UPPER BOUNDS ON VARIATION OF SPECTRAL SUBSPACES OF A HERMITIAN OPERATOR*

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*Based on joint works with S. Albeverio, V. Kostrykin, K. A. Makarov, and A. V. Selin

Outline

- Norm of an operator
- The abstract problem setup
  - *Maximal angle between subspaces*
  - *The questions we answer*
- Bounds on the shift of the spectrum (under off-diagonal perturbations)
- Review of known bounds on variation of spectral subspaces

We present rather general, abstract results that hold for operators on arbitrary Hilbert spaces. Surely, these results can be also applied to quantum-mechanical Hamiltonians.

Recalling of the operator norm definition

If V is a bounded linear operator on a Hilbert space $\mathfrak{H}$, its norm $\|V\|$ is given by

$$\|V\| = \sup_{\|f\|=1} \|Vf\| \qquad \text{(N.B.: } \sup = \text{least upper bound).}$$

For any $f \in \mathfrak{H}$ we have $\|Vf\| \leq \|V\| \|f\|$.

If V is a self-adjoint (i.e. Hermitian) operator on $\mathfrak{H}$, and

$$m_V = \min \operatorname{spec}(V) \text{ and } M_V = \max \operatorname{spec}(V),$$

then

$$\|V\| = \max\{|m_V|, |M_V|\}.$$

Example 1. $V = |\phi\rangle\kappa\langle\phi|$ with $\|\phi\| = 1$, $\kappa \in \mathbb{C} \Longrightarrow \|V\| = |\kappa|$.

Example 2. $\mathfrak{H} = L_2(\mathbb{R})$, $\quad (Vf)(x) = V(x)f(x)$ with $V(\cdot)$ a bounded function on $\mathbb{R}$. In this case $\|V\| = \sup\limits_{x\in\mathbb{R}} |V(x)|$.

The problem setup

Let A be a self-adjoint operator on a separable Hilbert space $\mathfrak{H}$. Assume that σ_0 is an isolated subset of $\mathrm{spec}(A)$, i.e.

$$d := \mathrm{dist}(\sigma_0, \sigma_1) > 0, \quad \text{where} \quad \sigma_1 = \mathrm{spec}(A) \setminus \sigma_0.$$

If V is a self-adjoint operator such that

$$\|V\| < \frac{d}{2} \qquad (*)$$

then the spectrum of the perturbed operator $L = A + V$ will also consist of two disjoint components ω_0 and ω_1:

$$\mathrm{spec}(L) = \omega_0 \cup \omega_1, \quad \omega_i = \mathrm{spec}(L) \cap \mathscr{O}_{\|V\|}(\sigma_i), \quad i = 0, 1.$$

Condition $(*)$ is sharp in the sense that, if $\|V\| > \frac{d}{2}$, the perturbed operator L may not have separated parts of the spectrum at all.

Assuming $(*)$, let

$$P = \mathsf{E}_A(\sigma_0) \text{ and } Q = \mathsf{E}_L(\omega_0),$$

the corresponding spectral projections of A and L.

For $P = \mathsf{E}_A(\sigma_0)$ and $Q = \mathsf{E}_L(\omega_0)$, we address the following question:

(i) Is it true that under the single spectral condition

$$\operatorname{dist}(\sigma_0, \sigma_1) = d > 0$$

the perturbation bound $\|V\| < d/2$ *necessarily implies*

$$\|P - Q\| < 1\,? \tag{$Q1$}$$

If not, then what is the best (largest) c *in*

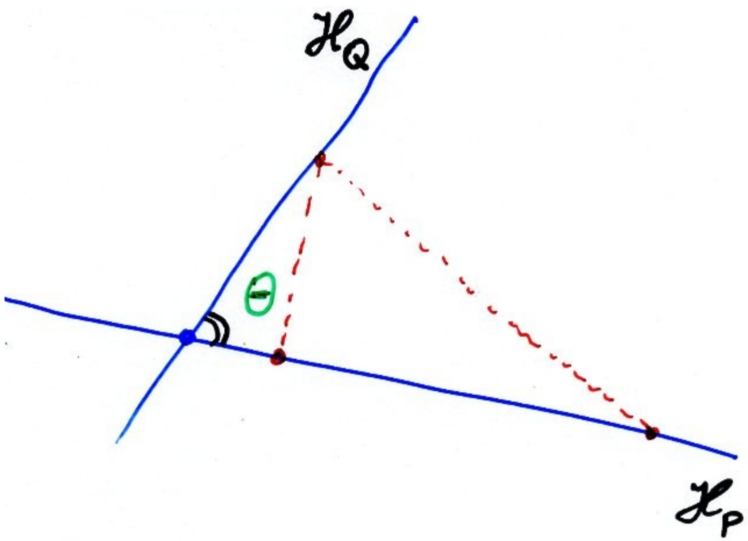
$$\|V\| < c\,d$$

ensuring $(Q1)$*?*

Geometrical interpretation. It is well known that

$$\|P-Q\| \leq 1$$

for any two orthogonal projections P and Q in the Hilbert space $\mathfrak{H}$.



