Minimal compact operators, subdifferential of the maximum eigenvalue and semi-definite programming

Tamara Bottazzi[a,b], Alejandro Varela[c,d]

[a] *Universidad Nacional de Río Negro. CITECCA, Sede Andina (8400) S.C. de Bariloche, Argentina.*
[b] *Consejo Nacional de Investigaciones Científicas y Técnicas, (1425) Buenos Aires, Argentina.*
[c] *Instituto Argentino de Matemática "Alberto P. Calderón", Saavedra 15 3er. piso, (C1083ACA) Buenos Aires, Argentina*
[d] *Instituto de Ciencias, Universidad Nacional de Gral. Sarmiento, J.M. Gutierrez 1150, (B1613GSX) Los Polvorines, Argentina*

Abstract

We formulate the issue of minimality of self-adjoint operators on a complex Hilbert space as a semi-definite problem, linking the work by Overton in [18] to the characterization of minimal hermitian matrices. This motivates us to investigate the relationship between minimal self-adjoint operators and the subdifferential of the maximum eigenvalue, initially for matrices and subsequently for compact operators. In order to do it we obtain new formulas of subdifferentials of maximum eigenvalues of compact operators that become useful in these optimization problems.

Additionally, we provide formulas for the minimizing diagonals of rank one self-adjoint operators, a result that might be applied for numerical large-scale eigenvalue optimization.

Keywords: Minimal operators, Subdifferential of eigenvalues, Moment of a subspace, Semi-definite programming.
2020 MSC: (Primary) 15A60, 47A12, 47B15, (Secondary) 47A05, 47A30, 51M15

1. Introduction and preliminaries

Let $B(H)$ and $K(H)$ be the spaces of linear bounded and compact operators defined on a complex Hilbert space H, respectively. We call $A \in B(H)$ a minimal operator if $\|A\| \leqslant \|A + D\|$, for all D diagonal in a fixed orthonormal basis $E = \{e_i\}_{i\in I}$ of H and $\|\cdot\|$ the operator norm. Note that when $A \in K(H)$, we can suppose that H is separable since there is only a numerable set $\{e_{i_k}\}_{k\in\mathbb{N}}$ such that $A(e_{i_k}) \neq 0$.

Email addresses: `tbotttazzi@unrn.edu.ar` (Tamara Bottazzi), `avarela@campus.ungs.edu.ar` (Alejandro Varela)

In particular, minimal compact self-adjoint operators are related with the distance to the subspace of diagonal self-adjoint operators, denoted by $\text{Diag}(K(H))^{sa}$, since for $A \in K(H)$ self-adjoint

$$\text{dist }(A, \text{Diag}(K(H))^{sa}) = \inf_{D \in \text{Diag}(K(H))} \|A + D\|.$$

Minimal operators allow the concrete description of geodesics in homogeneous spaces obtained as orbits of unitaries under a natural Finsler metric (see [11]). We use the superscript ^{sa} to note the subset of self-adjoint elements of a particular subset of $B(H)$.

In the case that $H = \mathbb{C}^n$, $B(H)$ is the space of complex square matrices of $n \times n$, that is $M_n(\mathbb{C})$. The matricial case of minimal operators was extensively studied in [1], [2] and [15].

In [7], [5] and [4] we studied minimal self-adjoint compact operators where it was stated that in general neither existence nor uniqueness of compact minimizing diagonals was granted. Some of these results were recently generalized to more general subalgebras of $K(H)$ and to C*-algebras in [23, 24].

The characterization of minimal self-adjoint matrices can be stated as a semidefinite programming problem [18]. Moreover, in [19] Overton develops several algorithms using the subdifferential of the maximum eigenvalue of a matrix, which is the set

$$\partial\lambda_{max}(A) = \left\{V \in M_n^{sa}(\mathbb{C}) : \lambda_{max}(Y) - \lambda_{max}(A) \geqslant \text{Re tr}(V(Y - A)),\ \forall\ Y \in M_n^{sa}(\mathbb{C})\right\}.$$

This subdifferential was also studied in [22] and is a powerful tool in cases of non-differentiable functions [9, 10].

The work of Overton in [18] and [19] motivated us to study the relation between minimal operators and subdifferentials, first for matrices, and then for compact operators.

In [3, 13, 21], the authors give useful expressions for the subdifferential of the norm operator and they relate this concept with the distance to some closed subsets in $B(H)$.

In the present work, we relate minimal operators with subdifferentials of the maximum eigenvalue and of the norm. We vinculate these concepts with the moment of the eigenspace of the maximum eigenvalue and the joint numerical range, which was developed in [16] for matrices, and [6] for compact operators.

Indeed, one of our main results is an explicit formulation for the largest eigenvalue subdifferential of a compact self-adjoint operator $A(x)$ with variable real diagonal x,

$$\partial\big(\lambda_{max}(A(x))\big) = \text{Diag}(\partial\lambda_{max}(A(x))) = m_{S_{max}},$$

in terms of $m_{S_{max}} = \text{co}\{|v|^2 : v \in S_{max}, \|v\| = 1\}$, the moment of the eigenspace related to the largest eigenvalue $\lambda_{max}(A(x))$ (see (3.2), (3.3) and Theorem 3.3). Additionally, when the smallest eigenvalue $\lambda_{min}(A(x))$ is negative, we give explicit formulas for $\partial\big(\lambda_{min}(A(x))\big)$ and vinculate $\partial\lambda_{max}$ and $\partial\lambda_{min}$ with the subdifferential of the spectral norm of $A(x)$. The above leads us to a new characterization of minimal self-adjoint compact operators that involves $\partial\big(\lambda_1(A(x))\big)$,

$\partial\|A(x)\|$, the intersection of moments of the maximum and minimum eigenvalues of $A(x)$ and the joint numerical range of a certain family of operators that has been studied in [6] and [16].

We first obtain the subdifferential formulas and the characterization of minimal operators when $A(x) \in M_n^{sa}(\mathbb{C})$. In order to extend it to the compact operator case, we needed some additional tools from non-smooth analysis and optimization. We used [9] and [10] as our main references of the topic.

The formula of the subdifferentials that we obtain can be applied to eigenvalues with multiplicity higher than one, but in case of a simple eigenvalue, our formula coincides with the definition of gradient and partial derivatives of the maximum eigenvalue of a matrix (see [17] and [14]). This may be useful to develop or improve algorithms for large-scale eigenvalue optimization.

The results we present in this paper are divided in three parts. Section 2 is devoted to state the minimality of self-adjoint matrices as a semi-definite problem, relating some of the results obtained by Overton in [18] with the main characterization theorems that appear in [2]. Inspired by [19], in Section 3 we study the subdifferential of the maximum eigenvalue, first for matrices and then for compact operators, and we link it with the moment of its eigenspace. In order to obtain these results we calculate new formulas of subdifferentials of eigenvalues of compact self-adjoint operators and operator norms (see Theorems 3.15 and 3.20). Finally, in section 4 we show explicit formulas for the minimizing diagonals for a given rank-one self-adjoint compact operator. These results might be used to improve some algorithms recently obtained for large-scale eigenvalue optimization problems (see [14]).

Next we introduce some additional definitions and notations.

A self-adjoint element $A \in B(H)$ is called positive if $\langle Ax, x\rangle \geqslant 0$ for all $x \in H$ and it is denoted by $A \geqslant 0$. For an operator $A \in B(H)$ we use $\ker(A)$ to denote the kernel of A and $|A|$ the modulus of A given by $(A^*A)^{1/2}$.

For every compact operator $A \in K(H)$, let $s_1(A), s_2(A), \cdots$ be the singular values of A, i.e. the eigenvalues of $|A|$ in decreasing order ($s_i(A) = \lambda_i(|A|)$, for each $i \in \mathbb{N}$) and repeated according to multiplicity. Let

$$\|A\|_1 = \sum_{i=1}^{\infty} s_i(A) = \operatorname{tr}|A|, \tag{1.1}$$

where $\operatorname{tr}(\cdot)$ is the trace functional, i.e.

$$\operatorname{tr}(A) = \sum_{j=1}^{\infty} \langle Ae_j, e_j\rangle \tag{1.2}$$

where e_j are the elements of a fixed orthonormal basis E. Observe that the series (1.2) converges absolutely and it is independent from the choice of basis and this coincides with the usual definition of the trace if H is finite-dimensional.

We define the usual ideal of trace class operators as

$$B_1(H) = \{A \in K(H) : \ \|A\|_1 < \infty\}. \tag{1.3}$$

2. The characterization of minimal matrices as a semidefinite-problem

Let $A_0 \in M_n^{sa}(\mathbb{C})$ and $\varphi : \mathbb{R}^n \to \mathbb{R}$ be the function given by

$$\varphi(x) = \max_{1 \leqslant i \leqslant n} |\lambda_i(A(x))|,$$

where $A(x) = A_0 + \operatorname{Diag}(x)$, $x \in \mathbb{R}^n$ and $\{\lambda_i(A(x))\}_{i=1}^n$ are its eigenvalues in decreasing order counted with multiplicity. We are interested in studying the following convex optimization problem:

$$\min_{x \in \mathbb{R}^n} \varphi(x). \tag{2.1}$$

Any solution of (2.1) gives us the spectral norm of a minimal matrix $A(x_0)$ and a best real diagonal approximation to the subspace of real diagonal matrices $\operatorname{Diag}(x_0)$ (may not be unique). In this case, we say that $A(x_0)$ is a minimal matrix, that is

$$\|A(x_0)\| \leqslant \|A(x)\|, \text{ for every } x \in \mathbb{R}^n.$$

When A_0 is a real symmetric matrix, this problem is a specific case of [18] and can be stated as

$$\min_{w \in \mathbb{R},\ x \in \mathbb{R}^n} w \text{ such that } -w \leqslant \lambda_i(A(x)) \leqslant w,\ 1 \leqslant i \leqslant n, \tag{2.2}$$

or equivalently

$$\min_{w \in \mathbb{R},\ x \in \mathbb{R}^n} w \text{ such that } \begin{cases} wI - A(x) \geqslant 0 \\ wI + A(x) \geqslant 0. \end{cases} \tag{2.3}$$

Problem (2.3) can be viewed as a Semi-Definite Programming (SDP) issue with two semidefinite constraints. Fletcher in [12] deals with a similar problem with only one semidefinite constraint.

If $A(x)$ is minimal, then there exist natural numbers $1 \leqslant s, t < n$ such that

$$\begin{cases} \lambda_i(A(x)) = \lambda_i & i = 1, 2, ..., n \\ \lambda_i = w & i = 1, 2, ..., t \\ \lambda_i = -w & i = n - s + 1, ..., n \\ w = \lambda_1 = ... = \lambda_t & > \lambda_{t+1} \geqslant ... \geqslant \lambda_{n-s} > \lambda_{n-s+1} = ... = \lambda_n = -w. \end{cases} \tag{2.4}$$

If $\{q_1, ..., q_n\}$ is an orthonormal set of eigenvectors corresponding to $\{\lambda_1, ..., \lambda_n\}$, we define

$$Q_1 = [q_1|...|q_t] \text{ and } Q_2 = [q_{n-s+1}|...|q_n], \tag{2.5}$$

matrices of $n \times t$ and $n \times s$, respectively.

Let $E_k = e_k \otimes e_k = e_k e_k^*$, with $\{e_k\}_{k=1}^m$ the canonical basis of $\mathbb{R}^m$ for any $m \in \mathbb{N}$.

The next result is a particular case of Theorem 3.2 in [18] applied to our context.

Proposition 2.1. *Let $A_0 \in \mathbb{R}^{n\times n}$, $A_0 = A_0^t$ and $x \in \mathbb{R}^n$. The following conditions are equivalent:*

1. *x is a solution of (2.2) (i.e: $A(x)$ is minimal).*
2. *$A(x)$ fulfills (2.4) and there exist semidefinite positive symmetric matrices U of $t \times t$ and V of $s \times s$ such that*
   - *$tr(U) + tr(V) = 1$,*
   - *$tr(Q_1^t E_k Q_1 U) - tr(Q_2^t E_k Q_2 V) = 0$, $k = 1, ..., n$.*

According to [8] we can convert an SDP complex problem into a real SDP, using the following result.

Lemma 2.2. *For every $Y \in M_n^{sa}(\mathbb{C})$,*

$$Y \geqslant 0 \text{ if and only if } \begin{bmatrix} \Re(Y) & -\Im(Y) \\ \Im(Y) & \Re(Y) \end{bmatrix} \geqslant 0, \tag{2.6}$$

(here $\Re(Y) = \frac{1}{2}(Y + \overline{Y})$ and $\Im(Y) = \frac{1}{2i}(Y - \overline{Y})$).

