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On applying the subspace perturbation theory to few-body Hamiltonians

Abstract We present a selection of results on variation of the spectral subspace of a Hermitian operator under a Hermitian perturbation and show how these results may work for few-body Hamiltonians.

Keywords Few-body problem · Binding energy shift · Variation of spectral subspace

1 Introduction

The subspace perturbation theory is a branch of the general theory of linear operators (see, e.g. [1; 8]) that studies variation of an invariant (in particular, spectral) subspace of an operator under an additive perturbation. In this small survey article we restrict the subject to Hermitian operators and follow the geometric approach that originates in the works by Davis [4; 5] and Davis and Kahan [6]. Within the Davis-Kahan approach, a bound on the variation of a spectral subspace has usually the form of a trigonometric estimate involving just two quantities: a norm of the perturbation operator and the distance between the relevant spectral subsets. We present only the estimates that are a priori in their nature and involve the distance between spectral sets of the unperturbed operator (but not of the perturbed one). The results valid for Hermitian operators of any origin are collected in Section 2. In Section 3 we give several examples that illustrate the meaning of the abstract results and show why these results might be useful already in the study of a few-body bound-state problem.

Through the whole material we will use only the standard operator norm. We recall that if $V$ is a bounded linear operator on a Hilbert space $H$, its norm is given by $\|V\| = \sup_{\|f\|=1} \|Vf\|$ where sup denotes the least upper bound. Thus, for any $|f\rangle \in \mathcal{H}$ we have $\|V|f\rangle\| \leq \|V\| \|f\|$. If $V$ is a Hermitian operator with $\min(\text{spec}(V)) = m_V$ and $\max(\text{spec}(V)) = M_V$ then $\|V\| = \max\{|m_V|, |M_V|\}$. In particular, if $V$ is separable of rank one, that is, if $V = \lambda \langle \phi | \phi \rangle$ with a normalized $|\phi\rangle \in \mathcal{H}$ and $\lambda \in \mathbb{R}$, then $\|V\| = |\lambda|$. Another example concerns the case where $\mathcal{H} = L^2(\mathbb{R})$ and $V$ is a bounded local potential, i.e. $\langle x | V | f \rangle = V(x)f(x)$ for any $|f\rangle \in \mathcal{H}$, with $V(\cdot)$ a bounded function on $\mathbb{R}$. In this case $\|V\| = \sup_{x \in \mathbb{R}} |V(x)|$.

2 The abstract problem setup and abstract results

Assume that $A$ is a Hermitian (or, equivalently, self-adjoint) operator on a separable Hilbert space $\mathcal{H}$. If $V$ is a bounded Hermitian perturbation of $A$ then the spectrum, $\text{spec}(H)$, of the perturbed operator $H = A + V$ is...
confined in the closed \( \|V\|\)-neighborhood \( \partial_{|V|}(\text{spec}(A)) \) of the spectrum of \( A \) (see, e.g., [8]). Hence, if a part \( \sigma \) of the spectrum of \( A \) is isolated from its complement \( \Sigma = \text{spec}(A) \setminus \sigma \), that is, if \[
 d := \text{dist}(\sigma, \Sigma) > 0, \]
then the spectrum of \( H \) is also divided into two disjoint components,
\[
\omega = \text{spec}(H) \cap \partial_{|V|}(\sigma) \quad \text{and} \quad \Omega = \text{spec}(H) \cap \partial_{|V|}(\Sigma),
\]
provided that \[
\|V\| < \frac{1}{2} d.
\] (3)

Under condition (3), one interprets the separated spectral components \( \omega \) and \( \Omega \) of the perturbed operator \( H \) as the results of the perturbation of the corresponding initial disjoint spectral sets \( \sigma \) and \( \Sigma \).

The transformation of the spectral subspace of \( A \) associated with the spectral set \( \sigma \) into the spectral subspace of \( H \) associated with the spectral set \( \omega \) may be studied in terms of the difference \( P - Q \) between the corresponding spectral projections \( P = E_{A}(\sigma) \) and \( Q = E_{H}(\omega) \) of \( A \) and \( H \). Of particular interest is the case where \( \|P - Q\| < 1 \). In this case the spectral projections \( P \) and \( Q \) are unitarily equivalent and the perturbed spectral subspace \( \Omega = \text{Ran}(Q) \) may be viewed as obtained by the direct rotation of the unperturbed spectral subspace \( \Psi = \text{Ran}(P) \) (see, e.g. [4, Sections 3 and 4]). Moreover, the quantity
\[
\theta(\Omega, \Psi) = \arcsin(\|P - Q\|)
\]
is used as a measure of this rotation. It is called the maximal angle between the subspaces \( \Omega \) and \( \Psi \). A short review of the concept of the maximal angle can be found, e.g. in [4, Section 2]; see also [6, B.14, 13].

