta'$ and $\gamma = \pi - \gamma'$ and check that these angles α, β and $\gamma \in (0, \pi/2)$ satisfy all the required conditions 1), 2) and 1') through 4') of Theorem 7.

If $\theta \in (\frac{3}{2}\pi, 2\pi)$, it is clear that if θ is close to $\frac{3}{2}\pi$, then the values of $\alpha(\theta), \beta(\theta)$ and $\gamma(\theta)$ defined as in Theorem 7 must be close to $\pi/2$. Then α, β and γ are right continuous in $\theta = \frac{3}{2}\pi$, i.e., $\lim_{\theta \to 3\pi/2^+} \alpha(\theta) = \lim_{\theta \to 3\pi/2^+} \beta(\theta) = \lim_{\theta \to 3\pi/2^+} \gamma(\theta) = \pi/2$. Similarly it can be proved that α, β and γ are left continuous in $\theta = \frac{3}{2}\pi$.

If $\theta \in (\pi, \frac{3}{2}\pi)$, then similar arguments as the ones made before (using the proven uniqueness, continuity and sum of α, β, γ of the previous case) prove that also in this case $\alpha + \beta + \gamma = \theta$.

If $\theta = \frac{3}{2}\pi$, choosing $\alpha = \beta = \gamma = \pi/2$, then obviously $\alpha + \beta + \gamma = \theta$, and because of the previous arguments α, β and γ are continuous functions of θ in the whole interval $(\pi, 2\pi)$.

Remark 8. *If $\theta \in (\pi, 2\pi)$ using the results and notations of the theorem above for a minimal matrix M with the structure of (4.10) and considering the cases $\mu \in (-\lambda, 0)$ (that is equivalent to $\theta \in (\frac{3}{2}\pi, 2\pi)$), or $\mu \in (0, \lambda)$ (that* *is equivalent to* $\theta \in (\pi, \frac{3}{2}\pi)$*), or* $\mu = 0$ *(that is equivalent to* $\theta = \frac{3}{2}\pi$*), then it can be proved that the unique angles* $\alpha \in (\pi/2, \frac{3}{4}\pi)$*,* $\beta \in (\pi/2, \frac{3}{4}\pi)$*,* $\gamma \in (\beta, \frac{3}{2}\pi - \beta)$ *from Theorem 7 must satisfy*

$$\alpha + \beta + \gamma = \theta\ ,\ \alpha = \frac{1}{2}\left(\pi - \arcsin\left(\frac{z^2 \sin(2\gamma)}{x^2}\right)\right)\ ,\ \beta = \frac{1}{2}\left(\pi - \arcsin\left(\frac{z^2 \sin(2\gamma)}{y^2}\right)\right).$$

Observe that the uniqueness of these angles in the specified intervals for each θ *and the conditions*

$$\alpha + \beta + \gamma = \theta,$$

$$x^2 \sin(2\alpha) = y^2 \sin(2\beta) = z^2 \sin(2\gamma),$$

$$(x \sin\alpha)^2 + (y \sin\beta)^2 + (z \sin\gamma)^2 \geqslant \left(\frac{xy\cos(\alpha)\cos(\beta)}{z\cos(\gamma)} + \frac{xz\cos(\alpha)\cos(\gamma)}{y\cos(\beta)} + \frac{yz\cos(\beta)\cos(\gamma)}{x\cos(\alpha)}\right)^2$$

imply that the root of

$$\frac{1}{2}\left(2\pi - \arcsin\left(\frac{z^2\sin(2\gamma)}{x^2}\right) - \arcsin\left(\frac{z^2\sin(2\gamma)}{y^2}\right)\right) + \gamma - \theta = 0$$

which is closer to $\gamma = \frac{3}{4}\pi$ *is the wanted solution.*

Remark 9. Algorithm.

