

Introduction to Quantum Mechanics: Part 2

1 Algebra of State Vectors

What does the State Vector mean?

“A state vector is not a property of a physical system, but rather represents an experimental procedure for preparing or testing one or more physical systems.”
F. Laloë[4] quoting A. Peres.[5]

There are other interpretations of the state vector: it may refer to an ensemble of identically prepared systems or even to a single system. Le Bellac (Quantum Physics, page 97 footnote) says

“... the state vector describes the physical reality of an individual quantum system. This point of view is far from universally shared... This diversity of viewpoints has no effect on the practical application of quantum mechanics.”

These state vectors like $|x\rangle$ are called “kets”, a name proposed by Dirac; it is part of the word “bracket”. This way of writing state vectors in Quantum Mechanics is called Dirac Notation.

1.1 Inner Product

With ordinary vectors the inner product can be written as $\mathbf{A} \cdot \mathbf{B}$ or $\mathbf{B} \cdot \mathbf{A}$ but with state vectors we define for each vector a “dual” vector.

There is a one-to-one correspondence between a vector and its dual vector. From a more mathematical perspective the dual vector provides a mapping from the ket vector onto complex numbers (the inner product). see Cohen-Tannoudji[6] page 110.

The dual vector corresponding to $c|\theta\rangle$ is $c^*\langle\theta|$.

Notice the complex conjugate of the constant c .

The inner products of the orthonormal basis states are $\langle x|x\rangle = 1$ and $\langle y|y\rangle = 1$ and $\langle y|x\rangle = 0$.

Suppose

$$|\psi\rangle = \lambda|x\rangle + \mu|y\rangle$$

$$\langle\psi| = \lambda^*\langle x| + \mu^*\langle y|$$

$$|\phi\rangle = \alpha|x\rangle + \beta|y\rangle$$

$$\langle\phi| = \alpha^*\langle x| + \beta^*\langle y|$$

where $|x\rangle$ and $|y\rangle$ are orthogonal and normalized.

Show that

$$\langle\psi|\phi\rangle = \langle\phi|\psi\rangle^*$$

we see that $\langle\psi|\psi\rangle$ is real.

2 Principles of Quantum Mechanics

2.1 Postulates - Preliminary Version

1. The state of a system is represented by a vector $|\Phi\rangle$. This is chosen to be normalized and $|\langle\Phi|\Phi\rangle|^2 = 1$. This is called the state vector of the system. $\langle\Phi|$ is the dual vector.

2. If $|\Phi\rangle$ and $|\Psi\rangle$ represent two physical states the probability amplitude for finding the system prepared in state Φ to be observed in the state Ψ is given by the inner product $\langle\Psi|\Phi\rangle$. The probability is the magnitude squared of the amplitude, $|\langle\Psi|\Phi\rangle|^2$.

After testing for state $|\Psi\rangle$ the system is in the state $|\Psi\rangle$ with the probability given above. Recall that a probability is a real number between 0 and 1.

2.2 Measurement

A system has been prepared in the state $|\Phi\rangle$. The state of the system after the testing or “measurement” is $|\Psi\rangle$ and we can take the point of view that the original state has been projected along this “direction” in the vector space.

This projection of the state after a measurement is sometimes called ”state-vector collapse” or wave function *collapse* or *reduction*.

This state-collapse is sometimes considered a postulate of Quantum Mechanics. In this perspective we do not discuss the details of the measurement process itself.

Suppose we prepare a state $|\Phi\rangle$ and expand it in a series of basis states $|x\rangle$.

$$|\Phi\rangle = \sum_x a_x |x\rangle$$

The a_x are the amplitudes for each basis state. The amplitude is $a_x = \langle x|\Phi\rangle$.

Mermin[7] says

“...the link between $|\Phi\rangle$ and the value of x revealed by the measurement is this: the probability of getting the output x is just $p_x = |a_x|^2$, where a_x is the amplitude of $|x\rangle$ in the expansion of $|\Phi\rangle$. This connection between amplitudes and the probabilities of measurement outcomes is known as the *Born rule*, after the physicist Max Born.”

