Integrated Course Ib
Theoretical quantum mechanics

lecture by
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Literature

– JUN J. SAKURAI, JIM NAPOLITANO: *Modern quantum mechanics*, Addison-Wesley, 2011
ISBN: 0-321-50336-8

– LEONARD I. SCHIFF: *Quantum mechanics*, McGraw-Hill, 1968
ISBN: 0-07-085643-5

– Any introductory book on quantum mechanics.

– RICHARD P. FEYNMAN, ROBERT B. LEIGHTON, MATTHEW L. SANDS: *Lectures on physics*

Contents

1 The Formalism and its interpretation

As any theory about physical phenomenons, quantum mechanics requires

i) kinematical aspects: The (mathematical) space where physical states are represented.

   Example from classical mechanics: points in phase space

ii) the definition of observables: Which quantities can be measured and how to represent them in the space of states?

   Example from classical mechanics: any function $f(\vec{r},\vec{p})$

   (This is more complicated in quantum mechanics.)

iii) an dynamical law: How do states evolve in "time"?

   Example from classical mechanics: Hamilton's equations determine $(\vec{q}(t), \vec{p}(t))$ depending on $(\vec{q}(t_0), \vec{p}(t_0))$.

1.1 The kinematical aspects of quantum mechanics

The FIRST POSTULATE says:

> "The state of a quantum mechanical system is represented as a normalized vector in a (complex) Hilbert space.
> Vectors, which differ only by a phase, represent the same state."

To understand what this means, we introduce some concepts:

a) *Hilbert space*: A (finite or infinite dimensional) complete vector space with a positive definite scalar product. Following Dirac, elements in the Hilbert space $\mathcal{H}$ are called *kets* and we represent them by $|\psi\rangle, |\phi\rangle \in \mathcal{H}$.

   For complex numbers $a,b \in \mathbb{C}$ also $a|\psi\rangle + b|\phi\rangle \in \mathcal{H}$ is a element of the Hilbert space.

   The sum is associative and the product by scalars is distributive.

b) *Scalar product*: The operation associating a complex number to each pair of states

$$\begin{aligned}\langle .,. \rangle : \mathcal{H} \times \mathcal{H} &\to \mathbb{C} \\ (|\psi\rangle, |\phi\rangle) &\mapsto \langle \psi,\phi \rangle\end{aligned}$$

   with the properties

$$\langle \eta, a\phi + b\psi \rangle = a\langle \eta,\phi \rangle + b\langle \eta,\psi \rangle \qquad \langle \psi,\phi \rangle = \langle \phi,\psi \rangle^*$$
$$\langle \psi,\psi \rangle \geq 0 \qquad \langle \psi,\psi \rangle = 0 \quad \Leftrightarrow \quad |\psi\rangle = 0$$

for $a,b \in \mathbb{C}$ and $|\phi\rangle, |\psi\rangle, |\eta\rangle \in \mathcal{H}$ is called the scalar product.

The *norm* of a state $|\psi\rangle$ is then defined as:

$$\|\psi\| := \||\psi\rangle\| := \sqrt{\langle\psi,\psi\rangle}$$

If $\||\psi\rangle\| = 1$, then $|\psi\rangle$ is said to be *normalized.*

c) *Phase*: Complex number $z \in \mathbb{C}$ with unit norm, that means $zz^* = 1$. It can be represented via a real number $\alpha \in \mathbb{R}$ as $z = e^{\mathbf{i}\alpha}$.

The physical state associated with $|\psi\rangle$ and $e^{\mathbf{i}\alpha}|\psi\rangle$ is THE SAME.

d) C*omplete basis*: A family of kets $(|\phi_i\rangle)_{i\in I\subseteq\mathbb{N}}$ such that for ALL states $|\psi\rangle \in \mathcal{H}$, there is a family of complex numbers $(c_i)_{i\in I\subseteq\mathbb{N}}$ (depending on $|\psi\rangle$) with:

$$|\psi\rangle = \sum_{i\in I} c_i |\phi_i\rangle$$

If $\langle\phi_i,\phi_j\rangle = \delta_{ij}$, then the basis is *complete* and *orthonormal.*