Proof. First define the block matrix $U = \frac{1}{\sqrt{2}} \begin{bmatrix} I_n & iI_n \\ iI_n & I_n \end{bmatrix}$, and observe that

$$UU^* = U^*U = \begin{bmatrix} I_n & 0 \\ 0 & I_n \end{bmatrix}.$$

Then,

$$U^* \begin{bmatrix} Y & 0 \\ 0 & \overline{Y} \end{bmatrix} U = \frac{1}{2} \begin{bmatrix} Y + \overline{Y} & i(Y - \overline{Y}) \\ -i(Y - \overline{Y}) & Y + \overline{Y} \end{bmatrix} = \begin{bmatrix} \Re(Y) & -\Im(Y) \\ \Im(Y) & \Re(Y) \end{bmatrix}.$$

Therefore, $\begin{bmatrix} \Re(Y) & -\Im(Y) \\ \Im(Y) & \Re(Y) \end{bmatrix}$ is unitary block equivalent to $\begin{bmatrix} Y & 0 \\ 0 & \overline{Y} \end{bmatrix}$ and

$$\begin{bmatrix} \Re(Y) & -\Im(Y) \\ \Im(Y) & \Re(Y) \end{bmatrix} \geqslant 0 \text{ if and only if } \begin{bmatrix} Y & 0 \\ 0 & \overline{Y} \end{bmatrix} \geqslant 0.$$

So, in order to prove (2.6), we only need to show that

$$Y \geqslant 0 \text{ if and only if } \begin{bmatrix} Y & 0 \\ 0 & \overline{Y} \end{bmatrix} \geqslant 0.$$

It is evident that the inequality

$$\begin{bmatrix} Y & 0 \\ 0 & \overline{Y} \end{bmatrix} \geqslant 0$$

implies $Y \geqslant 0$. On the other hand, if $Y \geqslant 0$, there exist a unitary $V \in M_n(\mathbb{C})$ such that $Y = V^* \text{Diag}(\lambda(Y))V$, with $\lambda_i(Y) \geqslant 0$, for every $i = 1, ..., n$. Then,

$$\overline{Y} = \overline{V}^* \text{Diag}(\overline{\lambda(Y)})\overline{V} = \overline{V}^* \text{Diag}(\lambda(Y))\overline{V} \geqslant 0,$$

since $\overline{V}$ is also unitary, and

$$\begin{bmatrix} Y & 0 \\ 0 & \overline{Y} \end{bmatrix} \geqslant 0.$$

□

Proposition 2.3. *Let $A_0 \in M_n^{sa}(\mathbb{C})$, $x \in \mathbb{R}^n$ and $\bar{A}[x] \in \mathbb{R}^{2n\times 2n}$ such that*

$$\bar{A}[x] = \begin{bmatrix} \Re(A_0) & -\Im(A_0) \\ \Im(A_0) & \Re(A_0) \end{bmatrix} + \begin{bmatrix} Diag(x) & 0 \\ 0 & Diag(x) \end{bmatrix}. \tag{2.7}$$

Then, we state problem (2.1) as the following real SDP

$$\min_{w\in\mathbb{R},\ x\in\mathbb{R}^n} w \text{ such that} \tag{2.8}$$

$$w \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} - \bar{A}[x] \geqslant 0 \text{ and } w \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} + \bar{A}[x] \geqslant 0. \tag{2.9}$$

Proof. By Lemma 2.2, linear matrix restrictions $wI - A(x) \geqslant 0$ and $wI + A(x) \geqslant 0$ are equivalent to conditions in (2.9).

□

If $\bar{A}[x]$ is a solution of (2.8) and (2.9), then there exist natural numbers $1 \leqslant \bar{s}, \bar{t} < 2n$ such that

$$\begin{cases} \lambda_i(\bar{A}[x]) = \lambda_i & i = 1, 2, ..., 2n \\ \lambda_i = w & i = 1, 2, ..., \bar{t} \\ \lambda_i = -w & i = n - \bar{s} + 1, ..., 2n \\ w = \lambda_1 = ... = \lambda_{\bar{t}} & > \lambda_{\bar{t}+1} \geqslant ... \geqslant \lambda_{2n-\bar{s}} > \lambda_{2n-\bar{s}+1} = ... = \lambda_{2n} = -w. \end{cases} \tag{2.10}$$

If $\{q_1, ..., q_{2n}\}$ is an orthonormal set of eigenvectors corresponding to $\{\lambda_1, ..., \lambda_{2n}\}$, we define

$$\bar{Q_1} = [q_1|...|q_{\bar{t}}] \text{ and } \bar{Q_2} = [q_{n-\bar{s}+1}|...|q_{2n}],, \tag{2.11}$$

matrices of $2n \times \bar{t}$ and $2n \times \bar{s}$, respectively.

Therefore, we arrive to the next result in relation with the study of

$$\min_{x\in\mathbb{R}^n} \|\bar{A}[x]\|. \tag{2.12}$$

Theorem 2.4 (SDP Complex into SDP real)**.** *Let $A_0 \in M_n^{sa}(\mathbb{C})$, $x \in \mathbb{R}^n$ and $\bar{A}[x] \in \mathbb{C}^{2n\times 2n}$ as in (2.7). The following conditions are equivalent:*

1. *x is a solution of (2.1) (i.e. $A(x)$ is a minimal matrix of $n \times n$).*
2. *$\|\bar{A}[x]\| \leqslant \|\bar{A}[y]\|$ for every $y \in \mathbb{R}^n$ (i.e., $(x, x) \in \mathbb{R}^{2n}$ is a solution of (2.12)).*
3. *Following the same notation as in Proposition 2.3, (2.10) and (2.11), there exist semidefinite positive symmetric matrices $\bar{U}$ of $\bar{t} \times \bar{t}$ and $\bar{V}$ of $\bar{s} \times \bar{s}$ such that*

- $tr(\bar{U}) + tr(\bar{V}) = 1$,
- $tr(\bar{Q_1}^t(E_k + E_{n-k})\bar{Q_1}\bar{U}) - tr(\bar{Q_2}^t(E_k + E_{n-k})\bar{Q_2}\bar{V}) = 0,\ k = 1, ..., n.$

Proof. It follows directly from the conversion of Problem (2.1) into a SDP real problem, as we did in Proposition 2.4. □

Theorem 2.4 indicates that $A(x)$ is minimal if and only if the real $2n \times 2n$ block matrix $\bar{A}[x]$ is a solution of the problem (2.12).

Observe that a solution $\bar{A}[x]$ of (2.12) is not necessarily a minimal matrix of $2n \times 2n$, since it can exist a $2n \times 2n$ best real diagonal approximant D such that

$$\|\bar{A}[0] + D\| < \|\bar{A}[x]\| \text{ with } D \neq \begin{bmatrix} \mathrm{Diag}(x) & 0 \\ 0 & \mathrm{Diag}(x) \end{bmatrix} = \sum_{k=1}^{n} x_k A_k,$$

where $A_k = E_k + E_{n-k}$ and

$$\begin{aligned} \bar{A}[x] &= \begin{bmatrix} \Re(A_0) & -\Im(A_0) \\ \Im(A_0) & \Re(A_0) \end{bmatrix} + x \sum_{k=1}^{n} e_k e_k^t + x \sum_{k=n+1}^{2n} e_k e_k^t \\ &= \begin{bmatrix} \Re(A_0) & -\Im(A_0) \\ \Im(A_0) & \Re(A_0) \end{bmatrix} + \sum_{k=1}^{n} x_k \underbrace{E_k + E_{n+k}}_{A_k} \\ &= \begin{bmatrix} \Re(A_0) & -\Im(A_0) \\ \Im(A_0) & \Re(A_0) \end{bmatrix} + \sum_{k=1}^{n} x_k A_k, \end{aligned}$$

However, $A(x)$ (with the same x) is a minimal matrix of $n \times n$.

Next, we obtain another characterization of the solution of problem (2.1) without converting it into a real SDP problem.

Theorem 2.5. *Let $A \in M_n^{sa}(\mathbb{C})$ and $x \in \mathbb{R}^n$. The following conditions are equivalent:*

a) $x = \mathrm{Diag}(A)$ *is a solution of* (2.2) *(i.e: $A = A(x)$ is minimal).*

b) *(Adapted to the more general case of $A \in M_n^{sa}(\mathbb{C})$ from [18, Theorem 3.2]) If $\{q_1, \ldots, q_n\}$ is an orthonormal basis of eigenvectors of A corresponding to the eigenvalues $\|A\| = \lambda_1 \geqslant \cdots \geqslant \lambda_n = -\|A\|$, $Q_1 = [q_1|\ldots|q_t]$, $Q_2 = [q_{n-s+1}|\ldots|q_n]$ are the $n \times t$ and $n \times s$ matrices whose columns correspond to the eigenvectors of λ_1 and λ_n respectively, then there exist semidefinite positive self-adjoint matrices $U \in \mathbb{C}^{t \times t}$ and $V \in \mathbb{C}^{s \times s}$ such that*

$$tr(U) + tr(V) = 1, \text{ and} \tag{2.13}$$

$$tr(Q_1^* E_k Q_1 U) - tr(Q_2^* E_k Q_2 V) = 0,\ \forall k = 1, ..., n. \tag{2.14}$$

c) *(Adapted from [23, Theorem 2.1.6] to the particular case of $W(H) = \mathrm{Diag}(M_n^{sa})$)*
There exists $X \in M_n(\mathbb{C})$ with $\mathrm{Diag}(X) = 0$ such that $AX = \|A\||X|$, where $|X| = (X^*X)^{1/2}$.

d) *(From [2, Theorem 2 (ii)]) Let E_+ (respectively E_-) be the spectral projection of A corresponding to the eigenvalue $\lambda_1 = \lambda_{max}(A)$ (respectively $\lambda_n = \lambda_{min}(A)$). Then there is a non-zero $X \in M_n^{sa}(\mathbb{C})$ such that*

$$\mathrm{Diag}(X) = 0,\ E_+X^+ = X^+,\ E_-X^- = X^- \ \ and \ \ tr(AX) = \|A\|\,\|X\|_1,$$

where $X^+ = \frac{|X|+X}{2}$ and $X^- = \frac{|X|-X}{2}$ (with $|X| = (X^2)^{1/2} \geqslant 0$).

Proof. The equivalences a) ⇔ c) ⇔ d) have already been proved in the provided citations. The equivalence with item b) is the only that needs a proof.
Let W be the unitary $n \times n$ matrix whose columns are the eigenvectors of A:

$$W = [Q_1|Q_2|R],$$

with $R = [q_{t+1}|\dots|q_{n-s}]$ (following the notation used in (2.5)) and Q_1, Q_2 from b).
Now consider the diagonal blocks of $t \times t$, $s \times s$ and $(n-t-s) \times (n-t-s)$ to define the following $n \times n$ self-adjoint matrix

$$X = W \cdot \begin{pmatrix} U & 0 & 0 \\ 0 & -V & 0 \\ 0 & 0 & 0 \end{pmatrix} \cdot W^*$$

using the positive semidefinite matrices U and V from b) of sizes $t \times t$ and $s \times s$ respectively.
Then using (2.14) it can be proved that $\mathrm{Diag}(X) = 0$. Moreover, using (2.13) and the fact that $U \geqslant 0$, $V \geqslant 0$ we obtain

$$\|X\|_1 = \mathrm{tr}|X| = \mathrm{tr}\left|W \cdot \begin{pmatrix} U & 0 & 0 \\ 0 & -V & 0 \\ 0 & 0 & 0 \end{pmatrix} \cdot W^*\right| = \mathrm{tr}\left(W \left|\begin{pmatrix} U & 0 & 0 \\ 0 & -V & 0 \\ 0 & 0 & 0 \end{pmatrix}\right| W^*\right) = \mathrm{tr}\left|\begin{pmatrix} U & 0 & 0 \\ 0 & -V & 0 \\ 0 & 0 & 0 \end{pmatrix}\right|$$
$$= \mathrm{tr}\begin{pmatrix} U & 0 & 0 \\ 0 & V & 0 \\ 0 & 0 & 0 \end{pmatrix} = 1.$$

And A can be diagonalized using W as

$$A = W \cdot \begin{pmatrix} \lambda_1 I_t & 0 & 0 \\ 0 & -\lambda_1 I_s & 0 \\ 0 & 0 & D_0 \end{pmatrix} \cdot W^*$$

where D_0 is the diagonal matrix with the eigenvalues of A distinct from λ_1 and $-\lambda_1 = \lambda_n$ (including multiplicity) and I_k denotes the $k \times k$ identity matrix.
Hence

$$A \cdot X = W \cdot \begin{pmatrix} \lambda_1 I_S & 0 & 0 \\ 0 & -\lambda_1 I_t & 0 \\ 0 & 0 & D_0 \end{pmatrix} \cdot W^* \cdot W \cdot \begin{pmatrix} U & 0 & 0 \\ 0 & -V & 0 \\ 0 & 0 & 0 \end{pmatrix} \cdot W^* = W \cdot \begin{pmatrix} \lambda_1 U & 0 & 0 \\ 0 & \lambda_1 V & 0 \\ 0 & 0 & 0 \end{pmatrix} \cdot W^*$$
$$= \lambda_1\, W \cdot \begin{pmatrix} U & 0 & 0 \\ 0 & V & 0 \\ 0 & 0 & 0 \end{pmatrix} \cdot W^* = \lambda_1 |X|$$

hold, which together with the fact that $\lambda_1 = \|A\|$ and item c) of Proposition 2.5 imply that A is a minimal matrix.