Paraphrasing Mermin

“ The postmeasurement state $|x\rangle$ contains no trace of the information present in the premeasurement state $|\Phi\rangle$. (beyond revealing that the amplitude $a_x \neq 0$) ... the state $|\Phi\rangle$ *collapses* or *is reduced* to the state $|x\rangle$ by the measurement.

An operator in Quantum Mechanics transforms a state into another state. A measurement is represented by an operator.

2.3 Expansion in basis states

A state $|\Phi\rangle$ can be expanded in a series of basis states:

$$|\Phi\rangle = |+\rangle\langle +|\Phi\rangle + |-\rangle\langle -|\Phi\rangle$$

In general

$$|\Phi\rangle = \sum_i |u_i\rangle\langle u_i|\Phi\rangle$$

where $|u_i\rangle$ are the basis states and $\langle u_i|\Phi\rangle$ are the expansion coefficient or amplitudes.

A linear combination of state vectors is (usually) a valid state vector.

The probability of $|\Phi\rangle$ being found in state $|u_i\rangle$ is $|\langle u_i|\Phi\rangle|^2$, the magnitude squared of the expansion coefficient (amplitude).

2.4 Mixture vs. Superposition

We must distinguish between a linear combination or *superposition* of states (sometimes called a *pure state*) and a *mixture* of states.

a) A beam of light polarized at 45 degrees (between x and y) can be described as an equal weighted **superposition** of x and y polarization states. $\frac{1}{\sqrt{2}}(|x\rangle + |y\rangle)$.

b) A beam of light formed by combining equal **intensities** of light polarized in the y direction and light polarized in the x direction (using mirrors, for example) is completely different and will give different results if you send it through a Polaroid analyzer in certain directions. This is called a **mixture**.

What is such a light beam called? What Polaroid directions will enable you to distinguish between these beams?

2.5 Matrix Representation

States in the two dimensional vector space and operators can be “represented” by two dimensional matrices. “Represented” means that the matrices will obey the same algebraic relationships as the abstract states and operators.

When we form a matrix representation we do this in a particular basis.

The states $|+\rangle$ and $|-\rangle$ can be represented as column matrices in the $+, -$ basis this way:

$$|+\rangle \text{ is represented by } \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |-\rangle \text{ is represented by } \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

In general a state $|\psi\rangle$ is represented by: $\begin{pmatrix} \langle +|\psi\rangle \\ \langle -|\psi\rangle \end{pmatrix}$

The dual vectors are represented by row matrices.

$$\langle +| \text{ is represented by } \begin{pmatrix} 1 & 0 \end{pmatrix} \quad \text{and} \quad \langle -| \text{ is represented by } \begin{pmatrix} 0 & 1 \end{pmatrix}$$

The dual of $\begin{pmatrix} a \\ b \end{pmatrix}$ is $\begin{pmatrix} a^* & b^* \end{pmatrix}$ and $\begin{pmatrix} a^* & b^* \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = |a|^2 + |b|^2$

Notice that the two basis states are normalized and orthogonal:

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 1 \quad \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 1 \quad \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0$$

Operators acting on such states will be represented by 2×2 matrices. for example:

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The operator S_z represents a Stern-Gerlach measurement (SGz) of the z component of spin. Similarly S_x represents a measurement (SGx) of the x component.

The most general normalized state is represented by

$$|\chi\rangle = \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \quad \text{where} \quad |\lambda|^2 + |\mu|^2 = 1$$

λ and μ are complex and can be parametrized by $\lambda = \cos \theta$ and $\mu = \sin \theta e^{i\delta}$.

We are sometimes casual about equating an operator to its matrix representation. They are different objects and more correctly a special symbol rather than an “=” should be used. In his notes McIntyre uses \doteq to mean “represented by”.

