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 $\| \ \|$ denotes the operator norm. Moreover, we generalize our techniques to some $n \times n$ cases.

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 fixed 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 $\| \ \|$ 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]. 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 $\mathcal{P}(n)$. Moreover, the natural questions and some particular examples that appear 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]).

Previous attempts to describe minimal matrices and their properties were done in [9] and for 3×3 matrices. In that paper, all 3×3 minimal matrices were parametrized. 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 recent approaches have been made 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 techniques can be extended.

In Section 3 we describe all the minimal diagonal matrices for a given Hermitian 3×3 matrix M where some of its off-diagonal entries are null. In this section some cases give infinite solutions.

Section 4 is devoted to the case of Hermitian matrices with non-zero off-diagonal entries. In this section we study separately the real matrices, and propose a decomposition in the general case (see Theorems 6

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and 7) that allows to find the unique closest diagonal matrix of a given Hermitian matrix M (see Remark 9) in this case.

The last section studies particular $n \times n$ types of Hermitian matrices where concrete minimal diagonals can be computed and some general properties. The continuity of the function that maps Hermitian matrices with null diagonals into its unique minimizing diagonal (when this is the case) is studied. Theorem 9 generalizes Theorem 3 and provides many examples of minimal matrices where its 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 here the spectrum of A, that is the (unordered) set of eigenvalues of A. We denote with $\|A\|$ the operator or spectral norm of $A \in M_n(\mathbb{C})$, that in case $A \in M_n^h(\mathbb{C})$ 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 with $\{e_i\}_{i=1}^n$ the canonical basis of $\mathbb{C}^n$. Given a matrix $A \in M_n(\mathbb{C})$, we denote with $A_{i,j}$ 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 with MN the usual matrix product, with $\mathrm{tr}(M)$ the usual (non-normalized) trace of M and with $C_i(M)$ the vector given by the i^{th} column of M.

For $(a_1, a_2, \ldots, a_n) \in \mathbb{R}^n$ we denote with $\mathrm{diag}(a_1, a_2, \ldots, a_n)$ 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 $\mathrm{Diag}(M)$ 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

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

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 belong to the closed ball $B_{\|M\|}(0) = \{D \in D_n(\mathbb{R}) : \|D\| \leqslant \|M\|\}$. This ball of $D_n(\mathbb{R})$ 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 $\|M\| = ||| \ [M] \ ||| = \min_{D \in D_n(\mathbb{R})} \|M + D\| = dist(M, D_n(\mathbb{R}))$.

Definition 2. *Let $M \in M_n^h(\mathbb{C})$ and $D \in D_n(\mathbb{R})$ 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 with $\sigma(M) = \{\lambda, \mu, -\lambda\}$ the spectrum of M, for $0 < \lambda = \|M\|$, $|\mu| \leqslant \lambda$ and $\mu = \mathrm{tr}(M)$.

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 with $M \circ N$ 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 with $A^t \in \mathbb{C}^{m\times n}$ its transpose, with $\operatorname{ran}(A)$ the range of the linear transformation A and with $\ker(A)$ 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, those 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 here for the sake of clarity.

Theorem 1. *Let $M^h_{3\times 3}(\mathbb{C})$ 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 module. That is, if for every e_i then $|\langle v_+, e_i\rangle| = |\langle v_-, e_i\rangle|$ 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 a pair of eigenvectors of $+\lambda$ and $-\lambda$ (respectively) such that their coordinates have the same module (see Remark 4 in [8]).

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

Theorem 2. *Let x, y, z 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 every 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 apparent 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 condition of Theorem 1 and M is minimal.

Cases 2 and 3 are proved in a similar way.

Let us consider now case 4. Note that in this case it can be computed the spectrum $\sigma(M) = \left\{\pm\frac{x^2y^2+x^2z^2+y^2z^2}{2xyz}\right\}$. 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 bigger than the sum of the two others). Under these hypothesis 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 by Theorem 1 M is minimal.