To prove the implication a) ⇒ b) we will use that the statement d) is equivalent to the condition of being a minimal matrix. Then given a minimal matrix $A \in M_n^{sa}(\mathbb{C})$ there exists X such that $\mathrm{Diag}(X) = 0$, $\mathrm{tr}(|X|) = \|X\| = 1$,

$\operatorname{tr}(AX) = \|A\|$, $E_+X = X$ and $E_-X = X$.
Now consider the unitary matrix $Q = [Q_1|Q_2|Q_3]$ constructed as follows. The $n \times t$ and $n \times s$ matrices $Q_1 = [v_1|\dots|v_t]$, $Q_2 = [v_{n-s+1}|\dots|v_n]$ are constructed with columns of eigenvectors corresponding to the eigenvalues $\lambda_1 = \|A\|$ and $\lambda_n = -\|A\|$, and $Q_3 = [v_{t+1}|\dots|v_{n-s}]$ is a $n \times (n-s-t)$ matrix with columns formed by eigenvectors of A that complete an orthonormal basis of $\mathbb{C}^n$.
Then, from the proof of (i) $\Rightarrow$ (ii) in [2, Theorem 2 (ii)] follows that there exists $Y \geqslant 0$, $Z \geqslant 0$ such that

$$X = Q \begin{pmatrix} Y & 0 & 0 \\ 0 & -Z & 0 \\ 0 & 0 & 0 \end{pmatrix} Q^* \quad \text{and} \quad A = Q \cdot \begin{pmatrix} \lambda_1 I_t & 0 & 0 \\ 0 & -\lambda_1 I_s & 0 \\ 0 & 0 & D_0 \end{pmatrix} \cdot Q^*.$$

Then since $\operatorname{tr}|X| = 1$ it must be

$$1 = \operatorname{tr}|X| = \operatorname{tr}\left(Q \left| \begin{pmatrix} Y & 0 & 0 \\ 0 & -Z & 0 \\ 0 & 0 & 0 \end{pmatrix} \right| Q^*\right) = \operatorname{tr}\begin{pmatrix} |Y| & 0 & 0 \\ 0 & |Z| & 0 \\ 0 & 0 & 0 \end{pmatrix} = \operatorname{tr}(Y+Z). \tag{2.15}$$

Moreover, using the expression $Q = [Q_1|Q_2|Q_3] = \begin{pmatrix} Q_1 & Q_2 & Q_3 \end{pmatrix}$ we can compute

$$X = \begin{pmatrix} Q_1 & Q_2 & Q_3 \end{pmatrix} \begin{pmatrix} Y & 0 & 0 \\ 0 & -Z & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} Q_1 \\ Q_2 \\ Q_3 \end{pmatrix}^* = Q_1 Y Q_1^* - Q_2 Z Q_2^*.$$

Hence, since $\operatorname{Diag}(X) = 0$ follows that

$$X_{k,k} = (Q_1 Y Q_1^* - Q_2 Z Q_2^*)_{k,k} = \operatorname{tr}(E_k (Q_1 Y Q_1^* - Q_2 Z Q_2^*) E_k) = 0, \ \forall k = 1, \dots, n$$

and therefore

$$0 = \operatorname{tr}\left(E_k (Q_1 Y Q_1^* - Q_2 Z Q_2^*)\right) = \operatorname{tr}\left(Q_1^* E_k Q_1 Y - Q_2^* E_k Q_2 Z\right) \tag{2.16}$$

Then considering $U = Y$ and $Z = V$ the equations (2.15) and (2.16) prove that item b) holds if A is minimal. □

Observe that the proof of Theorem 2.5 is different than the one made by Overton [18] and Fletcher [12], and it is related with the characterization of minimal self-adjoint matrices made in [2].

3. Subdifferential and moment of a subspace

Here we generalize some of the results developed by Overton in [19] to complex matrices and compact self-adjoint operators. Also, we relate the concept of subdifferential of the maximum eigenvalue with the moment of a subspace. In order to do this, it is necessary to state some particular definitions and previous results.

Recall that, given a subspace S of a separable Hilbert space H, the moment of S is defined by

$$m_S = \operatorname{co}\{|v|^2 : v \in S, \|v\| = 1\}, \tag{3.1}$$

where $v = (v_1, v_2, ...)$ are the coordinates of v any fixed basis of H, and $|v|^2 = \big(|v_1|^2, |v_2|^2, ...\big)$. In particular, if $H = \mathbb{C}^n$, by Proposition 3.2 in [16]

$$m_S = \text{Diag}\left(\{Y \in M_n^{sa}(\mathbb{C}) : Y \geqslant 0, \text{tr}(Y) = 1, Im(Y) \subset S\}\right), \tag{3.2}$$

and if H is an infinite dimensional Hilbert space, by Proposition 1 in [6]

$$m_S = \text{Diag}\left(\{Y \in B_1(H)^{sa} : Y \geqslant 0, \text{tr}(Y) = 1, Im(Y) \subset S\}\right). \tag{3.3}$$

On the other hand, consider a sequence $\mathbf{A} = \{A_j\}_{j=1}^{\infty}$ of self-adjoint compact operators or matrices A_j with bounded norm ($\|A_j\| \leqslant c$, for all j). We define the joint numerical range of $\mathbf{A}$ by

$$W(\mathbf{A}) = \left\{\{\text{tr}\left(\rho A_j\right)\}_{j=1}^{\infty} : \rho \in M_n^{sa}(\mathbb{C}) \wedge \text{tr}(\rho) = 1 \wedge \rho \geqslant 0\right\}, \tag{3.4}$$

when $\mathbf{A} \subset M_n^{sa}$, and

$$W(\mathbf{A}) = \left\{\{\text{tr}\left(\rho A_j\right)\}_{j=1}^{\infty} : \rho \in \mathcal{B}_1^{sa}(H) \wedge \text{tr}(\rho) = 1 \wedge \rho \geqslant 0\right\}, \tag{3.5}$$

when $\mathbf{A} \subset \mathcal{K}^{sa}(H)$.

For $E = \{e_j\}_{j=1}^{\infty}$ we will denote with $e_j \otimes e_j = E_j$, the rank-one orthogonal projections onto the subspaces generated by $e_j \in E$, for all $j \in \mathbb{N}$. We will be particularly interested in the study of $W(\mathbf{A})$ in the case of $\mathbf{A} = \mathbf{A_{S,E}} = \{P_S E_j P_S\}_{j=1}^{\infty}$ and S a finite dimensional subspace of H

$$W(\mathbf{A_{S,E}}) = \left\{\{\text{tr}\left(P_S E_j P_S \rho\right)\}_{j=1}^{\infty} : \rho \in \mathcal{B}_1(H),\ \rho \geqslant 0 \text{ and } \text{tr}(\rho) = 1\right\}. \tag{3.6}$$

Note that $W(\mathbf{A_{S,E}}) \subset \ell^1(\mathbb{R}) \cap \mathbb{R}^{\mathbb{N}}_{\geqslant 0}$. In this context, we will consider the set of its density operators

$$\mathcal{D}_S = \{Y \in \mathcal{B}_1(H) : P_S Y = Y \geqslant 0\ , \text{tr}(Y) = 1\} \tag{3.7}$$

(note that $P_S Y = Y P_S = P_S Y P_S$ for $Y \in \mathcal{D}_S$). If $\dim S < \infty$, the affine hull of $\mathcal{D}_S$ is also finite dimensional.

There exists a relation between the moment of a subspace and the joint numerical range of the particular family $\mathbf{A_{S,E}}$, as we illustrate in the next result.

Proposition 3.1 (Proposition 2 [6])**.** *The following are equivalent definitions of m_S, the moment of S (see (3.6)), with $\dim S = r < \infty$, related to a basis $E = \{e_i\}_{i=1}^{\infty}$ of H. Note the identification made between diagonal operators and sequences.*

a) $m_S = Diag(\mathcal{D}_S)$.
b) $m_S = co\left\{|v|^2 : v \in S \text{ and } \|v\| = 1\right\}$.
c) $m_S = \bigcup_{\{s^i\}_{i=1}^r \text{ o.n. set in } S} co\{|s^i|^2\}_{i=1}^r$.
d) $m_S = \{(tr(E_1 Y), \dots, tr(E_n Y), \dots) \in \ell^1(\mathbb{R}) : Y \in \mathcal{D}_S\}$.
e) $m_S = W(P_S E_1 P_S, \dots, P_S E_n P_S, \dots) \cap \left\{x \in \ell^1(\mathbb{R}) : x_i \geqslant 0 \text{ and } \sum_{i=1}^{\infty} x_i = 1\right\}$, *where P_S is the orthogonal projection onto S, and W is the joint numerical range (3.5).*

See [16, 6] for more properties about m_S in finite and infinite dimensional cases, respectively.

3.1. The finite dimensional case

Let $A \in M_n^{sa}(\mathbb{C})$, define $\lambda_{max}(A) = \lambda_1(A)$ and assume that it has multiplicity $s \geqslant 1$. Then, $\lambda_1 : M_n^{sa}(\mathbb{C}) \to \mathbb{R}$ is a convex function, since it can be written as the maximum of a set of linear functions,

$$\begin{aligned} \lambda_1(A) &= \max\{\langle Aq, q\rangle : q \in \mathbb{C}^n, \|q\| = 1\} = \max\{\operatorname{tr}(Aqq^*) : q \in \mathbb{C}^n, \|q\| = 1\} \\ &= \max\{\langle A, R\rangle_{tr} : \ R \in M_n^{sa}(\mathbb{C}), R \geqslant 0, \operatorname{tr}(R) = 1\}. \end{aligned} \tag{3.8}$$

The proof of the previous statement is done in Proposition 3.11 in a more general context.

Definition 3.2. For any convex function $f : \mathcal{X} \to \mathbb{R}$ defined on a Banach space $\mathcal{X}$, and $\mathcal{X}^*$ its dual, it can be defined the **subdifferential** of f at $x \in \mathcal{X}$ as

$$\partial f(x) = \{v \in \mathcal{X}^* : f(y) - f(x) \geqslant \operatorname{Re} v(y - x), \forall\ y \in \mathcal{X}\}, \tag{3.9}$$

as in [3].

In particular, if $\mathcal{X} = M_n^{sa}(\mathbb{C})$ and $f(\cdot) = \lambda_1(\cdot)$, the subdifferential at $x = A \in M_n^{sa}$ is

$$\partial\lambda_1(A) = \{V \in M_n^{sa}(\mathbb{C}) : \lambda_1(Y) - \lambda_1(A) \geqslant \operatorname{Re}\ \langle V, (Y - A)\rangle_{tr}\,,\ \forall\ Y \in M_n^{sa}(\mathbb{C})\}.$$

Then, using (3.8) and similar arguments than those in [19], the subdifferential of λ_1 at A is the set

$$\begin{aligned} \partial\lambda_1(A) &= \operatorname{co}\{qq^* : Aq = \lambda_1(A)q \text{ and } \|q\| = 1\} \\ &= \{Q_1 R_s Q_1^* : R_s \in M_s^{sa}(\mathbb{C}), R_s \geqslant 0, \operatorname{tr}(R_s) = 1\}, \end{aligned} \tag{3.10}$$

where the columns of Q_1 form an orthonormal set of s eigenvectors for $\lambda_1(A)$ (an orthonormal basis of the eigenspace of $\lambda_1(A)$). Observe that Q_1 depends on the matrix A.

