

State vectors in quantum mechanics¹

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1 Introduction

A state in quantum mechanics is represented by a vector in a space of vectors over the complex numbers. (That means that you can add two vectors or multiply one by a complex number.) A useful notation is to represent a state whose name is, say, ψ by $|\psi\rangle$. Conveniently, this allows us to represent a state whose name is, say, ψ_{nll_z} by $|nll_z\rangle$.

The space of states for quantum mechanics comes with an inner product that associates a complex number (ϕ, ψ) to two vectors ϕ and ψ . The inner product has two properties:

$$\begin{aligned}(\psi, \phi) &= (\phi, \psi)^* \\ (\phi, \alpha_1\psi_1 + \alpha_2\psi_2) &= \alpha_1(\phi, \psi_1) + \alpha_2(\phi, \psi_2) \quad .\end{aligned}\tag{1}$$

with the bracket notation, the inner product is $\langle\phi|\psi\rangle$. The space of states includes all vectors, but a physical state is represented by a state vector normalized to $\langle\psi|\psi\rangle = 1$.

The inner product has an interpretation using probabilities. Suppose you have a state $|\psi\rangle$ with $\langle\psi|\psi\rangle = 1$. Let $|\phi\rangle$ represent another state $\langle\phi|\phi\rangle = 1$. If you perform a measurement that determines if state $|\psi\rangle$ is in state $|\phi\rangle$, the probability that it is is $|\langle\phi|\psi\rangle|^2$.

2 Wave functions

If we consider the simple case of a single particle that can move in one dimension, then the state can be represented as a function ψ that takes a

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complex value $\psi(x)$ at position x . In this case, we add functions in the obvious way and the inner product is

$$\langle \phi | \psi \rangle = \int_{-\infty}^{\infty} dx \phi(x)^* \psi(x) . \quad (2)$$

The idea of state vectors is much more general than just the representation of single particle states in one dimension, but for the rest of these notes, we will use this case when an example is needed.

3 Expansion in a basis

One often uses an “orthonormal basis” $|n\rangle$ for the space of states. This means a set of vectors labeled by an integer n (or more generally a set of integers) with the property that

$$\langle n | m \rangle = \delta_{mn} \quad (3)$$

and the further property (called “completeness”) that any vector $|\psi\rangle$ can be expanded in the form

$$|\psi\rangle = \sum_n c_n |n\rangle . \quad (4)$$

Then $c_n = \langle n | \psi \rangle$ (show this) so

$$|\psi\rangle = \sum_n |n\rangle \langle n | \psi \rangle . \quad (5)$$

It is often useful to write the completeness relation as

$$1 = \sum_n |n\rangle \langle n| . \quad (6)$$

For example, the basis states $|n\rangle$ can be the harmonic oscillator energy eigenstates. One might call the corresponding wave functions $\Phi_n(x)$.

Sometimes we have a basis labeled by a continuous parameter instead of a discrete parameter. Suppose that the discrete parameter is s and takes values in $-\infty < s < \infty$. Then we can have basis states $|s\rangle$ with³

$$\langle s | r \rangle = \mathcal{N} \delta(s - r) \quad (7)$$

³Here $\mathcal{N}$ is a parameter that is often chosen to be 1, but this is sometimes not the most convenient choice.

and the further property (called “completeness”) that any vector $|\psi\rangle$ can be expanded in the form

$$|\psi\rangle = \frac{1}{\mathcal{N}} \int_{-\infty}^{\infty} ds \, c(s) |s\rangle . \quad (8)$$

Then $c(s) = \langle s|\psi\rangle$ (show this) so

$$|\psi\rangle = \frac{1}{\mathcal{N}} \int_{-\infty}^{\infty} ds \, |s\rangle \langle s|\psi\rangle . \quad (9)$$

It is often useful to write the completeness relation as

$$1 = \frac{1}{\mathcal{N}} \int_{-\infty}^{\infty} ds \, |s\rangle \langle s| . \quad (10)$$

4 Position basis

For the one dimensional example, consider states $|s\rangle$ represented by wave functions $|s\rangle \rightarrow \Phi_s$ with $\Phi_s(x) = \delta(x - s)$. The state $|s\rangle$ is definitely located at position s . To put this in a definitive fashion, note that $|s\rangle$ is an eigenfunction of the position operator X :

$$x|s\rangle = s|s\rangle . \quad (11)$$

The inner product is

$$\langle s|r\rangle = \delta(s - r) . \quad (12)$$

(You should prove this.) The completeness relations is

$$1 = \int_{-\infty}^{\infty} ds \, |s\rangle \langle s| . \quad (13)$$

If ψ is a state with wave function $\psi(x)$, we have

$$\langle x|\psi\rangle = \psi(x) . \quad (14)$$

(Show this.) Thus the usual wave function $\psi(x)$ is the component of $|\psi\rangle$ along the basis vector $|x\rangle$ the position basis.

