Theoretical Physics II B – Quantum Mechanics

Lecture 2

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1 State vectors & Hilbert space

Solutions to previous control questions

1.1 The properties are: closure, commutativity, associativity, distributive law, and closure under multiplication with a complex number

1.2 All done by direct calculation:

(a) $zz^* = a^2 + b^2 \geq 0$ and real.

(b) $z + z^* = 2a \ \in \mathbf{R}$.

(c) $(z_1 + z_2)^* = [a_1 + a_2 + (b_1 + b_2)i]^* = [a_1 + a_2 - (b_1 + b_2)i] = z_1^* + z_2^*$.

(d) $(z_1 z_2)^* = a_2 a_2 - b_1 b_2 - (a_1 b_2 + a_2 b_1)i = z_1^* z_2^*$.

(e) $|z_1 z_2| = |z_1||z_2|$ from relations above.

1.3 A set of vectors $\{|v_i\rangle\}$ are linearly independent, if it is impossible to represent one vector as linear combination of the others, i.e. if there are no constants c_i such that

$$|v_1\rangle = \sum_{i=2} c_i \; |v_i\rangle \; .$$

While this is th case for the first example - i.e. they are linearly independent; for the second choice of $|b\rangle$ one can write $|b\rangle = i\,|a\rangle$.

Why state vectors?

- Up to now, used the concept of wave (state) functions as mathematical representations for the state of a system.
- To further analyse properties, need many theorems from the theory of (complex) functions and integral transformations.
- Can formulate these theorems in terminology of vectors and vector calculus. Allows for simple interpretation of many properties of QM in n- or ∞-dimensional vector space.
- Caveat: This vector space is *purely abstract* and has *nothing in common with position space* of three real dimensions.
- However: Will try and represent ideas through sketches in 2-dimensional real space, where possible.

Ket-space as vector space

- Denote vectors by: $|\phi\rangle$, $|\chi\rangle$, ..., $|\uparrow\rangle$, $|\downarrow\rangle$, ..., $|\underline{r}\rangle$, $|\underline{p}\rangle$, ...
  (use quantum numbers etc. to label them)
- Kets form a *complex vector space* $\mathcal{V}$ *under addition*,
  if $\forall\,|\phi\rangle, |\chi\rangle, |\psi\rangle, \ldots \in \mathcal{V}$ the following properties are fulfilled:
  - Closure: $|\phi\rangle + |\chi\rangle \quad \in \mathcal{V}$.
  - Commutativity: $|\phi\rangle + |\chi\rangle = |\chi\rangle + |\phi\rangle$
  - Associativity: $|(\phi+\chi)\rangle + |\psi\rangle = |\phi\rangle + |(\chi+\psi)\rangle$.
  - Multiplication with a complex number $c \in \mathbf{C}$: $c\,|\phi\rangle = |(c\phi)\rangle$
    is "parallel" with $|\phi\rangle$: $|\phi\rangle \parallel |(c\phi)\rangle$
  - Distributive law: $c\,|(\phi+\chi)\rangle = c\,|\phi\rangle + c\,|\chi\rangle$.
- Introduce a *dual* space $\langle\phi|$, $\langle\chi|$, ..., $\langle\uparrow|$, $\langle\downarrow|$, ..., $\langle\underline{r}|$, $\langle\underline{p}|$, ...
  to define scalar products of vectors: $\langle\phi|\chi\rangle$.

Promoting vector spaces to Hilbert spaces

Note: In the lecture Hilbert spaces will be introduced as synonymous to the unitary space.
For a more precise definition, cf. the literature.

A vector space $\mathcal{V}$ is called a Hilbert space, if a scalar product of its vectors $\langle\phi|\chi\rangle$ can be defined such that

- $\forall\,|\phi\rangle\,,\,|\chi\rangle \in \mathcal{V}$: $\langle\phi|\chi\rangle = c$ with $c \in \mathbf{C}$ a complex number.
- In this, *sequence matters*: $\boxed{\langle\phi|\chi\rangle = c^* = \langle\chi|\phi\rangle^*}$
- Distributivity: $\langle\phi|\chi+\psi\rangle = \langle\phi|\chi\rangle + \langle\phi|\psi\rangle$
- Scaling with complex numbers $c \in \mathbf{C}$: $\langle\phi|(c\chi)\rangle = c\,\langle\phi|\chi\rangle$
  but: $\langle(c\phi)|\chi\rangle = c^*\,\langle\phi|\chi\rangle$
- Positive definite norm: $\langle\phi|\phi\rangle \geq 0 \longrightarrow ||\phi|| = \sqrt{\langle\phi|\phi\rangle}$

In addition one can define an

- Orthogonality criterion: $\langle\phi|\chi\rangle = 0 \longleftrightarrow \phi \perp \chi$

Note: In general, the Hilbert space are ∞-dimensional.