1. ***Case*** $M_{i,j} = 0$***, for some*** $i \neq j$*. If* M *is a Hermitian matrix with zero entries outside the diagonal, then the null diagonal is always minimizing for* M*.*
   If two entries outside the diagonal of M *are null, then there exist infinitely many other minimizing diagonals for* M *(see Proposition 2 for details).*
2. ***Case*** $M_{i,j} \neq 0$***, for*** $i \neq j$*. A given generic Hermitian matrix* M *with non-zero entries can be conjugated by diagonal unitary and permutation matrices (see Remark 6 and Proposition 3) to obtain a matrix with the structure*

   $$M_\theta = \begin{pmatrix} a & x\,e^{i\theta} & y \\ x\,e^{-i\theta} & b & z \\ y & z & c \end{pmatrix},\ \text{with } x \geqslant y \geqslant z > 0 \text{ and } \theta \in [0, 2\pi).$$

   Next we discuss how to find the minimizing diagonal matrices $Diag(a, b, c)$ *for* M_θ*.*

   (a) **Case** $\theta = 0$ **or** $\theta = \pi$**:** *in this the minimizing diagonal* $Diag(a, b, c)$ *can be computed writing:*

   $$a = \frac{D - 2|A|}{4xyz} \quad b = \frac{D - 2|B|}{4xyz} \quad c = \frac{D - 2|C|}{4xyz},$$

   where

   $$A = +x^2y^2 - y^2z^2 - z^2x^2 \quad B = -x^2y^2 - y^2z^2 + z^2x^2 \quad C = -x^2y^2 + y^2z^2 - z^2x^2$$

   $$\text{and } D = A + |A| + B + |B| + C + |C|.$$

   (b) **Case** $\theta = \frac{\pi}{2}$ **or** $\theta = \frac{3\pi}{2}$**:**
   In this case: $a = b = c = 0$*.*

   (c) **Case** $\theta \in (0, \frac{\pi}{2}) \cup (\frac{\pi}{2}, \pi)$**:**
   This case corresponds to the transpose of a matrix from the case where $\pi \leqslant \theta < 2\pi$ *that has the same minimizing diagonal. That is, if* $\theta \in (0, \frac{\pi}{2}) \cup (\frac{\pi}{2}, \pi)$*, then* $(2\pi - \theta) \in (\pi, \frac{3\pi}{2}) \cup (\frac{3\pi}{2}, 2\pi)$ *and the minimizing diagonal corresponding to* θ *is the same to the one corresponding to* $2\pi - \theta$*, which is described in the next case.*

(d) **Case** $\theta \in (\pi, \frac{3\pi}{2}) \cup (\frac{3\pi}{2}, 2\pi)$**:**
Let γ be the closest solution to $3/4\pi$ of the equation

$$\frac{1}{2}\left(2\pi - \arcsin\left(\frac{z^2\sin(2\gamma)}{x^2}\right) - \arcsin\left(\frac{z^2\sin(2\gamma)}{y^2}\right)\right) + \gamma - \theta = 0$$

(that can be easily approximated by a standard numerical method), and

$$\alpha = \frac{1}{2}\left(\pi - \arcsin\left(\frac{z^2\sin(2\gamma)}{x^2}\right)\right)\ ,\ \beta = \frac{1}{2}\left(\pi - \arcsin\left(\frac{z^2\sin(2\gamma)}{y^2}\right)\right).$$

Then the (approximated as much as needed) minimizing diagonal is

$$a = \frac{xy\cos(\alpha)\cos(\beta)}{z\cos(\gamma)}\ ,\ b = \frac{xz\cos(\alpha)\cos(\gamma)}{y\cos(\beta)}\ ,\ c = \frac{yz\cos(\beta)\cos(\gamma)}{x\cos(\alpha)}.$$

To obtain the minimal matrix corresponding to the original matrix M, inverse conjugation with the diagonal unitary and the permutation matrices which were used to obtain M_θ may be required. This inverse conjugation applied to the minimizing diagonal of M_θ gives the minimizing diagonal of M. Note that this operation can only change the order of the diagonal entries.

5 Some $n \times n$ cases

In this section we describe some general facts about minimal matrices and their minimizing diagonals, as well as the concrete minimizing diagonals for some particular $n \times n$ Hermitian matrices.

We include a result from [8] that will be used often. It generalizes Theorem 1 for $n > 3$. In this case convex hulls of orthonormal sets of eigenvectors may be needed instead of only one eigenvector for each eigenvalue $\lambda = \|M\| = \lambda_{\max}(M)$ and $-\lambda = -\|M\| = \lambda_{\min}(M)$ (see also Remark 2).

In the following corollary $\mathrm{co}(A)$ denotes the convex hull of the set A.