□

Remark 3. *From the previous theorem follows that in the first three cases the column (or row) of M with the 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 $\|C_3(M)\|_2^2$). This 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 verify 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

$$A = +x^2y^2 - y^2z^2 - z^2x^2 \quad B = -x^2y^2 - y^2z^2 + z^2x^2 \quad C = -x^2y^2 + y^2z^2 - z^2x^2$$
$$\text{and} \quad D = A + |A| + B + |B| + C + |C|$$

The proof of this statement follows after 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 hypothesis 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 chose* $0 \leqslant \theta \leqslant \pi$*) 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 than 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 its corresponding columns are also minimal.*

Proof. The proof follows after similar considerations as the ones done about the characteristic polynomials of the matrices in the previous Remark 5 or using conjugation of M_θ by permutation matrices or unitary diagonals. □

Remark 6. *Observe that if we search 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 its minimizing diagonal equal to the 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 an off-diagonal entry of the matrix is zero (see Proposition 2 and Theorem 2) and in the real case (see Theorem 3) we can also suppose that*

- $0 < \theta < \pi$ *(because the cases* $\theta = 0$ *or* $\theta = \pi$ *have the same minimizing diagonals that the real symmetric matrices and for other* $\theta \notin (0,\pi)$ *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 the above Proposition 3 and the previous Remark 5 prove that if two matrices have its off-diagonal entries with equal module (even if they are permuted in their positions) and if $\cos(\theta) = \cos(\alpha + \beta + \gamma)$ *(with* α, β, γ *as in (4.3) and* θ *as in (4.5)) then its 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 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 and that there are corresponding eigenvectors of $\pm\lambda$ that satisfy Theorem 1. Therefore (ii) holds.

(ii)⇒(i). If M is minimal there exist v_+ and v_- norm one eigenvectors of 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 null. 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) is direct from (ii)⇒(i) of Proposition 4.

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

(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 M_θ with zeros in its diagonal has eigenvalues $\{\pm\sqrt{x^2 + y^2 + z^2}, 0\}$. Then, calculating the corresponding eigenvectors of M_θ with zeros in its diagonal and using Theorem 1 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 not null 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 with v_δ a corresponding norm one 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 apparent 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 $aye^{-i\theta} + cye^{-i\theta} + xz = 0$, and then $a = -c$; 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 norm one eigenvectors v_λ, $v_{-\lambda}$ and v_μ such that*

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

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

Proof. Let us suppose first that $|\mu| < \lambda$. Then all eigenspaces have dimension one and any choice of norm one eigenvectors v_λ, $v_{-\lambda}$ corresponding to λ and $-\lambda$ verify Theorem 1. Then, using the same theorem, N is minimal, and Proposition 4 implies that $\mathrm{Diag}(N) = 0$. Therefore $\mathrm{Diag}(\mu\ (v_\mu \otimes v_\mu))$ =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 this eigenvectors and any other v_μ orthogonal to both of them. Then it can be proved similarly as above that they satisfy the claims 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 $\mu = a+b+c \neq 0$. Following the same notations of (3.9) and (3.10) of that paper 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 $\chi = \frac{c}{2(a+b+c)}$. Then, 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 done 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 $\{\lambda,\mu,-\lambda\}$ and 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 here 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 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 α, β, $\gamma \in [0,\pi]$ *such that:*

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

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

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

satisfy:

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

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

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 norm one 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 $S = \mu(v_\mu\otimes v_\mu)$ satisfies $\mathrm{Diag}(S) = \mathrm{Diag}(M)$ (even in the case $|\mu| = \lambda$). Let $v_\mu = (r,s,t)$, then it is apparent 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 norm one 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 than M and $\sigma(M_1) = \sigma(M)$. Now we will consider the cases $\mu = 0$ and $\mu \neq 0$.

- In 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 $\alpha = \beta = \gamma = \pi/2$ verify the requirements of the theorem and follows easily that N_1 is unitarily equivalent by means of diagonal matrices to M: $M = UN_1U^*$ for $U = \text{Diag}(i, -i, 1)$. In case $\theta = (2k + 1)\pi + \pi/2$, with $k \in \mathbb{Z}$, then the matrix M is the transpose as the one considered in the case when $\theta = 2k\pi + \pi/2$, 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 eigenvector of μ (because $v_\mu = (r, s, t)$ is eigenvector of 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 arrive at $x = y = 0$, also a contradiction. With similar arguments we can prove that, in any case considered, the supposition that one of the entries of M_1 is null leads to a contradiction.