Definition. Let $\mathcal{H}_P = \operatorname{Ran} P$ and $\mathcal{H}_Q = \operatorname{Ran} Q$. The quantity

$$\theta(\mathcal{H}_P, \mathcal{H}_Q) := \arcsin(\|P-Q\|)$$

is called the **maximal angle** between the subspaces $\mathcal{H}_P$ and $\mathcal{H}_Q$.

The concept of maximal angle is traced back at least to [Krein, Krasnoselsky, Milman (1948)]; [Dixmier (1949)].

Surely,

$$\|P-Q\| = \sin\big(\theta(\mathcal{H}_P, \mathcal{H}_Q)\big).$$

Definition. $\mathscr{H}_P$ and $\mathscr{H}_Q$ are in the **acute-angle case** if $\mathscr{H}_P \neq \{0\}$, $\mathscr{H}_Q \neq \{0\}$, and

$$\theta(\mathscr{H}_P, \mathscr{H}_Q) < \frac{\pi}{2}.$$

Thus, equivalent geometric formulation of the question (i):

Do the conditions $\operatorname{dist}(\sigma_0, \sigma_1) = d > 0$ *and* $\|V\| < d/2$ *always imply that the spectral subspaces of* A *and* L *associated with the respective unperturbed and perturbed spectral sets* σ_0 *and* ω_0 *are in the acute-angle case?*

Return to $P = \mathsf{E}_A(\sigma_0)$ and $Q = \mathsf{E}_L(\omega_0)$.

Provided $(Q1)$ is answered and, thus, it is established that $\|P - Q\| < 1$ holds, at least for

$$\|V\| < c\,d$$

with some constant $c < 1/2$, another important question arises:

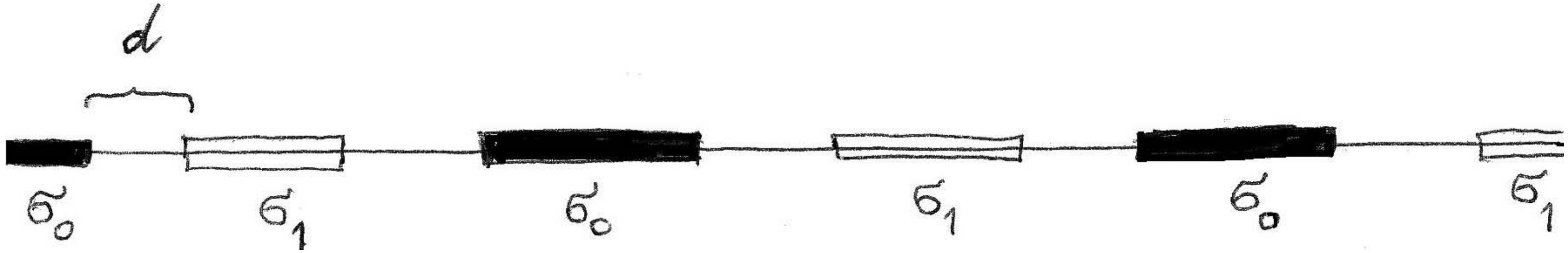
(ii) What function $M(x)$, $x \in [0, c)$, is best possible in the bound

$$\arcsin\big(\|P - Q\|\big) \le M\left(\frac{\|V\|}{d}\right) \text{ ?} \qquad (Q2)$$

