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 $\psi(\boldsymbol{r},t)$ or in momentum space as the Fourier transform of ψ:

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

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

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

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

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:

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

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

$$L_z = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \tag{5}$$

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

$$|L_z = +1\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \tag{6}$$

$$|L_z = 0\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \tag{7}$$

$$|L_z = -1\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \tag{8}$$

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 $\left\langle L_x^2\right\rangle$ in this state, we calculate

$$\begin{aligned}
\langle L_x\rangle &= \langle L_z = +1\,|L_x|\,L_z = +1\rangle && (9)\\
&= \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} && (10)\\
&= \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} && (11)\\
&= 0 && (12)
\end{aligned}$$

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

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

Now we have

$$\begin{aligned}
\left\langle L_x^2\right\rangle &= \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} \frac{1}{2} \begin{bmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} && (14)\\
&= \frac{1}{2} \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} && (15)\\
&= \frac{1}{2} && (16)
\end{aligned}$$

The uncertainty, or variance, is

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

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:

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

$$= -\lambda^3 + \lambda = 0 \tag{19}$$

$$\lambda = 0, \pm 1 \tag{20}$$

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

$$(L_x - \lambda I)\,|L_x = \lambda\rangle = 0 \tag{21}$$

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

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

For $\lambda = +1$ we have

$$-a + \frac{b}{\sqrt{2}} = 0 \tag{23}$$

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

$$\frac{b}{\sqrt{2}} - c = 0 \tag{25}$$

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

$$a = 1 \tag{26}$$

$$b = \sqrt{2} \tag{27}$$

$$c = 1 \tag{28}$$

Normalizing the eigenvector gives

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

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

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

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

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

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

(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

$$P(L_x=+1) = |\langle L_x=+1|L_z=-1\rangle|^2 \tag{33}$$
$$= \left(\frac{1}{2}\begin{bmatrix} 1 & \sqrt{2} & 1 \end{bmatrix}\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}\right)^2 \tag{34}$$
$$= \frac{1}{4} \tag{35}$$
$$P(L_x=0) = |\langle L_x=0|L_z=-1\rangle|^2 \tag{36}$$
$$= \left(\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 0 & -1 \end{bmatrix}\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}\right)^2 \tag{37}$$
$$= \frac{1}{2} \tag{38}$$
$$P(L_x=-1) = |\langle L_x=-1|L_z=-1\rangle|^2 \tag{39}$$
$$= \left(\frac{1}{2}\begin{bmatrix} 1 & -\sqrt{2} & 1 \end{bmatrix}\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}\right)^2 \tag{40}$$
$$= \frac{1}{4} \tag{41}$$

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

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

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

$$L_z^2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{43}$$

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

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

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

$$= \left(\begin{bmatrix}1\\0\\0\end{bmatrix}\begin{bmatrix}1 & 0 & 0\end{bmatrix} + \begin{bmatrix}0\\0\\1\end{bmatrix}\begin{bmatrix}0 & 0 & 1\end{bmatrix}\right)\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\\ \frac{1}{\sqrt{2}}\end{bmatrix} \tag{46}$$

$$= \begin{bmatrix}\frac{1}{2}\\ 0\\ \frac{1}{\sqrt{2}}\end{bmatrix} \tag{47}$$

We can normalize this state to get

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

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

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

where the δ_i are real numbers. For example

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

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

$$P(L_x=0) = |\langle L_x=0|\psi\rangle|^2 \tag{51}$$

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

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

$$= \frac{1}{8}\left|e^{i\delta_1} - e^{i\delta_3}\right|^2 \tag{54}$$

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

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

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