

PH101: Physics 1

Module 3: Introduction to Quantum Mechanics

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Postulates of Quantum Mechanics and the Question of Measurement

The story so far

- Einstein and de Broglie together wrote down the mathematical formulae that explained the meaning of wave particle duality

$$\text{Wave property} = \frac{h}{\text{Particle property}} \left\{ \begin{array}{l} \lambda = \frac{h}{p} \\ T = \frac{h}{E} \end{array} \right.$$

- Schrodinger used this to write down the expression for the probability amplitude of a matter wave with well defined momentum and energy (but not well defined position) in terms of its particle-like properties and using this he derived the wave equation for matter waves – **the Schrodinger Equation**
- Schrodinger used the superposition principle (or the concept of a wave packet) and the above matter wave to generate a state that corresponds to a particle with nearly well defined momentum and nearly well defined position thereby showing the way to recover classical physics from quantum mechanics.

Postulates of Quantum Mechanics

As the subject progressed, it became clear that a list of “Rules of the game” had to be urgently written down so that further progress could quickly be made. These rules go by the name of “Postulates of Quantum Mechanics” and they summarize what was known at that time (around 1927). The point of view contained in these postulates is known as the *Copenhagen Interpretation* of Quantum Mechanics since it was started by Neils Bohr and Werner Heisenberg working together in Copenhagen, Denmark between 1925-27.

1) State postulate: The state* of a quantum particle is described by a “wave function” which is denoted by $\psi(x, t)$ which is in general, a complex number and has the following meaning: $|\psi(x, t)|^2 dx$ is the probability of finding that particle between positions x and $x + dx$ at some time t . This is unlike in classical physics where the state of the particle is uniquely specified by prescribing its position x and momentum p (or velocity).

**The state of a system at a given time both in classical and quantum physics refers to that minimum amount of information needed to describe what this is at a later time assuming one knows all the forces etc that are acting in the system (i.e. the dynamics).*

2) Observables: While position is described by just a number x other physical quantities (known as “observables”) are described by operators (derivatives with respect to x, y, z if the particle moves in 3 dimensions e.g.).

Of this, the most important is the (linear) momentum $p = -i \hbar \frac{\partial}{\partial x}$. Since in this way of doing things, if x – the position has a well defined value, the momentum p cannot be a number with a well defined value. It has to be something that acts on the given state and leads to a number which could be the most probable value (or expectation value) for this quantity. Other observables such as angular momentum, kinetic energy etc. may be generated using the above correspondence. The average or “expected” value of an observable A is determined through the formula

$$\langle A \rangle = \int dx \psi^*(x, t) A \psi(x, t)$$

3) The measurement postulate: Measurement of the value of an observable in a quantum state in general yields a different result each time the measurement is performed (imagine n -copies of the same state and the same measurement being performed on all copies). All that quantum mechanics can predict are the values of these outcomes and the probabilities (or frequencies) with which they are seen. No one can know which of these outcomes will be seen in a specific attempt at measurement.

4) Collapse postulate: In general, it is not possible in quantum mechanics to perform measurements on a physical system without altering the state of the system. When a measurement of a certain physical quantity is performed, the state of the system changes abruptly to a new state where the quantity just measured has a well defined value equal to the outcome of the measurement.

e.g. You make a measurement of the position of the electron in a hydrogen atom. The state of the electron now abruptly changes to a new state such that subsequent measurements of the position made immediately afterwards yield the same result for the position. In classical physics this is not surprising. In quantum physics the position of the electron in general has a range of values with the corresponding probabilities - but having measured the position once, any measurements of position made immediately after this will not lead to new values for the position.

5) Non-commutativity: In general any two measurements are not commutative i.e. the answers depend on the order in which they are made.