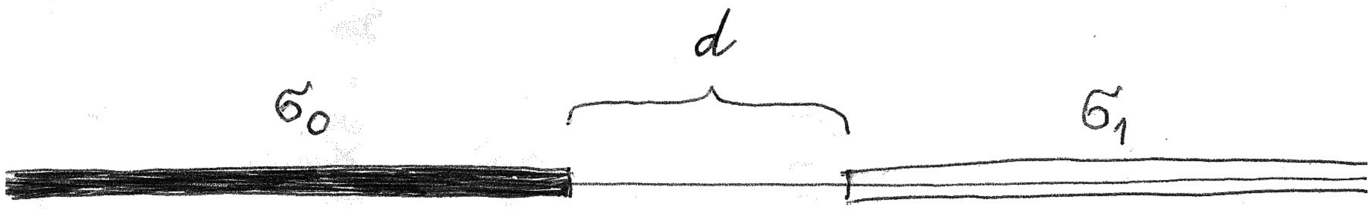
The estimating function M in $(Q2)$ is required to be universal in the sense that it should be the same for all self-adjoint A and V for which the conditions $\operatorname{dist}(\sigma_0, \sigma_1) = d > 0$ and $\|V\| < c\,d$ hold.

Under the assumption that $\mathrm{spec}(A) = \sigma_0 \cup \sigma_1$ ***and*** $\sigma_0 \cap \sigma_1 = \emptyset$ ***one distinguishes the following three cases*:**

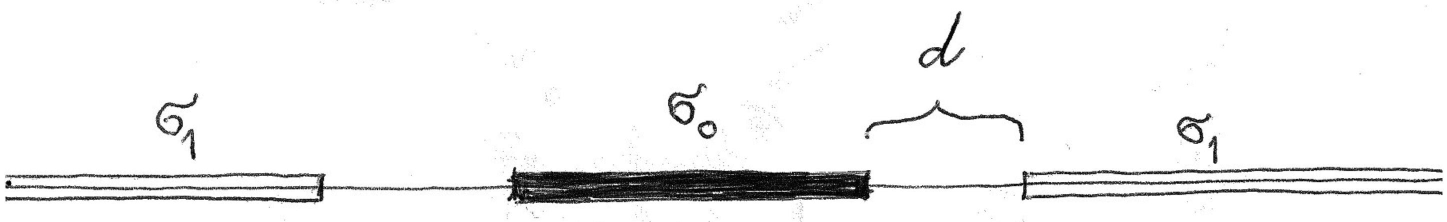
Generic case **(G)**: The only condition $\mathrm{dist}(\sigma_0, \sigma_1) = d > 0$.



Special case **(S1)**: σ_0 and σ_1 are subordinated, $\mathrm{conv}(\sigma_0) \cap \mathrm{conv}(\sigma_1) = \emptyset$.



Special case **(S2)**: One of the sets σ_0 and σ_1 lies in a finite gap of the other one, say $\mathrm{conv}(\sigma_0) \cap \sigma_1 = \emptyset$.



Known answers in the case of general s.a. perturbations

Recall, we assume $\mathrm{spec}(A) = \sigma_0 \cup \sigma_1$, $\mathrm{dist}(\sigma_0, \sigma_1) = d > 0$, $\|V\| < \frac{d}{2}$, $\omega_0 = \mathrm{spec}(L) \cap \mathscr{O}_{\|V\|}(\sigma_0)$, and $P = \mathsf{E}_A(\sigma_0)$, $Q = \mathsf{E}_L(\omega_0)$.

(S1 & S2) The best constant c is equal just to $1/2$. The optimal function M is

$$M(x) = \frac{1}{2}\arcsin(2x), \quad x \in [0, 1/2).$$

That is, for any s.a. V such that $\|V\| < d/2$ one has the (sharp) bound

$$\arcsin\|P - Q\| \le \frac{1}{2}\arcsin\frac{2\|V\|}{d} < \frac{\pi}{4}.$$

This is the essence of Davis-Kahan $\sin 2\theta$ Theorem, 1970.

(G) The subspaces $\mathrm{Ran}(P)$ and $\mathrm{Ran}(Q)$ are in the acute-angle case,

$$\|P-Q\|<1, \quad \text{provided} \quad \|V\|<c_{\mathrm{S}}\,d, \quad c_{\mathrm{S}}=0.454839\ldots$$

