

POSTULATES OF QUANTUM MECHANICS - STATES AND MEASUREMENTS

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Different books give different sets of postulates on which non-relativistic quantum mechanics is based. Most sources that I've seen, however, do tend to agree on the essentials, so we'll run through those here.

In classical mechanics, the path of a particle is, in the Hamiltonian formalism, described by specifying its position $x(t)$ and momentum $p(t)$ as functions of time. Both the position and momentum are specified precisely at all times. In quantum mechanics, the state of a particle is specified by a vector (ket) $|\psi(t)\rangle$ in a Hilbert space. This vector can be expressed either in position space as a wave function $\psi(\mathbf{r}, t)$ or in momentum space as the Fourier transform of ψ :

$$\phi(\mathbf{p}, t) = \int d^3r \psi(\mathbf{r}, t) e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} \quad (1)$$

The probability of finding the particle in the infinitesimal spatial volume d^3r centred at location \mathbf{r} is $|\psi(\mathbf{r}, t)|^2 d^3r$, and the probability of the particle's momentum being in the infinitesimal volume d^3p centred at momentum \mathbf{p} is $|\phi(\mathbf{p}, t)|^2 d^3p$.

The time dependence of $\psi(\mathbf{r}, t)$ is assumed to be given by the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V(\mathbf{r}) \psi \quad (2)$$

In classical mechanics, any dynamical variable ω is a function of the two phase-space coordinates x and p : $\omega = \omega(x, p)$. In quantum mechanics, the spatial coordinate x is replaced by a Hermitian operator X and the momentum p is replaced by the differential operator $P = -i\hbar \nabla$ which we discussed earlier. The classical dynamical variable $\omega(x, p)$ becomes a Hermitian operator $\Omega(X, P)$, where x and p in $\omega(x, p)$ are replaced by their corresponding operators X and P .

In classical mechanics, it is assumed that (in principle) any dynamical variable ω may be measured with arbitrary precision without changing the state of the particle. In quantum mechanics, every physically measurable

quantity is assumed to have a Hermitian operator associated with it. If we wish to measure the value of a variable represented by the Hermitian operator Ω , we must determine the eigenvalues ω_i and corresponding eigenvectors $|\omega_i\rangle$ of Ω , then express the state $|\psi\rangle$ as a linear combination of the $|\omega_i\rangle$. Then the best we can do is to state that the particular eigenvalue ω_i will be measured with probability $|\langle\omega_i|\psi\rangle|^2$. After the measurement, the state $|\psi\rangle$ 'collapses' to become the state $|\omega_i\rangle$. The only possible outcomes of a measurement of Ω are its eigenvalues; no intermediate values are possible. The collapse of the wave function is an ideal case. In practice, if a measurement of a physical quantity (associated with the Hermitian operator Ω , say) produces a value ω_i , the wave function (state vector) of the system is changed, but it may not actually become an eigenvector of Ω due to side effects of the measurement. For example, if we have a particle in a state $|x\rangle$ which is an eigenstate of the position operator X , then the idea of collapse of the wave function might lead us to expect that a measurement of position would yield precisely x and leave the system unchanged, since it was already in an eigenstate of position. However, in order to measure the position of a particle, we need interact with the particle, perhaps by bouncing a photon off it. A photon can determine the position of something only to within a location roughly equal to its wavelength, so to get a precise position measurement, we would need a photon of very short wavelength, which corresponds to a very high frequency, and thus to a very large momentum. Bouncing such a photon off a particle is bound to have some effect on the particle's state.

To illustrate these postulates, suppose we have the following three operators on a complex 3-d Hilbert space:

$$L_x = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \quad (3)$$

$$L_y = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{bmatrix} \quad (4)$$

$$L_z = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \quad (5)$$

Since L_z is diagonal, its eigenvalues can be read off from the diagonal elements as $0, \pm 1$, so these are the possible values of L_z that could be obtained in a measurement. Also because L_z is diagonal, its eigenvectors are

$$|L_z = +1\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad (6)$$

$$|L_z = 0\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \quad (7)$$

$$|L_z = -1\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \quad (8)$$

Suppose we start with the state $|L_z = +1\rangle$ in which $L_z = +1$, and we want to measure L_x in this state. To find the expectation values $\langle L_x \rangle$ and $\langle L_x^2 \rangle$ in this state, we calculate

$$\langle L_x \rangle = \langle L_z = +1 | L_x | L_z = +1 \rangle \quad (9)$$

$$= [1 \ 0 \ 0] \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad (10)$$

$$= \frac{1}{\sqrt{2}} [1 \ 0 \ 0] \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \quad (11)$$

$$= 0 \quad (12)$$

To get $\langle L_x^2 \rangle$ we first find the operator

$$L_x^2 = \frac{1}{2} \begin{bmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix} \quad (13)$$