Let $A(x) = A_0 + \operatorname{Diag}(x) = A_0 + \sum_{j=1}^n x_k e_k e_k^*$, with $A_0 \in M_n^{sa}(\mathbb{C})$, $\{e_k\}_{k=1}^n$ a fixed orthonormal basis of $\mathbb{C}^n$ and $x \in \mathbb{R}^n$. The maximum eigenvalue of $A(x)$, $\lambda_1(A(x)) = \lambda_{max}(A(x))$, is a map from $\mathbb{R}^n$ to $\mathbb{R}$. Observe that $\lambda_1(A(x))$ is a composition of a smooth function $A(\cdot)$ and a convex map $\lambda_1(\cdot)$. Moreover, for every k, the partial derivatives of A are

$$\frac{\partial A}{\partial x_k}(x) = e_k e_k^*.$$

Adapting Theorem 3 in [19] to the self-adjoint case, the subdifferential of $\lambda_1(A(x))$ is

$$\begin{aligned} \partial\left(\lambda_1(A(x))\right) = \{v \in \mathbb{R}^n :\ & v_k = \langle R_s, Q_1(x)^* e_k e_k^* Q_1(x)\rangle_{tr}\,, \\ & R_s \in M_s^{sa}(\mathbb{C}), R_s \geqslant 0, \operatorname{tr}(R_s) = 1\}, \end{aligned} \tag{3.11}$$

where s is the multiplicity of $\lambda_1(A(x))$ and the columns of $Q_1(x)$ form an orthonormal basis of eigenvectors for $\lambda_1(A(x))$. Note that $Q_1(x)$ depends on $A(x)$ and

$$v_k = \langle R_s, Q_1(x)^* e_k e_k^* Q_1(x)\rangle_{tr} = \operatorname{tr}(R_s Q_1(x)^* e_k e_k^* Q_1(x)) \geqslant 0,$$

for every k, since R_s and $Q_1(x)^* e_k e_k^* Q_1(x)$ are semidefinite positive matrices.

Using (3.11), we obtain the following characterization of the subdifferential.

Theorem 3.3. *Let $A(x) = A_0 + \mathrm{Diag}(x)$, with $A_0 \in M_n^{sa}(\mathbb{C})$ and $x \in \mathbb{R}^n$, and S_1 be the eigenspace of $\lambda_1(A(x))$. Then*

$$\partial\big(\lambda_1(A(x))\big) = \mathrm{Diag}(\partial\lambda_1(A(x))) = m_{S_1}, \tag{3.12}$$

where m_{S_1} is the moment of the eigenspace S_1 and we have identified diagonal matrices with vectors in the last equality.

Proof. Suppose $\lambda_1(A(x)) = \lambda_{max}(A(x))$ has multiplicity s and S_1 is the eigenspace of $\lambda_1(A(x))$ with a fixed orthonormal basis of eigenvectors $\{q_1(x), ..., q_s(x)\}$. If $Q_1(x) = \big[q_1(x)|...|q_s(x)\big] \in \mathbb{C}^{n\times s}$. By (3.11), any $v \in \partial\lambda_1(A(x))$ has coordinates

$$v_k = \mathrm{tr}\left(R_s Q_1(x)^* e_k e_k^* Q_1(x)\right) = \mathrm{tr}\left(Y(x) e_k e_k^*\right) = \langle Y(x)e_k, e_k\rangle = Y_{kk},$$

with $R_s \in M_s^{sa}(\mathbb{C})$, $R_s \geqslant 0$, $\mathrm{tr}(R_s) = 1$, for every $k = 1, ..., n$. Then, $v = (v_1, v_2, ..., v_n) = \mathrm{Diag}(Y(x))$ with $Y(x) = Q_1(x) R_s Q_1(x)^* \in \partial\lambda_1(A(x))$ satisfies

- $Y(x) = Y(x)^* \geqslant 0$,
- $\mathrm{tr}(Y(x)) = \mathrm{tr}(Q_1(x)R_sQ_1(x)^*) = \mathrm{tr}(R_sQ_1(x)^*Q_1(x)) = \mathrm{tr}(R_s) = 1$, and
- $\mathrm{Im}(Y(x)) \subset S_1$. Indeed, for every $h \in \mathbb{C}^n$ note that

$$Y(x)h = Q_1(x)\left(\underbrace{R_sQ_1(x)^*h}_{w}\right) = Q_1(x)w \in S_1,$$

  with w a column vector of s coordinates.

Therefore, by (3.2)

$$v = \mathrm{Diag}(Y(x)) = \mathrm{Diag}\left(Q_1(x)R_sQ_1(x)^*\right) \in m_{S_1}.$$

On the other hand, take any $v \in m_{S_1}$. Then, it can be written as

$$v = \left(\mathrm{tr}(e_1e_1^*Y), \mathrm{tr}(e_2e_2^*Y), ..., \mathrm{tr}(e_ne_n^*Y)\right),$$

with $Y = Y^* \geqslant 0$, $\mathrm{tr}(Y) = 1$ and $Im(Y) \subset S_1$. In terms of the orthogonal decomposition $\mathbb{C}^n = S_1 \oplus S_1^\perp$, given by the matrix $Q = \big[Q_1(x) \quad Q_2(x)\big]$ (Q_2 is a matrix whose columns form an orthonormal set for $S_1^\perp$ and Q is a unitary matrix), Y is defined by

$$Y = Q\begin{bmatrix} V & 0 \\ 0 & 0 \end{bmatrix} Q^* = Q_1(x)VQ_1(x)^*$$

with $V \in M_s^{sa}(\mathbb{C})$, $1 = \mathrm{tr}(Y) = \mathrm{tr}(V)$ and $V \geqslant 0$. Therefore, $v \in \partial\lambda_1(A(x))$. □

Corollary 3.4. *Under the assumptions of Theorem 3.3, if $\lambda_1(A(x))$ has multiplicity one (i.e., $s = 1$), then*

$$\partial\lambda_1(A(x)) = \{|v|^2 : A(x)v = \lambda_1(A(x))v, \|v\| = 1\},$$

$\lambda_1(A(x))$ is derivable and $\frac{\partial\lambda_1}{\partial x_k}(x) = |v_k|^2$ for every $k = 1, 2, \ldots n$.

The next result gives a concrete formula to the directional derivative of $\lambda_1(A(x))$ and appears in [19], but here we include an explicit proof for the self-adjoint case.

Proposition 3.5. *Let $A(x) = A_0 + \mathrm{Diag}(x)$, with $A_0 \in M_n^{sa}(\mathbb{C})$ and $x \in \mathbb{R}^n$. Suppose $\lambda_1(A(x)) = \lambda_{max}(A(x))$, has multiplicity s, with a corresponding orthonormal basis of eigenvectors $\{q_1(x), ..., q_s(x)\}$ and $Q_1(x) = \left[q_1(x)|...|q_s(x)\right]$. Then the directional derivative of λ_1 at $x \in \mathbb{R}^n$ in the direction $w \in \mathbb{R}^n$ that is defined by*

$$\lambda_1'(x, w) = \lim_{t\to 0^+} \frac{\lambda_1(x + tw) - \lambda_1(A(x))}{t}$$

is the largest eigenvalue of

$$B(w) = \sum_{k=1}^{n} w_k Q_1(x)^* e_k e_k^* Q_1(x).$$

Proof. Recall that $\lambda_1(A(x)) = \lambda_1 \circ A(x)$, is a composition of a smooth map $A(x)$ with a convex function λ_1. Then, for every $w \in \mathbb{R}^n$

$$\lambda_1'(x, w) = \max_{v\in\partial\lambda_1(A(x))} \langle v, w\rangle,$$

since the generalized derivative and generalized gradient coincide with the directional derivative and subdifferential, respectively (see Proposition 2.2.7 in [9]). Therefore,

$$\begin{aligned}
\lambda_1'(x, w) &= \max\left\{\sum_{k=1}^{n} v_k w_k : v_k = \langle R_s, Q_1(x)^* e_k e_k^* Q_1(x)\rangle_{tr}, R_s \in M_s^{sa}(\mathbb{C}), R_s \geqslant 0, \mathrm{tr}(R_s) = 1\right\} \\
&= \max\left\{\left\langle R_s, \sum_{k=1}^{n} w_k Q_1(x)^* e_k e_k^* Q_1(x)\right\rangle_{tr} : R_s \in M_s^{sa}(\mathbb{C}), R_s \geqslant 0, \mathrm{tr}(R_s) = 1\right\} \\
&= \max\left\{\langle R_s, B(w)\rangle_{tr} : R_s \in M_s^{sa}(\mathbb{C}), R_s \geqslant 0, \mathrm{tr}(R_s) = 1\right\} \\
&= \lambda_1(B(w)),
\end{aligned}$$

where the last equality is due to (3.8). □

Lemma 3.6. *Let $A(x) = A_0 + \mathrm{Diag}(x)$, with $A_0 \in M_n^{sa}(\mathbb{C})$ and $x \in \mathbb{R}^n$, $\lambda_n(A(x))$ be the minimum eigenvalue of $A(x)$ and S_n its corresponding eigenspace. Then,*

$$\partial\lambda_n(A(x)) = \partial\lambda_n(x) = -m_{S_n}. \tag{3.13}$$

Proof. Since $\lambda_n(A(x)) = -\lambda_1(-A(x))$ for any $A(x) \in M_n^{sa}(\mathbb{C})$, then

$$\begin{aligned}\partial\lambda_n(A(x)) &= -\partial\lambda_1(-A(x)) \\ &= -\operatorname{Diag}\left(\operatorname{co}\{uu^* : \|u\| = 1,\ -A(x)u = \lambda_1(-A(x))u\}\right) \\ &= -\operatorname{Diag}\left(\operatorname{co}\{uu^* : \|u\| = 1,\ A(x)u = \lambda_n(A(x))u\}\right) \\ &= -m_{S_n}.\end{aligned}$$

□

The subdifferential of the spectral norm of a matrix A is

$$\begin{aligned}\partial\|A\| &= \operatorname{co}\{uv^* : Au = \|A\|v \text{ and } \|u\| = \|v\| = 1\} \\ &= \{VR_tW^* : R_t \in M_t^{sa}(\mathbb{C}), R_t \geqslant 0, \operatorname{tr}(R_t) = 1\},\end{aligned} \tag{3.14}$$

where V, W are unitary matrices of the singular value decomposition of A, i.e. $A = V\operatorname{Diag}(s(A))W^*$ and $s_1(A) = \|A\|$. The proof of (3.14) appears first in [22] for the real case and, more recently for the complex case, in [3] and [13].

The subdifferential (3.14) can be closely related with the subdifferentials of λ_1 and λ_n in some cases, as we observe in the next statement.

Remark 3.7. The expression in (3.14) for any $A(x) = A_0 + \operatorname{Diag}(x)$, with $A \in M_n^{sa}(\mathbb{C})$ and $x \in \mathbb{R}^n$ is

$$\partial\|A(x)\| = \operatorname{co}\{uu^* : A(x)u = \|A(x)\|u \text{ and } \|u\| = 1\}. \tag{3.15}$$

Let $\lambda_n(A(x))$ and $\lambda_1(A(x))$ be the minimum and maximum eigenvalue of $A(x)$, respectively. Considering (3.15) and Lemma 3.6, it is evident that

$$\partial\|A(x)\| = \begin{cases} \partial\lambda_1(A(x)) & \text{if} \quad \|A(x)\| = \lambda_1(A(x)) \\ \partial\lambda_n(A(x)) & \text{if} \quad \|A(x)\| = -\lambda_n(A(x)) = |\lambda_n(A(x))| \\ \operatorname{co}\left(\partial\lambda_1(A(x)) \cup \partial\lambda_n(A(x))\right) & \text{if} \quad \|A(x)\| = -\lambda_n(A(x)) = \lambda_1(A(x)). \end{cases}$$

Theorem 3.8. *Let $A(x) = A_0 + \operatorname{Diag}(x)$, with $A_0 \in M_n^{sa}(\mathbb{C})$ and $x \in \mathbb{R}^n$ such that $\lambda_1(A(x)) = -\lambda_n(A(x))$. Then, the following statements are equivalent,*

(1) $0 \in \partial\|A(x)\|$.
(2) $0 \in \partial\lambda_1(A(x)) + \partial\lambda_n(A(x))$.
(3) $m_{S_1} \cap m_{S_n} \neq \varnothing$, *where S_1 and S_n are the eigenspaces of $\lambda_1(A(x))$ and $\lambda_n(A(x))$, respectively.*
(4) $W\left(\{P_{S_1}e_ie_i^*P_{S_1}\}_{i=1}^n\right) \cap W\left(\{P_{S_n}e_ie_i^*P_{S_n}\}_{i=1}^n\right) \neq \{0\}$.
(5) *$A(x)$ is minimal.*

Proof. The equivalences (3) ⇔ (4) ⇔ (5) have already been proved in [16].