Example: Dealing with bras and kets

Assume $|\phi_1\rangle$ and $|\phi_2\rangle$ are **orthonormal**, i.e.

$$\langle\phi_1|\phi_2\rangle = \langle\phi_2|\phi_1\rangle^* = 0 \quad \text{and} \quad \langle\phi_1|\phi_1\rangle = \langle\phi_2|\phi_2\rangle = 1\,.$$

Two linearly independent states of a physical system are given by

$$|\psi_1\rangle = 4i\,|\phi_1\rangle - 12i\,|\phi_2\rangle \quad \text{and} \quad |\psi_2\rangle = |\phi_1\rangle - 6i\,|\phi_2\rangle\ .$$

- What is the associated bra, $\langle\psi_1|$?

$$\langle\psi_1| = (4i)^*\,\langle\phi_1| - (12i)^*\,\langle\phi_2| = -(4i)\,\langle\phi_1| + (12i)\,\langle\phi_2|\ .$$

- Determine $|\psi_1+\psi_2\rangle$ and $\langle\psi_1+\psi_2|$:

$$\begin{aligned} |\psi_1+\psi_2\rangle &= (1+4i)\,|\phi_1\rangle - 18i\,|\phi_2\rangle \\ \langle\psi_1+\psi_2| &= (1+4i)^*\,\langle\phi_1| - (18i)^*\,\langle\phi_2| = (1-4i)\,\langle\phi_1| + 18i\,\langle\phi_2|\ . \end{aligned}$$

Example (continued)

- Calculate $\langle\psi_1|\psi_2\rangle$.

$$\begin{aligned}\langle\psi_1|\psi_2\rangle &= \left(-4i\,\langle\phi_1| + 12i\,\langle\phi_2|\right)\left(|\phi_1\rangle - 6i\,|\phi_2\rangle\right)\\ &= -4i\,\langle\phi_1|\phi_1\rangle + 12i\,\langle\phi_2|\phi_1\rangle - 24\,\langle\phi_1|\phi_2\rangle + 72\,\langle\phi_2|\phi_2\rangle = 72 - 4i\,.\end{aligned}$$

- Show, by direct calculation, that indeed $\langle\psi_2|\psi_1\rangle = \langle\psi_1|\psi_2\rangle^*$.

$$\begin{aligned}\langle\psi_2|\psi_1\rangle &= \left(\langle\phi_1| + 6i\,\langle\phi_2|\right)\left(4i\,|\phi_1\rangle - 12i\,|\phi_2\rangle\right)\\ &= 4i\,\langle\phi_1|\phi_1\rangle - 24\,\langle\phi_2|\phi_1\rangle - 12i\,\langle\phi_1|\phi_2\rangle + 72\,\langle\phi_2|\phi_2\rangle = 72 + 4i\,.\end{aligned}$$

Note that this relation would hold also true without $|\phi_1\rangle$ and $|\phi_2\rangle$ being ortthonormal.

Base vectors

- The decomposition of a vector $|\phi\rangle$ into a set of base vectors $\{|v_k\rangle\}$ depends on the *dimension* N of the corresponding vector space $\mathcal{V}$: there are N vectors $|v_k\rangle$:

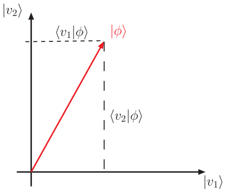
$$|\phi\rangle = \sum_{k=1}^{N} \phi_k |v_k\rangle \ ,$$

  where the *components* ϕ_k of the vector $|\phi\rangle$ with respect to the base $\{|v_k\rangle\}$ are complex numbers.
- The index k enumerates the base vectors, just as in the linear algebra lectures you've encountered so far.

