

Lecture notes FY2045 Quantum Mechanics I

— 3 General formulation of Quantum Mechanics

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1 Motivation

So far we have worked in the position representation, where a system is described by the wavefunction $\Psi(\mathbf{r}, t)$. We also briefly looked at the function $\Phi(\mathbf{p}, t)$ which appeared when expanding Ψ in terms of momentum eigenfunctions. Analogous to $|\Psi|^2$, the interpretation of $|\Phi|^2$ is as a probability density in *momentum space*. Moreover, it is possible to formulate quantum mechanics in momentum space, where Φ is the *momentum space wavefunction*.

In fact, there are multiple ways of formulating a quantum theory. This lead Dirac to suggest and introduce a notation which could help with the development of the theory, and provide a unified way of treating different quantities.¹ We will now turn to this more general description, known as Dirac's bra-ket notation, or simply Dirac notation.

2 Dirac's bra-ket notation

In Dirac notation, a quantum mechanical state of a system is described by a state vector $|\Psi\rangle$ in a complex, linear vector space \mathcal{H} called Hilbert space. The dimension of the vector space can be finite or infinite. $|\Psi\rangle$ is a function of time — $|\Psi\rangle = |\Psi(t)\rangle$.

For each vector $|a\rangle$, we define the dual vector $\langle a|$ in the dual space \mathcal{H}^* ,

$$|a\rangle \xleftrightarrow{\text{dual}} \langle a|,$$

so that we can define a *scalar product*

$$\langle a| \cdot |b\rangle \equiv \langle a|b\rangle. \quad (1)$$

This is a complex number,² and has the property

$$\langle a|b\rangle = \langle b|a\rangle^*, \quad (2)$$

where $*$ denotes complex conjugation.³ Moreover,

$$c|a\rangle \xleftrightarrow{\text{dual}} c^* \langle a|, \quad c \in \mathbb{C}. \quad (3)$$

We call $|\cdot\rangle$ a *ket*, and $\langle \cdot|$ a *bra*, as in $\langle \text{bra} | \text{ket} \rangle$ — from *bracket*.

3 Interpretation

How should we think of these abstract vectors? Let's consider a double slit experiment with electrons.

See also Compendium 10.1 by Øverbø or Ch. 6.1 in Hemmer.

¹ "In mathematical theories the question of notation, while not of primary importance, is yet worthy of careful consideration, since a good notation can be of great value in helping the development of a theory, by making it easy to write down those quantities or combinations of quantities that are important, and difficult or impossible to write down those that are unimportant." — Dirac (1939).

² See Renou *et al.* (2023, 2021) for a discussion of whether quantum mechanics has to be formulated using complex numbers and how to test this experimentally, and Wu *et al.* (2022) for a recent experimental refutation of so-called *real quantum mechanics*.

³ This reminds us of

$$\int dx \psi_1^*(x) \psi_2(x) = \left[\int dx \psi_2^*(x) \psi_1(x) \right]^*.$$

3.1 Example — Electron double slit experiment

We want to describe the probability amplitude⁴ of an electron leaving the source at s , and arriving at the detector at position x , see fig. 1. With our new notation, we can write this as

$$\underbrace{\langle \text{Particle arrives at } x |}_{\text{Final condition}} \underbrace{|\text{Particle leaves } s \rangle}_{\text{Initial condition}} \equiv \langle x | s \rangle.$$

However, this can happen in two ways:

$$\langle x | s \rangle = \langle x | s \rangle_{\text{through 1}} + \langle x | s \rangle_{\text{through 2}}.$$