In the case of an uncountably infinite vector space the basis $(|q\rangle)_{q\in\mathbb{R}}$ can be written as a function of a real variable. The representation of $|\psi\rangle$ then is an infinite sum, that is an integral

$$|\psi\rangle = \int \psi(q)|q\rangle\,\mathrm{d}q$$

and a complete and orthonormal basis is characterized by $\langle q,q'\rangle = \delta(q-q')$.

e) *Adjoint*: For each Hilbert space $\mathcal{H}$ there is another Hilbert space $\mathcal{H}^*$ called *dual*, with elements $\langle f| \in \mathcal{H}^*$, which are LINEAR FUNCTIONALS acting on $\mathcal{H}$:

$$\begin{aligned}\langle f| : \mathcal{H} &\to \mathbb{C}\\ |\psi\rangle &\mapsto \langle f|\psi\rangle\end{aligned}$$

$\langle\psi|\phi\rangle$ is called *bracket.* Riesz theorem says, that there is a ONE TO ONE correspondence between $\mathcal{H}$ and $\mathcal{H}^*$:

$$\underset{|\psi\rangle\in\mathcal{H}}{\forall}\ \underset{\langle\psi|\in\mathcal{H}^*}{\exists}\ \underset{|\phi\rangle\in\mathcal{H}}{\forall}\ :\ \langle\psi|\phi\rangle = \langle\psi,\phi\rangle, \|\langle\psi|\| = \||\psi\rangle\|$$

The so associated $\langle\psi|$ is the *adjoint* of $|\psi\rangle$, called *bra*, and we write:

$$\begin{aligned}{}^\dagger : \mathcal{H} &\to \mathcal{H}^*\\ |\psi\rangle &\mapsto (|\psi\rangle)^\dagger = \langle\psi|\end{aligned}$$

The function † is semilinear, that means for $a,b \in \mathbb{C}$ and $|\psi\rangle, |\phi\rangle \in \mathcal{H}$ is:

$$(a|\psi\rangle + b|\phi\rangle)^\dagger = a^*\langle\psi| + b^*\langle\phi|$$

f) *Representation*: Assume that $(|\phi_i\rangle)_{i\in I\subseteq\mathbb{N}}$ (respectively $(|q\rangle)_{q\in\mathbb{R}}$) is a complete orthonormal basis. The ket $|\psi\rangle$ is said to "be represented" in that basis by associating:

discrete case | continous case

$$|\psi\rangle \mapsto \begin{pmatrix} \langle\phi_1|\psi\rangle \\ \langle\phi_2|\psi\rangle \\ \vdots \end{pmatrix} \in \mathbb{C}^{|I|} \qquad\qquad |\psi\rangle \mapsto \langle q|\psi\rangle =: \psi(q)$$

$$\langle\psi| \mapsto \begin{pmatrix} \langle\phi_1|\psi\rangle^* \\ \langle\phi_2|\psi\rangle^* \\ \vdots \end{pmatrix} \in \mathbb{C}^{|I|} \qquad\qquad \langle\psi| \mapsto \langle q|\psi\rangle^* = \psi(q)^*$$

This $\psi(q)$ is the wave function.

g) *Exterior product*: The object $|\phi\rangle\langle\psi| : \mathcal{H} \to \mathcal{H}$ is a linear operator acting on $|\eta\rangle \in \mathcal{H}$ defined by

$$(|\phi\rangle\langle\psi|)\,|\eta\rangle := \underbrace{\langle\psi|\eta\rangle}_{\in\mathbb{C}}|\phi\rangle$$

with the adjoint:

$$(|\phi\rangle\langle\psi|)^\dagger := |\psi\rangle\langle\phi|$$

Example from linear algebra:

$$\vec{v} = (v_1, \ldots, v_n)^T \qquad\qquad \vec{u} = (u_1, \ldots, u_n)^T$$

$$\vec{v}^T\vec{u} = \sum_{i=1}^{n} v_i u_i$$

$$\vec{u}\vec{v}^T = \begin{pmatrix} u_1v_1 & \ldots & u_1v_n \\ \vdots & \ddots & \vdots \\ u_nv_1 & \ldots & u_nv_n \end{pmatrix}$$

