Quantum States

The physical state of a quantum-mechanical system is represented by a vector in a Hilbert space, sometimes called the "state vector." In Dirac notation, we represent the state vector by the "ket" $|\Psi\rangle$.

We can represent the state vector by its components using any complete set of orthonormal basis states, the same way we do with ordinary vectors. If the basis set is discrete, we write

$$|\Psi\rangle = \sum_{n=1}^{\infty} c_n |n\rangle, \tag{1}$$

where the vector "components" c_n can be found from taking the inner product of Eq. (1) with the mth "bra" state:

$$\langle m|\Psi\rangle = \sum_{n=1}^{\infty} c_n \langle m|n\rangle = \sum_{n=1}^{\infty} c_n \delta_{mn} = c_m. \tag{2}$$

This result lets us re-write the original sum as:

$$|\Psi\rangle = \sum_{n=1}^{\infty} |n\rangle\langle n|\Psi\rangle. \tag{3}$$

Removing the ket from both sides of the equation gives us the completeness relation,

$$\hat{I} = \sum_{n=1}^{\infty} |n\rangle\langle n|. \tag{4}$$

If the basis is continuous, the sum is replaced by an integral:

$$|\Psi\rangle = \int_{-\infty}^{\infty} c(q)|q\rangle. \tag{5}$$

Again, the coefficients $c(q)$ are found from the inner product:

$$\langle q'|\Psi\rangle = \int_{-\infty}^{\infty} c(q)\langle q'|q\rangle = \int_{-\infty}^{\infty} c(q)\delta(q-q') = c(q') \tag{6}$$

where the Kronecker delta of Eq. (2) has been replaced by the Dirac delta function.

Two examples of continuous basis states are the eigenstates of the position operator X, defined by $\hat{X}|x\rangle = x|x\rangle$, and the eigenstates of the momentum operator P, defined by $\hat{P}|p\rangle = p|p\rangle$. The relations equivalent to Eq. (3) are:

$$|\Psi\rangle = \int_{-\infty}^{\infty} |x\rangle\langle x|\Psi\rangle \tag{7}$$

$$|\Psi\rangle = \int_{-\infty}^{\infty} |p\rangle\langle p|\Psi\rangle \tag{8}$$

For these two basis sets, the coefficients have special names. The first is the wavefunction:

$$\Psi(x,t) \equiv \langle x | \Psi \rangle \tag{9}$$

while the second is its Fourier transform, which Griffiths calls:

$$\Phi(p,t) \equiv \langle p | \Psi \rangle \tag{10}$$

where I have included the time-dependence explicitly.

To take the inner product between any two arbitrary quantum states, we need to know their coefficients in some basis. For a discrete basis, the result is

$$\langle \Phi | \Psi \rangle = \sum_{n=1}^{\infty} \langle \Phi | n \rangle \langle n | \Psi \rangle \tag{11}$$

If we work in a continuous basis, the sum becomes an integral. Let's use the position eigenstate basis. Then the result is:

$$\langle \Phi | \Psi \rangle = \int_{-\infty}^{\infty} \langle \Phi | x \rangle \langle x | \Psi \rangle dx = \int_{-\infty}^{\infty} \Phi^*(x,t) \Psi(x,t) dx \tag{12}$$

The result on the far right-hand side is the way you first learned to take the inner product of two wavefunctions.

Physical Observables

Physical observables are represented by Hermitian operators, which have a number of important properties:

      i) their eigenvalues are real
      ii) they have a complete set of eigenstates
      iii) eigenstates with different eigenvalues are orthogonal
      iv) eigenstates with the same eigenvalue can be made orthogonal by using the
         Gram-Schmidt procedure

There is one catch in infinite-dimensional vector spaces. When the spectrum is continuous, the eigenstates are not normalizable – i.e. they are not in our Hilbert space. Fortunately that doesn't matter, because we can still use them as basis vectors in the ways described above.

If we measure any physical observable, the measurement yields one of the eigenvalues of the corresponding operator. Let's call the operator $\hat{A}$ and define the eigenstates and eigenvalues by

$$\hat{A} | a_n \rangle = \alpha_n | a_n \rangle \tag{13}$$

If the eigenvalue spectrum is discrete, the probability to obtain the nth eigenvalue as a result of the measurement is

$$P(\alpha_n) = |\langle a_n | \Psi \rangle|^2 . \tag{14}$$

If the eigenvalue is degenerate, i.e. there are several states with the same eigenvalue, then the probability to obtain that eigenvalue in a measurement is

$$P(\alpha_n) = \sum_{j=1}^{g_n} \left| \left\langle a_n^j \middle| \Psi \right\rangle \right|^2 \tag{15}$$

where the eigenstates $\left| a_n^j \right\rangle$ all share the same eigenvalue α_n, and g_n is the number of those states.

