

BOUNDS ON THE SHIFTS OF BINDING ENERGIES
AND VARIATION OF THE SPECTRAL SUBSPACES
OF FEW-BODY HAMILTONIANS*

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First, we present rather general, **abstract results** that hold for operators on **arbitrary Hilbert spaces**.

Then we will turn to **quantum-mechanical** (in particular **few-body**) Hamiltonians.

We start with recalling one definition that is needed through the whole material.

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

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

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

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

then

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

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

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

The abstract problem setup

Let A be a **self-adjoint** operator on a Hilbert space \mathfrak{H} such that

$$\text{spec}(A) = \sigma_0 \cup \sigma_1, \quad \text{dist}(\sigma_0, \sigma_1) = d > 0.$$

The spectral subspaces of A :

$$\mathfrak{H}_0 = \text{Ran } E_A(\sigma_0), \quad \mathfrak{H}_1 = \text{Ran } E_A(\sigma_1).$$

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

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

We focus on the problem of **variation of the spectral subspaces under off-diagonal perturbations (i.e. potentials in the case)**

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

Comment: Why off-diagonal perturbations?

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

$$V_{\text{diag}} = \begin{pmatrix} P_0 V|_{\mathfrak{H}_0} & 0 \\ 0 & P_1 V|_{\mathfrak{H}_1} \end{pmatrix} \quad \text{and} \quad V_{\text{off}} = \begin{pmatrix} 0 & P_0 V|_{\mathfrak{H}_1} \\ P_1 V|_{\mathfrak{H}_0} & 0 \end{pmatrix},$$

where P_0 and P_1 are the orthogonal projections onto \mathfrak{H}_0 and \mathfrak{H}_1 , respectively, $P_0 = E_A(\sigma_0)$ and $P_1 = E_A(\sigma_1)$.

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

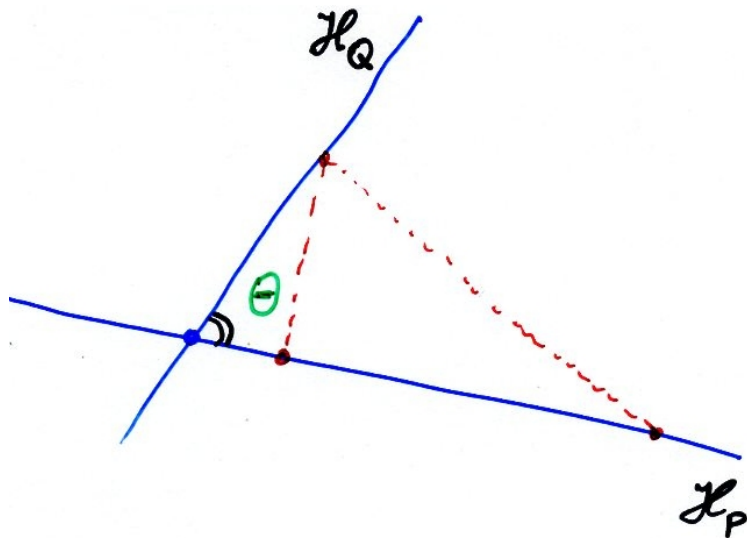
The action of the off-diagonal part V_{off} is completely nontrivial: it may change the spectrum and does change the spectral subspaces. Thus, the *core of the perturbation theory for invariant subspaces is in the study of their variation under off-diagonal perturbations.*

The bounds on variation of the spectral subspaces will be given in terms of the **maximal angle between two subspaces**.

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 $\mathcal{H}_P = \text{Ran } P$ and $\mathcal{H}_Q = \text{Ran } Q$. 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,

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

One is interested in the case where the “rotation angle” from an unperturbed spectral subspace to the perturbed one is acute (i.e. the maximal angle θ between them is smaller than 90°).

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

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

that is, if $\|P - Q\| < 1$.

MAIN QUESTIONS:

- (i) What is an **optimal** requirement on $\|V\|$ ($= \|B\|$) that guarantees that V does not close the gaps between σ_0 and σ_1 (and, thus, $\text{dist}(\sigma'_0, \sigma'_1) > 0$)?
- (ii) What then can be said about **variation of the spectral subspace**, say, \mathfrak{H}_0 : Is it then true that the unperturbed and perturbed spectral subspaces \mathfrak{H}_0 and \mathfrak{H}'_0 are in the acute-angle case, i.e.