Corollary 3. ***[8, Corollary 3]*** *Let $M \in M^h_{n\times n}(\mathbb{C})$ be a non-zero matrix such that its maximum and minimum eigenvalues satisfy $\lambda_{\max}(M) + \lambda_{\min}(M) = 0$ and let S_+ (respectively S_-) be the spectral eigenspace corresponding to $\lambda_{\max}(M)$ (respectively $\lambda_{\min}(M)$).*

Then the following properties are equivalent

(a) *M is minimal.*
(b) *There exist orthonormal sets $\{v_i\}_{i=1}^r \subset S_+$ and $\{v_j\}_{j=r+1}^{r+s} \subset S_-$ such that*

$$co\big(\{v_i \circ \overline{v_i}\}_{i=1}^r\big) \cap co\left(\{v_j \circ \overline{v_j}\}_{j=r+1}^{r+s}\right) \neq \varnothing.$$

The minimizing diagonals of a fixed matrix $M \in M^h_n(\mathbb{C})$ form a convex set. Suppose that D_0, D_1 are minimizing diagonals for M and $t \in [0, 1]$, then

$$\begin{aligned} \|M + tD_0 + (1-t)D_1\| &= \|tM + (1-t)M + tD_0 + (1-t)D_1\| \\ &\leqslant \|t(M + D_0)\| + \|(1-t)(M + D_1)\| \\ &\leqslant \|M + D\|, \quad \text{for all } D \in D_n(\mathbb{R}). \end{aligned} \tag{5.1}$$

Therefore, the convex combination $tD_0 + (1-t)D)_1$ is also a minimizing diagonal for M.

The following remark shows that the set of matrices with infinitely many different minimizing diagonals is neither open, nor closed in $M^h_n(\mathbb{C})$. The same property holds for its complement in $M^h_n(\mathbb{C})$ (the set of matrices that have a unique minimizing diagonal).

Remark 10. *The set of matrices that have infinitely many minimizing diagonals is not open in $M_n^h(\mathbb{C})$. Consider for example the matrices $M_m = \begin{pmatrix} 0 & 1/m & x \\ 1/m & 0 & 0 \\ \overline{x} & 0 & 0 \end{pmatrix}$, for $m \in \mathbb{N}$ and $x \in \mathbb{C}$, $x \neq 0$. Each M_m has a unique minimizing diagonal (see Proposition 1) but their limit:*

$$\lim_{m\to\infty} M_m = \begin{pmatrix} 0 & 0 & x \\ 0 & 0 & 0 \\ \overline{x} & 0 & 0 \end{pmatrix}$$

has infinitely many minimizing diagonals (see Proposition 2).

Moreover, the matrices $M_m = \begin{pmatrix} 0 & 1/m & 0 \\ 1/m & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$, for $m \in \mathbb{N}$ have infinitely many minimizing diagonals (see Proposition 2) but satisfy $\lim_{m\to\infty} M_m = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$. Since the zero matrix obviously has only one minimizing diagonal, the set of matrices with infinitely many minimizing diagonals is neither closed.

The same examples prove that the set of matrices with a unique minimizing diagonal is neither closed nor open.

Despite the previous remark, there are large sets of matrices with a unique minimizing diagonal that are open in $M_n^h(\mathbb{C})$ (such as that of matrices in $M_3^h(\mathbb{C})$ with at least two non-zero off-diagonal entries, see Proposition 1). The following proposition proves the continuity of the map that evaluated on the off-diagonal part of a matrix gives its unique minimizing diagonal.

Recall that $\mathrm{Diag}(M)$ is the diagonal matrix with the same diagonal as M. Now consider the map

$$\mathcal{O} : M_n^h(\mathbb{C}) \to M_n^h(\mathbb{C}) \text{ , such that } \mathcal{O}(M) = M - \mathrm{Diag}(M).$$

$\mathcal{O}$ puts zeros in the diagonal of $M \in M_n^h(\mathbb{C})$.

Proposition 9. *Let $M \in M_n^h(\mathbb{C})$ a matrix with a unique minimizing diagonal $d_{min}(M)$ and $\mathcal{O}(M) = M - Diag(M)$.*

1. *If $M_m \in M_n^h(\mathbb{C})$, with $m \in \mathbb{N} \cup \{0\}$ satisfies the condition that each M_m has a unique minimizing diagonal $d_{min}(M_m)$ such that $\lim_{m\to\infty} \mathcal{O}(M_m) = \mathcal{O}(M_0)$, then*

$$\lim_{m\to\infty} d_{min}(M_m) = d_{min}(M_0).$$

2. *Let $B \subset M_n^h(\mathbb{C})$ be the open subset of matrices that have only one minimizing diagonal. Then $d_{min} : \mathcal{O}(B) \to D_n(\mathbb{R})$ is a continuous map.*