1.2 Observables and measurements in quantum mechanics

What can be observed and how measurements affect quantum states is encoded into the following two POSTULATES:

> "Observables in quantum mechanics are represented by LINEAR HERMITIAN OPERATORS on $\mathcal{H}$."
>
> "The results of a measurement of the physical quantity represented by an observable can only take values belonging to the SPECTRUM of the observable. Just after measurement, that gives one of the eigenvalues of the observable, the state belongs to corresponding eigenspace.“

a) $\hat{A}: \mathcal{H} \to \mathcal{H}$ is a *linear* operator if and only if:

$$\hat{A}\left(a\left|\psi\right\rangle + b\left|\phi\right\rangle\right) = a\hat{A}\left|\psi\right\rangle + b\hat{A}\left|\phi\right\rangle$$

For every linear operator $\hat{A}$ there is the identity:

$$\left\langle\psi\middle|\hat{A}\phi\right\rangle =: \left\langle\phi\middle|\hat{A}^\dagger\psi\right\rangle^*$$

$\hat{A}^\dagger$ is called the *adjoint* of $\hat{A}$. If and only if $\hat{A} = \hat{A}^\dagger$ then $\hat{A}$ is called HERMITIAN.

b) The *spectrum* of an operator $\hat{Q}$ is defined by a set of numbers Q_i, called *eigenvalues*, that fulfill the equation:

$$\hat{Q}\left|Q_i\right\rangle = Q_i\left|Q_i\right\rangle$$

The $\left|Q_i\right\rangle$ are the corresponding eigenvectors. If there is more than one eigenvector for the same eigenvalue then the spectrum is called *degenerated* and the different eigenvectors are denoted by $\left|Q_i^{(d)}\right\rangle$ with $d \in D \subseteq \mathbb{N}$.

Hermitian operators have REAL eigenvalues and ORTHOGONAL eigenvectors.

That means, if $\hat{A} = \hat{A}^\dagger$, $\hat{A}\left|a_i\right\rangle = a_i\left|a_i\right\rangle$, then $a_i = a_i^*$ and $\left\langle a_i\middle|a_j\right\rangle = 0$ if $i \neq j$.

If the eigenvectors are normalized, then we can write $\left\langle a_i\middle|a_j\right\rangle = \delta_{ij}$.

c) The *spectrum decomposition* of a Hermitian operator ($\hat{A} = \hat{A}^\dagger$)

discrete case	continous case
$\hat{A}\left\|a_i\right\rangle = a_i\left\|a_i\right\rangle$	$\hat{A}\left\|a\right\rangle = a\left\|a\right\rangle$

is given by:

$$\hat{A} = \sum_{i\in I} a_i\left|a_i\right\rangle\left\langle a_i\right| \qquad\qquad \hat{A} = \int a\left|a\right\rangle\left\langle a\right|\mathrm{d}a$$

In linear algebra a symmetric matrix $M = M^T$ with eigenvalues m_i for $i \in \{1,\ldots,n\}$ can be written as:

$$M = \begin{pmatrix} m_1 & 0 & \ldots & 0 \\ 0 & m_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \ldots & 0 & m_n \end{pmatrix} = m_1\begin{pmatrix} 1 & 0 & \ldots & 0 \\ 0 & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \ldots & 0 & 0 \end{pmatrix} + \ldots + m_n\begin{pmatrix} 0 & 0 & \ldots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & 0 & 0 \\ 0 & \ldots & 0 & 1 \end{pmatrix}$$

d) The *unit operator* $\hat{I}$ defined by

$$\underset{\left|\phi\right\rangle\in\mathcal{H}}{\forall} : \hat{I}\left|\phi\right\rangle = \left|\phi\right\rangle$$

can be written as

discrete case	continous case
$\hat{I} = \sum_{i\in I}\left\|a_i\right\rangle\left\langle a_i\right\|$	$\hat{I} = \int\left\|a\right\rangle\left\langle a\right\|\mathrm{d}a$

where $(\left|a_i\right\rangle)_{i\in I\subseteq\mathbb{N}}$ (respectively $(\left|a\right\rangle)_{a\in\mathbb{R}}$) is a complete orthonormal basis.