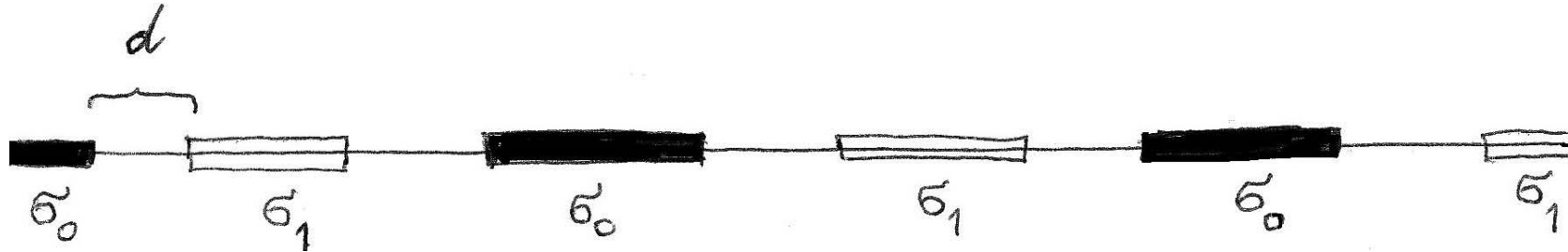
$$\theta(\mathfrak{H}_0, \mathfrak{H}'_0) < \frac{\pi}{2} ?$$

And what is a **(sharp) bound** on $\theta := \theta(\mathfrak{H}_0, \mathfrak{H}'_0)$ in terms of $\|V\|$ and $d = \text{dist}(\sigma_0, \sigma_1)$?

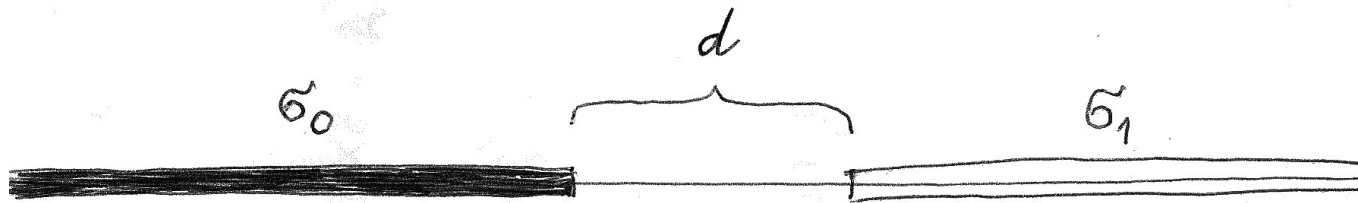
Recall, $\theta(\mathfrak{H}_0, \mathfrak{H}'_0)$ stands for the maximal angle between the unperturbed and perturbed spectral subspaces $\mathfrak{H}_0 = \text{Ran } E_A(\sigma_0)$ and $\mathfrak{H}'_0 = \text{Ran } E_{A+V}(\sigma'_0)$.

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

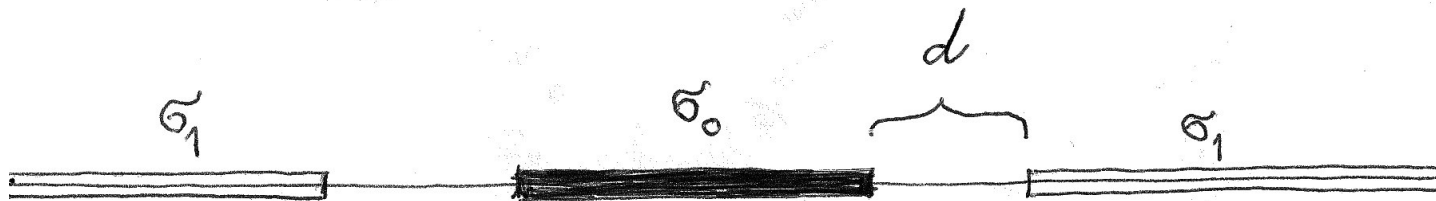
Generic case (G): The only condition $\text{dist}(\sigma_0, \sigma_1) = d > 0$.