Proof. 1) If $\lim_{m\to\infty} \mathcal{O}(M_m) = \mathcal{O}(M_0)$, then $d_{min}(M_m)$ must be bounded for all $m \in \mathbb{N}$. This holds because, since $d_{min}(M_m) + \mathcal{O}(M_m)$ is minimal, then $\|d_{min}(M_m) + \mathcal{O}(M_m)\| \leqslant \|\mathcal{O}(M_m)\|$ and therefore

$$\begin{aligned}\|d_{min}(M_m)\| &= \|d_{min}(M_m) \pm \mathcal{O}(M_m)\| \leqslant \|d_{min}(M_m) + \mathcal{O}(M_m)\| + \|\mathcal{O}(M_m)\| \\ &\leqslant 2\|\mathcal{O}(M_m)\|.\end{aligned}$$

The claim that $d_{min}(M_m)$ is bounded follows since $\{\mathcal{O}(M_m)\}_{n\in\mathbb{N}}$ is a convergent sequence.

Then, as $\{d_{min}(M_m)\}_{m\in\mathbb{N}}$ belongs to a compact set, we can choose a subsequence $\{M_{m_k}\}_{k\in\mathbb{N}}$ such that $d_{min}(M_{m_k})$ converges to a real diagonal D_0.

We will prove first that $D_0 = d_{min}(M_0)$. Given $\varepsilon > 0$, we can choose $k_0 \in \mathbb{N}$ such that $\|\mathcal{O}(M_0) - \mathcal{O}(M_{m_k})\| < \varepsilon$ and $\|d_{min}(M_{m_k}) - D_0\| < \varepsilon$, for all $k \geqslant k_0$. Then

$$\begin{aligned}\|\mathcal{O}(M_0) + D_0\| &= \|\mathcal{O}(M_0) + D_0 \pm (\mathcal{O}(M_{m_k}) + d_{min}(M_{m_k}))\| \\ &= \|\mathcal{O}(M_0) - \mathcal{O}(M_{m_k}) + D_0 - d_{min}(M_{m_k}) + \mathcal{O}(M_{m_k}) + d_{min}(M_{m_k})\| \\ &< 2\varepsilon + \|\mathcal{O}(M_{m_k}) + d_{min}(M_{m_k})\| \\ &\leqslant 2\varepsilon + \|\mathcal{O}(M_{m_k}) + D\| = 2\varepsilon + \|\mathcal{O}(M_{m_k}) \pm \mathcal{O}(M_0) + D\| \\ &< 3\varepsilon + \|\mathcal{O}(M_0) + D\|\end{aligned}$$

for every real diagonal D and $\varepsilon > 0$. Then $\|\mathcal{O}(M_0) + D_0\| \leqslant \|\mathcal{O}(M_0) + D\|$ for every real diagonal D, which proves that D_0 is a minimizing diagonal for M_0, and therefore $D_0 = d_{min}(M_0)$.

Note that the previous argument also proves that if D_1 is the limit of any convergent subsequence of $\{d_{min}(M_m)\}_{m\in\mathbb{N}}$, then it must be $D_1 = D_0 = d_{min}(M_0)$. Then, using that $\{d_{min}(M_m)\}_{m\in\mathbb{N}}$ is bounded, the whole sequence $\{M_m\}_{m\in\mathbb{N}}$ satisfies $\lim_{m\to\infty} d_{min}(M_m) = D_0 = d_{min}(M_0)$.

2) Note that if $B \subset M_n^h(\mathbb{C})$ is open and $\mathcal{O}(B) = \{\mathcal{O}(M) : M \in B\}$, then $\mathcal{O}(B)$ is open in $\mathcal{O}\left(M_n^h(\mathbb{C})\right)$ since $\mathcal{O} : M_n^h(\mathbb{C}) \to M_n^h(\mathbb{C})$ is a projection and $d_{min} : \mathcal{O}(B) \to D_n(\mathbb{R})$ is a well defined map. By 1) $d_{min} : \mathcal{O}(B) \to D_n(\mathbb{R})$ is continuous.