2.6 Eigenstates and Measurements

Sakurai[3] quotes P. A. M. Dirac, one of the founders of modern quantum mechanics and comments:

“A measurement always causes the system to jump into an eigenstate of the dynamical variable that is being measured”

What does all this mean? We interpret Dirac’s words as follows: Before a measurement of observable A is made the system is assumed to be represented by some linear combination...

$$|\Phi\rangle = \sum_i c_i |u_i\rangle = \sum_i |u_i\rangle \langle u_i | \Phi \rangle$$

where the $|u_i\rangle$ are the eigenstates of an operator A corresponding to what is being measured.

“When the measurement is performed the system is ‘thrown into’ one of the eigenstates, say $|u'\rangle$ of the observable A

When the measurement causes $|\Phi\rangle$ to change into $|u'\rangle$ it is said that A is measured to be u' . It is in this sense that the result of a measurement yields one of the eigenvalues of the observable being measured.”

If $A|u'\rangle = u'|u'\rangle$ we say that $|u'\rangle$ is an eigenstate or eigenvector of the operator A and u' , a number, is the eigenvalue.

The probability for finding the system in the state $|u'\rangle$ after the measurement or equivalently for measuring u' is $|\langle u' | \Phi \rangle|^2$ as we have seen before.

2.7 Averages and Expectation Values

If we make measurements on a collection of identically prepared systems (an *ensemble*) what will be the average of the measured values?

The average of a collection of values (even in everyday situations) is

$$\text{Ave} = \sum_i \text{Value}_i \times \text{Probability}_i$$

The average is $\sum_i a_i |\langle a_i | \Phi \rangle|^2$ where a_i are the possible measured values.

This can be written $\sum_i a_i \langle \Phi | a_i \rangle \langle a_i | \Phi \rangle = \langle \Phi | \mathcal{A} | \Phi \rangle$ since $\mathcal{A} = \sum_i |a_i\rangle a_i \langle a_i|$

a_i is the eigenvalue of \mathcal{A} in the state $|a_i\rangle$ which is an eigenstate of \mathcal{A} $\mathcal{A}|a_i\rangle = a_i|a_i\rangle$

The expectation value of an operator A in the state $|\Phi\rangle$ is $\langle A \rangle = \langle \Phi | A | \Phi \rangle$.

This is the average value of the results of measurements of A on an ensemble of identically prepared systems $|\Phi\rangle$

Example: The average value of the z component of spin for a system in state $|\Phi\rangle$ is the expectation value of S_z that is: $\langle S_z \rangle = \langle \Phi | S_z | \Phi \rangle$

2.8 Conjugate Operators

An operator A transforms a state $|\psi\rangle$ into a new state $|\psi'\rangle$. We write $|\psi'\rangle = A|\psi\rangle$.

The operator which transforms the corresponding dual state (the “bra” in Dirac’s language) is written as A^\dagger . Then $\langle \psi' | = \langle \psi | A^\dagger$.

From $\langle \psi' | \phi \rangle = \langle \phi | \psi' \rangle^*$ we obtain the important result

$$\langle \psi | A^\dagger | \phi \rangle = \langle \phi | A | \psi \rangle^*$$

The Hermitian conjugate of A is A^\dagger . see Cohen-Tannoudji[6] p. 118.

3 x basis states for Spin $\frac{1}{2}$

Using SG devices prepare the states $|+\rangle_x$ and $|-\rangle_x$.

Select the state $|+\rangle_x$ and measure $|+\rangle$ and $|-\rangle$ with a SGz device.

What is the probability of observing the output in the $+z$ direction?

The probability amplitude is $\langle + | + \rangle_x$.

The probability or amplitude squared is $|\langle + | + \rangle_x|^2$. We observe a probability of 1/2.

Write $|+\rangle_x$ as a linear combination of orthonormal z basis states:

$$|+\rangle_x = a|+\rangle + b|-\rangle$$

where a and b are in general complex.

Then we see that $\langle +|+\rangle_x = a$ and we require $|a|^2 = \frac{1}{2}$ to agree with the experiment.

so we find $a = \frac{1}{\sqrt{2}} e^{i\alpha}$.

We will choose (by convention) $\alpha = 0$ so $a = \frac{1}{\sqrt{2}}$. Similarly for b .