  Then 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 $\alpha, \beta, \gamma \in [0, \pi]$ and from Proposition 6 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 $M_{\theta_1} = M_{-\theta} = (M_\theta)^t$, 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 have been defined before and putting $N = N_1$ and $S = S_1$ the items (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 not null. This claim follows after considering the following cases.

- As seen in the proof of (2) 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 all not null and $\mu \neq 0$ ($\theta \neq k\pi + \pi/2$, $k \in \mathbb{Z}$), since we are supposing $\lambda = \|M\| = \|M_0\|$ follows that $\text{Im}((M_0)_{1,2}) = x\sin\alpha = \lambda\zeta \neq 0$, $\text{Im}((M_0)_{1,3}) = y\sin\beta = \lambda\psi \neq 0$ and $\text{Im}((M_0)_{2,3}) = z\sin\gamma = \lambda\xi \neq 0$. 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

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

and $\lambda^2 = (x\sin\alpha)^2 + (y\sin\beta)^2 + (z\sin\gamma)^2$.

Pick v_μ as in (4.9). Then $S_{1,2} = x\cos\alpha = ((a+b+c)(v_\mu \otimes v_\mu))_{1,2} = \frac{\mu zy \sin\gamma \sin\beta}{\lambda^2}$. 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 apparent 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 again 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 which proves 4).

Items 3) and 4) imply 5) because since M is minimal, then $\mathrm{tr}(M)$ is an eigenvalue of M and therefore $\mathrm{tr}(M)^2 \leqslant \|M\|^2$.

□

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

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

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

and α, β, γ, 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) follows that $NS = 0$ and $SN = 0$. Furthermore S has rank one and N rank two. Then $\mathrm{ran}(S) = \ker(N)$ and $\ker(S) = \mathrm{ran}(N)$ and $\sigma(S) = \{0, \mathrm{tr}(S)\}$. Therefore if we call

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

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

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

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

then 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) $Diag(N + S) = Diag(M)$
b) *If* $v \in \ker(N)$ *with* $v \in \mathbb{R}^3$ *and* $\|v\| = 1 \Rightarrow S = (a + b + c)\,(v \otimes v)$
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') $x^2 \sin(2\alpha) = y^2 \sin(2\beta) = z^2 \sin(2\gamma)$
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 θ, x, y, z fixed 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 α,β,$\gamma \in [\pi/2, 2\pi]$. If we consider $\mu < 0$ ($\mu = 0$ corresponds to $\theta = 3\pi/2$ that as Corollary 2 states it has the same minimizing diagonals than 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

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

and with 1'), if we denote with $k = x_c x_s = y_c y_s = z_c z_s$ we can prove that

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

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 $x_c x_s = y_c y_s \wedge y \leqslant x$ then $\sin(\beta) < \sin(\alpha)$, $y_s < x_s$ then $x_s \leqslant |x_c| < |y_c|$ and then
$$k^2 = x_s^2 x_c^2 < y_c^2 x_c^2 < \left(x_c^2 y_c^2 + x_c^2 z_c^2 + y_c^2 z_c^2\right),$$
which contradicts (4.13).

b) $\beta \in (\pi/2, \alpha]$:
(i) if $\beta \in [3/4\pi, \alpha]$ then $|y_s| \leqslant |y_c| \leqslant |x_c|$ and 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) 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 then