□

Corollary 4. *Let M_θ be as in (4.5). Then the entries of the unique minimizing diagonal of M_θ define a continuous function of x, y, z and θ:*

$$d : \mathbb{R}^3_{\neq 0} \times [0, \pi] \to \mathbb{R}^3, \quad d(x, y, z, \theta) = (d_{min}(M_\theta)_{1,1}, d_{min}(M_\theta)_{2,2}, d_{min}(M_\theta)_{3,3})\,.$$

Proof. The proof follows considering the map $d_{min} : \mathcal{O}(\{M_\theta : \theta \in [0, \pi], \text{ and } x, y, z \neq 0\}) \to D_n(\mathbb{R})$ and Proposition 9. □

Theorem 8. *If $M \in M_n^h(\mathbb{C})$ is such that $diag(M) = 0$ and $Re(M_{i,j}) = 0$, for all i, j, then M is minimal.*

Proof. Let us suppose that v_λ is an eigenvector of $\lambda = \|M\|$. Then, it is clear that $-\lambda \in \sigma(M)$ and that the vector $\overline{v_\lambda}$ is an eigenvector of $-\lambda$. Since $|(v_\lambda)_i| = |(\overline{v_\lambda})_i|$ for every i, a generalization of Theorem 1 (see Corollary 3) proves that M is minimal. □

In the next theorem for $M \in \mathbb{C}^{n\times n}$ we denote by $C_j(M)$ the j^{th} column of M, by $M_{\check{j}}$ the matrix in $\mathbb{C}^{(n-1)\times(n-1)}$ obtained after taking out the j^{th} column and row of M and by $v_{\check{j}}$ the element of $\mathbb{C}^{n-1}$ obtained after taking out the j^{th} entry of $v \in \mathbb{C}^n$.

Theorem 9. *For $N \in M_n^h(\mathbb{C})$ and $k \in \mathbb{N}$ such that $1 \leqslant k \leqslant n$. Suppose that N satisfies the following properties:*

1) *the k^{th} column $C_k(N)$ satisfies that its k^{th} entry $(C_k(N))_k = N_{k,k} = 0$,*
2) *$C_j(N) \cdot C_k(N) = 0$, for all $j \neq k$,*
3) *$\|N_{\check{k}}\| \leqslant \|C_k(N)\|_2$.*

Then N is a minimal matrix with $\|N\| = \|C_k(N)\|_2$. Moreover, if each i^{th} entry $(C_k(N))_i = N_{i,k} \neq 0$, for all $i \neq k$, then the diagonal of N is the only one which makes N a minimal matrix.

Proof. Let us denote by $c_k = \|C_k(N)\|_2$, by $\{e_i\}_{i=1,\ldots,n}$ the canonical basis of $\mathbb{C}^n$ and define

$$v_+ = \frac{1}{\sqrt{2}\,c_k}\left(C_k(N) + c_k\, e_k\right) \quad \text{and} \quad v_- = \frac{1}{\sqrt{2}\,c_k}\left(-C_k(N) + c_k\, e_k\right).$$

Direct calculations show that $\|v_+\|_2 = \|v_-\|_2 = 1$, $Nv_+ = c_k\, v_+$, $Nv_- = -c_k\, v_-$ and $v_+ \cdot v_- = 0$.

Let v be an eigenvector of N, with $\|v\|_2 = 1$ and eigenvalue $\sigma \neq \pm c_k$. It is clear that v is orthogonal to v_+, v_-, $e_k = \frac{1}{\sqrt{2}}(v_+ + v_-)$ and $C_k(N) = c_k\sqrt{2}\, v_+ - c_k\, e_k$. Then $|\sigma| = \|Nv\|_2 = \|N_{\check{k}}\, v_{\check{k}}\|_2 \leqslant \|N_{\check{k}}\| \leqslant c_k$. Therefore, $\|N\| = c_k = \|C_k(N)\|_2$ and since $|v_+ \cdot e_i| = |v_- \cdot e_i|$, for all $i = 1, \ldots, n$, then N is a minimal matrix (by Corollary 3).

Now suppose that $(C_k(N))_i = N_{i,k} \neq 0$, for all $i \neq k$. Then property (**??**) implies that $N_{j,j} = -\frac{(C_j(N))_{\check{j}}\cdot(C_k(N))_{\check{j}}}{N_{j,k}}$, for all $j \neq k$ (with the notation set before the statement of this theorem) and $N_{j,j} \in \mathbb{R}$ since N is Hermitian. Moreover, a direct computation proves that if we an entry on the diagonal not equal to $N_{j,j} = -\frac{(C_j(N))_{\check{j}}\cdot(C_k(N))_{\check{j}}}{N_{j,k}}$ and denote by N' this new matrix, then $\|N'\, C_k(N)\|_2 > \|C_k(N)\|_2$, which proves that the diagonal of N is the only one that makes it minimal. □

Note that the column $C_k(N)$ of the previous theorem must satisfy $\|C_k(N)\| \geqslant \|C_j(N)\|$, for all j.