(1)⇔(3) If $0 \in \partial\|A(x)\|$ and $\lambda_1(A(x)) = -\lambda_n(A(x))$, then using Remark 3.7

$$0 \in \operatorname{co}\left(\partial\lambda_1(A(x)) \cup \partial\lambda_n(A(x))\right) = \operatorname{co}\left(m_{S_1} \cup -m_{S_n}\right)$$

and there exist $\alpha \in (0,1)$, $Y_0 \in \{Y \in M_n^{sa}(\mathbb{C}) : Y \geqslant 0, \mathrm{tr}(Y) = 1, \mathrm{Im}(Y) \subset S_1\}$ and $Z_0 \in \{Z \in M_n^{sa}(\mathbb{C}) : Z \geqslant 0, \mathrm{tr}(Z) = 1, \mathrm{Im}(Z) \subset S_n\}$ such that $0 = \alpha \mathrm{Diag}(Y) + (1-\alpha)\mathrm{Diag}(-Z)$. Using that $\mathrm{tr}(Y) = \mathrm{tr}(Z) = 1$ we obtain that $\alpha = \frac{1}{2}$ and then $\mathrm{Diag}(Y) = \mathrm{Diag}(Z)$. Therefore, $m_{S_1} \cap m_{S_n} \neq \varnothing$.

The converse implication can be proved reversing the previous steps.

To prove (2)⇔(3) we can use the formulas $\partial\big(\lambda_1(A(x))\big) = m_{S_1}$ and $\partial\lambda_n(A(x)) = -m_{S_n}$ from (3.12) and (3.13). Then it is trivial that $m_{S_1} \cap m_{S_n} \neq \varnothing$ if and only if $0 \in m_{S_1} - m_{S_n} = \partial\lambda_1(A(x)) + \partial\lambda_n(A(x))$. □

3.2. The compact operator case

Lemma 3.9. *Let $B_1(H)$ be the ideal of trace class operators. Then,*

$$\mathrm{co}\left(\{hh^* : h \in H, \|h\| = 1\}\right) = \{Y \in B_1(H) : Y \geqslant 0,\ tr(Y) = 1\},$$

Proof. If $\sum_j a_j h^j (h^j)^*$ is a convex combination of unitary vectors $h^j \in H$, then it fulfills that is a semidefinite positive compact operator with $\mathrm{tr}\left(\sum_j a_j h^j (h^j)^*\right) = \sum_j a_j = 1$. On the other hand, every $Y \in B_1(H)^{sa}$, with $Y \geqslant 0$ and $\mathrm{tr}(Y) = 1$ can be written as a (maybe infinite) convex combination of rank one operators. □

Definition 3.10. Given a Banach space $\mathcal{X}$, a function $f : \mathcal{X} \to \mathbb{R}$ is said to be regular at $x \in \mathcal{X}$ if

1. for all v, the usual one-sided derivative
$$f'(x,v) = \lim_{t \to 0^+} \frac{f(x+tv) - f(x)}{t}$$
exists.
2. For all v, $f'(x,v)$ coincides with the general derivative.

To see more details of this definition, see [10] and [9].

Proposition 3.11. *Let $A \in K(H)^{sa}$ and*

$$\lambda_{max}(A) = \max\{\lambda \in \mathbb{R} :\ A - \lambda I \text{ is not invertible}\} \tag{3.16}$$

be the maximum of the spectrum of A, then the following statements hold.

1. *If $\lambda_{max}(A) \neq 0$, then $\lambda_{max}(A)$ is an eigenvalue of A and it has finite multiplicity.*
2. *The following are equivalent forms to describe $\lambda_{max}(A)$,*

$$\lambda_{\max}(A) = \max_{\|h\|=1} \langle Ah, h\rangle \tag{3.17}$$
$$= \max\{tr(Ahh^*) : \|h\| = 1\} = \max\{\langle A, hh^*\rangle_{tr} :\ \|h\| = 1\} \tag{3.18}$$
$$= \max\{\langle A, Y\rangle_{tr} :\ Y \in B_1(H)^{sa}, Y \geqslant 0, tr(Y) = 1\}. \tag{3.19}$$

3. *$\lambda_{\max} : K(H)^{sa} \to \mathbb{R}$ is a convex function and is Lipschitz near A and regular in the sense of Definition 3.10.*

4. *As a particular case of Lemma 3.9, we define the set*

$$\mathcal{D}_{S_{\max}} = co\left(\{qq^* : q \in H, Aq = \lambda_{\max}(A)q, \|q\| = 1\}\right). \tag{3.20}$$

Then,

$$\mathcal{D}_{S_{\max}} = \{Y \in B_1(H)^{sa} : Y \geqslant 0, E_+Y = YE_+,\ tr(Y) = 1\}, \tag{3.21}$$

where E_+ is the orthogonal projection onto the eigenspace of $\lambda_{\max}(A)$. Moreover, if $\lambda_{\max}(A) \neq 0$, then

$$\mathcal{D}_{S_{\max}} = \{Q_{\max} R_s Q_{\max}^* : R_s \in M_s^{sa}(\mathbb{C}), R_s \geqslant 0, tr(R_s) = 1\}, \tag{3.22}$$

where s is the multiplicity of $\lambda_{\max}$ and the columns of $Q_{\max}$ form an orthonormal basis of eigenvectors of $\lambda_{\max}$.

Proof. 1. It is a well-known fact of the spectrum of compact operators.

2. Equality (3.17) holds since for any λ eigenvalue of A and $v \in S_\lambda$, $v \neq 0$, $Av = \lambda_{\max}(A)v$ and $\langle Av, v\rangle = \lambda \langle v, v\rangle \in \mathbb{R}$. Then,

$$\lambda_{\max}(A) \geqslant \max\{\lambda \in \mathbb{R} : \exists v \in H \text{ such that } Av = \lambda v\} = \max\left\{\frac{\langle Av, v\rangle}{\langle v, v\rangle} : v \in H\right\}$$
$$= \max_{\|h\|=1} \langle Ah, h\rangle.$$

(3.18) follows from the equality $\langle Ah, h\rangle = \mathrm{tr}(Ahh^*)$, and (3.19) is due to Lemma 3.9, since maximizing a linear function (the trace) over a set gives the same result as maximizing it over its convex hull.

3. By (3.17), if $A, B \in K(H)^{sa}$ and $t \in [0, 1]$, then

$$\begin{aligned}\lambda_{\max}(tA + (1-t)B) &= \max_{\|h\|=1} \langle (tA + (1-t)B)h, h\rangle = \max_{\|h\|=1} \left[t\langle Ah, h\rangle + (1-t)\langle Bh, h\rangle\right] \\ &\leqslant t \max_{\|h\|=1} \langle Ah, h\rangle + (1-t) \max_{\|h\|=1} \langle Bh, h\rangle \\ &= t\lambda_{\max}(A) + (1-t)\lambda_{\max}(B).\end{aligned}$$

Therefore, $\lambda_{\max} : K(H)^{sa} \to \mathbb{R}$ is a convex function. On the other hand, $\lambda_{\max}$ is bounded above on a neighborhood of $A = A^*$ (since $\lambda_{\max}(A) \leqslant \|A\| < \infty$ for all $A \in B(H)$), so by [9] (Prop. 2.2.6 and 2.3.6), $\lambda_{\max}$ is Lipschitz near A and regular.

4. The first equality is evident, since any $Y \geqslant 0$, such that $E_+Y = YE_+$ and $\mathrm{tr}(Y) = 1$ can be written as

$$Y = \sum_{i=1}^{s} a_i qq^*,$$

where $\sum_{i=1}^{s} a_i = 1$, $a_i \geqslant 0$ for every i, and $\{q_i\}_{i=1}^{s}$ is an orthonormal basis of the eigenspace $S_{\max}$ of A. If $\lambda_{\max}(A) \neq 0$, then $s < \infty$ and we can define $Q_{\max} = [q_1|q_2|...|q_s]$ and $R_s = \mathrm{Diag}\left(\{a_i\}_{i=1}^{s}\right) \in M_s^{sa}(\mathbb{C})$, such that

$$Y = Q_{\max} R_s Q_{\max}^*.$$

□

For $\lambda_{\max} : K(H)^{sa} \to \mathbb{R}$, it can be defined the subdifferential at $A \in K(H)^{sa}$, using (3.9), as

$$\partial\lambda_{\max}(A) = \{Y \in B_1(H)^{sa} : \lambda_{\max}(B) - \lambda_{\max}(A) \geqslant \text{Re tr}(Y(B-A)), \forall\, B \in K(H)^{sa}\}, \tag{3.23}$$

In the next result, we obtain more useful expressions of $\partial\lambda_{\max}$.

Proposition 3.12. *If $A \in K(H)^{sa}$, $\lambda_{max}(A)$ has multiplicity $s \geqslant 1$ and $\mathcal{D}_{S_{\max}}$ is as in (3.20), then the subdifferential of $\lambda_{\max}(A)$ is the set*

$$\begin{aligned} \partial\lambda_{\max}(A) &= \mathcal{D}_{S_{\max}} \\ &= \{Y \in B_1(H)^{sa} : Y \geqslant 0, E_+Y = YE_+,\ tr(Y) = 1\}, \end{aligned} \tag{3.24}$$

where E_+ is the orthogonal projection onto the eigenspace of $\lambda_{\max}(A)$. In particular, if $\lambda_{\max}(A) \neq 0$, then

$$\partial\lambda_{\max}(A) = \{Q_{\max} R_s Q^*_{\max} : R_s \in M_s^{sa}(\mathbb{C}), R_s \geqslant 0, tr(R_s) = 1\}, \tag{3.25}$$

where the columns of $Q_{\max}$ form an orthonormal basis of eigenvectors for $\lambda_{\max}$.

Proof. As a consequence of (3.18), the subdifferential of $\lambda_{\max}$ at A can be expressed as

$$\partial\lambda_{\max}(A) = \text{co}\{qq^* : Aq = \lambda_{\max}(A)q \text{ and } \|q\| = 1\}.$$

Then the formulations of $\partial\lambda_{\max}(A)$ in (3.24) and (3.25) follow directly from (3.21) and (3.22), respectively.

□

Definition 3.13. Let $\mathcal{X}$ and $\mathcal{Y}$ be Banach spaces. A function $F : \mathcal{X} \to \mathcal{Y}$ is strictly differentiable at $x \in \mathcal{X}$ if there exists a continuous linear operator from $\mathcal{X}$ to $\mathcal{Y}$, denoted by $D_sF(x)$, such that

$$\lim_{x' \to x, t \to 0^+} \frac{F(x' + tv) - F(x')}{t} = \text{Re tr}\left(D_sF(x), v\right), \tag{3.26}$$

for every $v \in \mathcal{X}$. The operator $D_sF(x)$ is the strict differential of F at x.

Lemma 3.14. *Let $c_0(\mathbb{R}) = c_0$ be the space of real sequences that converge to 0 and*

$$A(x) = A_0 + \text{Diag}(x) = A_0 + \sum_{k \in \mathbb{N}} x_k e_k e_k^* \tag{3.27}$$

be an affine function with $A_0 \in K(H)^{sa}$ fixed and $x \in c_0$.

1. *For every k,*

$$\frac{\partial A}{\partial x_k}(x) = e_k e_k^*.$$

and $A(\cdot)$ is a smooth function

2. $A : c_0 \to K(H)^{sa}$ *is strictly differentiable at* x *and*

$$D_s A(x) = \sum_{j\in\mathbb{N}} x_k e_k e_k^* = Diag(x) \in D(K(H)^{sa}),$$

where $D_s A$ *is the map defined in* (3.26).

