**Project description**

In this project, a quantum system (say, nucleus, atom or molecule) is modeled by a Hamiltonian of finite rank (see [1] for a discussion of the rank two case that is already quite interesting). The Hilbert space may be chosen as $\mathcal{H} = \mathbb{C}^n$ and the Hamiltonian itself may be viewed as an $n \times n$ Hermitian number matrix $H_0$. Effect of an external field is reproduced by adding to $H_0$ a Hermitian matrix $V$ of the same dimension $n \times n$, that is, the total (perturbed) Hamiltonian reads $H = H_0 + V$. It is well known that the perturbation $V$ cannot shift the eigenvalues of $H_0$ more than the norm $\|V\|$ (which is the maximum over the set of absolute values of all eigenvalues of $V$). Assume that the eigenvalues of $H_0$ are grouped in two disjoint sets $\sigma$ and $\Sigma$, that the distance between $\sigma$ and $\Sigma$ equals $d > 0$, and that $V$ satisfies the bound $\|V\| < d/2$. Clearly, in this case the spectrum of the perturbed Hamiltonian $H = H_0 + V$ will also consist of two disjoint sets of eigenvalues that originate from the sets $\sigma$ and $\Sigma$. We denote these sets by $\omega$ and $\Omega$, respectively. Now denote by $\mathcal{P}$ the linear span of the eigenvectors of $H_0$ belonging to the eigenvalues from $\sigma$ and let $\mathcal{Q}$ be the linear span of eigenvectors of $H$ corresponding to the eigenvalues from $\omega$. If $P$ and $Q$ are orthogonal projections in $\mathcal{H}$ whose ranges are $\mathcal{P}$ and $\mathcal{Q}$, respectively, the quantity

$$\theta = \arcsin(\|P - Q\|)$$

is called the maximal angle between the subspaces $\mathcal{P}$ and $\mathcal{Q}$.

We note that the maximal angle $\theta$ is a natural geometric characteristic for position of the subspaces $\mathcal{P}$ and $\mathcal{Q}$ with respect to one another. In particular, if $\mathcal{P}$ and $\mathcal{Q}$ are one-dimensional, that is, they are the spans of some unit vectors $p$ and $q$, respectively, then $\theta$ coincides just with the acute angle between $p$ and $q$, $\theta = \arccos(|\langle p, q \rangle|)$. Thus, if $p$ is a bound state of the unperturbed system (i.e. $p$ is an eigenvector of the Hamiltonian $H_0$) and $q$ of the perturbed one (i.e. $p$ is an eigenvector of the Hamiltonian $H$), the quantity $\cos^2 \theta = |\langle p, q \rangle|^2$ provides us with the probability of the system to remain still in the state $p$ after the external field $V$ has been applied. Surely, a relevant physical interpretation of a similar probabilistic kind is available for $\theta$ in case of larger dimensions of $\mathcal{P}$ and $\mathcal{Q}$.

It is known that if the set $\sigma$ lies in a gap of the set $\Sigma$ then the following sharp bound holds:

$$\theta \leq \frac{1}{2} \arcsin \left( \frac{2\|V\|}{d} \right), \quad \text{whenever} \quad \|V\| < \frac{d}{2}.$$  

This bound is the essence of the celebrated Davis-Kahan $\sin 2\theta$ Theorem [2] (also see [3]). This bound is universal in the sense that it is independent of the dimension $n$ and the structure of the Hermitian matrices $A$ and $V$; only the condition $\|V\| < d/2$ is important.

For generic disposition of the spectral sets $\sigma$ and $\Sigma$ (when nothing is known on the mutual position of these sets except for their disjointness) no sharp estimate of the form

$$\theta \leq M \left( \frac{\|V\|}{d} \right)$$  

(1)
is available in the literature. One may look through [3] to become familiar with the best current bounds for the estimating function \( M(x) \) on the right-hand side of (1).

The project is aimed at obtaining bounds on the maximal angle \( \theta \) between the unperturbed and perturbed spectral subspaces \( \mathcal{P} \) and \( \Omega \) in some particular cases that are not covered by the Davis-Kahan \( \sin 2 \theta \) Theorem. The problem is assumed to be solved for dimensions \( n = 4, 5 \) and, perhaps, \( n = 6 \) by performing computer calculations. The goal is to obtain bounds of the form (1) with approximate numerical functions \( M(x) \).

Also, it would be great to consider, in the same way and for the same dimensions \( n \), a version of the problem where the perturbation matrix \( V \) is off-diagonal with respect to the orthogonal decomposition \( \mathcal{H} = \mathcal{P} \oplus \mathcal{P}^\perp \). One may consult [4] on the current status of the subspace perturbation theory for off-diagonal perturbations.

References


Possible number of students involved

This project may involve up to two students. One of them would solve the problem for generic (not structured) perturbations \( V \) and the other one for off-diagonal \( V \). Participants of the project could combine their efforts in preparing the basic part of the computer code to compute eigenvalues and eigenvectors of a Hermitian matrix.

Prerequisites for participation in the project

A knowledge of linear algebra and quantum mechanics is required. A participant should also have an experience in computer programming allowing him/her to solve the basic problems of linear algebra. Programming language would essentially be a choice of the participant.

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