Theorem 10. *Let $M \in M_n^h(\mathbb{C})$ be such that $v, w \in \mathbb{C}^n$ are unit norm eigenvectors corresponding to the eigenvalues $\lambda_{\max} = \|M\|$ and $\lambda_{\min} = -\|M\|$ respectively, that satisfy $v \circ \overline{v} = w \circ \overline{w}$ and $v_i \neq 0$, for all $i = 1, \dots, n$. Then M is a minimal matrix and it has only one minimizing real diagonal.*

Proof. First note that since $v \circ \overline{v} = w \circ \overline{w}$, with v and w unit norm eigenvectors of $\|M\|$ and $-\|M\|$ respectively, then the matrix M must be minimal (see Corollary 3).

Let $D \in D_n(\mathbb{R})$ be any real diagonal matrix with $D_{i,i} = d_i$, $i = 1, 2, \dots, n$. Direct calculations (using that v and w are unit norm eigenvectors of M corresponding to eigenvalues $\|M\|$ and $-\|M\|$ respectively) show that

$$\begin{aligned}\|(M+D)v\|^2 &= \|\|M\|v + Dv\|^2 = \sum_{i=1}^{n} |v_i|^2 \left(\|M\| + d_i\right)^2 \\ &= \sum_{i=1}^{n} \left(|v_i|^2\|M\|^2 + 2|v_i|^2\|M\|d_i + |v_i|^2 d_i^2\right) \\ &= \|M\|^2 + 2\|M\| \sum_{i=1}^{n} |v_i|^2 d_i + \sum_{i=1}^{n} |v_i|^2 d_i^2\end{aligned} \tag{5.2}$$

and

$$\begin{aligned}\|(M+D)w\|^2 &= \| - \|M\|w + Dw\|^2 = \sum_{i=1}^{n} |w_i|^2 \left(-\|M\| + d_i\right)^2 \\ &= \sum_{i=1}^{n} \left(|w_i|^2\|M\|^2 - 2|w_i|^2\|M\|d_i + |w_i|^2 d_i^2\right) \\ &= \|M\|^2 - 2\|M\| \sum_{i=1}^{n} |w_i|^2 d_i + \sum_{i=1}^{n} |w_i|^2 d_i^2.\end{aligned} \tag{5.3}$$

Next we consider three cases depending on the size of $\|(M+D)v\|$ and conclude that in all possible cases $M + D$ cannot be a minimal matrix unless $D = 0$:

1) $\|(M+D)v\| > \|M\|$:
In this case $M + D$ cannot be a minimal matrix since the norm of $M + D$ in a single vector (of norm one) is strictly greater than the matrix norm of M.
2) $\|(M+D)v\| < \|M\|$:
Using the formula (5.2) $\|(M+D)v\| < \|M\|$ implies that

$$-2\|M\| \sum_{i=1}^{n} |v_i|^2 d_i > \sum_{i=1}^{n} |v_i|^2 d_i^2.$$

But $v \circ \overline{v} = w \circ \overline{w}$, which implies that $|v_i|^2 = |w_i|^2$, for every $i = 1, \dots, n$. Therefore, it follows that

$$-2\|M\| \sum_{i=1}^{n} |w_i|^2 d_i > \sum_{i=1}^{n} |w_i|^2 d_i^2.$$

Then

$$\|M\|^2 - 2\|M\| \sum_{i=1}^{n} |w_i|^2 d_i + \sum_{i=1}^{n} |w_i|^2 d_i^2 > \|M\|^2 + \sum_{i=1}^{n} |w_i|^2 d_i^2 + \sum_{i=1}^{n} |w_i|^2 d_i^2$$

and using the equality (5.3) we obtain that

$$\|(M+D)w\|^2 > \|M\|^2 + \sum_{i=1}^{n} \|M\||w_i|^2 d_i^2 + \sum_{i=1}^{n} |w_i|^2 d_i^2 \geqslant \|M\|^2.$$

Then $\|(M+D)w\|^2 > \|M\|^2$ and similar arguments to those of 1), but using the vector w instead of v, lead to the fact that $M + D$ cannot be a minimal matrix.