Among various questions being answered within the subspace perturbation theory, the first and rather basic question is on whether the condition (3) is sufficient for the bound
\[
\theta(\Omega, \Psi) < \frac{\pi}{2}
\]
(4)
to hold, or, in order to secure (4), one should impose a stronger requirement \( \|V\| < c d \) with some \( c < \frac{1}{2} \). More precisely, the question is as follows.

(i) What is the best possible constant \( c_{s} \) in the inequality \( \|V\| < c_{s} d \) ensuring the spectral subspace variation bound (4)?

Another, practically important question concerns the maximal possible size of the subspace variation:

(ii) What function \( M : [0, c_{s}) \rightarrow [0, \frac{\pi}{2}) \) is best possible in the bound
\[
\theta(\Omega, \Psi) \leq M \left( \frac{\|V\|}{d} \right) \quad \text{for} \quad \|V\| < c_{s} d?
\]
(5)

Both the constant \( c_{s} \) and the estimating function \( M \) are required to be universal in the sense that they should not depend on the Hermitian operators \( A \) and \( V \) involved.

By now, the problems (i) and (ii) have been completely solved only for the particular spectral dispositions where one of the sets \( \sigma \) and \( \Sigma \) lies in a finite or infinite gap of the other set, say, \( \sigma \) lies in a gap of \( \Sigma \). In this case
\[
c_{s} = \frac{1}{2} \quad \text{and} \quad M(x) = \frac{1}{2} \arcsin(2x).
\]
(6)

This is the essence of the Davis-Kahan \( \sin 2\theta \) theorem in [4].

In the generic case (where no assumptions are done on the mutual position of the sets \( \sigma \) and \( \Sigma \)), the strongest known answers to the questions (i) and (ii) are the recent ones given by Seelmann [16], within the approach developed in [3]; see also the earlier works [10] and [13]. In particular, [16, Theorem 1] implies that the generic optimal constant \( c_{s} \) satisfies inequality \( c_{s} > 0.454839 \). For the best upper estimate on the function \( M \) in the bound (5) we also refer to [16]. Here we only notice that for sure \( \theta(\Omega, \Psi) \leq \frac{1}{4} \arcsin \frac{2\|V\|}{d} \) whenever \( \|V\| \leq \frac{1}{4} d \) (see [4, Remark 4.4]; cf. [13, Corollary 2]).

Now recall that, under the assumption (1), a bounded operator \( V \) is said to be off-diagonal with respect to the partition \( \text{spec}(A) = \sigma \cup \Sigma \) if it anticommutes with the difference \( J = P - P^\perp \) of the spectral projections \( P = E_{A}(\sigma) \) and \( P^\perp = E_{A}(\Sigma) \), that is, if \( VJ = -JV \). The problems like (i) and (ii) have also been addressed in the case of off-diagonal Hermitian perturbations. When considering such a perturbation, one should first
take into account that the requirements ensuring the disjointness of the corresponding perturbed spectral components \( \omega \) and \( \Omega \) originating in \( \sigma \) and \( \Sigma \) are much weaker than condition (5). In particular, if the sets \( \sigma \) and \( \Sigma \) are subordinated, say \( \max(\sigma) < \min(\Sigma) \), then for any \( \|V\| \) no spectrum of \( H = A + V \) enters the open interval between \( \max(\sigma) \) and \( \min(\Sigma) \) (see, e.g., [17, Remark 2.5.19]). In such a case the maximal angle between the unperturbed and perturbed spectral subspaces admits a sharp bound of the form (5) with \( M(x) = \frac{1}{2} \arctan(2x), x \in [0, \infty) \). This is the consequence of the celebrated Davis-Kahan tan2\( \theta \) theorem (also, cf. the extensions of the tan2\( \theta \) theorem in [2] [4] [14]). Furthermore, if it is known that the set \( \sigma \) lies in a finite gap of the set \( \Sigma \) then the disjointness of the perturbed spectral components \( \omega \) and \( \Omega \) is ensured by the (sharp) condition \( \|V\| < \sqrt{2d} \). The same condition is optimal for the bound (4) to hold. Both these results have been established in [13]. The explicit expression for the best possible function \( M \) in the corresponding estimate (5), \( M(x) = \arctan x, x \in [0, \sqrt{2}] \), was found in [2] [4]. As for the generic spectral disposition with no restrictions on the mutual position of \( \sigma \) and \( \Sigma \), the condition \( \|V\| \leq \sqrt{2d} \) has been proven to be optimal in order to guarantee that the gaps between \( \sigma \) and \( \Sigma \) do not close under an off-diagonal \( V \) and, thus, that \( \text{dist}(\sigma, \Omega) > 0 \). The proof was first given in [12, Theorem 1] for bounded \( A \) and then in [17, Proposition 2.5.22] for unperturbed \( A \). The best published lower bound \( c_{\ast} > 0.675989 \) for the generic optimal constant \( c_{\ast} \) in the off-diagonal case has been established in [13]. Paper [13] also contains the strongest known upper estimate for the optimal function \( M \) in the corresponding bound (5) (see [13, Theorem 6.2 and Remark 6.3]).