3. $D_s A : c_0 \to K(H)^{sa}$ *satisfies that its adjoint* $D_s A^* : K(H)^{sa} \to c_0$*, is*

$$D_s A(C) = \mathrm{Diag}(C) = \mathrm{Diag}\left(\{\langle Ce_i, e_i\rangle\}_{i\in\mathbb{N}}\right), \ \textit{for every } C \in K(H)^{sa}.$$

Proof. The proof of item 1 is direct, since each partial derivative of A is a constant function. Then, for every $x \in c_0$ the differential $D_s A$ is

$$D_s A(x) = \sum_{j\in\mathbb{N}} x_k e_k e_k^* = \mathrm{Diag}\,(x) \in D(K(H)^{sa}).$$

Additionally, if A is a smooth function, then it is strictly differentiable ([9], p. 32) and $D_s A(x)$ is the strict derivative of A at x. The adjoint $D_s A^* : K(H)^{sa} \to c_0$ fulfills

$$D_s A^*(C)x = \mathrm{Re}\ \mathrm{tr}(C^* D_s A(x)),\ \forall\ C \in K(H)^{sa},\ \forall\ x \in c_0.$$

Then, for each $E_{ij} = e_i e_j^*$

$$D_s A^*(E_{ij})x = \mathrm{Re}\ \mathrm{tr}(E_{ij} D_s A(x)) = \mathrm{Diag}(x),$$

and for every $C \in K(H)^{sa}$ and e_i

$$D_s A^*(C)e_i = \mathrm{Re}\ \mathrm{tr}(C D_s A(e_i)) = C_{ii}.$$

Basically, $D_s A^*$ is the pinching operator, which extracts the main diagonal of every $C \in K(H)^{sa}$ (with respect to the orthonormal prefixed basis $\{e_i\}_{i\in\mathbb{N}}$ of H), that is

$$D_s A^*(C) = \mathrm{Diag}(C) = \mathrm{Diag}\left(\{\langle Ce_i, e_i\rangle\}_{i\in\mathbb{N}}\right).$$

□

We are now in position to state one of the main results of this subsection.

Theorem 3.15. *Let* $\lambda_{\max} : K(H)^{sa} \to \mathbb{R}$ *and* $A : c_0 \to \mathbb{R}$ *be the functions defined in* (3.16) *and* (3.27)*, respectively. Consider the composition map* $\lambda_{\max} \circ A : c_0 \to \mathbb{R}$*, given by* $\lambda_{\max} \circ A(x) = \lambda_{\max}(A(x))$*. Let* s *be the multiplicity of* $\lambda_{\max}(A(x))$ *and* $S_{\max}$ *the eigenspace of* $\lambda_{\max}(A(x))$*.*

Then, the subdifferential of $\lambda_{\max}(A(x))$ *at* $x \in c_0$ *is*

$$\begin{aligned} \partial\big(\lambda_{\max}(A(x))\big) &= \mathrm{Diag}\left(\mathcal{D}_{S_{\max}}\right) \\ &= \mathrm{Diag}(\partial\lambda_{\max}(A(x))) \\ &= m_{S_{\max}}, \end{aligned} \tag{3.28}$$

where $m_{S_{\max}}$ *is the moment of the eigenspace* $S_{\max}$ *(see* (3.1)*).*

In particular, if $\lambda_{\max}(A(x)) \neq 0$

$$\partial\big(\lambda_{\max}(A(x))\big) = \operatorname{Diag}\left(\{Q_{\max}(x) R_s Q_{\max}(x)^* : R_s \in M_s^{sa}(\mathbb{C}), R_s \geqslant 0, tr(R_s) = 1\}\right), \tag{3.29}$$

where the columns of $Q_{\max}(x)$ *form an orthonormal set of eigenvectors for* $\lambda_{\max}(A(x))$.

Proof. Let $x \in c_0$. As it was proved in Lemma 3.14, $A(x)$ is a smooth function and, particularly, strictly differentiable at x. Furthermore, by Proposition 3.11, $\lambda_{\max}$ is convex, Lipschitz near $A(x)$ and regular (in the sense of Definition 3.10). Therefore, by Theorem 2.3.10 (Chain rule) and Remark 2.3.11 in [9],

$$\partial\big(\lambda_{\max}(A(x))\big) = \partial\left(\lambda_{\max} \circ A\right)(x) = DA^* \partial \lambda_{\max}(A(x)),$$

where DA^* is the adjoint of DA. By Lemma 3.14, $DA^* : K(H)^{sa} \to c_0$ fulfills that

$$DA^*(C) = \operatorname{Diag}(C) = \operatorname{Diag}\left(\{\langle Ce_i, e_i\rangle\}_{i \in \mathbb{N}}\right).$$

By (3.24),

$$\partial \lambda_{\max}(A(x)) = \mathcal{D}_{S_{\max}} = \{Y(x) \in B_1(H)^{sa} : Y(x) \geqslant 0, E_+ Y(x) = Y(x) E_+,\ \operatorname{tr}(Y(x)) = 1\},$$

Combining the above,

$$\partial\big(\lambda_{\max}(A(x))\big) = \operatorname{Diag}\left(\partial \lambda_{\max}(A(x))\right) = \operatorname{Diag}\left(\mathcal{D}_{S_{\max}}\right) = m_{S_{\max}},$$

where the last equality is due to Proposition 3.1.

On the other hand, if $\lambda_{\max}(A(x)) \neq 0$, by (3.25)

$$\partial \lambda_{\max}(A(x)) = \{Q_{\max}(x) R_s Q_{\max}(x)^* : R_s \in M_s^{sa}(\mathbb{C}), R_s \geqslant 0, \operatorname{tr}(R_s) = 1\},$$

where s is the multiplicity of $\lambda_{\max}(A(x))$, and the columns of $Q_{\max}(x)$ form an orthonormal set of eigenvectors for $\lambda_{\max}(x)$. In this case, we obtain the following equality

$$\partial\big(\lambda_{\max}(A(x))\big) = DA^* \partial \lambda_{\max}(A(x)) = \operatorname{Diag}\{Q_{\max} R_s Q_{\max}^* : R_s \in M_s^{sa}(\mathbb{C}), R_s \geqslant 0, \operatorname{tr}(R_s) = 1\}.$$

□

Corollary 3.16. *Under the assumptions of Theorem 3.15, the following formula holds*

$$\partial \lambda_{\max}(x) = \{v \in c_0 : v_k = tr\left(R_s Q_{\max}(x)^* e_k e_k^* Q_{\max}(x)\right), \forall k \in \mathbb{N}\}.$$

Proof. By the mentioned Theorem and its proof, any $v \in \partial \lambda_{\max}(x)$

$$v = \operatorname{Diag}(Q_{\max}(x) R_s Q_{\max}(x)^*),$$

where $R_s \in M_s^{sa}(\mathbb{C})$, $R_s \geqslant 0$, $\operatorname{tr}(R_s) = 1$ and the columns of $Q_{\max}(x)$ form an orthonormal set of eigenvectors for $\lambda_{\max}(x)$. Then, the coordinates of v are

$$v_k = (Q_{\max}(x) R_s Q_{\max}(x)^*)_{kk} = \operatorname{tr}\left(Q_{\max}(x) R_s Q_{\max}(x)^* e_k e_k^*\right) = \operatorname{tr}\left(R_s Q_{\max}(x)^* e_k e_k^* Q_{\max}(x)\right).$$

for every $k \in \mathbb{N}$. □

Recently, in [21], the author gave the following explicit expression for the subdifferential of the operator norm of $A \in B(H)$ such that $\operatorname{dist}(A, K(H)) < \|A\|$,

$$\partial\|A\| = \overline{\text{co}}\ \{uv^* : u, v \in H, Au = \|A\|v \text{ and } \|u\| = \|v\| = 1\}, \tag{3.30}$$

where the closure of the convex hull $\overline{\text{co}}$ is in the operator norm.

When $A(x)$ is compact self-adjoint but not semi-definite, we obtain analogous results as Lemma 3.6 and Remark 3.7, since $\lambda_{\max}(A(x))$ and $\lambda_{\min}(A(x))$ are real eigenvalues of $A(x)$ with finite multiplicity. We compile these facts in the next proposition and we omit the proof, which is similar to the matricial case (see Lemma 3.6 and Remark 3.7).

Proposition 3.17. *Let $A(x) = A_0 + \operatorname{Diag}(x)$, with $A_0 \in K(H)^{sa}$ and $x \in c_0$, be such that $A(x)$ is such that $\lambda_{min}(A(x)) < 0 < \lambda_{max}(A(x))$. Then the following properties hold.*

1. *If $\lambda_{min}(A(x))$ is the minimum eigenvalue of $A(x)$ and S_{min} its corresponding eigenspace, then*

$$\partial\big(\lambda_{min}(A(x))\big) = \partial\lambda_{min}(x) = -m_{S_{min}}. \tag{3.31}$$

2. *The equivalent expression of equation (3.30) in this case is*

$$\partial\left(\|A(x)\|\right) = co\{uu^* : A(x)u = \|A(x)\|u \text{ and } \|u\| = 1\}. \tag{3.32}$$

3. *Considering (3.31) and (3.32), it is evident that*

$$\partial\big(\|A(x)\|\big) = \begin{cases} \partial\lambda_{\max}(A(x)) & \text{if } \ \|A(x)\| = \lambda_{\max}(A(x)) \\ \partial\lambda_{min}(A(x)) & \text{if } \ \|A(x)\| = -\lambda_{min}(A(x)) = |\lambda_{min}(A(x))| \\ \operatorname{co}\big(\partial\lambda_{\max}(A(x)) \cup \partial\lambda_{min}(A(x))\big) & \text{if } \ \|A(x)\| = -\lambda_{min}(A(x)) = \lambda_{\max}(A(x)). \end{cases}$$

Proposition 3.18. *Let $K \in K(H)^{sa}$ be such that $K \leqslant 0$, with $\dim(ker(K)) = \infty$ and $Y, Z \in B_1(H)$ that satisfy $YP_{S_{\lambda_{\min}(K)}} = Y$, $ZP_{\ker(K)} = Z$, $Y \geqslant 0$, $Z \geqslant 0$, $tr(Y) = tr(Z) = 1$ and $\operatorname{Diag}(Y) = \operatorname{Diag}(Z)$. Then $A = K + \frac{\|K\|}{2}I$ is a minimal operator.*

Proof. Observe that $K \leqslant 0$ implies that $-\lambda_{min}(K) = |\lambda_{min}(K)| = \|K\|$ and hence $S_{\lambda_{min}(K)} = S_{-\|K\|}$.

Now consider the spectral projection $P_{\lambda_{min}(K)} = P_{\|K\|}$ on the eigenspace $S_{\lambda_{min}(K)} = S_{-\|K\|}$ corresponding to the eigenvalue $\lambda_{min}(K) = \|K\|$ and the orthogonal projection onto the kernel of K denoted by $P_{\ker(K)}$. Note that then $A = -\|K\|P_{-\|K\|} + R + \frac{\|K\|}{2}I$ with R orthogonal to $P_{-\|K\|}$. Hence we can obtain the following equalities

$$\begin{aligned} \operatorname{tr}(YA) &= \operatorname{tr}\left(Y\left(K + \frac{\|K\|}{2}I\right)\right) = \operatorname{tr}\left(YP_{-\|K\|}K + \frac{\|k\|}{2}Y\right) = \operatorname{tr}\left(-\|K\|Y + \frac{\|k\|}{2}Y\right) \\ &= \operatorname{tr}\left(\frac{-\|k\|}{2}Y\right) = -\frac{\|K\|}{2}, \end{aligned} \tag{3.33}$$

$$\mathrm{tr}(ZA) = \mathrm{tr}\left(ZK + \frac{\|K\|}{2}Z\right) = \mathrm{tr}\left(ZP_{\ker(K)}K + \frac{\|k\|}{2}Z\right) = \mathrm{tr}\left(0 + \frac{\|k\|}{2}Z\right) \underset{(3.34)}{=} \frac{\|K\|}{2}.$$

Now consider $X = \frac{Z-Y}{2} \in B_1(H)$ with null diagonal, and define ψ in the dual of $B(H)$ as $\psi(W) = \mathrm{tr}(XW)$. Then ψ satisfies

- $\psi(XD) = 0$ for every diagonal operator D since $\mathrm{Diag}(X) = 0$,
- $\psi(A) = \frac{1}{2}\mathrm{tr}\left(ZK + \frac{\|K\|}{2}Z\right) - \frac{1}{2}\mathrm{tr}\left(YK + \frac{\|K\|}{2}Y\right) = \frac{1}{2}\left(\frac{\|K\|}{2} - \left(-\frac{\|K\|}{2}\right)\right) = \frac{\|K\|}{2} = \|A\|$, where we have used (3.33) and (3.34), and
- $$\begin{aligned}\|X\|_1 = \mathrm{tr}(|X|) = \mathrm{tr}\left(\left|\frac{Z-Y}{2}\right|\right) &= \frac{1}{2}\mathrm{tr}\left((Z^2 - YZ - ZY + Y^2)^{1/2}\right)\\ &= \frac{1}{2}\mathrm{tr}\left((Z^2+Y^2)^{1/2}\right) = \frac{1}{2}\mathrm{tr}(Z+Y) = 1\end{aligned}$$
  where we have used that Y and Z act on orthogonal subspaces.