Now we have

$$\langle L_x^2 \rangle = [1 \ 0 \ 0] \frac{1}{2} \begin{bmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad (14)$$

$$= \frac{1}{2} [1 \ 0 \ 0] \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} \quad (15)$$

$$= \frac{1}{2} \quad (16)$$

The uncertainty, or variance, is

$$\Delta L_x = \sqrt{\langle L_x^2 \rangle - \langle L_x \rangle^2} = \frac{1}{\sqrt{2}} \quad (17)$$

To find the possible values of L_x and their probabilities, we need to find the eigenvalues and eigenvectors of L_x , which we can do in the L_z basis, since this basis is given by the three vectors in 6. The eigenvalues are found in the usual way from the determinant:

$$\begin{vmatrix} -\lambda & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -\lambda & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & -\lambda \end{vmatrix} = -\lambda \left(\lambda^2 - \frac{1}{2} \right) - \frac{1}{\sqrt{2}} \left(\frac{-\lambda}{\sqrt{2}} \right) \quad (18)$$

$$= -\lambda^3 + \lambda = 0 \quad (19)$$

$$\lambda = 0, \pm 1 \quad (20)$$

The eigenvectors can be found in the usual way, by solving

$$(L_x - \lambda I) |L_x = \lambda\rangle = 0 \quad (21)$$

where the ket takes on the three possible values of λ successively. We let

$$|L_x = \lambda\rangle = \begin{bmatrix} a \\ b \\ c \end{bmatrix} \quad (22)$$

For $\lambda = +1$ we have

$$-a + \frac{b}{\sqrt{2}} = 0 \quad (23)$$

$$\frac{1}{\sqrt{2}} (a - \sqrt{2}b + c) = 0 \quad (24)$$

$$\frac{b}{\sqrt{2}} - c = 0 \quad (25)$$

Only two of these three equations are independent, so we can set $a = 1$ and solve for b and c to get

$$a = 1 \quad (26)$$

$$b = \sqrt{2} \quad (27)$$

$$c = 1 \quad (28)$$

Normalizing the eigenvector gives

$$|L_x = +1\rangle = \frac{1}{2} \begin{bmatrix} 1 \\ \sqrt{2} \\ 1 \end{bmatrix} \quad (29)$$

The other two eigenvectors can be found the same way, with the result

$$|L_x = 0\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} \quad (30)$$

$$|L_x = -1\rangle = \frac{1}{2} \begin{bmatrix} 1 \\ -\sqrt{2} \\ 1 \end{bmatrix} \quad (31)$$

Note that these eigenvectors are orthonormal.

Now that we have the eigenvectors of L_x we can answer the following question. If we start with the state $|L_z = -1\rangle$ and measure L_x , what are the possible outcomes and the probability of each?

First, we need to express $|L_z = -1\rangle$ in terms of the eigenvectors of L_x which we can do by solving three simultaneous linear equations, and we find

$$|L_z = -1\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = \frac{1}{2} (|L_x = +1\rangle + |L_x = -1\rangle) - \frac{1}{\sqrt{2}} |L_x = 0\rangle \quad (32)$$

(You can verify this by direct substitution.) Thus all 3 possible values of L_x can result from a measurement, and the probability of each is

$$P(L_x = +1) = |\langle L_x = +1 | L_z = -1 \rangle|^2 \quad (33)$$

$$= \left(\frac{1}{2} [1 \quad \sqrt{2} \quad 1] \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right)^2 \quad (34)$$

$$= \frac{1}{4} \quad (35)$$

$$P(L_x = 0) = |\langle L_x = 0 | L_z = -1 \rangle|^2 \quad (36)$$

$$= \left(\frac{1}{\sqrt{2}} [1 \quad 0 \quad -1] \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right)^2 \quad (37)$$

$$= \frac{1}{2} \quad (38)$$

$$P(L_x = -1) = |\langle L_x = -1 | L_z = -1 \rangle|^2 \quad (39)$$

$$= \left(\frac{1}{2} [1 \quad -\sqrt{2} \quad 1] \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right)^2 \quad (40)$$

$$= \frac{1}{4} \quad (41)$$

Now suppose we start with the state, written in the L_z basis:

$$|\psi\rangle = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \quad (42)$$