If the spectrum is continuous, the probability to obtain a result in the interval $[q_a, q_b]$ is

$$P[q_a, q_b] = \int_{q_a}^{q_b} \left| c(q) \right|^2 dq = \int_{q_a}^{q_b} \left| \left\langle q \middle| \Psi \right\rangle \right|^2 dq \tag{16}$$

When we complete a measurement corresponding to the operator $\hat{A}$ and obtain the nth eigenvalue of $\hat{A}$ as our result, then the measurement causes the quantum system to "collapse" into the corresponding eigenstate of $\hat{A}$. Repeated measurements of $\hat{A}$ will produce the same result as the preceding measurement. If we then measure a second observable represented by another Hermitian operator $\hat{B}$ with $\left[\hat{A}, \hat{B}\right] = 0$, then the measurement of $\hat{B}$ does not change further measurements of $\hat{A}$, because the eigenstates of $\hat{B}$ are also eigenstates of $\hat{A}$. If, on the other hand, $\left[\hat{A}, \hat{B}\right] \neq 0$, then the measurement of $\hat{B}$ will disturb the system and will change the result of a further measurement of $\hat{A}$. In this case $\hat{A}$ and $\hat{B}$ are said to represent "incompatible observables."

If our Hilbert space has a finite number of dimensions N, it is convenient to choose a basis and represent quantum states by column vectors whose entries are the vector components in that basis. Operators are represented by matrices, with matrix elements defined by $\hat{A}_{mn} = \left\langle m \middle| \hat{A} \middle| n \right\rangle$. For example, the ket $\left| \Psi \right\rangle$ in a 3-dimensional Hilbert space and the operator $\hat{A}$ acting on that space would be represented by:

$$\left| \Psi \right\rangle \rightarrow \begin{pmatrix} \langle 1 | \Psi \rangle \\ \langle 2 | \Psi \rangle \\ \langle 3 | \Psi \rangle \end{pmatrix} \qquad \hat{A} \rightarrow \begin{pmatrix} \langle 1|\hat{A}|1 \rangle & \langle 1|\hat{A}|2 \rangle & \langle 1|\hat{A}|3 \rangle \\ \langle 2|\hat{A}|1 \rangle & \langle 2|\hat{A}|2 \rangle & \langle 2|\hat{A}|3 \rangle \\ \langle 3|\hat{A}|1 \rangle & \langle 3|\hat{A}|2 \rangle & \langle 3|\hat{A}|3 \rangle \end{pmatrix} \tag{17}$$

Where the basis states are $\left| 1 \right\rangle$, $\left| 2 \right\rangle$, and $\left| 3 \right\rangle$. The bra associated with $\left| \Psi \right\rangle$ is represented by the row vector:

$$\left\langle \Psi \right| \rightarrow \begin{pmatrix} \langle \Psi | 1 \rangle & \langle \Psi | 2 \rangle & \langle \Psi | 3 \rangle \end{pmatrix} \tag{18}$$

Notice that the elements of the bra are the complex conjugates of the elements of the ket.

You find the eigenvectors and eigenvalues of $\hat{A}$ using the matrix rules you know well; let's label them the usual way: $\hat{A} \left| a_n \right\rangle = \alpha_n \left| a_n \right\rangle$. All the rules above follow: If your system is in the state $\left| \Psi \right\rangle$, then a measurement of $\hat{A}$ will then produce the result α_n with

probability $\left| \langle a_n | \Psi \rangle \right|^2$. The average (expectation) value of $\hat{A}$ can be calculated two ways (the first is easier to calculate, but the second contains more information):

$$\langle \hat{A} \rangle = \langle \Psi | \hat{A} | \Psi \rangle = \sum_{n=1}^{N} \alpha_n \left| \langle a_n | \Psi \rangle \right|^2. \tag{19}$$

The Hamiltonian

The Hamiltonian $\hat{H}$ is a special operator. It not only represents the energy of the system, but it determines the time evolution of the quantum states. Let's represent the eigenvectors and eigenvalues of $\hat{H}$ by

$$\hat{H} | n \rangle = E_n | n \rangle \tag{20}$$

If the energy spectrum is discrete, we first write the initial quantum state as:

$$| \Psi(t = 0) \rangle = \sum_{n=1}^{\infty} c_n | n \rangle. \tag{21}$$

where

$$c_n = \langle n | \Psi(t = 0) \rangle \tag{22}$$

Then the state for all future times has the following time dependence:

$$| \Psi(t) \rangle = \sum_{n=1}^{\infty} c_n | n \rangle \exp\left(\frac{-iE_n t}{\hbar} \right). \tag{23}$$

Written in terms of wavefunctions, the previous expressions become:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) \exp\left(\frac{-iE_n t}{\hbar} \right), \tag{24}$$

where

$$\psi_n(x) \equiv \langle x | n \rangle \text{ and } c_n = \int_{-\infty}^{\infty} \psi_n^*(x) \Psi(x, t = 0) dx. \tag{25}$$