

The Essentials of Quantum Mechanics

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In classical mechanics, a particle has an exact, sharply defined position and an exact, sharply defined momentum at all times. Quantum mechanics is a *different* fundamental formalism, in which observables such as position and momentum are not real numbers but operators; consequently there are uncertainty relations, e.g. $\Delta x \Delta p \gtrsim \hbar$, which say that as some observables become more sharply defined, others become more uncertain. Experiments show that quantum mechanics, not classical mechanics, is the correct description of nature.

Here is a summary of the essentials of quantum mechanics, focussing on the case of a single non-relativistic particle (eg an electron) in one dimension. This is not a complete review of everything you need to know: it is a quick outline of the basics to help you get oriented with this challenging subject.

1. *States.* The state of the system is given by a *wavefunction* $\psi(x)$. The wavefunction is complex, and gives the amplitude for finding the particle at position x . The probability density is the square modulus of the amplitude, so in one dimension the probability to find the particle located between x and $x + dx$ is

$$P(x)dx = |\psi(x)|^2 dx . \quad (1)$$

This means that if you start off with an “ensemble” of identical copies of the system, all with the same wavefunction $\psi(x)$, and in each member you measure the position of the particle, then you will get different results from different members of the ensemble. The probability of getting particular answers is given by (1). A physical state must be normalized, so that all the probabilities add up to 1:

$$\int |\psi(x)|^2 dx = 1 . \quad (2)$$

However, for some purposes we will find it convenient to use unnormalized states.

2. *Operators.* Each observable corresponds to a linear operator. A linear operator is something that acts on a state and gives another state, ie it changes one function into another.

$$\begin{array}{ll} \text{position operator } \hat{x} & \text{defined by } \hat{x}\psi(x) = x\psi(x) \\ \text{momentum operator } \hat{p} & \text{defined by } \hat{p}\psi(x) = -i\hbar \frac{\partial\psi}{\partial x} \end{array} \quad (3)$$

For example, when the position operator acts on the state $\psi(x) = 1/(a^2+x^2)$, it gives $x/(a^2+x^2)$, while the momentum operator gives $2i\hbar x/(a^2+x^2)^2$.

Linearity means that an operator \hat{Y} acts on a sum of two states in the obvious way:

$$\hat{Y}(\psi(x) + \phi(x)) = \hat{Y}\psi(x) + \hat{Y}\phi(x) \quad (4)$$

3. *Expectation values.* The expectation value of an observable Y in a normalized state ψ is

$$\langle \psi | \hat{Y} | \psi \rangle = \int_{-\infty}^{\infty} \psi^*(x) \hat{Y} \psi(x) dx \quad (5)$$

This means that if you have an ensemble of identical copies of the system, all with the same wavefunction $\psi(x)$, then when you measure the value of the observable Y in all the members, the average value that you get is $\langle \psi | \hat{Y} | \psi \rangle$ (sometimes written $\langle \hat{Y} \rangle_{\psi}$, or even $\langle \hat{Y} \rangle$, if it is obvious from the context which state to use).

So the average position of a particle in a normalized state $\psi(x)$ is

$$\langle \psi | \hat{x} | \psi \rangle = \int_{-\infty}^{\infty} \psi^*(x) \hat{x} \psi(x) dx = \int_{-\infty}^{\infty} \psi^*(x) x \psi(x) dx = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx \quad (6)$$

which is just what you would expect from Eq. (1).

4. *Eigenvalues and eigenstates.* Each operator \hat{Y} has a set of eigenvalues y which are the possible values you can get on doing a measurement of Y . Any measurement of Y *must* yield one of the eigenvalues. Each eigenvalue y is associated with an eigenstate $\phi_y(x)$, which is the state for which the value of Y is exactly y , with no uncertainty. So if you create an ensemble of systems that are all in the same state, namely the Y -eigenstate $\phi_y(x)$, then when you measure the value of the observable Y , each member of the ensemble will give you the same answer, namely y . You can find the eigenstates and eigenvalues of an operator from the eigenvalue equation,

$$\hat{Y} \phi_y(x) = y \phi_y(x) \quad (7)$$

This equation says that if $\phi_y(x)$ is the eigenstate with eigenvalue y , then acting on $\phi_y(x)$ with the operator \hat{Y} just gives the same state back, but multiplied by the eigenvalue y . Physically, $\phi_y(x)$ is the state in which the observable Y has the definite value y . Note that the eigenvalues of an operator that corresponds to an observable are always real, since they are possible values of that physical observable.

For example, the eigenstates of the momentum operator are plane waves $\psi_p(x) = e^{ipx/\hbar}$:

$$\hat{p} e^{ipx/\hbar} = -i\hbar \frac{\partial}{\partial x} e^{ipx/\hbar} = p e^{ipx/\hbar} \quad (8)$$

The eigenstates of the position operator are δ -functions, $\psi_{x_1}(x) = \delta(x - x_1)$. The function $\delta(x - x_1)$ is zero everywhere except at $x = x_1$ where it is infinite, so $\hat{x} \delta(x - x_1) = x \delta(x - x_1) = x_1 \delta(x - x_1)$. (The formal definition of the δ -function is: $\int \delta(x - x_1) f(x) dx = f(x_1)$ for any function f .)