e) The *projection* of $|\psi\rangle$ along a basis vector $|a_i\rangle$ (respectively $|a\rangle$) is:

discrete case	continous case
$(\|a_i\rangle \langle a_i\|) \|\psi\rangle = \langle a_i\|\psi\rangle \|a_i\rangle$	$(\|a\rangle \langle a\|) \|\psi\rangle = \langle a\|\psi\rangle \|a\rangle$

f) The *algebra* of the operators $\hat{Q}_1$ and $\hat{Q}_2$ is:

$$\left(\hat{Q}_1\hat{Q}_2\right)|\psi\rangle := \hat{Q}_1\left(\hat{Q}_2|\psi\rangle\right) \neq \left(\hat{Q}_2\hat{Q}_1\right)|\psi\rangle$$
$$\left(\hat{Q}_1\hat{Q}_2\right)^\dagger := \hat{Q}_2^\dagger\hat{Q}_1^\dagger$$

The *commutator* is defined by:

$$\left[\hat{Q}_1,\hat{Q}_2\right] := \hat{Q}_1\hat{Q}_2 - \hat{Q}_2\hat{Q}_1$$

It is bilinear and has the properties:

i) It is antisymmetric:

$$\left[\hat{Q}_1,\hat{Q}_2\right] = -\left[\hat{Q}_2,\hat{Q}_1\right]$$

ii) Jacobi identity:

$$\left[\hat{Q}_1,\left[\hat{Q}_2,\hat{Q}_3\right]\right] + \left[\hat{Q}_2,\left[\hat{Q}_3,\hat{Q}_1\right]\right] + \left[\hat{Q}_3,\left[\hat{Q}_1,\hat{Q}_2\right]\right] = 0$$

iii) Leibniz identity:

$$\left[\hat{Q}_1,\hat{Q}_2\hat{Q}_3\right] = \hat{Q}_2\left[\hat{Q}_1,\hat{Q}_3\right] + \left[\hat{Q}_1,\hat{Q}_2\right]\hat{Q}_3$$

Due to these identities the commutator is analogous to the classical Poisson bracket.
Two observables $\left(\hat{A} = \hat{A}^\dagger, \hat{B} = \hat{B}^\dagger\right)$ are called *compatible* if and only if $\left[\hat{A},\hat{B}\right] = 0$.
Theorem: If $\hat{A}$ and $\hat{B}$ are compatible then there exists a basis $(|k_i\rangle)_{i\in I\subseteq\mathbb{N}}$ such that:

$$\hat{A}|k_i\rangle = a_i|k_i\rangle$$
$$\hat{B}|k_i\rangle = b_i|k_i\rangle$$

Therefore the states $|k_i\rangle$ have well defined properties (a_i,b_i).

g) i) The *matrix representation* of an operator WITH RESPECT TO THE BASIS $(|a_i\rangle)_{i\in\{1,\ldots,n\}}$ (respectively $(|q\rangle)_{q\in\mathbb{R}}$) is:

discrete case

$$\hat{Q} \to \begin{pmatrix} \langle a_1|\hat{Q}|a_1\rangle & \ldots & \langle a_1|\hat{Q}|a_n\rangle \\ \vdots & \ddots & \vdots \\ \langle a_n|\hat{Q}|a_1\rangle & \ldots & \langle a_n|\hat{Q}|a_n\rangle \end{pmatrix} = \left(\langle a_i|\hat{Q}|a_j\rangle\right)_{ij} =: Q_{ij}$$

continuous case

$$\hat{Q} \to \langle q|\hat{Q}|q'\rangle = Q\left(q,q'\right)$$

ii) The *trace* of $\hat{Q}$ is defined by

discrete case	continuous case
$\mathrm{Tr}\left(\hat{Q}\right) = \sum_{i=1}^{n} \langle a_i \| \hat{Q} \| a_i \rangle$	$\mathrm{Tr}\left(\hat{Q}\right) = \int Q\left(q,q\right) \mathrm{d}q$

ans is independent of the basis.

