Lecture notes FY2045 Quantum Mechanics I — 3 General formulation of Quantum Mechanics

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1 Motivation

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

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.

[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 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 $\mathcal{H}^*$,

$$|a\rangle \overset{dual}{\longleftrightarrow} \langle a|,$$

so that we can define the *scalar product* (or inner product) of vectors $|a\rangle$ and $|b\rangle$[2]

$$\langle a||b\rangle \equiv \langle a|b\rangle. \tag{1}$$

This is a complex number,[3] and has the property

$$\langle a|b\rangle = \langle b|a\rangle^*, \tag{2}$$

where * denotes complex conjugation.[4] Moreover,

$$c|a\rangle \overset{dual}{\longleftrightarrow} c^*\langle a|, \quad c \in \mathbb{C}. \tag{3}$$

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

[2] For abstract vector spaces it is common to use the notation $\langle\cdot,\cdot\rangle$ for the inner product rather than the dot operator $\cdot$. We can therefore write

$$\langle|a\rangle, |b\rangle\rangle = \langle a|b\rangle,$$

which illustrates both why Dirac named the vectors as he did, and why the Dirac notation is so convenient.

[3] 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 Avella (2022) for a synopsis of recent experimental results refuting so-called *real quantum mechanics*.

[4] This reminds us of

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

3 Interpretation

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

3.1 Example — Electron double slit experiment

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

We want to describe the probability amplitude[5] 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

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

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

$$\langle x|\psi\rangle = \psi(x). \tag{4}$$

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:

[5] The probability is the absolute square of the probability amplitude.

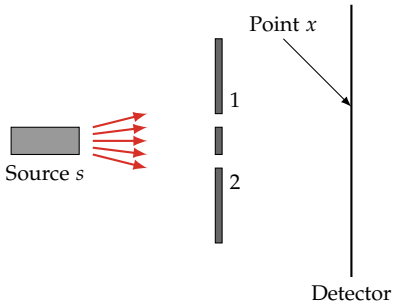

Figure 1: Electrons are sent from the source at s towards the two slits (1 and 2), and are detected by the detector at some position x.

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, the 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,

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

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

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

Here,[6]

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

is a *completeness relation*,[7] which can be used to express a vector in terms of different sets of complete basis vectors.

[6] 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*.

[7] In Cartesian coordinates it reads

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

such that

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

as expected.

4.2 Completeness relations for Hilbert space vectors

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

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

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

$$\langle k|m\rangle = \delta_{km}, \tag{8}$$

such that

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

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

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

Hence, we arrive at the *completeness relation*

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

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 *operator*.

If basis vectors form an uncountable set, instead of $\langle k'|k\rangle = \delta_{k'k}$, we use[8]

$$\langle k'|k\rangle = \delta(k - k') \tag{11}$$

and get the completeness relation

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

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

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 What is Hilbert space?

See Griffiths pp. 92-93.

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

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

with an inner product of two functions in Hilbert space

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

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

$$\langle f_n|f_m\rangle = \delta_{nm}. \tag{15}$$

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"[9], called a *rigged Hilbert space*. These states do not represent possible physical states, but "are still very useful".[9]

[9] See Griffiths and Schroeter (2018) p. 100.

6 Operators

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

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

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

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

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

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

The operators have the following properties

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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