The amplitude $\langle x | s \rangle_{\text{through 1}}$ is the product of amplitude from s to 1, $\langle 1 | s \rangle$, and from 1 to x , $\langle x | 1 \rangle$:

$$\langle x | s \rangle_{\text{through 1}} = \langle x | 1 \rangle \langle 1 | s \rangle,$$

and similarly for from s to x through 2. Hence, we can write

$$\begin{aligned} \langle x | s \rangle &= \langle x | 1 \rangle \langle 1 | s \rangle + \langle x | 2 \rangle \langle 2 | s \rangle = \sum_{\text{slit}=1,2} \langle x | \text{slit} \rangle \langle \text{slit} | s \rangle \\ &= \langle x | \underbrace{\left[\sum_{\text{slit}=1,2} |\text{slit} \rangle \langle \text{slit}| \right]}_{\equiv 1} | s \rangle. \end{aligned}$$

We have found a *completeness relation*,

$$\sum_{\text{slit}=1,2} |\text{slit} \rangle \langle \text{slit}| = 1.$$

3.2 Relation to wavefunction

How can we then understand a state $|\psi\rangle$ and relate it to the wavefunction we are used to? The wavefunction gives the probability amplitude of finding a particle at position x . With the new notation

$$\langle \text{Particle is at } x | \text{Particle is in state } \psi \rangle$$

or simply

$$\langle x | \psi \rangle = \psi(x). \quad (4)$$

This is exactly our wavefunction! For instance, the wavefunction for an energy eigenstate with quantum number n is

$$\langle x | \psi_n \rangle = \psi_n(x).$$

If $|x\rangle$ is the state were a particle is at position x , and $|\psi_n\rangle$ is an energy eigenstate with energy E_n , $\langle x | \psi_n \rangle$ is the probability amplitude of finding the particle in eigenstate $|\psi_n\rangle$ at position x . Hence:

This section is based on Ch. 3 of Vol. III in the Feynman Lectures, Feynman *et al.* (1963)

⁴ The probability is the absolute square of the probability amplitude.

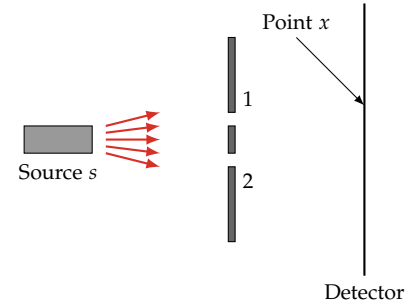


Figure 1: Electrons are sent from the source at s towards the two slits (1 and 2), and are detected by the detector at some position x .

The wavefunction

$$\psi(x) = \langle x | \psi \rangle$$

is the “component of the Hilbert space vector $|\psi\rangle$ in the $|x\rangle$ -direction”, or the projection of $|\psi\rangle$ on the basis vector $|x\rangle$.

There is, therefore, a one-to-one correspondence between wavefunction and state vector,

$$\begin{aligned}\psi(x) &\Leftrightarrow |\psi\rangle, \\ \psi_n(x) &\Leftrightarrow |\psi_n\rangle = |n\rangle = |E_n\rangle, \\ \psi_{x'}(x) &\Leftrightarrow |x'\rangle,\end{aligned}$$

etc. However, they are *different objects*, belonging to different vector spaces.

Other examples are

- $\langle p | \psi \rangle$ — projection on momentum basis vector,
 - $\langle \psi_n | \psi \rangle$ — projection on energy basis vector,
- etc. This requires that the sets of vectors are complete!

4 Completeness

Before looking at completeness for the state vectors in Hilbert space, let's take a look at the analogous case of ordinary vectors in 3D space.

4.1 Analogy — vectors in \mathbb{R}^3

An ordinary vector is often written down in terms of components in a Cartesian coordinate system,

$$\mathbf{A} = A_x \hat{\mathbf{e}}_x + A_y \hat{\mathbf{e}}_y + A_z \hat{\mathbf{e}}_z = \sum_i A_i \hat{\mathbf{e}}_i. \quad (5)$$

The components, A_i , depends on our choice of orthonormal basis vectors $\hat{\mathbf{e}}_i$. However, the vector \mathbf{A} itself is *independent of basis*! This means that we could write it in terms of other basis vectors, for instance in spherical coordinates,

$$\mathbf{A} = A_r \hat{\mathbf{e}}_r + A_\theta \hat{\mathbf{e}}_\theta + A_\phi \hat{\mathbf{e}}_\phi = \sum_i A'_i \hat{\mathbf{e}}'_i.$$