So we find that

$$|+\rangle_x = \frac{1}{\sqrt{2}} (|+\rangle + |-\rangle)$$

3.1 Operators

Matrix Representation

An operator transforms a state. $A|\psi\rangle = |\phi\rangle$. Expand the states in the z basis.

$$|\psi\rangle = |+\rangle\langle +|\psi\rangle + |-\rangle\langle -|\psi\rangle$$

$$|\phi\rangle = |+\rangle\langle +|\phi\rangle + |-\rangle\langle -|\phi\rangle$$

Then $A|\psi\rangle = |\phi\rangle$ becomes

$$A(|+\rangle\langle +|\psi\rangle + |-\rangle\langle -|\psi\rangle) = |+\rangle\langle +|\phi\rangle + |-\rangle\langle -|\phi\rangle$$

Take the inner product with $\langle +|$ and also with $\langle -|$

$$\langle +|A|+\rangle\langle +|\psi\rangle + \langle +|A|-\rangle\langle -|\psi\rangle = \langle +|\phi\rangle$$

$$\langle -|A|+\rangle\langle +|\psi\rangle + \langle -|A|-\rangle\langle -|\psi\rangle = \langle -|\phi\rangle$$

Write this as a matrix equation.

$$\begin{pmatrix} \langle +|A|+\rangle & \langle +|A|-\rangle \\ \langle -|A|+\rangle & \langle -|A|-\rangle \end{pmatrix} \begin{pmatrix} \langle +|\psi\rangle \\ \langle -|\psi\rangle \end{pmatrix} = \begin{pmatrix} \langle +|\phi\rangle \\ \langle -|\phi\rangle \end{pmatrix}$$

Average value

The operator A is associated with the measurement of an observable. Expand operator A , as a spectral decomposition in terms of projection operators on basis states.

$$A = |+\rangle a_+ \langle +| + |-\rangle a_- \langle -|$$

where a_+ and a_- are the measured values of the observable in each of the two basis states.

For components of spin $a_+ = \frac{\hbar}{2}$ and $a_- = -\frac{\hbar}{2}$

Evaluate

$$\langle \psi|A|\psi\rangle = \langle \psi|+\rangle \langle +|\psi\rangle a_+ + \langle \psi|-\rangle \langle -|\psi\rangle a_- = P_+ a_+ + P_- a_-$$

where P_+ and P_- are the probabilities for finding each of the basis states.

This is the **average** value of the measured quantity in the state $|\psi\rangle$. It is called the expectation value of A and is often written as $\langle A \rangle$.

In general the average is $\sum_n P_n a_n$ where n labels the basis states.

Eigenvalues

A is diagonal in this basis. The diagonal elements of A are the eigenvalues of A and the states $|+\rangle$ and $|-\rangle$ are the eigenstates of A . Notice that $A|+\rangle = a_+|+\rangle$. If the system to be measured is in an eigenstate of the operator A then the state is not changed as a result of the measurement. If it is in a linear superposition of states then after the measurement it “collapses” into one of the eigenstates.

3.2 Spin Operators

The operators corresponding to measurements of the components of spin $\frac{1}{2}$ written in the z basis are :

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Of course the S_z operator is diagonal in the z basis.

The eigenstates of S_z are $|+\rangle_z = |+\rangle$ and $|-\rangle_z = |-\rangle$

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The eigenstates of S_x are $|+\rangle_x = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$ and $|-\rangle_x = \frac{1}{\sqrt{2}}(|+\rangle - |-\rangle)$

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \text{and} \quad \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

The eigenstates of S_y are $|+\rangle_y = \frac{1}{\sqrt{2}}(|+\rangle + i|-\rangle)$ and $|-\rangle_y = \frac{1}{\sqrt{2}}(|+\rangle - i|-\rangle)$

