Name of the project coordinator: **Alexander K. Motovilov**

Project title: **Bounds on rotation of eigenstates of a few-level system by an external field**

JINR Laboratory: **BLTP**

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 $\mathfrak{H} = \mathbb{C}^n$ 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 σ and Σ, that the distance between σ and Σ 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 σ and Σ. We denote these sets by ω and Ω, respectively.

Now denote by $\mathfrak{P}$ the linear span of the eigenvectors of H_0 belonging to the eigenvalues from σ and let $\mathfrak{Q}$ be the linear span of eigenvectors of H corresponding to the eigenvalues from ω. If P and Q are orthogonal projections in $\mathfrak{H}$ whose ranges are $\mathfrak{P}$ and $\mathfrak{Q}$, respectively, the quantity

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

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

We note that the maximal angle θ is a natural geometric characteristic for position of the subspaces $\mathfrak{P}$ and $\mathfrak{Q}$ with respect to one another. In particular, if $\mathfrak{P}$ and $\mathfrak{Q}$ are one-dimensional, that is, they are the spans of some unit vectors p and q, respectively, then θ coincides just with the acute angle between p and q, $\theta = \arccos\bigl(|\langle p, q\rangle|\bigr)$. 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 θ in case of larger dimensions of $\mathfrak{P}$ and $\mathfrak{Q}$.

It is known that if the set σ lies in a gap of the set Σ then the following sharp bound holds:

$$\theta \le \frac{1}{2}\arcsin\frac{2\|V\|}{d}, \quad \text{whenever} \quad \|V\| < \frac{d}{2}.$$

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 σ and Σ (when nothing is known on the mutual position of these sets except for their disjointness) no sharp estimate of the form

$$\theta \le M\left(\frac{\|V\|}{d}\right) \tag{1}$$

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 θ between the unperturbed and perturbed spectral subspaces $\mathfrak{P}$ and $\mathfrak{Q}$ 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 $\mathfrak{H} = \mathfrak{P} \oplus \mathfrak{P}^{\perp}$. One may consult [4] on the current status of the subspace perturbation theory for off-diagonal perturbations.

References

[1] http://en.wikipedia.org/wiki/Two-state_quantum_system

[2] C. Davis and W. M. Kahan, *The rotation of eigenvectors by a perturbation. III*, SIAM J. Numer. Anal. **7** (1970), 1–46

[3] S. Albeverio and A. K. Motovilov, *Sharpening the norm bound in the subspace perturbation theory*, Compl. Anal. Oper. Theory, Online First (DOI: 10.1007/s11785-012-0245-7); arXiv:1112.0149

[4] S. Albeverio and A. K. Motovilov, *The a priori* $\tan\theta$ *theorem for spectral subspaces*, Integr. Equ. Oper. Theory, **73**:3 (2012), 413–430; arXiv:1012.1569

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.

More info on the project coordinator

Full name:	Motovilov, Alexander Konstantinovich
Position:	Head of Sector
Degree:	Doctor of Physical and Mathematical Sciences
JINR Division:	Bogoliubov Laboratory of Theoretical Physics, Department of Nuclear Theory
Personal webpage	http://theor.jinr.ru/˜motovilv