This proves that ψ is a witness of the minimality of A with respect to the diagonal operators, and hence A is minimal (see Section 5 and in particular Proposition 5.1 of [20] and Remark 9 of [7]). ☐

Example 3.19. We describe here a concrete case where Proposition 3.18 can be applied. Given $h \in H$, $\|h\| = 1$, consider the rank one and hence compact operator $K = -hh^\star \leqslant 0$ with $|h_j|^2 \leqslant \frac{1}{2}$ and $h_j \neq 0$ for all $j \in \mathbb{N}$. Then $A = K + \frac{1}{2}I$ is minimal as can also be proved using Theorem 4.4(2) since A is minimal if and only if $-A$ is.

Now we can prove a similar result as that obtained in Theorem 3.8 for matrices.

Theorem 3.20. *Let $A(x) = A_0 + \mathrm{Diag}(x)$, with $A_0 \in K^{sa}(H)$ and $x \in c_0$ such that $\lambda_{\max}(A(x)) = -\lambda_{\min}(A(x))$. Then, the following statements are equivalent,*

(1) $0 \in \partial\big(\|A(x)\|\big)$.
(2) $0 \in \partial\lambda_{\max}(A(x)) + \partial\lambda_{\min}(A(x))$.
(3) $m_{S_{\max}} \cap m_{S_{\min}} \neq \varnothing$, *where $S_{\max}$ and $S_{\min}$ are the eigenspaces of $\lambda_{\max}(A(x))$ and $\lambda_{\min}(A(x))$, respectively.*
(4) $W\left(\{P_{S_{\max}} e_i e_i^* P_{S_{\max}}\}_{i=1}^{\infty}\right) \cap W\left(\{P_{S_{\min}} e_i e_i^* P_{S_{\min}}\}_{i=1}^{\infty}\right) \neq \{(0,\dots,0,\dots)\}$.
(5) *There exists $m \in \mathbb{N}$, concrete C^*-isomorphisms $U_{S_{\max}} : M_{\dim(S_{\max})} \to P_{S_{\max}} B(H) P_{S_{\max}}$ and $U_{S_{\min}} : M_{\dim(S_{\min})} \to P_{S_{\min}} B(H) P_{S_{\min}}$ (for example, as defined in Proposition 10 and subsection 5.1 of [6]), matrices $\{B_j\}_{j=1}^m \subset M^{sa}_{\dim(S_{\max})}(\mathbb{C})$ and $\{C_j\}_{j=1}^m \subset M^{sa}_{\dim(S_{\min})}(\mathbb{C})$ with $B_j = U^{-1}_{S_{\max}}(P_{S_{\max}} e_j e_j^* P_{S_{\max}})$, $C_j = U^{-1}_{S_{\min}}(P_{S_{\min}} e_j e_j^* P_{S_{\min}})$ such that*
$$W(\{B_j\}_{j=1}^m) \cap W(\{C_j\}_{j=1}^m) \neq \{(0,\dots,0)\}.$$
(6) *$A(x)$ is minimal.*

Proof. The equivalences (3) ⇔ (4) ⇔ (5) ⇔ (6) have already been proved in [6, Proposition 12 and Theorem 4].

(1)⇔(3) If $0 \in \partial\|A(x)\|$ and $\lambda_{\max}(A(x)) = -\lambda_{\min}(A(x))$, then using Proposition 3.17,

$$0 \in \operatorname{co}\left(\partial\lambda_{\max}(A(x)) \cup \partial\lambda_n(A(x))\right) = \operatorname{co}\left(m_{S_{\max}} \cup -m_{S_{\min}}\right)$$

and, with the same steps used on the proof of the (1)⇔(3) equivalence in Theorem 3.8, follows that $m_{S_{\max}} \cap m_{S_{\min}} \neq \emptyset$. The converse can be proved similarly.

To prove (2)⇔(3) we can use the formulas $\partial\lambda_{\max}(A(x)) = m_{S_{\max}}$ and $\partial\lambda_{\min}(A(x)) = -m_{S_{\min}}$ proved in Theorem 3.15 and Proposition 3.17. Then it is trivial that $m_{S_{\max}} \cap m_{S_{\min}} \neq \emptyset$ if and only if $0 \in m_{S_{\max}} - m_{S_{\min}} = \partial\lambda_{\max}(A(x)) + \partial\lambda_{\min}(A(x))$. □

Remark 3.21. Observe that item (5) of Theorem 3.20 allows the use of joint numerical ranges of finite self-adjoint matrices to decide the minimality of the compact operator.

4. Minimizing diagonals for rank one self-adjoint operators

Any rank-one self-adjoint (compact) operator $R \in B(H)^{sa}$ is a positive scalar multiple of an orthogonal projection $hh^* \in B(H)$ with $h \in H$ and $\|h\| = 1$. Then, D_0 is a minimizing diagonal of hh^* if and only if rD_0 is a minimizing diagonal of $rhh^* = R$. In this subsection we will describe explicitly diagonals $D_0 \in B(H)$ (in a fixed orthonormal basis $E = \{e_j\}_{j\in J}$ of H) such that $\|hh^* + D_0\| \leqslant \|hh^* + D\|$, for every diagonal (with respect to E) $D \in B(H)$. We will call them minimizing diagonals of hh^* in the E basis. We can suppose that $|h_j| > 0$, $\forall j$ and for numerable j, since otherwise we can work in a closed subspace of H. In this context $(h_1, h_2, \dots, h_n, \dots) \in H$, with h_j denotes the coordinates of h in the fixed orthogonal basis E. As mentioned, the results can be easily translated to general rank-one self-adjoint operators.

Let us consider $h \in H$ with $\|h\| = 1$ and the rank one projection $hh^* \in B(H)$. We will explicitly describe diagonals $D_0 \in B(H)$ (in a fixed orthonormal basis $E = \{e_j\}_{j\in J}$ of H) such that $\|hh^* + D_0\| \leqslant \|hh^* + D\|$, for every diagonal (with respect to E) $D \in B(H)$. We will call them minimizing diagonals of hh^* in the E basis. We can suppose that $|h_j| > 0$, $\forall j$ and for numerable j, since otherwise we can work in a closed subspace of H. In this context $(h_1, h_2, \dots, h_n, \dots) \in H$, with h_j denotes the coordinates of h in the fixed orthogonal basis E.

The following is a slight generalization of the sufficient part of [1, Theorem 2.2] and its proof follows the same idea.

Lemma 4.1. *Let $\mathcal{A}$ be a C^*-algebra, $\mathcal{B} \subset \mathcal{A}$ a C^*-subalgebra, H a Hilbert space and $\rho : \mathcal{A} \to B(H)$ a representation of $\mathcal{A}$, and there exists $\xi \in H$, $\|\xi\|_H^2 = 1$, $Z \in \mathcal{A}$ such that $\langle \rho(Z)\xi, \rho(D)\xi \rangle = 0$ $\forall D \in \mathcal{B}$, $\rho(Z^*Z)\xi = \|Z\|^2\xi$ then*

$$\|Z\| \leqslant \|Z + D\| \ , \forall D \in \mathcal{B}.$$

That is, Z is a minimal element with respect to $\mathcal{B}$.

Proof. Observe that for every $D \in \mathcal{B}$

$$\begin{aligned}\|Z+D\|^2 &\geqslant \langle \rho(Z+D)\xi, \rho(Z+D)\xi\rangle \\ &= \langle \rho(Z)\xi, \rho(Z)\xi\rangle + \langle \rho(Z)\xi, \rho(D)\xi\rangle + \langle \rho(D)\xi, \rho(Z)\xi\rangle + \langle \rho(D)\xi, \rho(D)\xi\rangle \\ &\geqslant \langle \rho(Z)\xi, \rho(Z)\xi\rangle = \langle \rho(Z)^*\rho(Z)\xi, \xi\rangle = \langle \rho(Z^*Z)\xi, \xi\rangle \\ &= \|Z\|^2\langle \xi, \xi\rangle = \|Z\|^2\end{aligned}$$

and therefore $\|Z\| \leqslant \|Z+D\| \forall D \in \mathcal{B}$. ☐

We include here a result adapted to our needs.

Lemma 4.2. *Let Z be an operator of $B(H)$, and $\xi \in B_2(H)$ (a Hilbert-Schmidt operator) with $tr(\xi^*\xi) = 1$ such that $Z^*Z\xi = \|Z\|^2\xi$, $tr(Z\xi(D\xi)^*) = tr(Z\xi\xi^*D^*) = 0$, $\forall D \in Diag(B(H))$ (the algebra of diagonal operators in a fixed basis), then*

$$\|Z\| \leqslant \|Z+D\|, \ \forall D \in Diag(B(H)).$$

Proof. The proof is also motivated in the previous lemma.

$$\begin{aligned}\|Z+D\| &\geqslant \operatorname{tr}\left((Z+D)\xi\left((Z+D)\xi\right)^*\right) = \operatorname{tr}(Z^*Z\xi\xi^* + Z\xi\xi^*D^* + D\xi\xi^*Z^* + D^*D\xi\xi^*) \\ &= \operatorname{tr}(Z^*Z\xi\xi^*) + 0 + 0 + \operatorname{tr}(D^2\xi\xi^*) \geqslant \operatorname{tr}(Z^*Z\xi\xi^*) = \operatorname{tr}(\|Z\|^2\xi\xi^*) = \|Z\|^2\operatorname{tr}(\xi\xi^*) = \|Z\|^2\end{aligned}$$

for all $D \in \operatorname{Diag}(B(H))$. ☐

The next result follows directly from [15, Theorem 9] and [5, Theorem 2]. We state it here for the sake of clarity.

Theorem 4.3. *Let $T \in B(H)^{sa}$ be described as an infinite matrix by $(T_{ij})_{i,j\in\mathbb{N}}$ in a fixed basis. Suppose that T satisfies that*

a) there exists $j_0 \in \mathbb{N}$ satisfying $T_{j_0,j_0} = 0$, with $T_{j_0,n} \neq 0$, for all $n \neq j_0$,

b) if $T^{(j_0)}$ is the operator T with zero in its j_0th-column and j_0th-row then

$$\|col_{j_0}(T)\| \geqslant \left\|T^{(j_0)}\right\|$$

(where $\|col_{j_0}(T)\|$ denotes the Hilbert norm of the j_0th-column of T), and

c) $\langle col_{j_0}(T), c_n(T)\rangle = 0$ for each $n \in \mathbb{N}$, $n \neq j_0$.

Then,

1. $\|T\| = \|col_{j_0}(T)\|$.
2. *T is minimal, that is*

$$\|T\| = \inf_{D\in\operatorname{Diag}(B(H)^{sa})} \|T+D\| = \inf_{D\in\operatorname{Diag}(K(H))} \|T+D\|,$$

and $D = \operatorname{Diag}\left(\{T_{nn}\}_{n\in\mathbb{N}}\right)$ is the unique bounded minimal diagonal operator for T.

Next, we introduce equivalent conditions for a rank one orthogonal projector in $B(H)$ to achieve minimality.

Theorem 4.4. *Let h be an element of H with $\|h\|_2 = 1$ and $h = (h_1, h_2, \dots, h_n, \dots)$ in a fixed basis E of H. Then,*

(1) if there exists j_0 such that $|h_{j_0}|^2 > 1/2$ then

$$hh^* - \operatorname{Diag}(1 - |h_{j_0}|^2, \dots, 1 - |h_{j_0}|^2, |h_{j_0}|^2, 1 - |h_{j_0}|^2, \dots) =$$

$$= hh^* + (|h_{j_0}|^2 - 1)I + (1 - 2|h_{j_0}|^2)\ e_{j_0} e_{j_0}^*$$

is a minimal matrix and is unique if $h_j \neq 0\ \forall j$.

(2) and if $|h_j|^2 \leqslant 1/2$ for every j then $D_0 = -\frac{1}{2}I$ is a minimizing diagonal for hh^*. Moreover, if $h_j \neq 0\ \forall j$, then this minimizing diagonal is unique (see also Corollary 4.6).

Proof. Recall that the diagonal of $hh^* \in H$ is $\operatorname{Diag}(hh^*) = \{|h_1|^2, |h_2|^2, \dots, |h_n|^2, \dots\}$ and hh^* is a trace class positive operator (a projection or rank one) with $\operatorname{tr}(hh^*) = \sum_{j\in\mathbb{N}} |h_j|^2 = 1$ and hence a Hilbert-Schmidt operator with $\|hh^*\|_2 = \operatorname{tr}(hh^*(hh^*)^*) = \operatorname{tr}(hh^*) = 1$. We would also consider that the indexes j belong to $\mathbb{N}$ although they could be finite in which case the proof is similar. We would also suppose that the coordinates $h_j \neq 0$ for all $j \in \mathbb{N}$ since otherwise the entire j-th row and column of hh^* must be null and we can reorder the basis and take those j away.

