Theoretical Physics II B – Quantum Mechanics

Lecture 3

Frank Krauss

February 11, 2014

1. Linear operators

Solutions to previous control questions

2.1 Two vectors being orthogonal: $\langle\phi|\chi\rangle = 0.$
Two vectors being parallel: $|\phi\rangle = c\,|\chi\rangle$ with $c \in \mathbf{C}$. Therefore $\langle\phi|\chi\rangle = \langle c\chi|\chi\rangle = c^*$. But $|c|^2 = 1$ since $1 = \langle\phi|\phi\rangle = \langle c\chi|c\chi\rangle = c^*c = |c|^2$. This means that $|c| = 1$ and, in general $c = e^{i\gamma}$ with $\gamma \in \mathbf{R}$, a real number.
Thus: $\langle\phi|\chi\rangle = e^{-i\gamma}$

2.2(a) $|\phi\rangle = \frac{|v_1\rangle + i|v_2\rangle}{\sqrt{2}}$, $|\chi\rangle = \frac{|v_1\rangle - i|v_2\rangle}{\sqrt{2}}$

$$\begin{aligned}
\langle\phi|\phi\rangle &= \frac{1}{2}|\left(|v_1\rangle + i\,|v_2\rangle\right)|^2 = \frac{1}{2}\left(\langle v_1| - i\,\langle v_2|\right)\left(|v_1\rangle + i\,|v_2\rangle\right) = 1\\
\langle\chi|\chi\rangle &= \frac{1}{2}|\left(|v_1\rangle - i\,|v_2\rangle\right)|^2 = \frac{1}{2}\left(\langle v_1| + i\,\langle v_2|\right)\left(|v_1\rangle - i\,|v_2\rangle\right) = 1\\
\langle\phi|\chi\rangle &= \frac{1}{2}\left(\langle v_1| - i\,\langle v_2|\right)\left(|v_1\rangle - i\,|v_2\rangle\right) = 0
\end{aligned}$$

Solutions to previous control questions

2.2(b) $|\phi\rangle = \int\limits_a^b \mathrm{d}k\; e^{ik}\;|v_k\rangle,\; |\chi\rangle = \int\limits_a^b \mathrm{d}k\; e^{2ik}\;|v_k\rangle.$

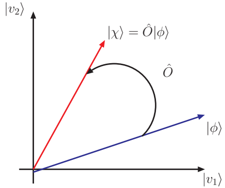
$$
\begin{aligned}
\langle\phi|\phi\rangle &= \int\limits_a^b \mathrm{d}k\mathrm{d}k' e^{i(k'-k)}\,\langle v'_k|v_k\rangle = \int\limits_a^b \mathrm{d}k = b-a\\
\langle\chi|\chi\rangle &= \int\limits_a^b \mathrm{d}k\mathrm{d}k' e^{2i(k'-k)}\,\langle v'_k|v_k\rangle = \int\limits_a^b \mathrm{d}k = b-a\\
\langle\phi|\chi\rangle &= \int\limits_a^b \mathrm{d}k\mathrm{d}k' e^{i(2k-k')}\,\langle v'_k|v_k\rangle = \int\limits_a^b \mathrm{d}k e^{ik} = i\left(e^{ia}-e^{ib}\right)\,.
\end{aligned}
$$

Operators

- In Dirac notation, operators $\hat{O}$ map vectors $|\phi\rangle$ onto vectors $|\chi\rangle$:

$$|\phi\rangle \xrightarrow{\hat{O}} |\chi\rangle = \hat{O}\,|\phi\rangle = \left|\hat{O}\phi\right\rangle$$

- Operators mapping vectors onto themselves are denoted by $\hat{\mathbf{1}}$, the **identity operator**.



- Note: operators act on objects in vector spaces, i.e. vectors. Therefore, for their proper definition it is important to state in which space they act (operate).