3) $\|(M+D)v\| = \|M\|$:
If $\|(M+D)v\| = \|M\|$, then using (5.2) we obtain that $2\|M\| \sum_{i=1}^n |v_i|^2 d_i + \sum_{i=1}^n |v_i|^2 d_i^2 = 0$, and therefore

$$\sum_{i=1}^n |v_i|^2 d_i^2 = -2\|M\| \sum_{i=1}^n |v_i|^2 d_i. \tag{5.4}$$

Next we consider two possible sub-cases.

(a) Case $\sum_{i=1}^n |v_i|^2 d_i^2 = 0$.
This assumption implies that $d_i = 0$, for all $i = 1, \ldots, n$, since we assumed that $v_i \neq 0$, for all i. Then $D = 0$.

(b) Case $\sum_{i=1}^n |v_i|^2 d_i^2 > 0$.
In this case, the equality (5.4) implies that $-2\|M\| \sum_{i=1}^n |v_i|^2 d_i > 0$. Therefore,

$$-2\|M\| \sum_{i=1}^n |w_i|^2 d_i + \sum_{i=1}^n |w_i|^2 d_i^2 > 0$$

follows after replacing $|v_i|$ with $|w_i|$. Then

$$\|M+D\|^2 \geqslant \|(M+D)w\|^2 = \|M\|^2 - 2\|M\| \sum_{i=1}^n |w_i|^2 d_i + \sum_{i=1}^n |w_i|^2 d_i^2 > \|M\|^2,$$

where we applied (5.3) in the only equality. This strict inequality implies that $M + D$ cannot be a minimal matrix.

After considering the cases 1), 2) and 3) we obtained that either $M + D$ is not minimal, or D must be the zero matrix. Therefore, the diagonal of M is the only one that makes it a minimal matrix. □

The following proposition is probably known, but we include a proof here for the sake of completeness.

Proposition 10. *Let $X \in M_n(\mathbb{C})$ and $M_X \in M_{2n}(\mathbb{C})$ be the block matrix defined by $M_X = \begin{pmatrix} 0 & X \\ X^* & 0 \end{pmatrix}$. Then M_X is a minimal matrix.*

Moreover, if there exists a norming eigenvector of M_X such that all its coordinates are non-zero, the zero diagonal is the only minimizing diagonal for M_X.

Proof. It is obvious that M_X satisfies $\|M_X\| = \|X\|$. Let $\begin{pmatrix} \xi \\ \eta \end{pmatrix} \in \mathbb{C}^{2n\times 1}$ be a column vector with $\xi, \eta \in \mathbb{C}^n$. If $\begin{pmatrix} \xi \\ \eta \end{pmatrix}$ is an eigenvector of the corresponding eigenvalue λ of M_X, a direct calculation shows that $X\eta = \lambda\xi$ and $X^*\xi = \lambda\eta$. Then $\begin{pmatrix} \xi \\ -\eta \end{pmatrix}$ must be an eigenvector of M_X with corresponding eigenvalue $-\lambda$. As a consequence, since $\pm\|X\|$ are eigenvalues of M_X, we can suppose without loss of generality that $\|X\|$ has an eigenvector, that we will denote with $v = \begin{pmatrix} \xi \\ \eta \end{pmatrix}$ (with all its coordinates non-zero) and $-\|X\|$ has an eigenvector of the form $w = \begin{pmatrix} \xi \\ -\eta \end{pmatrix}$. This is enough to prove that M_X is a minimal matrix because $v \circ \overline{v} = w \circ \overline{w}$ (see for example Corollary 3).

Then we are under the assumptions of Theorem 10 and, therefore, since there exists a norming eigenvector with none of its coordinates equal to zero, there exists a unique minimizing diagonal (in this case the zero diagonal). □

Remark 11. *In the general case, the uniqueness of the minimizing diagonal in Proposition 10 may not hold. Consider for example the case when $X = \begin{pmatrix} 0 & x \\ 0 & 0 \end{pmatrix}$, for $x \in \mathbb{C}\setminus\{0\}$. Then M_X is minimal (using for example Corollary 3) but $Diag(0, c, c, 0)$ is also a minimizing diagonal for M_X, for every $c \in \mathbb{R}$, $|c| \leqslant |x|$.*

Corollary 5. *If $X \in M_{n\times n}(\mathbb{C})$ and $C \in M^h_{m\times m}(\mathbb{C})$ with $\|C\| \leqslant \|X\|$, then any block matrix of the form*

$$M_{X,1} = \begin{pmatrix} 0 & X & 0 \\ X^* & 0 & 0 \\ 0 & 0 & C \end{pmatrix}, \quad M_{X,2} = \begin{pmatrix} 0 & 0 & X \\ 0 & C & 0 \\ X^* & 0 & 0 \end{pmatrix} \quad \text{or} \quad M_{X,3} = \begin{pmatrix} C & 0 & 0 \\ 0 & 0 & X \\ 0 & X^* & 0 \end{pmatrix}$$

is a minimal matrix.