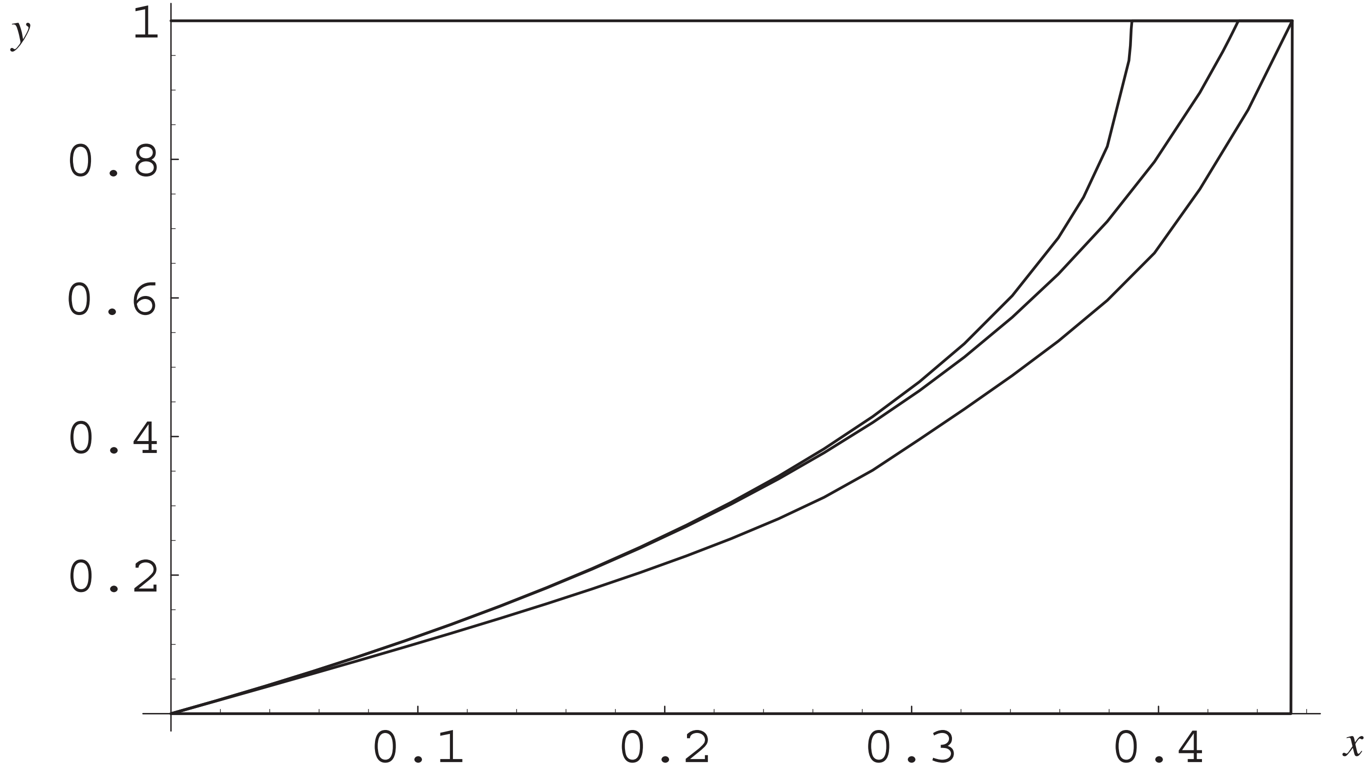
[*A. Seelmann (2013)*], based on [*S. Albeverio, A.K.M. (2011)*]; Seelmann also gives the best known expression for $M(x)$]

In particular, there is a new $\sin 2\theta$ bound

$$\arcsin\|P-Q\| \le \frac{1}{2}\arcsin\frac{\pi\|V\|}{d} < \frac{\pi}{4} \quad \text{if} \quad \|V\|<\frac{1}{\pi}d$$

[*S. Albeverio, A.K.M. (2011)*].

It remains the strongest known bound for $\|V\| \le \dfrac{4}{\pi^2+4}d$.



Graphs of the functions $\frac{2}{\pi}M_{\rm KMM}(x)$ [Kostrykin Makarov AKM, 2003], $\frac{2}{\pi}M_{\rm MS}(x)$ [Makarov Seelmann, 2010], $\frac{2}{\pi}M_{\rm AM}(x)$ [Albeverio AKM, 2011], and $\frac{2}{\pi}M_{\rm S}(x)$ [Seelmann, 2013]. The upper curve depicts the graph of $\frac{2}{\pi}M_{\rm KMM}(x)$, the intermediate curve is the graph of $\frac{2}{\pi}M_{\rm MS}(x)$, and the lower curve represents the graphs of both $\frac{2}{\pi}M_{\rm AM}(x)$ and $\frac{2}{\pi}M_{\rm S}(x)$ (indistinguishable in this picture).