We take a measurement of L_z^2 and obtain +1. The operator L_z^2 is given by squaring 5:

$$L_z^2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (43)$$

This has a degenerate eigenvalue $\lambda = +1$, so the most we can say about the state $|\psi\rangle$ after the measurement is that it is projected onto the subspace

$a \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} + b \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$. That is, the state after the measurement is given by

$$|\psi\rangle_{after} = \mathbb{P}_{L_z=\pm 1} |\psi\rangle_{before} \quad (44)$$

$$= [|L_z = +1\rangle \langle L_z = +1| + |L_z = -1\rangle \langle L_z = -1|] \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \quad (45)$$

$$= \left(\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} [1 \ 0 \ 0] + \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} [0 \ 0 \ 1] \right) \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \quad (46)$$

$$= \begin{bmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{\sqrt{2}} \end{bmatrix} \quad (47)$$

We can normalize this state to get

$$|\psi\rangle_{after} = \frac{2}{\sqrt{3}} \begin{bmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{\sqrt{2}} \end{bmatrix} \quad (48)$$

Thus if we measure L_z immediately after the measurement of L_z^2 above, we get $L_z = +1$ with probability $\frac{1}{3}$ and $L_z = -1$ with probability $\frac{2}{3}$.

Finally, suppose we have a state $|\psi\rangle$ with the probabilities of measurements of L_z given as $P(L_z = 1) = \frac{1}{4}$, $P(L_z = 0) = \frac{1}{2}$ and $P(L_z = -1) = \frac{1}{4}$. Since these probabilities are given by $|\langle L_z = \lambda | \psi \rangle|^2$ for each of the three possible values of λ , and the vectors $|L_z = \lambda\rangle$ are orthonormal, the most general form for $|\psi\rangle$ is

$$|\psi\rangle = \frac{e^{i\delta_1}}{2} |L_z = 1\rangle + \frac{e^{i\delta_2}}{\sqrt{2}} |L_z = 0\rangle + \frac{e^{i\delta_3}}{2} |L_z = -1\rangle \quad (49)$$

where the δ_i are real numbers. For example

$$|\langle L_z = 1 | \psi \rangle|^2 = \left| \frac{e^{i\delta_1}}{2} \right|^2 = \frac{1}{4} \quad (50)$$

While the presence of a phase factor in a solitary state doesn't affect the physics of that state, if we have a sum of states, each with its own (different) phase factor, we can't ignore these phase factors. For example, if we measure L_x in this state and want the probability that $L_x = 0$, we have, using 30

$$P(L_x = 0) = |\langle L_x = 0 | \psi \rangle|^2 \quad (51)$$

$$= \left| \frac{1}{\sqrt{2}} [1 \ 0 \ -1] \left(\frac{e^{i\delta_1}}{2} |L_z = 1\rangle + \frac{e^{i\delta_2}}{\sqrt{2}} |L_z = 0\rangle + \frac{e^{i\delta_3}}{2} |L_z = -1\rangle \right) \right|^2 \quad (52)$$

$$= \left| \frac{1}{\sqrt{2}} [1 \ 0 \ -1] \left(\frac{e^{i\delta_1}}{2} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} + \frac{e^{i\delta_2}}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} + \frac{e^{i\delta_3}}{2} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right) \right|^2 \quad (53)$$

$$= \frac{1}{8} |e^{i\delta_1} - e^{i\delta_3}|^2 \quad (54)$$

$$= \frac{1}{8} |1 - e^{i(\delta_3 - \delta_1)}|^2 \quad (55)$$

The last line will have a different result for different values of the phase factors δ_1 and δ_3 , so they can't be ignored.

PINGBACKS

Pingback: Schrödinger equation and propagators

Pingback: Time-dependent propagators

Pingback: Postulates of quantum mechanics - Schrödinger equation and propagators