Linear operators

Linear operators fulfil:

- $\hat{O}\,|\phi+\chi\rangle = \hat{O}\,|\phi\rangle + \hat{O}\,|\chi\rangle$
- $\hat{O}\,|c\phi\rangle = c\hat{O}\,|\phi\rangle\ \forall\ c \in \mathcal{C}$

for all kets in the Hilbert space $\mathcal{H}$.
In addition, they have the following properties:

- Sum of operators: $(\hat{L}+\hat{M})\,|\phi\rangle = \hat{L}\,|\phi\rangle + \hat{M}\,|\phi\rangle$
- Product of operators: $(\hat{L}\hat{M})\,|\phi\rangle = \hat{L}(\hat{M}\,|\phi\rangle) = \hat{L}\,\left|\hat{M}\phi\right\rangle$

  Note: Sequence matters! By convention in the line above, $\hat{M}$ is applied before $\hat{L}$ is applied to the result of this operation:

$$\hat{L}\hat{M}\,|\phi\rangle \neq \hat{M}\hat{L}\,|\phi\rangle\ .$$

Representations of linear operators

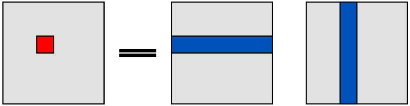
In order to numerically calculate with specific linear operators, it is important to interpret it. To this end, remember that

linear operators can be represented by matrices.

Calculating with linear operators

- Summing two operators happens component-wise: If $\hat{C} = \hat{A} + \hat{B}$, then $C_{ij} = A_{ij} + B_{ij}$.
- Two operators are multiplied according to the rules of matrix multiplication. Using component notation this means that if $\hat{C} = \hat{A}\hat{B}$, then $C_{ik} = \sum\limits_j A_{ij} B_{jk}$, where the sum runs over all j.

  In order to obtain the element in the ith row and the kth column, the components of the ith row of the first matrix are multiplied with those in the kth column of the second matrix, and the resulting products are added:

  
- Using the same rules for the product $\hat{A}\,|a\rangle$ it can easily be shown that the first two definitions on the previous slide are satisfied.

Constructing a specific representation

The representation of an operator is always with respect to a base. To construct it, consider the action of an operator $\hat{O}$ when applied onto a set of base vectors $\{|v_k\rangle\}$. Each of these vectors is mapped onto a new vector, $|a\rangle$, namely $|a\rangle = \hat{O}\,|v_k\rangle$, which typically is not a base vector. However, expanding it in the base vectors yields

$$|a\rangle = \sum_{k'=1}^{N} |v'_k\rangle \langle v'_k|a\rangle = \sum_{k'=1}^{N} |v'_k\rangle \left\langle v'_k \left| \hat{O} \right| v_k \right\rangle ,$$

which allows to identify the matrix components of the operator as

$$O_{k'k} = \left\langle v'_k \left| \hat{O} \right| v_k \right\rangle$$

and it becomes clear that the $\hat{O}$ can be represented as an $N \times N$ matrix.

Special properties and operators

- The trace of an operator, $\mathrm{Tr}\left(\hat{O}\right)$, is defined as the sum over its diagonal elements, $\mathrm{Tr}\left(\hat{O}\right) = \sum\limits_i O_{ii}$.
- $\hat{O}^{-1}$ is the **inverse** of $\hat{O}$, if $\hat{O}^{-1}\hat{O} = \hat{O}\hat{O}^{-1} = \hat{\mathbf{1}}$.
  Properties:
  - $\left(\hat{O}^{-1}\right)^{-1} = \hat{O}$;
  - $\left(c\hat{O}\right)^{-1} = \frac{1}{c}\,\hat{O}^{-1}\ \forall c \in \mathbf{C}$;
  - $\left(\hat{L}\hat{M}\right)^{-1} = \hat{M}^{-1}\hat{L}^{-1}$.

    This property follows from $\left(\hat{L}\hat{M}\right)\left(\hat{L}\hat{M}\right)^{-1} = \hat{1}$ by multiplying from the left first with $\hat{L}^{-1}$ and then with $\hat{M}^{-1}$.
  - If $\hat{O}$ and, consequently, $\hat{O}^{-1}$ depend on a parameter t,

$$\frac{\mathrm{d}\hat{O}^{-1}(t)}{\mathrm{d}t} = -\hat{O}^{-1}\frac{\mathrm{d}\hat{O}(t)}{\mathrm{d}t}\hat{O}^{-1}\,.$$

Special operators: Adjoint operator

- $\hat{O}^\dagger$ is the **adjoint** of $\hat{O}$, if for any scalar product $\langle\phi|\hat{O}\chi\rangle = \langle\phi\hat{O}^\dagger|\chi\rangle$.
- When represented as a matrix, $\hat{O}^\dagger$ emerges from $\hat{O}$ by transposing and complex-conjugating its matrix components.
- Properties of adjoint operators:
  - $\left(\hat{O}^\dagger\right)^\dagger = \hat{O}$;
  - $\left(\hat{O}^{-1}\right)^\dagger = \left(\hat{O}^\dagger\right)^{-1}$;
  - $\left(c\hat{O}\right)^\dagger = c^*\,\hat{O}^\dagger\ \forall c \in \mathbf{C}$;
  - $\left(\hat{O}+\hat{Q}\right)^\dagger = \hat{O}^\dagger + \hat{Q}^\dagger$;
  - $\left(\hat{O}\hat{Q}\right)^\dagger = \hat{Q}^\dagger\hat{O}^\dagger$.