Even though, generally, the components $\hat{A}_i \neq \hat{A}'_i$, the vector \mathbf{A} is still the same. We can relate the basis vectors to the components using the scalar products:

$$\hat{\mathbf{e}}_i \cdot \mathbf{A} = \hat{\mathbf{e}}_i \cdot \sum_j A_j \hat{\mathbf{e}}_j = \sum_j A_j \underbrace{\hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j}_{\delta_{ij}} = A_i.$$

Inserting this into the decomposition of \mathbf{A} [eq. (5)], we get

$$\mathbf{A} = \sum_i \hat{\mathbf{e}}_i A_i = \sum_i \hat{\mathbf{e}}_i (\hat{\mathbf{e}}_i \cdot \mathbf{A}) = \underbrace{\left[\sum_i (\hat{\mathbf{e}}_i \hat{\mathbf{e}}_i \cdot) \right]}_{=1} \mathbf{A}. \quad (6)$$

Here,⁵

$$1 = \sum_i (\hat{\mathbf{e}}_i) \hat{\mathbf{e}}_i.$$

is a *completeness relation*,⁶ which can be used to express a vector in terms of different sets of complete basis vectors.

4.2 Completeness relations for Hilbert space vectors

In an n -dimensional vector space, we can choose n linearly independent basis vectors $|1\rangle, |2\rangle, |3\rangle, \dots$, and write

$$|\psi\rangle = \sum_{k=1}^n c_k |k\rangle, \quad c_k \in \mathbb{C}. \quad (7)$$

We assume the basis vectors are orthogonal and with length 1;

$$\langle k|m\rangle = \delta_{km}, \quad (8)$$

such that

$$\langle m|\psi\rangle = \sum_{k=1}^n c_k \langle m|k\rangle = c_m. \quad (9)$$

Inserting this into the expansion of $|\psi\rangle$ in eq. (7), we get

$$|\psi\rangle = \sum_{k=1}^n \underbrace{\langle k|\psi\rangle}_{\in \mathbb{C}} |k\rangle = \sum_{k=1}^n |k\rangle \langle k|\psi\rangle = \underbrace{\left[\sum_{k=1}^n |k\rangle \langle k| \right]}_{=1} \cdot |\psi\rangle.$$

Hence, we arrive at the *completeness relation*

$$\sum_{k=1}^n |k\rangle \langle k| = 1 \quad (\text{discrete case}). \quad (10)$$

Notice that the order of the bra and ket matters:

$\langle a b\rangle$	— inner product, a complex number,
$ a\rangle\langle b $	— outer product, an <i>operator</i> .

If basis vectors form an uncountable set, instead of $\langle k'|k\rangle = \delta_{k'k}$, we use⁷

$$\langle k'|k\rangle = \delta(k - k') \quad (11)$$

and get the completeness relation

$$\int dk |k\rangle \langle k| = 1 \quad (\text{continuous case}). \quad (12)$$

An arbitrary vector $|\Psi\rangle$ may therefore be expanded in terms of different basis sets, for instance

$$\begin{aligned} |\Psi\rangle &= \sum_n c_n |\psi_n\rangle = \sum_n \langle \psi_n | \Psi \rangle |\psi_n\rangle, \\ |\Psi\rangle &= \int dp \Phi(p) |p\rangle = \int dp \langle p | \Psi \rangle |p\rangle, \\ |\Psi\rangle &= \int dx' c(x') |x'\rangle = \int dx' \langle x' | \Psi \rangle |x'\rangle. \end{aligned}$$

⁵ It's more correct to write this as

$$1 = \sum_i \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_i,$$

where \otimes denotes the *outer product*.