Special case (S2): σ_0 and σ_1 are subordinated, $\text{conv}(\sigma_0) \cap \text{conv}(\sigma_1) = \emptyset$.



Special case (S3): One of the sets σ_0 and σ_1 lies in a finite gap of the other one, say $\text{conv}(\sigma_0) \cap \sigma_1 = \emptyset$.



Review of the results for self-adjoint $V = \begin{pmatrix} 0 & B \\ B^* & 0 \end{pmatrix}$

(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); $\frac{\sqrt{3}}{2} = 0.866025\dots$

$$\theta < \frac{\pi}{2} \quad \text{whenever} \quad \|V\| < c_{\text{MS}} d, \quad c_{\text{MS}} = 0.675989\dots$$

[*K.A. Makarov, A. Seelmann (2010)*]

(S2) For any $\|V\|$ the initial gap between σ_0 and σ_1 remains in $\rho(L)$.
The sharp bound for θ :

$$\tan 2\theta \leq \frac{2\|V\|}{d} \quad \Longleftrightarrow \quad \theta \leq \frac{1}{2} \arctan \frac{2\|V\|}{d} \quad \left(< \frac{\pi}{4} \right).$$

(The *Davis-Kahan tan2θ Theorem, 1970*)

(S3) [*V.Kostrykin, K.A.Makarov, A.K.M. (2005)*]: Gaps between σ_0 and σ_1 remain open and $\theta < \frac{\pi}{2}$ whenever $\|V\| < \sqrt{2}d$ (sharp);

$$\tan \theta \leq \frac{\|V\|}{d} \quad [S. Albeverio, A.V. Selin, A.K.M. (2006, 2012)]$$

(see [*Integr. Equation Operator Theory 73 (2012), 413*]).

Bounds on position of the perturbed spectrum

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

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

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

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

(S2) The gap between σ_0 and σ_1 remains in $\rho(A + V)$.

(S3) $\sigma'_0 \in O_{r_V}(\sigma_0)$. The gaps between $O_{r_V}(\sigma_0)$ and σ_1 remain in $\rho(A + V)$.

Applications to Schrödinger operators (in particular to few-body Hamiltonians)

Let $A = H_0 + V_0$ be the Schrödinger operator with H_0 the kinetic energy and V_0 the "main" potential (combining, say, two-body forces). Let V be an additional interaction (say, three-body forces), and

$$H = A + V.$$

1. Suppose that E_0 is the g.s. energy (simple eigenvalue) of A , and ψ_0 the g.s. wave function, $A\psi_0 = E_0\psi_0$ ($\|\psi_0\| = 1$).

Set $\text{spec}(A) = \sigma_0 \cup \sigma_1$ with $\sigma_0 = \{E_0\}$ and $\sigma_1 = \text{spec}(A) \setminus \{E_0\}$ ($\neq \emptyset$).

If $2\|V\| < d := \text{dist}(E_0, \sigma_1)$ then there is g.s. (E'_0, ψ'_0) for H ,

$$H\psi'_0 = E'_0\psi'_0.$$

We claim that $|\langle \psi'_0, \psi_0 \rangle| = \cos \theta$ with $\theta < \pi/4$ such that

$$\sin 2\theta \leq \frac{2\|V\|}{d}.$$

This is the consequence of the Davis-Kahan $\sin 2\theta$ Theorem (1970).

If, in addition, V is off-diagonal then, for **any arbitrary large** $\|V\|$, **NO** spectrum of H enters the gap between E_0 and σ_1 , and

$$|\langle \psi'_0, \psi_0 \rangle| = \cos \theta$$

with

$$\tan 2\theta \leq \frac{2\|V\|}{d}.$$

In particular, we have:

$$|\langle \psi'_0, \psi_0 \rangle|^2 \geq \frac{1}{2} \left(1 + \frac{d}{\sqrt{d^2 + 4\|V\|^2}} \right) \quad \left(> \frac{1}{2} \right)$$

(Probability of the system to remain in the initial ground state ψ_0 .)