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} \quad \text{and} \quad \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

$$\sin 2a = 2 \sin a \cos a \quad \cos 2a = \cos^2 a - \sin^2 a$$

$$\sin(a \pm b) = \sin a \cos b \pm \cos a \sin b \quad \cos(a \pm b) = \cos a \cos b \mp \sin a \sin b$$

$$\cos^2 a - \sin^2 b = \cos(a + b) \cos(a - b)$$

$$\sin^2 a - \sin^2 b = \sin(a + b) \sin(a - b)$$

$$\cos^2 a - \cos^2 b = -\sin(a + b) \sin(a - b)$$

Direction of the Stern-Gerlach to prepare a state

Example

A beam of atoms is prepared in the state $|\psi\rangle = \cos\frac{\theta}{2}|+\rangle + \sin\frac{\theta}{2}|-\rangle$

The state which is orthogonal to this state is $|\psi_{\perp}\rangle = \sin\frac{\theta}{2}|+\rangle - \cos\frac{\theta}{2}|-\rangle$

This is an eigenstate of the spin operator $S_{\theta} = \cos\theta S_z + \sin\theta S_x$ (derived below).

The average value of the x component of spin is $\frac{\hbar}{2} \sin\theta$ and the average value of the z component is $\frac{\hbar}{2} \cos\theta$. The average value of the y component is 0.

In what direction does the spin point on the average?

In what direction should a Stern-Gerlach device be oriented to prepare these states?

For the particular values $\theta = 0, \frac{\pi}{2}, \pi$ check that the state and the averages agree with what you expect. Which way would you say that the spin points for these cases?

Rewrite the states in the z basis using the matrix representation.

$$|\psi\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix} \quad |\psi_{\perp}\rangle = \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \end{pmatrix}$$

$$|\psi\rangle\langle\psi| = \begin{pmatrix} \cos^2\frac{\theta}{2} & \cos\frac{\theta}{2}\sin\frac{\theta}{2} \\ \cos\frac{\theta}{2}\sin\frac{\theta}{2} & \sin^2\frac{\theta}{2} \end{pmatrix}$$

$$|\psi_{\perp}\rangle\langle\psi_{\perp}| = \begin{pmatrix} \sin^2\frac{\theta}{2} & -\cos\frac{\theta}{2}\sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2}\sin\frac{\theta}{2} & \cos^2\frac{\theta}{2} \end{pmatrix}$$

$$|\psi\rangle\langle\psi| - |\psi_{\perp}\rangle\langle\psi_{\perp}| = \begin{pmatrix} \cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2} & 2\cos\frac{\theta}{2}\sin\frac{\theta}{2} \\ 2\cos\frac{\theta}{2}\sin\frac{\theta}{2} & -\cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2} \end{pmatrix}$$

$$S_{\theta} = \frac{\hbar}{2} \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix} = \frac{\hbar}{2} (S_z \cos\theta + S_x \sin\theta)$$

Eigenstates, Directions, and Averages

The Stern-Gerlach device has a magnetic field direction at an angle θ with the z axis in the x, z plane. Compare with expectations for $\theta = 0$, $\theta = \frac{\pi}{2}$, $\theta = \pi$.

Check that $|\psi\rangle$ is an eigenstate of S_θ with eigenvalue $+\frac{\hbar}{2}$.

$$S_\theta|\psi\rangle = \frac{\hbar}{2} \begin{pmatrix} \cos \theta & \sin \theta \\ \sin \theta & -\cos \theta \end{pmatrix} \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} \cos \theta \cos \frac{\theta}{2} + \sin \theta \sin \frac{\theta}{2} \\ \sin \theta \cos \frac{\theta}{2} - \cos \theta \sin \frac{\theta}{2} \end{pmatrix}$$

$$S_\theta|\psi\rangle = \frac{\hbar}{2}|\psi\rangle = \frac{\hbar}{2} \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{pmatrix}$$

Evaluate the average value (expectation value) $\langle\psi|S_\theta|\psi\rangle = \langle S_\theta\rangle$.

$$\langle S_\theta\rangle = \begin{pmatrix} \cos \frac{\theta}{2} & \sin \frac{\theta}{2} \end{pmatrix} \frac{\hbar}{2} \begin{pmatrix} \cos \theta & \sin \theta \\ \sin \theta & -\cos \theta \end{pmatrix} \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{pmatrix}$$

References

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