5 Momentum basis

For the one dimensional example, consider states $|k\rangle$ represented by wave functions $|k\rangle \rightarrow \Phi_k$ with

$$\Phi_k(x) = e^{ikx} . \quad (15)$$

The state $|k\rangle$ has momentum k . To put this in a definitive fashion, note that $|k\rangle$ is an eigenfunction of the momentum operator P :

$$P|k\rangle = k|k\rangle . \quad (16)$$

The inner product is

$$\langle k'|k\rangle = 2\pi\delta(k' - k) . \quad (17)$$

This formula is well known to those who know it. Let's look at it. It says

$$\int dx e^{-ik'x} e^{ikx} = 2\pi\delta(k' - k) . \quad (18)$$

In turn, this says that for any function $\tilde{f}(k)$ we have

$$\frac{1}{2\pi} \int dk \int dx e^{-ik'x} e^{ikx} \tilde{f}(k) = \tilde{f}(k') \quad (19)$$

or

$$\int dx e^{-ik'x} \left\{ \int \frac{dk}{2\pi} e^{ikx} \tilde{f}(k) \right\} = \tilde{f}(k') . \quad (20)$$

Now its more familiar. We start with a function $\tilde{f}(k)$. We define it's Fourier transform (from k to x) as

$$f(x) = \int \frac{dk}{2\pi} e^{ikx} \tilde{f}(k) . \quad (21)$$

Then $\tilde{f}(k)$ is given by the Fourier transform from x to k ,

$$\tilde{f}(k') = \int dx e^{-ik'x} f(x) . \quad (22)$$

That's the standard inversion formula for Fourier transforms. Our inner product formula is a restatement of this inversion formula.

The completeness relation is

$$1 = \int_{-\infty}^{\infty} \frac{dk}{2\pi} |k\rangle\langle k| . \quad (23)$$

If ψ is a state with wave function $\psi(x)$, we have

$$\langle k|\psi\rangle = \tilde{\psi}(k) , \quad (24)$$

where $\tilde{\psi}(k)$ is the Fourier transform of $\psi(x)$. (Show this.) Thus the usual Fourier transformed wave function $\tilde{\psi}(k)$ is the component of $|\psi\rangle$ along the basis vector $|k\rangle$ the momentum basis.

There is real physics in this, not just mathematics of Fourier analysis. If a state on a particle in one dimension is represented by a state ψ , then $\langle x|\psi\rangle$ is the amplitude for the particle to be at position x and $\langle k|\psi\rangle$ is the amplitude for the particle to have momentum k . These are components of the state vector in two different bases.

6 Operators and their adjoints

We often need to consider operators that act on the states. An operator A that acts on a state $|\psi\rangle$ produces a new state vector $A|\psi\rangle$. The operators considered in quantum mechanics are (almost always) linear operators. This means that if $|\psi\rangle = \alpha|\phi_1\rangle + \beta|\phi_2\rangle$ then $A|\psi\rangle = \alpha A|\phi_1\rangle + \beta A|\phi_2\rangle$.

For every operator A there is an “adjoint” operator $A^\dagger$. The definition is related to the inner product. If we temporarily use the (ψ, ϕ) notation for the inner product, the definition is

$$(A\psi, \phi) = (\psi, A^\dagger\phi) \quad (25)$$

for all vectors ψ and ϕ . It is a little difficult to express this in the bracket notation. If $|\psi'\rangle = A|\psi\rangle$ then

$$\langle\psi'|\phi\rangle = \langle\psi|A^\dagger|\phi\rangle . \quad (26)$$

Many operators useful in quantum mechanics are self-adjoint

$$A^\dagger = A . \quad (27)$$

A self-adjoint operator is often called “hermitian.” In fact, all operators that represent observables, such as the energy operator or hamiltonian, the momentum, and the angular momentum, are self-adjoint.

Let A be a self-adjoint operator and consider its eigenvectors $|a\rangle$:

$$A|a\rangle = a|a\rangle . \quad (28)$$

Then the eigenvalues must be real and eigenvectors corresponding to different eigenvalues must be orthogonal.

To show this, lets revert to the mathematicians notation for the inner product and say that ψ_a is an eigenvector with $A\psi_a = a\psi_a$. Then

$$\begin{aligned} a^*(\psi_a, \psi_a) &= (a\psi_a, \psi_a) = (A\psi_a, \psi_a) = (\psi_a, A^\dagger\psi_a) \\ &= (\psi_a, A\psi_a) = (\psi_a, a\psi_a) = a(\psi_a, \psi_a) , \end{aligned} \quad (29)$$

so $a^* = a$. Furthermore, if $A\psi_a = a\psi_a$ and if $A\psi_b = b\psi_b$ then

$$\begin{aligned} a(\psi_a, \psi_b) &= (a\psi_a, \psi_b) = (A\psi_a, \psi_b) = (\psi_a, A^\dagger\psi_b) \\ &= (\psi_a, A\psi_b) = (\psi_a, b\psi_b) = b(\psi_a, \psi_b) , \end{aligned} \quad (30)$$

so that

$$(a - b)(\psi_a, \psi_b) = 0 . \quad (31)$$

Thus either $a - b = 0$ or else $(\psi_a, \psi_b) = 0$.

It is a theorem, but not so easy to prove, that the eigenvectors corresponding to a self-adjoint operator form a complete basis for the space of states.

Another important class of operators are the “unitary” operators. A linear operator U is unitary if

$$(U\psi, U\phi) = (\psi, \phi) \quad (32)$$

for all vectors ψ and ϕ . In other words, $(\psi, U^\dagger U\phi) = (\psi, \phi)$ for all vectors ψ and ϕ . This implies that $U^\dagger U$ is the unit operator. In other words,

$$U^\dagger = U^{-1} . \quad (33)$$

For example, the operator that rotates vectors through angle $|\vec{\theta}|$ about an axis in the direction $\vec{\theta}$, $U(\vec{\theta})$, is unitary. Then the property $(U\psi, U\phi) = (\psi, \phi)$ says that if you do a quantum measurement on the rotated system you get the same result as if you did the measurement on the unrotated system.