Off-diagonal perturbations

Let $\mathfrak{H}_0 = \mathrm{Ran}(P) = \mathrm{Ran}(\mathsf{E}_A(\sigma_0))$ and $\mathfrak{H}_1 = \mathrm{Ran}(P^\perp) = \mathrm{Ran}(\mathsf{E}_A(\sigma_1))$.

One can decompose any bounded V into the sum $V = V_{\mathrm{diag}} + V_{\mathrm{off}}$ of the diagonal and off-diagonal (w.r.t. $\mathfrak{H} = \mathfrak{H}_0 \oplus \mathfrak{H}_1$) parts

$$V_{\mathrm{diag}} = \begin{pmatrix} PV\big|_{\mathfrak{H}_0} & 0 \\ 0 & P^\perp V\big|_{\mathfrak{H}_1} \end{pmatrix} \quad \text{and} \quad V_{\mathrm{off}} = \begin{pmatrix} 0 & PV\big|_{\mathfrak{H}_1} \\ P^\perp V\big|_{\mathfrak{H}_0} & 0 \end{pmatrix},$$

The subspaces $\mathfrak{H}_0$ and $\mathfrak{H}_1$ remain invariant under V_{diag} and, hence, under $A + V_{\mathrm{diag}}$. Therefore, for the diagonal perturbations the problem reduces to the perturbation of spectra only.

The action of the off-diagonal part V_{off} is completely nontrivial: it may change the spectrum and does change the spectral subspaces. Thus, the *core of the perturbation theory for invariant subspaces is in the study of their variation under off-diagonal perturbations*.

A 2×2 operator block matrix representation of A w.r.t. the decomposition $\mathfrak{H}=\mathfrak{H}_0\oplus\mathfrak{H}_1$:

$$A=\begin{pmatrix} A_0 & 0\\ 0 & A_1\end{pmatrix},\quad A_0=A\big|_{\mathfrak{H}_0},\quad A_1=A\big|_{\mathfrak{H}_1}.$$

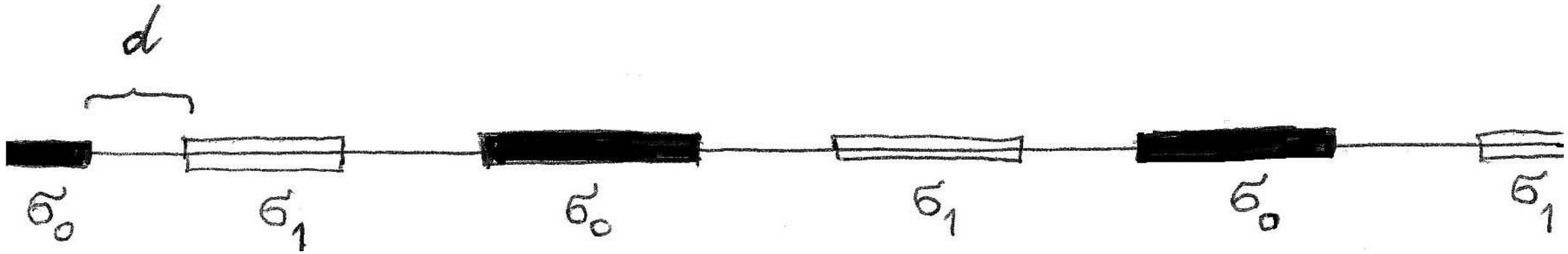
Now we focus on the problem of variation of the spectral subspaces under off-diagonal perturbations

$$V=\begin{pmatrix} 0 & B\\ B^* & 0\end{pmatrix}\qquad (\|V\|=\|B\|).$$

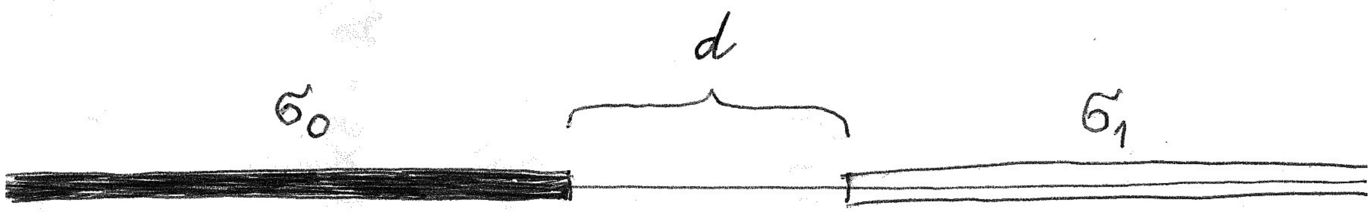
Perturbed operator:

$$L=A+V=\begin{pmatrix} A_0 & B\\ B^* & A_1\end{pmatrix}.$$

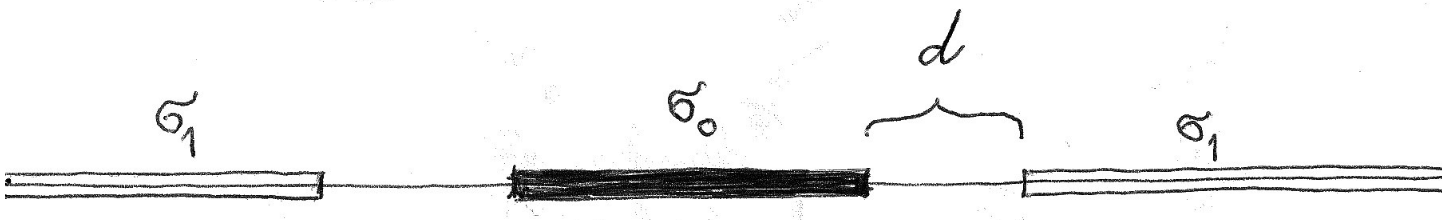
Generic case (**G**): The only condition $\mathrm{dist}(\sigma_0, \sigma_1) = d > 0$.



Special case (**S1**): σ_0 and σ_1 are subordinated, $\mathrm{conv}(\sigma_0) \cap \mathrm{conv}(\sigma_1) = \varnothing$.



Special case (**S2**): One of the sets σ_0 and σ_1 lies in a finite gap of the other one, say $\mathrm{conv}(\sigma_0) \cap \sigma_1 = \varnothing$.



Bounds on position of the perturbed spectrum

(G) [*V.Kostrykin, K.A.Makarov, A.K.M., 2007*, bounded A], [*C. Tretter, 2009*, unbounded A]:

$$\omega_i \subset O_{r_V}(\sigma_i), \quad i = 0, 1,$$

where $O_{r_V}(\sigma_i)$ denotes the closed r_V-neighborhood of σ_i with

$$r_V = \|V\| \tan\left(\frac{1}{2}\arctan\frac{2\|V\|}{d}\right) < \|V\|.$$

(S1) The gap between σ_0 and σ_1 remains in $\rho(A+V)$.

(S2) $\omega_0 \in O_{r_V}(\sigma_0)$. The gaps between $O_{r_V}(\sigma_0)$ and σ_1 remain in $\rho(A+V)$.

We ask the same questions (i) and (ii).

Known results for off-diagonal self-adjoint $V=\begin{pmatrix} 0 & B \\ B^* & 0 \end{pmatrix}$

(S1) For any $\|V\|$ the initial gap between σ_0 and σ_1 remains in $\rho(L)$. In this case $c_{\text{best}} = +\infty$ and $M(x) = \dfrac{1}{2}\arctan(2x)$. The sharp bound for the maximal angle:

$$\arcsin\|P-Q\| \le \frac{1}{2}\arctan\frac{2\|V\|}{d} \quad \left(<\frac{\pi}{4}\right).$$

(The Davis-Kahan $\tan 2\theta$ Theorem, 1970)

Estimates like that in $\tan 2\theta$ Theorem (but in terms of quadratic forms of A and V) have been obtained also for some unbounded V (see [A.K.M., A.V.Selin, IEOT **56** (2006), 511], [L. Grubišić, V. Kostrykin, K. A. Makarov, K. Veselić, J. Spectr. Theory **3** (2013), 83]).

(S2) [*V.Kostrykin, K.A.Makarov, A.K.M. (2005)*]: Gaps between σ_0 and σ_1 remain open whenever $\|V\| < \sqrt{2}d$ (sharp).

In this case also $c_{\text{best}} = \sqrt{2}$ in the answer to question (i), while $M(x) = \arctan x$. The sharp bound for the maximal angle reads:

$$\arcsin\|P - Q\| \leq \arctan\frac{\|V\|}{d}$$

[*S. Albeverio, A.V. Selin, A.K.M. (2006, 2012)*]

(for the final result see [S. Albeverio, A.K.M., IEOT **73** (2012), 413]).

(G) [*V.Kostrykin, K.A.Makarov, A.K.M. (2007)*]: Gaps between σ_0 and σ_1 remain open whenever $\|V\| < \frac{\sqrt{3}}{2} d$ (sharp); $\frac{\sqrt{3}}{2} = 0.866025\ldots$.