Furthermore, necessarily

$$E'_0 \leq E_0$$

and

$$E_0 - E'_0 \leq \|V\| \tan \left(\frac{1}{2} \arctan \frac{2\|V\|}{d} \right) \quad (< \|V\|).$$

2. Suppose that

$$\sigma_0 = \{E_0, E_1, \dots, E_n\}$$

consists of the $n+1$ lowest eigenvalues of A and let $\sigma_1 = \text{spec}(A) \setminus \sigma_0$ be the remainder of the spectrum of A .

Denote by \mathfrak{H}_0 the spectral subspace of A associated with σ_0 , i.e. the linear span of the corresponding eigenvectors.

Assume that $2\|V\| < d := \text{dist}(\sigma_0, \sigma_1)$ and σ'_0 combines the eigenvalues of $H = A + V$ that stem from the eigenvalues of A contained in σ_0 .

Then

$$\theta \leq \frac{1}{2} \arcsin \frac{2\|V\|}{d} \quad \left(\implies \theta < \frac{\pi}{4} \right),$$

where, recall, $\theta := \theta(\mathfrak{H}_0, \mathfrak{H}'_0)$ is the maximal angle between \mathfrak{H}_0 and the spectral subspace of $H = A + V$ associated with σ'_0 .

If, in addition, V is off-diagonal, then, for **any arbitrary large** $\|V\|$, **NO** spectrum of H enters the gap between E_{n+1} ($= \max(\sigma_0)$) and σ_1 , and

$$\theta \leq \frac{1}{2} \arctan \frac{2\|V\|}{d}.$$

Moreover, necessarily

$$E'_0 \leq E_0$$

and

$$E_0 - E'_0 \leq \|V\| \tan \left(\frac{1}{2} \arctan \frac{2\|V\|}{d} \right) \quad (< \|V\|).$$

Estimates of such a kind (but in terms of quadratic forms of A and V) may be done even for some **unbounded** V (see [A.K.M., A.V.Selin, Integral Equations Operator Theory **56** (2006), 511], [L. Grubišić, V. Kostrykin, K. A. Makarov, K. Veselić, arXiv:1006.3190 (2010)]).

3. Suppose that

$$\sigma_0 = \{E_{n+1}, E_{n+2}, \dots, E_{n+k}\}, \quad n \geq 0, k \geq 1,$$

is a set of consecutive eigenvalues of A and $\sigma_1 = \text{spec}(A) \setminus \sigma_0$.

Notice that there are eigenvalues E_0, E_1, \dots, E_n of A lying to the left of σ_0 . Also there is a part of $\text{spec}(A)$ lying to the right of σ_0 .

Assume that

$$\|V\| < \frac{d}{2} \quad (d = \text{dist}(\sigma_0, \sigma_1)),$$

and σ'_0 consists of the eigenvalues of $H = A + V$ that result from the eigenvalues of A contained in σ_0 . Then $\theta = \theta(\mathfrak{H}_0, \mathfrak{H}'_0) < \frac{\pi}{4}$ and

$$\sin 2\theta \leq \frac{2\|V\|}{d}.$$

This follows again from the Davis-Kahan $\sin 2\theta$ Theorem.

If V is off-diagonal then the bound may be essentially strengthened:

- The gaps between σ_0 and σ_1 remain open whenever condition

$$\|V\| < \sqrt{2}d$$

is satisfied.

- Moreover, under this condition

$$\tan \theta \leq \frac{\|V\|}{d}.$$

This is corollary of the a priori $\tan \theta$ Theorem [*S. Albeverio, A.V. Selin, A.K.M. (2006, 2012)*].

Conclusions

- We have found new sharp norm bounds on rotation of spectral subspaces of a self-adjoint operator under off-diagonal perturbations.
- We have also established optimal bounds on the shift of the spectrum under off-diagonal perturbations.
- The maximal angle bounds obtained allow one to derive the corresponding bounds on variation of spectral subspaces under non-off-diagonal (generic) perturbations.
- The general results have been 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.