3 Applications to few-body problems

Throughout this section we suppose that the “unperturbed” Hamiltonian \( A \) has the form \( A = H_0 + V_0 \) where \( H_0 \) stands for the kinetic energy operator of an \( N \)-particle system in the c.m. frame and the potential \( V_0 \) includes only a part of all interactions that are present in the system (say, only two-body forces if \( N = 3 \)). The perturbation \( V \) is assumed to describe the remaining part of the interactions (say, three-body forces for \( N = 3 \); instead, if all the interparticle interactions are already included in \( V_0 \), it may only describe the effect of external fields). We consider the case where \( V \) is a bounded operator. Surely, both \( A \) and \( V \) are assumed to be Hermitian. In order to apply to \( H = A + V \) the abstract results mentioned in the previous section, one only needs to know the norm of the perturbation \( V \) and a few very basic things on the spectrum of the operator \( A \).

We start our discussion with the simplest example illustrating the sin\( 2\theta \) and tan2\( \theta \) theorems from [4].

Example 3.1 Suppose that \( E_0 \) is the ground-state (g.s.) energy of the Hamiltonian \( A \). Assume, in addition, that the eigenvalue \( E_0 \) is simple (this is typical for a ground state) and let \( |\psi_0\rangle \) be the normalized g.s. wave function, i.e. \( A|\psi_0\rangle = E_0|\psi_0\rangle \), \( \|\psi_0\| = 1 \). Set \( \sigma = \{E_0\}, \Sigma = \text{spec}(A) \setminus \{E_0\} \) and \( d = \text{dist}(\sigma, \Sigma) = \min(\Sigma) - E_0 \) (we remark that the set \( \Sigma \) is definitely not empty since it should contain at least the essential spectrum of \( A \)). If the norm of \( V \) is such that the condition (3) holds, then the g.s. energy \( E_0 \) of the total Hamiltonian \( H = A + V \) is also a simple eigenvalue with a g.s. vector \( |\psi_0\rangle \), \( \|\psi_0\| = 1 \). The g.s. energy \( E_0 \) lies in the closed \( \|V\| \)-neighborhood of the g.s. energy \( E_0 \), that is, \( E_0 - E_0' \leq \|V\| \). The corresponding spectral projections \( P = \Pi_{E_0}(\sigma) \) and \( Q = \Pi_{E_0}(\omega) \) of \( A \) and \( H \) associated with the one-point spectral sets \( \sigma = \{E_0\} \) and \( \omega = \{E_0'\} \) read as \( P = |\psi_0\rangle \langle \psi_0| \) and \( Q = |\psi_0\rangle \langle \psi_0'| \). One verifies by inspection that \( \arcsin \left( \frac{|P - Q|}{\|P - Q\|} \right) = \arccos \left( |\langle \psi_0| \psi_0'\rangle| \right) \), which means that the maximal angle \( \theta(P, Q) \) between the one-dimensional spectral subspaces \( \mathbb{P} = \text{span}(P) \) and \( \mathbb{Q} = \text{span}(Q) \) is, of course, nothing but the angle between the g.s. vectors \( |\psi_0\rangle \) and \( |\psi_0'\rangle \). Then the Davis-Kahan sin\( 2\theta \) theorem (see (5) and (6)) implies that \( \arccos \left( |\langle \psi_0| \psi_0'\rangle| \right) \leq \frac{1}{2} \arcsin \frac{2\|V\|}{d} \). This bound on the rotation of the ground state under the perturbation \( V \) is sharp. In particular, it implies that under condition (3) the angle between \( |\psi_0\rangle \) and \( |\psi_0'\rangle \) can never exceed 45\( ^{\circ} \).

If, in addition, it is known that the perturbation \( V \) is off-diagonal with respect to the partition \( \text{spec}(A) = \sigma \cup \Sigma \) then for any (arbitrarily large) \( \|V\| \) no spectrum of \( H \) enters the gap between the g.s. energy \( E_0 \) and the remaining spectrum \( \Sigma \) of \( A \). Moreover, there are the following sharp universal bounds for the perturbed g.s. energy \( E_0' \):

\[
E_0 - \varepsilon_V \leq E_0' \leq E_0,
\]

where

\[
\varepsilon_V = \|V\| \tan \left( \frac{1}{2} \arctan \frac{2\|V\|}{d} \right) < \|V\| \tag{7}
\]