Thus, in an answer to the question ((i)) one necessarily has the following upper bound

$$c^* \le \frac{\sqrt{3}}{2}.$$

The latest published answer to the question (i):

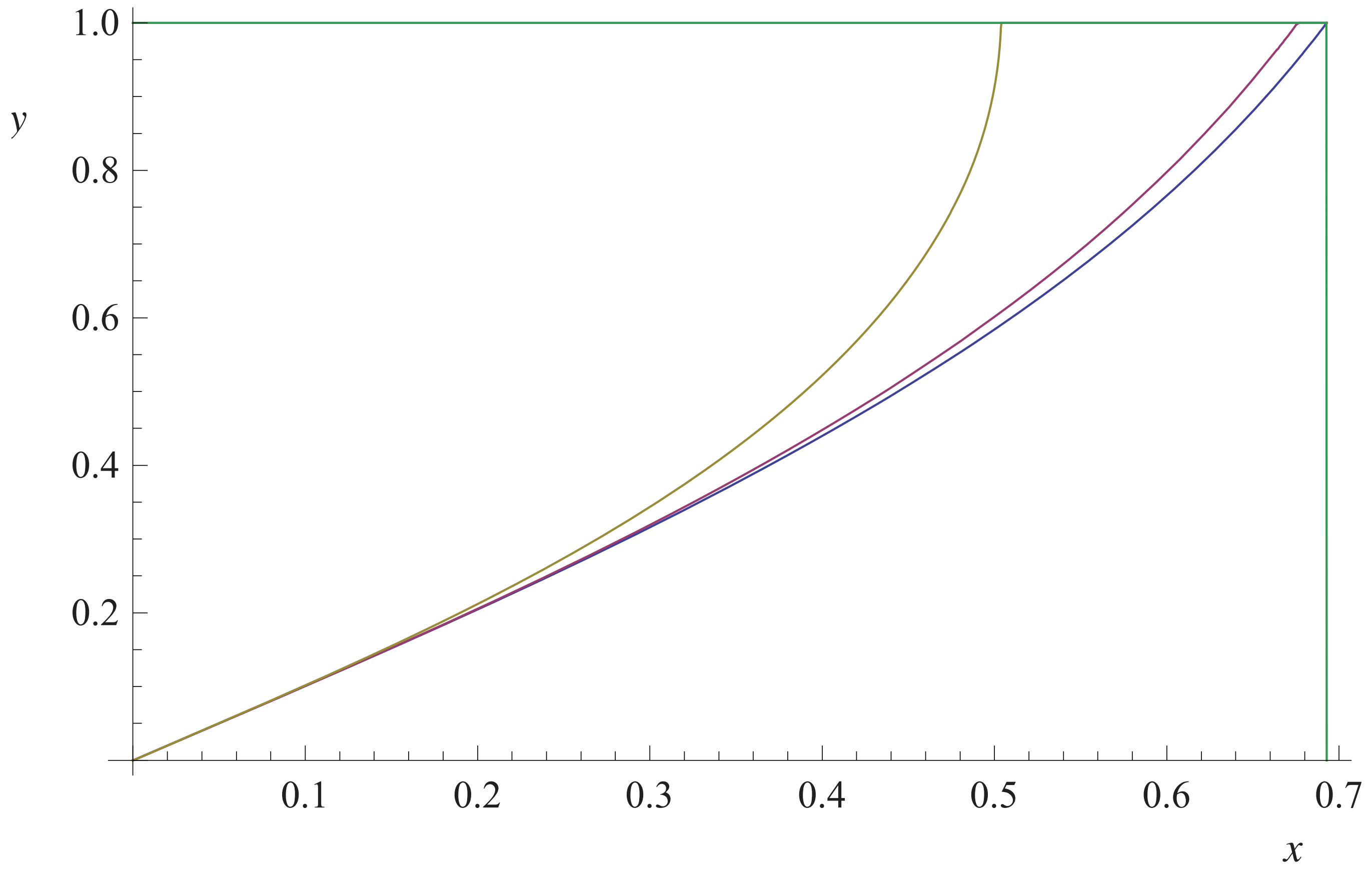
$$\|P - Q\| < 1 \quad \text{whenever} \quad \|V\| < c^* d, \quad c^* \ge 0.69407\ldots$$

[*A.Seelmann (2014)*]

The previous best published estimates for c^*:

$c^* \ge 0.6928\ldots$ [S. Albeverio, A.K.M. (2014)]
$c^* \ge 0.6759\ldots$ [K.A. Makarov, A. Seelmann (2010)]
$c^* \ge 0.5032\ldots$ [V.Kostrykin, K.A. Makarov, A.K.M. (2007)].