⁶ In Cartesian coordinates it reads

$$1 = (\hat{\mathbf{e}}_x) \hat{\mathbf{e}}_x + (\hat{\mathbf{e}}_y) \hat{\mathbf{e}}_y + (\hat{\mathbf{e}}_z) \hat{\mathbf{e}}_z,$$

such that

$$\begin{aligned} \mathbf{A} &= 1 \mathbf{A} \\ &= [(\hat{\mathbf{e}}_x) \hat{\mathbf{e}}_x + (\hat{\mathbf{e}}_y) \hat{\mathbf{e}}_y + (\hat{\mathbf{e}}_z) \hat{\mathbf{e}}_z] \mathbf{A} \\ &= A_x \hat{\mathbf{e}}_x + A_y \hat{\mathbf{e}}_y + A_z \hat{\mathbf{e}}_z, \end{aligned}$$

as expected.

⁷ Notice that this is similar to the δ -function normalization introduced previously for functions with continuous eigenvalues.

5 What is Hilbert space?

In quantum mechanics we refer to the Hilbert \mathcal{H} space as the set of *square-integrable functions* on a specified interval

See Griffiths pp. 92-93.

$$f(x) \text{ such that } \int_a^b dx |f(x)|^2 < \infty, \quad (13)$$

with an inner product of two functions in Hilbert space

$$\langle f|g \rangle = \int_a^b dx f^*(x)g(x). \quad (14)$$

Mathematicians call this space $L^2(a, b)$.

If $f, g \in \mathcal{H}$, the existence of the inner product is guaranteed by the Schwartz inequality

$$|\langle f|g \rangle| \leq \sqrt{\langle f|f \rangle} \sqrt{\langle g|g \rangle},$$

with $\langle f|f \rangle \geq 0$ and real. f is normalized if $\langle f|f \rangle = 1$. A set of functions $\{f_n\}$ is orthonormal if

$$\langle f_n|f_m \rangle = \delta_{nm}. \quad (15)$$

Completeness: For all $f \in \mathcal{H}$, we can write

$$f(x) = \sum_n c_n f_n(x) \longleftrightarrow |f\rangle = \sum_n c_n |f_n\rangle,$$

where

$$c_n = \langle f_n|f \rangle = \int dx f_n^*(x)f(x).$$

Eigenfunctions of continuous eigenvalues The position and momentum space vectors $|x\rangle$ and $|p\rangle$ **do not** satisfy the orthonormality condition in eq. (15), but are rather δ -function normalized

$$\langle x'|x \rangle = \delta(x - x').$$

This means that the eigenfunctions of \hat{x} and \hat{p} (with real eigenvalues) **do not** live in Hilbert space, but in the nearby “suburbs”⁸, called a *rigged Hilbert space*. These states do not represent possible physical states, but “are still very useful”.⁸

⁸ See Griffiths and Schroeter (2018) p. 100.

6 Operators

An operator \hat{A} is defined as a map

$$\hat{A} : \mathcal{H} \rightarrow \mathcal{H}, \quad \hat{A}|a\rangle = |c\rangle,$$

that is,

$$\text{operator} \cdot \text{vector} = \text{new vector}.$$

The *adjoint* or *Hermitian conjugate* operator \hat{A}^\dagger of \hat{A} is defined by

$$\underbrace{\langle a|\hat{A}^\dagger|b \rangle}_{\in \mathbb{C}} = \langle b|\hat{A}|a \rangle^* \quad \forall |a\rangle, |b\rangle \in \mathcal{H}. \quad (16)$$

The dual vector of $\hat{A}|a\rangle$ is $\langle a|\hat{A}^\dagger$.

The operators have the following properties

See Compendium 10.2 by Øverbø, Hemmer Ch. 6.3, and Griffiths Ch. 3.3.

1. $(\hat{A}^\dagger)^\dagger = \hat{A}$
2. $(\alpha \hat{A})^\dagger = \alpha^* \hat{A}$
3. $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger \hat{A}^\dagger$
4. Hermitian or self-adjoint operator: $\hat{A}^\dagger = \hat{A} \Rightarrow \langle a|\hat{A}|a\rangle \in \mathbb{R}$.

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