Moreover, any minimizing diagonal for any of the $M_{X,i}$, for $i = 1, 2, 3$, can be permuted in order to construct a minimizing diagonal for the other two.

Proof. Let us consider first $M_{X,1}$, with $\|C\| \leqslant \|X\|$. Observe that $\|M_{X,C}\| = \max\left\{\left\|\begin{pmatrix} 0 & X \\ X^* & 0 \end{pmatrix}\right\|, \|C\|\right\} = \max\{\|X\|, \|C\|\} = \|X\|$ since $\|C\| \leqslant \|X\|$. Therefore, $M_{X,1}$ is a minimal matrix because $M_X = \begin{pmatrix} 0 & X \\ X^* & 0 \end{pmatrix}$ always is (see Theorem 10).

The matrices $M_{X,2}$ and $M_{X,3}$ (with $\|C\| \leqslant \|X\|$) can be obtained from $M_{X,1}$ after left and right multiplication by certain unitary matrices. Then those are also minimal matrices since the operator norm is unitarily invariant. For example, if I_j is the $j \times j$ identity matrix, and U the unitary matrix defined by $U = \begin{pmatrix} I_n & 0 & 0 \\ 0 & 0 & I_m \\ 0 & I_n & 0 \end{pmatrix}$, then

$$UM_{X,1}U^* = \begin{pmatrix} 0 & 0 & X \\ 0 & C & 0 \\ X^* & 0 & 0 \end{pmatrix} = M_{X,2}.$$

And using the same unitary matrix U, and every diagonal $D = \begin{pmatrix} D_1 & 0 & 0 \\ 0 & D_2 & 0 \\ 0 & 0 & D_3 \end{pmatrix}$,

$$UDU^* = \begin{pmatrix} D_1 & 0 & 0 \\ 0 & D_3 & 0 \\ 0 & 0 & D_2 \end{pmatrix} = D'$$

(with the entries of D' being a permutation of those of D). Then any minimizing diagonal D for $M_{X,1}$ can be permuted to a minimizing diagonal D' for $M_{X,2}$ since for any diagonal D, $U(M_{X,1} + D)U^* = UM_{X,1}U^* + UDV^* = M_{X,2} + D'$ holds, with

$$\|M_{X,1} + D\| = \|U(M_{X,1} + D)U^*\| = \|M_{X,2} + D'\|.$$

Therefore, if U is as described, then D is a minimizing diagonal of $M_{X,1}$ if and only if $D' = UDU^*$ is a minimizing diagonal for $M_{X,2} = UM_{X,1}U^*$.

Similar considerations allow us to prove that $M_{X,3}$ is a minimal matrix and any of its minimizing diagonals can be permuted to obtain a minimizing diagonal of the other two. □

Theorem 11. *If $M \in M_n(\mathbb{C})$ is a minimal matrix and $E_{h,k} \in M_n(\mathbb{C})$ is the identity matrix with the h and k rows permuted, then the matrix $E_{h,k}ME_{h,k}$ is also minimal (observe that the matrix $E_{h,k}ME_{h,k}$ is the matrix M with the rows h, k permuted and the columns h, k permuted afterwards).*

Proof. This result can be proved using that $E_{h,k}ME_{h,k}$ is unitarily equivalent to M or using that they have the same characteristic polynomial (see the proof of the 3×3 case in Proposition 3).

□

Corollary 6. *If $X_k \in M_{n_k \times n_k}(\mathbb{C})$ with $k = 1, \dots m$, then any block matrix of the form*

$$M = \begin{pmatrix} 0 & X_1 & 0 & 0 & 0 & \dots & 0 & 0 \\ X_1^* & 0 & 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & X_2 & 0 & \dots & 0 & 0 \\ 0 & 0 & X_2^* & 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \dots & 0 & X_m \\ 0 & 0 & 0 & 0 & 0 & \dots & X_m^* & 0 \end{pmatrix}$$

and any of the matrices obtained by one permutation of block rows followed by another permutation of the respective block columns is a minimal matrix.

Proof. The proof follows by applying Corollary 5 and Theorem 11. □

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