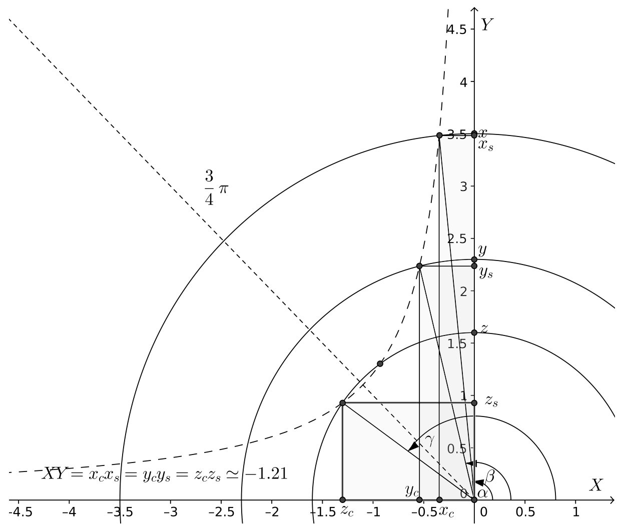

FIGURE 1. The corresponding α, β and γ for $\theta = 6.$, $x = 3.5$, $y = 2.3$ and $z = 1.6$.

$|x_s + x_c| \geqslant |y_s + y_c|$, 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).

Then $\alpha \notin (\frac{3}{4}\pi, \pi)$ 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 $\beta \notin (\frac{3}{4}\pi, \pi)$ and therefore $\beta \in (\pi/2, \frac{3}{4}\pi]$, and that $\gamma \in [\beta, \frac{3}{2}\pi - \beta] \subset [\pi/2, \pi]$ (see Figure 1).

Uniqueness:

The angles α and β are unique in this intervals because they must fulfil 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 fulfil 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 of that item, then $\lambda^2 = \|M\| = (x \sin\alpha)^2 + (y \sin\beta)^2 + (z \sin\gamma)^2 = (x \sin\alpha)^2 + (y \sin\beta)^2 + (z \sin\gamma')^2$, 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 trace the definition of these angles given in 4.8 of Theorem 6, it can be seen that it is a continuous application with respect to θ (and also with respect to x,y,z).

The sum of α, β, and γ gives θ:

Since $\theta \in (\frac{3}{2}\pi, 2\pi)$, $\alpha(\theta), \beta(\theta) \in (\pi/2, \frac{3}{4}\ \pi)$, $\gamma(\theta) \in \big(\beta(\theta), \frac{3}{2}\pi - \beta(\theta)\big)$ then $3/2\ \pi \leqslant \alpha(\theta) + \beta(\theta) + \gamma(\theta) \leqslant 9/4\ \pi$. Then using that $\cos(\alpha(\theta) + \beta(\theta) + \gamma(\theta)) = \cos(\theta)$ 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 $\theta = \frac{3}{2}\pi$, $x \geqslant y \geqslant z > 0$ then $\sigma(M_{3\pi/2}) = \{\lambda, 0, -\lambda\}$ (see Corollary 2). $M_{3\pi/2}$ has the same null minimizing diagonals than 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 with α', β' and γ' the solutions which existence was proved in Theorem 7, then it is enough to take $\alpha = \pi - \alpha'$, $\beta = \pi - \beta'$ and $\gamma = \pi - \gamma'$ and verify 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 apparent that if θ is close to $\frac{3}{2}\pi$ then the values of $\alpha(\theta), \beta(\theta)$ and $\gamma(\theta)$ defined as in the previous 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 considerations 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 considerations 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 previous theorem 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 under the conditions

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

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

$$(x \sin\alpha)^2 + (y \sin\beta)^2 + (z \sin\gamma)^2 \geqslant$$

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

imply that the root of

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

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 infinite other minimizing diagonals for M (see Proposition 2 for details).

(2) ***Case*** $M_{i,j} \neq 0$ ***for*** $i \neq j$. *Given a generic Hermitian matrix M with non zero entries it can be conjugated with diagonal unitary and permutation matrices (see Remark 6 and Proposition 3) to obtain a matrix with the structure*

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

We discuss next 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 that the one corresponding to $2\pi - \theta$ that is described in the following 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

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

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

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

To obtain the minimal matrix corresponding to the original matrix M, then the inverse conjugation with diagonal unitary and permutation matrices 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 its minimizing diagonals and the concrete minimizing diagonals for some particular $n \times n$ Hermitian matrices.

We include here 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 for each eigenvalue $\lambda = \|M\| = \lambda_{\max}(M)$ and $-\lambda = -\|M\| = \lambda_{\min}(M)$ (see also Remark 2).