Note that the eigenstates of the position and momentum operators are *not normalizable*, so they are not themselves physically allowed states for a system, but they are the building blocks for allowed states, since you can build normalizable states out of them, e.g. wavepackets.

5. *Resolving a state into eigenstates.* The eigenstates of any operator \hat{Y} form a *complete orthonormal basis* of states, so you can write any state $\psi(x)$ in terms of them:

$$\psi(x) = \sum_y A_y \phi_y(x) \quad \text{or} \quad \psi(x) = \int A(y) \phi_y(x) dy \quad (9)$$

A_y or $A(y)$ is the amplitude for the value of the observable Y for a particle in the state $\psi(x)$ to be y . So when you make a measurement of the observable \hat{Y} on a system in the state $\psi(x)$:

$$\begin{aligned} \text{discrete eigenvalues:} & \quad |A_y|^2 = \text{probability to get the value } y \\ \text{continuous eigenvalues:} & \quad |A(y)|^2 dy = \text{probability to get } y \text{ to } y + dy \end{aligned} \quad (10)$$

The only question is: for a given state ψ , how do you express it in terms of eigenstates of Y , i.e. how do you calculate the coefficients A_y or $A(y)$? Actually, thanks to the orthonormality property this is easy: you multiply the state by the complex conjugate of the eigenstate of \hat{Y} with eigenvalue y , and integrate:

$$A_y \quad \text{or} \quad A(y) = \int \phi_y(x)^* \psi(x) dx . \quad (11)$$

Using (10) you then know the probability of getting any of the allowed values when you perform a measurement of Y on a particle in state ψ . This follows from the orthonormality property of the eigenstates:

$$\int \phi_{y_1}(x)^* \phi_{y_2}(x) dx = \begin{cases} \delta(y_1 - y_2) & \text{continuous eigenvalue spectrum} \\ \delta_{y_1, y_2} & \text{discrete eigenvalue spectrum} \end{cases} \quad (12)$$

6. *Measurement.* If a system has been prepared in a state $\psi(x)$, and you measure the value of some observable Y in that system, then

- The result of your measurement is one of the eigenvalues of the corresponding operator \hat{Y} .
- The probability to get any particular value (y_m , say) is given by the amount of the corresponding eigenstate $\phi_{y_m}(x)$ that is contained in $\psi(x)$ (see item 5 above).
- After you have made the measurement, the wavefunction of the system is changed: it is now $\phi_{y_m}(x)$, the eigenstate of \hat{Y} corresponding to the value of \hat{Y} that you obtained. So if you immediately measure Y again you will get the same answer as before. This is the “collapse of the wavefunction” that gives rise to apparent paradoxes like “Schrödinger’s cat”.

7. *The uncertainty principle.* Now you can see (qualitatively) how the uncertainty principle arises. The eigenstates of one operator are not in general the same as the eigenstates of a different operator. So when you make a state with a definite value of one observable, it will in general not have a definite value of the other observables. For example, a plane wave, which is an eigenstate of the momentum operator, has a definite value of the momentum. But plane waves are completely spread out in space, so the plane wave contains all eigenstates of the position operator, so the position is then completely uncertain.

8. *Time evolution.* The evolution through time of a state is determined by the energy operator, usually called the “Hamiltonian” \hat{H} , via the “time-dependent Schrödinger equation”:

$$\hat{H}\psi = i\hbar \frac{\partial\psi}{\partial t} \quad (13)$$

For a spinless non-relativistic particle of mass m in a one-dimensional potential $V(x)$ the Hamiltonian is

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \quad (14)$$

9. *Energy eigenstates.* Because time evolution is so important, the energy eigenstates are particularly important. As you would expect from (7), these are defined by

$$\hat{H}\psi_E(x) = E\psi_E(x) \quad (15)$$

which is called the “time-independent Schrödinger equation”, but is really just the standard equation for the Hamiltonian (i.e. energy) operator’s eigenvalues and eigenstates. You can apply the time-dependent Schrödinger

equation to the energy eigenstates, and show that they have simple time dependence: they oscillate at a frequency determined by their energy.

$$\psi_E(x, t) = \psi_E(x, 0)e^{-iEt/\hbar} \quad (16)$$

So the easiest way to evolve a state forward in time is to resolve it into energy eigenstates, and let each eigenstate oscillate at its own frequency:

$$\begin{aligned} \psi(x, 0) &= \sum_E A_E \psi_E(x) \\ \Rightarrow \psi(x, t) &= \sum_E A_E \psi_E(x) e^{-iEt/\hbar} \end{aligned} \quad (17)$$

The tricky part of this is that you have to calculate the eigenstates and corresponding eigenvalues of the Hamiltonian. This is not always easy to do, but once it is done you have solved the system: you know exactly how it will behave.