(1) We will use Theorem 4.3 to prove that under the hypothesis $|h_{j_0}|^2 > 1/2$ the infinite matrix

$$m = hh^* + (|h_{j_0}|^2 - 1)I + (1 - 2|h_{j_0}|^2)\ e_{j_0} e_{j_0}^*$$

is minimal. The diagonal of m is

$$\operatorname{Diag}(m) = (|h_1|^2 + |h_{j_0}|^2 - 1\ ,\ |h_2|^2 + |h_{j_0}|^2 - 1, \dots, \overbrace{\ 0\ }^{j_0}, |h_{j_0+1}|^2 + |h_{j_0}|^2 - 1, \dots).$$

Observe first that if $k \neq j_0$, since $\sum_j |h_j|^2 = 1$, then $m_{k,k} = |h_k|^2 + |h_{j_0}|^2 - 1 = -(1 - |h_k|^2 - |h_{j_0}|^2) = -\sum_{j\neq k, j_0} |h_j|^2$ and that $m_{j_0,j_0} = |h_{j_0}|^2 + (|h_{j_0}|^2 - 1) + (1 - 2|h_{j_0}|^2) = 0$. With these elements in the diagonal a direct computation shows that the columns $\operatorname{col}_k(m)$ and $\operatorname{col}_{j_0}(m)$ are orthogonal for $k \neq j_0$ (the elements of the diagonal were chosen for this purpose).

Now consider the rank one operator $p_h^{(j_0)} = h^{(j_0)}\left(h^{(j_0)}\right)^*$, where $h^{(j_0)}$ equals h except in the j_0 entry where there is a zero. Then its spectrum is $\sigma\left(p_h^{(j_0)}\right) = \{0, \|h^{(j_0)}\|^2\} = \{0, 1 - |h_{j_0}|^2\}$ and hence using functional calculus $\sigma\left(p_h^{(j_0)} + (|h_{j_0}|^2 - 1)I^{(j_0)}\right) = \{|h_{j_0}|^2 - 1, 0\}$, where $I^{(j_0)}$ is the identity matrix with a 0 in the j_0, j_0 entry. Hence, denoting with $\text{col}_{j_0}(m)$ the j_0-column of m, we have that

$$\begin{aligned}\|m^{(j_0)}\| = \left\|p_h^{(j_0)} + (|h_{j_0}|^2 - 1)I^{(j_0)}\right\| = 1 - |h_{j_0}|^2 = \sqrt{1-|h_{j_0}|^2}\sqrt{1-|h_{j_0}|^2} \\ \leqslant \sqrt{1-|h_{j_0}|^2}|h_{j_0}| = \|\text{col}_{j_0}(m)\| \qquad (4.1)\end{aligned}$$

where we used that $\sqrt{1-|h_{j_0}|^2} < |h_{j_0}| \Leftrightarrow 1/2 < |h_{j_0}|^2$ and that $\text{col}_{j_0}(m) = \overline{h_{j_0}} h^{(j_0)}$ then $\|\text{col}_{j_0}(m)\| = |h_{j_0}|\|h^{(j_0)}\| = |h_{j_0}|\sqrt{\sum_{j\neq j_0}|h_j|^2} = \sqrt{1-|h_{j_0}|^2}$. Therefore, considering that $\text{col}_k(m) \perp \text{col}_{j_0}(m)$ for $k \neq j_0$ and that $\|m^{(j_0)}\| \leqslant \|\text{col}_{j_0}(m)\|$ (see (4.1)) hold and Theorem 4.3 we can conclude that m is a minimal matrix. Hence $\text{Diag}(1-|h_{j_0}|^2, \dots, 1-|h_{j_0}|^2, |h_{j_0}|^2, 1-|h_{j_0}|^2, \dots)$ is the closest diagonal to hh^* if $h_j \neq 0$ for all j.

(2) This item could be proved using Proposition 3.18 but we include here a proof using other techniques regarding this special case. First we will show that there exists an element $k \in (\text{span}\{h\})^\perp \subset H$ such that $|h_j| = |k_j|$ $\forall j \in \mathbb{N}$. This can be done considering an infinite polygon in the $\mathbb{C}$ plane with sides $|h_j|^2$ that starts and ends in $(0,0)$. This can be constructed if and only if $|h_j|^2 \leqslant 1/2$, $\forall j \in \mathbb{N}$. Then define a collection of angles $-\pi/2 < \theta_j \leqslant \pi/2$, for $j \in \mathbb{N}$, of the corresponding sides of length $|h_j|^2$ with respect to the positive real axis required in order to obtain the mentioned closed polygon. With these notations we obtain that

$$\sum_{j\in\mathbb{N}} e^{i\theta_j}|h_j|^2 = 0$$

since the origin is where the polygon ends. Now, if $h_j = |h_j|e^{i\alpha_j}$, for $j \in \mathbb{N}$, we have that

$$0 = \sum_{j\in\mathbb{N}} e^{i\theta_j}|h_j|^2 = \sum_{j\in\mathbb{N}} e^{i\alpha_j}|h_j|e^{i(\theta_j-\alpha_j)}|h_j| = \langle h, k\rangle \qquad (4.2)$$

for $k = \sum_{j\in\mathbb{N}} |h_j|e^{-i(\theta_j-\alpha_j)}e_j$. Hence $k \in (\text{span}\{h\})^\perp$, satisfies that $|k_j| = |h_j|$ $\forall j \in \mathbb{N}$ and hence $\|k\|^2 = \sum_{j\in\mathbb{N}}|k_j|^2 = \sum_{j\in\mathbb{N}}|h_j|^2 = 1$.
Then hh^* is a rank one projector with eigenvectors h and k with corresponding eigenvalues 1 and 0 ($hh^*h = h$ and $hh^*k = h\langle k, h\rangle = 0$). Then the operator $Z = hh^* - \frac{1}{2}I$ has eigenvalues $\frac{1}{2}$ and $\frac{-1}{2}$ with corresponding eigenvectors h and k (where $I \in B(H)$ denotes the identity operator).
Now consider the operator $Z = hh^* - \frac{1}{2}I$. Observe that the diagonal of Z is $\left(|h_1|^2 - 1/2, |h_2|^2 - 1/2, \dots, |h_n|^2 - 1/2, \dots\right)$ in the fixed basis and that if we choose $\xi = \frac{1}{\sqrt{2}}(hh^* + kk^*)$ then $Z\xi = \frac{1}{2\sqrt{2}}(hh^* - kk^*)$ and $Z^*Z\xi = ZZ\xi = (\frac{1}{2})^2\frac{1}{\sqrt{2}}(hh^* + kk^*) = \|Z\|^2\xi$. Moreover, using that $Z\xi^2 = \frac{1}{4}(hh^* - kk^*)$ and that the diagonal of $hh^* - kk^*$ is null, follows that $\text{tr}(Z\xi(D\xi)^*) = \text{tr}(Z\xi^2D^*) = \frac{1}{4}\text{tr}((hh^* - kk^*)D^*) = 0$. Now we can apply Lemma 4.2 with our defined $Z = hh^* - \frac{1}{2}I$ and $\xi = \frac{1}{\sqrt{2}}(hh^* + kk^*)$ to prove that Z is a minimal operator with respect to $Diag(B(H))$.

□

Remark 4.5. Note that the minimizing diagonals for a rank one operator, as stated in Theorem 4.4, are bounded but not compact.

Next we show that the uniqueness of the minimizing diagonal fails if h has any zero coordinate.

Corollary 4.6. *Let $h \in H$ such that $|h_j| \leqslant 1/2$ for all $j \in \mathbb{N}$, and suppose that there exists $j_0 \in \mathbb{N}$ such that $h_{j_0} = 0$. Then, $hh^* \pm \frac{1}{2} e_{j_0} e_{j_0}^*$ are minimal operators.*

Proof. By item 2 of Theorem 4.4, $-\frac{1}{2} I$ is a minimizing diagonal for hh^* and $\|hh^* - \frac{1}{2} I\| = \frac{1}{2}$. Now consider $hh^* \pm \frac{1}{2} e_{j_0} e_{j_0}^*$, with h as in the hypothesis. Then,

$$\frac{1}{2} = \left\| \left(hh^* \pm \frac{1}{2} e_{j_0} e_{j_0}^* \right) e_{j_0} \right\| = \left\| C_{j_0} \left(hh^* \pm \frac{1}{2} e_{j_0} e_{j_0}^* \right) \right\| \leqslant \left\| hh^* \pm \frac{1}{2} e_{j_0} e_{j_0}^* \right\|$$

and for each $j \neq j_0$,

$$\left\| C_j \left(hh^* \pm \frac{1}{2} e_{j_0} e_{j_0}^* \right) \right\| = \sqrt{|h_j|^4 + \sum_{k \neq j} |h_j|^2 |h_k|^2} = \sqrt{|h_j|^4 + |h_j|^2 (1 - |h_j|^2)} = |h_j| \leqslant \frac{1}{2}.$$

Also, observe that

$$C_{j_0} \left(hh^* \pm \frac{1}{2} e_{j_0} e_{j_0}^* \right) \perp C_j \left(hh^* \pm \frac{1}{2} e_{j_0} e_{j_0}^* \right)$$

for every $j \neq j_0$. Then, by Corollary 6.3 in [4],

$$\left\| C_{j_0} (hh^* \pm \frac{1}{2} e_{j_0} e_{j_0}^*) \right\| = \left\| hh^* \pm \frac{1}{2} e_{j_0} e_{j_0}^* \right\| = \frac{1}{2} = \left\| hh^* - \frac{1}{2} I \right\|,$$

therefore $hh^* \pm \frac{1}{2} e_{j_0} e_{j_0}^*$ are minimal operators. □

The following is a related result with a different approach that provides conditions under which a diagonal matrix D is minimal related to a rank-one operator.

Lemma 4.7. *Let $h \in H$ such that $\|h\| = 1$ and $D \in D(B(H)^{sa})$. If there exists $j_0 \in \mathbb{N}$ such that*

1. $\|hh^* - D\| = \|(hh^* - D) e_{j_0}\| = \|C_{j_0}(hh^* - D)\|$.
2. $|h_{j_0}|^2 = D_{j_0, j_0}$.

Then, $hh^* - D$ is minimal with $C_j(hh^* - D) \perp C_{j_0}(hh^* - D)$ for every $j \neq j_0$.

Moreover, if $h_j \neq 0$ for all $j \in \mathbb{N}$, then D is the unique minimizing diagonal and its entries are defined as

$$D_{jj} = |h_j|^2 - \overline{h_j} h_{j_0} (1 - |h_j|^2), \text{ for every } j \neq j_0. \tag{4.3}$$

Proof. The minimality of $hh^* - D$ is a direct consequence of Lemma 6.1 in [4], since

$$(hh^* - D)_{j_0,j_0} = |h_{j_0}|^2 - D_{j_0,j_0} = 0.$$

Moreover, if $c_{j_0}(hh^* - D)_j = (hh^* - D)_{j,j_0} \neq 0$ for all $j \neq j_0$, then $hh^* - D$ has a unique minimizing diagonal defined by

$$(hh^* - D)_{j,j} = -\frac{\left\langle c_j(hh^* - D)_{\check{j}}, c_{j_0}(hh^* - D)_{\check{j}} \right\rangle}{(hh^* - D)_{j,j_0}}, \text{ for } j \neq j_0,$$

where $c_k(X)_{\check{l}} \in H \ominus \text{gen}\{e_l\}$ is the element obtained after taking off the l^{th} entry of $c_k(X) \in H$. Then, for $j \neq j_0$

$$\begin{aligned}
(hh^* - D)_{j,j} &= -\frac{\left\langle c_j(hh^* - D)_{\check{j}}, c_{j_0}(hh^* - D)_{\check{j}} \right\rangle}{(hh^* - D)_{j,j_0}} \\
|h_j|^2 - D_{jj} &= \sum_{i \neq j} |h_i|^2 \overline{h_j} h_{j_0} + \overline{h_j} h_{j_0} \left(|h_{i_0}|^2 - D_{i_0,i_0} \right) \\
|h_j|^2 - D_{jj} &= \sum_{i \neq j} |h_i|^2 \overline{h_j} h_{j_0} \\
D_{jj} &= |h_j|^2 - \sum_{i \neq j} |h_i|^2 \overline{h_j} h_{j_0} \\
D_{jj} &= |h_j|^2 - \overline{h_j} h_{j_0} (1 - |h_j|^2)
\end{aligned}$$

□

5. Funding

Partially supported by Grants CONICET (PIP 0525), ANPCyT (PICT 2015-1505 and 2017-0019).

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