(see [12, Lemma 1.1] and [17, Proposition 2.5.21]). At the same time, the Davis-Kahan tan2\( \theta \) theorem [6] implies that \( \arccos \left( |\langle \psi_0| \psi_0'\rangle| \right) \leq \frac{1}{2} \arcsin \frac{2\|V\|}{d} < \frac{\pi}{4} \).
With a minimal change, the above consideration is extended to the case where the initial spectral set \( \sigma \) consists of the \( n+1 \) lowest binding energies \( E_0 \leq E_1 \leq \ldots \leq E_n \), \( n \geq 1 \), of \( A \). We only want to underline that if \( V \) is off-diagonal than for any \( \| V \| \) the whole perturbed spectral set \( \omega \) of \( H = A + V \) originating from \( \sigma \) will necessarily lie in the interval \( [E_0 - \varepsilon, \ E_0] \) where the shift \( \varepsilon \) is given by (7), while the interval \( (E_n, \min(\Sigma)) \) will contain no spectrum of \( H \). Furthermore, the tan \( 2\theta \)-theorem-like estimates for the maximal angle between the spectral subspaces \( \mathcal{P} = \text{Ran}(E_A(\sigma)) \) and \( \Omega = \text{Ran}(E_H(\omega)) \) may be done even for some unbounded \( V \) (but, instead of \( d \) and \( \| V \| \), in terms of quadratic forms involving \( A \) and \( V \)), see 2(13).

Along with the sin \( 2\theta \) theorem, our second example also illustrates the tan \( \theta \) bound proven in 2(14).

**Example 3.2** Assume that \( \sigma = \{E_{n+1},E_{n+2},\ldots,E_{n+k}\}, n \geq 0, \ k \geq 1 \), is the set of consecutive binding energies of \( A \) and \( \Sigma = \text{spec}(A) \setminus \sigma = \Sigma_+ \cup \Sigma_- \) where \( \Sigma_+ \) is the increasing sequence of the energy levels \( E_0,E_1,\ldots,E_n \) of \( A \) that are lower than \( \min(\sigma) \); \( \Sigma_- \) denotes the remaining part of the spectrum of \( A \), i.e. \( \Sigma_+ = \text{spec}(A) \setminus (\sigma \cup \Sigma_-) \). Together with (1), this assumption means that the set \( \sigma \) lies in the finite gap \( (\max(\Sigma_-),\min(\Sigma_+)) \) of the set \( \Sigma \). Under the single condition (3), not much can be said about the location of the perturbed spectral sets \( \omega \) and \( \Omega \), except for (2), but the Davis-Kahan sin \( 2\theta \) theorem still well applies to this case and, thus, we again have the bound \( \theta(\mathcal{P},\mathcal{Q}) \leq \frac{1}{2} \arcsin \frac{2\|V\|}{d} < \frac{\pi}{4} \).

Much stronger conclusions can be done if the operator \( V \) is off-diagonal with respect to the partition \( \text{spec}(A) = \sigma \cup \Sigma \). As it was already mentioned in Section 2, for off-diagonal \( V \) the gap-non-closing condition reads as \( \| V \| < \sqrt{d} \) (and even a weaker but more detail condition \( \| V \| < \sqrt{dD} \) with \( D = \min(\Sigma_+) - \max(\Sigma_-) \) is allowed, see [11,13]). In this case the lower bound of the spectrum of the operator \( H = A + V = E_0 - \varepsilon_V \) where the maximal possible energy shift \( \varepsilon_V \), \( \varepsilon_V < d \), is given again by (7). Furthermore, \( \omega \subset [E_{n+1} - \varepsilon_V,E_{n+2} + \varepsilon_V] \) and the open intervals \( (E_n,E_{n+1} - \varepsilon_V) \) and \( (E_{n+1} + \varepsilon_V,\min(\Sigma_+)) \) contain no spectrum of \( H \). For tighter enclosures for \( \omega \) and \( \Omega \) involving, say, the the gap length \( D \) we refer to [11,12,17]. In the case under consideration, the sharp bound for the rotation of the spectral subspace \( \mathcal{P} = \text{Ran}(E_A(\sigma)) \) is given by \( \theta(\mathcal{P},\mathcal{Q}) \leq \arccos \frac{2\|V\|}{dD} \) (see 2, Theorem 1; cf. 14, Theorem 2). However, if the value of \( D \) is known and \( \| V \| < \sqrt{dD} \), then a more detail and stronger but still optimal estimate for \( \theta(\mathcal{P},\mathcal{Q}) \) involving \( D \) is available (see 2, Theorem 4.1).

Both Examples 3.1 and 3.2 show how one may obtain a bound on the variation of the spectral subspace prior to any calculations with the total Hamiltonian \( H \). To perform this, only the knowledge of the values of \( d \) and \( \| V \| \) is needed. Furthermore, if \( V \) is off-diagonal, with just these two values one can also provide the stronger estimates (via \( \varepsilon_V \)) for the binding energy shifts.

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