Therefore the equation

$$\hat{Q} |\psi\rangle = |\phi\rangle$$

can be written in this basis by:

i) Multiplying $\langle a_i|$ from the left: $\langle a_i| \hat{Q} |\phi\rangle = \langle a_i|\phi\rangle$

ii) Insert an unit operator after $\hat{Q}$:

$$\langle a_i| \hat{Q}\hat{I} |\phi\rangle = \langle a_i| \hat{Q} \left(\sum_{j=1}^{n} |a_j\rangle \langle a_j| \right) |\phi\rangle = \sum_{j=1}^{n} \langle a_i| \hat{Q} |a_j\rangle \langle a_j|\psi\rangle = \langle a_i|\phi\rangle$$

This is the component form of the vector equation:

$$\begin{pmatrix} Q_{11} & \dots & Q_{1n} \\ \vdots & & \vdots \\ Q_{n1} & \dots & Q_{nn} \end{pmatrix} \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_n \end{pmatrix} = \begin{pmatrix} \phi_1 \\ \vdots \\ \phi_n \end{pmatrix}$$

The continuous version is

$$\int Q\left(q,q'\right) \psi\left(q'\right) \mathrm{d}q' = \phi\left(q\right)$$

with $Q\left(q,q'\right) := \langle q| \hat{Q} |q\rangle$, $\psi\left(q'\right) = \langle q'|\psi\rangle$ and $\phi\left(q\right) = \langle q|\phi\rangle$.

h) Change of basis and unitary transformations.

i) An operator $\hat{U}$ is called *unitary* if and only if $\hat{U}^T = \hat{U}^{-1}$.

ii) Unitary transformations ("transformation" is the same as "operator") preserve scalar products. For $|\psi\rangle, |\phi\rangle \in \mathcal{H}$ we define:

$$|\psi'\rangle := \hat{U} |\psi\rangle \qquad\qquad |\phi'\rangle := \hat{U} |\phi\rangle$$

Then the scalar product is the same:

$$\langle \psi' | \phi' \rangle = \langle \psi|\phi\rangle$$

iii) Unitary transformations represent changes of the basis.

$$|\psi\rangle = \hat{I} |\psi\rangle = \left(\sum_i |a_i\rangle \langle a_i| \right) |\psi\rangle = \sum_{i\in I} \langle a_i|\psi\rangle |a_i\rangle$$

$$\langle b_i|\psi\rangle = \sum_{j\in I} \langle b_i|a_j\rangle \langle a_j|\psi\rangle$$

$$\begin{pmatrix} \psi_1^{(b)} \\ \vdots \\ \psi_N^{(b)} \end{pmatrix} = \mathbb{U} \cdot \begin{pmatrix} \psi_1^{(a)} \\ \vdots \\ \psi_N^{(a)} \end{pmatrix}$$
$$[\mathbb{U}]_{ij} = U_{ij} = \langle b_i | a_j \rangle$$

iv) For operators the transformations are:

$$\begin{aligned} Q_{ij}^{(b)} &= \langle b_i | \hat{Q} | b_j \rangle = \langle b_i | \hat{I}\hat{Q}\hat{I} | b_j \rangle = \sum_{l,m \in I} \langle b_i | a_l \rangle \langle a_l | \hat{Q} | a_m \rangle \langle a_m | b_j \rangle = \\ &= \sum_{l,m \in I} U_{il} Q_{lm}^{(a)} U_{mj} = \sum_{l,m} U_{il} Q_{lm}^{(a)} (U_{jm})^* \\ \mathbb{Q}^{(b)} &= \mathbb{U}\mathbb{Q}^{(a)}\mathbb{U}^\dagger \end{aligned}$$

2 „Simple“ applications

3 Symmetries in quantum mechanics (Angular momentum)

4 Perturbation theory (time-independent)

5 Perturbation theory (time-dependent)

6 Many-particle systems

7 Scattering theory

Appendix

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