Observe that in the following corollary $\text{co}(A)$ 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 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*

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

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 infinite 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 with unique minimizing diagonals).

Remark 10. *The set of matrices that have infinite 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 infinite 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 infinite 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 null matrix has obviously only one minimizing diagonal, the set of matrices with infinite minimizing diagonals is neither closed.

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

Despite the previous remark, there are big sets of matrices with unique minimizing diagonal that are open in $M_n^h(\mathbb{C})$ (such as the one 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 $\text{Diag}(M)$ is the diagonal matrix with the same diagonal of M. Consider now the map

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

$\mathcal{O}$ 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 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 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 an 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

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

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 hole 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. The previous item (1) proves that $d_{min} : \mathcal{O}(B) \to D_n(\mathbb{R})$ is continuous.

□

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

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

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 apparent 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 with $C_j(M)$ the j^{th} column of M, with $M_{\check{j}}$ the matrix in $\mathbb{C}^{(n-1)\times(n-1)}$ resulting after taking off the j^{th} column and row of M and with $v_{\check{j}}$ the element of $\mathbb{C}^{n-1}$ obtained after taking off the j^{th} entry of $v \in \mathbb{C}^n$.

Theorem 9. *Let $N \in M_n^h(\mathbb{C})$ and $k \in \mathbb{N}$ fixed 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 $j \neq k$, and*
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 $(C_k(N))_i = N_{i,k} \neq 0$, $\forall i \neq k$, then the diagonal of N is the only one that makes N a minimal matrix.

Proof. Let us denote with $c_k = \|C_k(N)\|_2$, with $\{e_i\}_{i=1,\dots,n}$ 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 apparent 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 $i = 1,\dots,n$, then N is a minimal matrix (by Corollary 3).

Now suppose that $(C_k(N))_i = N_{i,k} \neq 0$, $\forall i \neq k$. Then property (2) 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 mentioned previous to the statement of this theorem) and $N_{j,j} \in \mathbb{R}$ since N is Hermitian. Moreover, a direct computation proves that if we choose a diagonal i^{th} entry different from $N_{j,j} = -\frac{(C_j(N))_{\check{j}} \cdot (C_k(N))_{\check{j}}}{N_{j,k}}$ and call with 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 verify $\|C_k(N)\| \geqslant \|C_j(N)\|$ for all j.

Theorem 10. *Let $M \in M_n^h(\mathbb{C})$ be such that $v, w \in \mathbb{C}^n$ are norm one eigenvectors of 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 norm one 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 $D_{i,i} = d_i$, $i = 1, 2, \ldots, n$. Direct calculations (using that v and w are norm one eigenvectors of M of 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), then $\|(M+D)v\| < \|M\|$ 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 $i = 1, \ldots, n$. Therefore, 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 considerations as those in the case (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 $\sum_{i=1}^{n}|v_i|^2d_i^2=0$.
This assumption implies that $d_i=0$ for all $i=1,\dots,n$, because we are supposing that $v_i\neq 0$, for all i . Then $D=0$.

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

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

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

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

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 null 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 $M_X\in M_{2n}(\mathbb{C})$ 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 with all its coordinates not null, the zero diagonal is the only minimizing diagonal for M_X.

Proof. It is apparent that M_X satisfies $\|M_X\|=\|X\|$. Let $\begin{pmatrix}\xi\\\eta\end{pmatrix}\in\mathbb{C}^{2n\times 1}$ represent 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 not null) and $-\|X\|$ another 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 null, 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 of $X=\begin{pmatrix}0&x\\0&0\end{pmatrix}$ for $x\in\mathbb{C}\backslash\{0\}$. 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*

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

is a minimal matrix.

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

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 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 with the same unitary 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 precise permutation of those of D). Then any minimizing diagonal D for $M_{X,1}$ can be permuted into a minimizing diagonal D' for $M_{X,2}$ because for any diagonal D, $U(M_{X,1} + D)U^* = UM_{X,1}U^* + UDV^* = M_{X,2} + D'$ holds, with

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

And 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 in 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 from one permutation of block rows followed by another permutation of the respective block columns is a minimal matrix.

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

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