  In general, moving an operator, acting on a ket, to act on the bra (and vice versa) essentially translates it into its adjoint.

Special operators: Hermitean operators

An operator $\hat{H}$ is called **self-adjoint** or **Hermitean** if $\hat{H}^\dagger = \hat{H}$.
This means that all diagonal elements are real numbers: $H_{ii} \in \mathbf{R}$.
Properties of Hermitean operators include:

- $\left\langle \phi \middle| \hat{H} \middle| \chi \right\rangle = \left\langle \phi\hat{H}|\chi \right\rangle = \left\langle \phi|\hat{H}\chi \right\rangle$, following from its definition.
- $\left\langle \phi \middle| \hat{H} \middle| \phi \right\rangle \in \mathbf{R}$, a real number for **all** kets $|\phi\rangle$.
- $\forall$ Hermitean operators $\hat{H}$, $\hat{K}$:
  - $\hat{H} + \hat{K}$, $\left\{\hat{H},\, \hat{K}\right\} \equiv \left[\hat{H},\, \hat{K}\right]_+ \equiv \hat{H}\hat{K} + \hat{K}\hat{H}$, $i\left[\hat{H},\, \hat{K}\right]$ are Hermitean;
  - $\forall r \in \mathbf{R}$: $r\hat{H}$ is Hermitean;
  - $\hat{H}^n$, $\mathrm{d}\hat{H}(t)/\mathrm{d}t$ are Hermitean;
  - $\forall$ operators $\hat{A}$: $\hat{A}\hat{H}\hat{A}^\dagger$ is Hermitean.
- Note: If, in some representation all entries of an Hermitean operator $\hat{H}$ are real, the corresponding matrix is **symmetric**: $H_{ij} = H_{ji}$.

Special operators: Unitary operators

An operator $\hat{U}$ is called **unitary** if $\hat{U}^\dagger = \hat{U}^{-1}$.
Properties of unitary operators include:

- $\hat{U}^\dagger\hat{U} = \hat{U}\hat{U}^\dagger = \hat{\mathbf{1}}$
- $\left\langle \hat{U}\chi | \hat{U}\phi \right\rangle = \left\langle \chi | \hat{U}^\dagger\hat{U} | \phi \right\rangle = \langle\chi|\phi\rangle$. In other words:

> Under unitary transformations, $|\psi\rangle \to \hat{U}\,|\psi\rangle$, scalar products are invariant. In particular, orthogonal vectors stay orthogonal.

- $a\hat{U}$ is unitary if $aa^* = 1$;
- $\hat{U}^n$ is unitary if $n > 0$ or $-n \in \mathbf{N}$;
- $\hat{U}\hat{V}$ is unitary for all unitary operators $\hat{U}$ and $\hat{V}$.

Learning outcomes

- Operators and linear operators and their representation as matrices.
- Special operators (inverse, adjoint, Hermitean, unitary) and their properties.

Control questions

3.1 Show that

(a) $a\hat{U}$ is unitary if $aa^* = 1$ and $\hat{U}$ is unitary;

(b) $\hat{U}\hat{V}$ is unitary for all unitary operators $\hat{U}$ and $\hat{V}$;

(c) The unitarity of the matrix $\hat{V} = \frac{1}{\sqrt{|\alpha|^2+|\beta|^2}}\begin{pmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{pmatrix}$, where α, β are arbitrary complex numbers.

3.2 The trace of an operator, $\mathrm{Tr}\left(\hat{O}\right)$, is defined as the sum over its diagonal elements, $\mathrm{Tr}\left(\hat{O}\right) = \sum\limits_i O_{ii}$.

(a) What are the matrix elements of the unit operator $\hat{\mathbf{1}}$? Calculate its trace in an N-dimensional Hilbert space.

(b) Express the product of two operators $\hat{L}$ and $\hat{M}$ using component notation, and show that $\mathrm{Tr}(\hat{L}\hat{M}) = \mathrm{Tr}(\hat{M}\hat{L})$.