Universität Regensburg, Fakultät für Physik
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Übungen zur Quantenmechanik für LA und Nanoscience
Blatt 1 (für die Übungen in der Woche 23.-27.10.)

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1 Finite-dimensional vector spaces, scalar products, and Hermitian matrices

Below, $\vec{u}$ and $\vec{v}$ denote complex N-dimensional vectors, i.e., $\vec{u}, \vec{v} \in \mathbb{C}^N$, while A and B denote $N \times N$ complex matrices, i.e., $A, B \in \mathbb{C}^{N\times N}$. The canonical scalar product of two such vectors is given by

$$\langle u|v\rangle = \vec{u}^\dagger \cdot \vec{v} = \sum_{n=1}^{N} u_n^* v_n \,,$$

where $\vec{u}^\dagger := (\vec{u}^T)^*$. A matrix is called Hermitian if $A = (A^T)^* =: A^\dagger$.

a) Show that A is Hermitian if and only if $\langle Au|v\rangle = \langle u|Av\rangle$ for all $\vec{u}, \vec{v}$.

b) Show for Hermitian A and B that the product AB is Hermitian if and only if $[A, B] = 0$. $[A, B] := AB - BA$ is called the commutator of A and B.

c) Show that $BAB^\dagger$ is Hermitian for Hermitian A and arbitrary B.

2 Finite-dimensional vector spaces and eigenspaces of Hermitian matrices

Let $\vec{u}, \vec{v} \in \mathbb{C}^N$ and $A, B \in \mathbb{C}^{N\times N}$ as above.

a) Give an argument why a Hermitian $N \times N$ matrix A has exactly N eigenvalues. Show that all eigenvalues are real.

b) Take A to be Hermitian with nondegenerate eigenvalues (i.e., all eigenvalues are distinct). Show that the eigenvectors to different eigenvalues are orthogonal.

   Remark: The most important consequence of the last two results is that the eigenvectors form an orthogonal basis of $\mathbb{C}^N$. A more general theorem states that even in the degenerate case a full orthogonal set of N eigenvectors can be *chosen* that form such a basis.

c) The space spanned by a complete set of linearly independent eigenvectors w.r.t. a given eigenvalue λ is called its eigenspace $\mathrm{Eig}(A, \lambda)$. What is the dimension of this eigenspace?

d) Let A be Hermitian and $\{\vec{e}_n; n = 1, \ldots, N\}$ be a corresponding orthonormal eigenbasis. Explain the notions “orthonormal” and “eigenbasis”. Expand an arbitrary vector $\vec{u}$ in this basis. Give an explicit expression for the expansion coefficients in terms of the scalar product.

3 Matrix properties

a) Given a square matrix A, show that

$$\det(e^A) = e^{\operatorname{tr} A} \,.$$

   Hint: This equality can be proven for any square matrix, but for simplicity you can assume that A is diagonalizable.

b) Given a generic linear operator A, show that the operator $A^\dagger A$ has real and non-negative eigenvalues only.

4 Infinite-dimensional spaces: A scalar product for square-integrable functions

The vector space $\mathbb{H}$ of square-integrable functions $\{\psi : \mathbb{R}^N \to \mathbb{C}\}$ may be endowed with a sesquilinear scalar product $\mathbb{H} \times \mathbb{H} \to \mathbb{C}$ via

$$\langle \psi_1 | \psi_2 \rangle := \int d^N x \, \psi_1^*(\vec{x}) \psi_2(\vec{x}) \, .$$

a) Explain the mathematical notions "square integrable" and "sesquilinear scalar product".

b) Show that the definition above satisfies all the requirements of a sesquilinear scalar product, i.e., show that

- for square integrable ψ_1 and ψ_2, the scalar product is finite,
- the scalar product is (anti-) linear in its arguments, and
- the scalar product is positive semidefinite ($\langle \psi | \psi \rangle \geq 0$).

Bonus question: Discuss under what conditions the scalar product is positive definite, i.e., $\langle \psi | \psi \rangle \geq 0$ with equality if and only if $\psi = 0$.