Orthonormal base

- Assume *orthonormal* base vectors: $\langle v_k | v_l \rangle = \delta_{kl}$
- To extract the components ϕ_l, multiply $|\phi\rangle = \sum\limits_{k=1}^{N} \phi_k \, |v_k\rangle$ from left with $\langle v_l|$:

$$\langle v_l|\phi\rangle = \sum_{k=1}^{N} \phi_k \, \langle v_l|v_k\rangle = \phi_l$$



- This yields the decomposition

$$|\phi\rangle = \sum_{k=1}^{N} |v_k\rangle \, \langle v_k|\phi\rangle$$

If every $|\phi\rangle \in \mathcal{V}$ can be decomposed as above, the base $\{|v_k\rangle\}$ is called a *complete orthonormal base*.

Rewriting scalar products

- Extent the equation above, $|\phi\rangle = \sum_{k=1}^{N} |v_k\rangle \langle v_k|\phi\rangle$ to the "bra"-space:

$$\langle\chi| = \sum_{k=1}^{N} \langle\chi|v_k\rangle \langle v_k|$$

- Then scalar products can be written in components as:

$$\begin{aligned}\langle\chi|\phi\rangle &= \left[\sum_{l=1}^{N} \langle\chi|v_l\rangle \langle v_l|\right] \left[\sum_{k=1}^{N} |v_k\rangle \langle v_k|\phi\rangle\right] \\ &= \sum_{l,k=1}^{N} \langle\chi|v_l\rangle \underbrace{\langle v_l|v_k\rangle}_{\delta_{kl}} \langle v_k|\phi\rangle = \sum_{k=1}^{N} \langle\chi|v_k\rangle \langle v_k|\phi\rangle\end{aligned}$$

- Using the rules of matrix multiplication, you may think of bras as row vectors, while kets are column vectors.

Continous bases

- Kets $|\phi\rangle$ living in an infinitely-dimensional Hilbert space can be expanded in **continous base vectors** $|v(k)\rangle$ through

$$|\phi\rangle = \int \mathrm{d}k\, \phi(k)\, |v(k)\rangle \ ,$$

where the continous components $\phi(k)$ of the vector $|\phi\rangle$ with respect to the base $\{|v(k)\rangle\}$ are now complex-valued functions, given by

$$\phi(k) = \int \mathrm{d}k\ \langle v(k)|\phi\rangle \ .$$

- For the base vectors to form an orthonormal base, they must satisfy an extension of $\langle v_k|v_l\rangle = \delta_{kl}$, namely

$$\langle v(k)|v(l)\rangle = \delta(k-l)\,.$$

Products of (position & momentum space) wave functions

- Wave functions in position or momentum space are postulated to be square integrable. In Dirac notation (bras and kets) one could interpret them as the components of the state vector $|\psi\rangle$ decomposed into position or momentum space base vectors, denoted as $|\underline{r}\rangle$ or $|\underline{p}\rangle$:

$$\psi(\underline{r}) = \langle\underline{r}|\psi\rangle \quad \text{and} \quad \psi(\underline{p}) = \langle\underline{p}|\psi\rangle$$

  In this case, the Hilbert space is ∞-dimensional, with

$$\langle\underline{r}|\underline{r}'\rangle = \delta(\underline{r}-\underline{r}')\,.$$

- Following the logic above:

$$\int \mathrm{d}\underline{r}\mathrm{d}\underline{r}'\,\langle\phi|\underline{r}\rangle\,\langle\underline{r}'|\psi\rangle = \int \mathrm{d}\underline{r}\,\langle\phi|\underline{r}\rangle\,\langle\underline{r}|\psi\rangle = \int \mathrm{d}\underline{r}\,\phi^*(\underline{r})\psi(\underline{r}) = \langle\phi|\psi\rangle$$

Learning outcomes

- Dirac notation: bras and kets.
- Kets as vectors in a vector space and their properties.
- Scalar products and their properties in Hilbert space.
- Formal decomposition into base vectors, with scalar products as components.
- Scalar products as sums/products over components.

Control questions

At the end of each lecture, there will be some control questions. Try to solve them as part of your preparation for the next lecture.

2.1 What is the general result for the scalar product of two parallel (orthogonal) normalised (unit-length) vectors in Hilbert space?

2.2 Assuming an orthonormal base $\{|v_k\rangle\}$, calculate the norms and scalar product $\langle\phi|\chi\rangle$ of the vectors

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

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