"Evolution" of the answer to question (ii) [on $M(x)$] in case of off-diagonal V.



Off-diagonal case. Graphs of the functions $\frac{2}{\pi}M_{\mathrm{KMM}}(x)$ [Kostrykin Makarov AKM, 2007], $\frac{2}{\pi}M_{\mathrm{MS}}(x)$ [Makarov Seelmann, 2010], and $\frac{2}{\pi}M_{\mathrm{AM}}(x)$ [Albeverio AKM, 2014]. The upper curve depicts the graph of $\frac{2}{\pi}M_{\mathrm{KMM}}(x)$, the intermediate curve is the graph of $\frac{2}{\pi}M_{\mathrm{MS}}(x)$, and the lower curve represents the graph of $\frac{2}{\pi}M_{\mathrm{AM}}(x)$.

Ideas of the proof

- Triangle inequality for the maximal angle between subspaces.

  Lemma [L.G.Brown, 1993] *Let $\mathfrak{P}$, $\mathfrak{Q}$, and $\mathfrak{R}$ be three arbitrary subspaces of the Hilbert space $\mathfrak{H}$. The following inequality holds:*

  $$\theta(\mathfrak{P},\mathfrak{Q}) \le \theta(\mathfrak{P},\mathfrak{R}) + \theta(\mathfrak{R},\mathfrak{Q}).$$

- Generic a priori $\sin 2\theta$ estimate for the maximal angle.

  Theorem [S.Albeverio, A.K.M., 2011]. *Assume for a self-adjoint A the spectral case (G). Suppose that V is s.a., off-diagonal, and $\|V\| < \frac{1}{\pi}d$. Then*

  $$\theta(\mathfrak{H}_0,\mathfrak{H}_0') \le \frac{1}{2}\arcsin\frac{\pi\|V\|}{d},$$

  where $d = \operatorname{dist}(\sigma_0,\sigma_1)$ and $\mathfrak{H}_0 = \operatorname{Ran}(\mathsf{E}_A(\sigma_0))$, $\mathfrak{H}_0' = \operatorname{Ran}(\mathsf{E}_{A+V}(\omega_0))$.

- Consider the consecutive operators $L_{t_i} = A + t_i V$, $i = 0, 1, \ldots, n$, $0 = t_0 < t_1 < t_2 < \ldots < t_n = 1$ and arrive at the optimization problem

$$\arcsin\big(\|P - Q\|\big) \le \frac{1}{2} \inf_{n,\,\{t_i\}_{i=0}^n} \sum_{j=0}^{n-1} \arcsin \frac{\pi(t_{j+1} - t_j)\|V\|}{\operatorname{dist}\big(\omega_0(t_j), \omega_1(t_j)\big)}, \qquad (M)$$

where t_i, $i = 1, 2, \ldots, n-1$, should be chosen such that

$$0 < \frac{(t_{j+1} - t_j)\|V\|}{\operatorname{dist}\big(\omega_0(t_j), \omega_1(t_j)\big)} \le \frac{1}{\pi}.$$

In case of generic (non-off-diagonal) V we have

$$\operatorname{dist}\big(\omega_0(t_j), \omega_1(t_j)\big) \ge d - 2\|V\|t_j. \qquad (d - gen)$$

If V is off-diagonal then

$$\operatorname{dist}\big(\omega_0(t_j), \omega_1(t_j)\big) \ge 2d - \sqrt{d^2 + 4t_j^2\|V\|^2}. \qquad (d - off)$$

For non-off-diagonal V, a first bound from above for the r.h.s. of (M) has been obtained in [S.Albeverio, A.K.M. 2011], with the help of $(d - gen)$. Complete optimization for the r.h.s. of (M) with $(d - gen)$ has been done in [A.Seelmann 2013].

In [Albeverio A.K.M., 2014] and [Seelmann, 2014] the bound $(d - off)$ has been employed.

Conclusions

- We have reviewed the best known norm bounds on rotation of spectral subspaces of a self-adjoint operator under a perturbation.
- The general results may be applied to quantum-mechanical (in particular, to few-body) Hamiltonians.
- The spectral shift and subspace variation bounds may be employed to verify the quality of numerical calculations. They may be used to give the corresponding upper estimates prior the actual calculations.