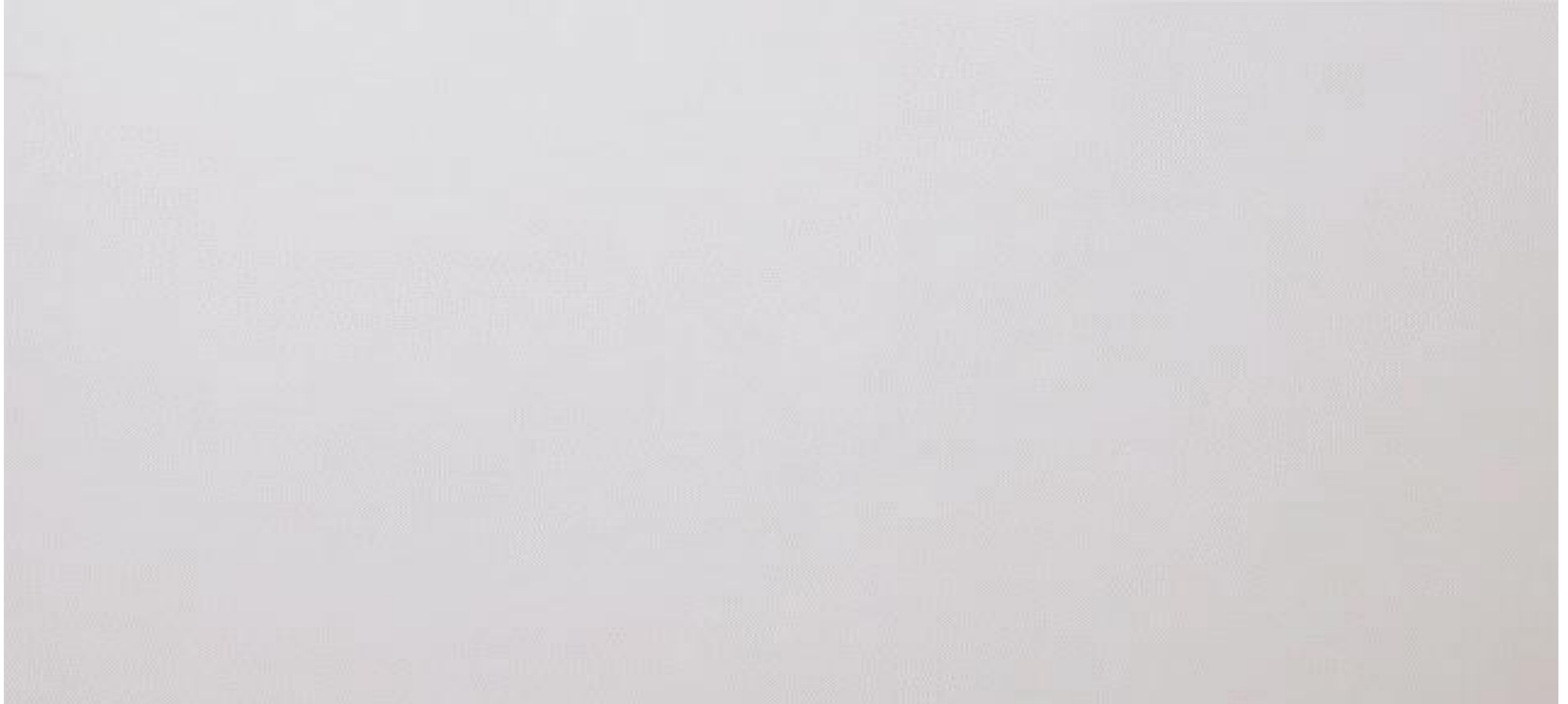
e.g. Imagine I measure the momentum of an electron in the hydrogen atom and then measure its position and note down the readings. I choose another hydrogen atom and reverse the order in which I make the measurements i.e. I first measure the position. But now I may or may not get the same value for the position I got when I did it with the earlier specimen. I keep choosing new specimens (all in the same state as the first specimen) and keep making position measurements until I get the outcome of the first specimen. Then I immediately measure the momentum. In classical physics the value of the momentum that I measured in the new specimen will be the same as in the first specimen but not so in the quantum world. This is called non-commutativity.

6) Evolution postulate: The state of a system in quantum mechanics evolves (changes in time) consistent with **Schrodinger's equation** until interrupted by a measurement.

$$i \hbar \frac{\partial}{\partial t} \psi(x, t) = \left(- \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t) \right) \psi(x, t)$$

Some conceptual difficulties with the probabilistic interpretation

- Schrodinger's cat paradox



The time-independent Schrodinger equation

Basis states of the Hamiltonian: In the Schrodinger equation we encountered an

expression $\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x, t)\right)$. This is called the Hamiltonian operator or Hamiltonian for short. It acts on functions of x (and possibly t) and gives other functions as the end result. We denote the Hamiltonian by the symbol H .

$$H = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x, t)\right)$$

Consider the case when the potential energy is independent of time i.e. we write $V(x)$ instead of $V(x, t)$. Just as in rigid bodies, the moment of inertia matrix \mathbf{I} had specific directions e_1, e_2 and e_3 so that $\mathbf{I} e_j = I_j e_j$ called eigenvectors, we could also ask if there are special functions $\varphi_j(x)$ that have the eigenvector property.

$$H\varphi_j(x) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\varphi_j(x) = E_j \varphi_j(x)$$

The time-independent Schrodinger equation

Then the functions $\varphi_j(x)$ would be analogous to finding the “principal directions” of the Hamiltonian. Just as in rigid bodies the three directions e_1, e_2 and e_3 were linearly independent and any other vector may be expressed as a linear combination of these directions viz. $v = \sum_j c_j e_j$ here too we may write for any function $\psi(x, t)$,

$$\psi(x, t) = \sum_j c_j(t) \varphi_j(x)$$

Specifically we want $\psi(x, t)$ to obey Schrodinger's equation. This means,

$$i \hbar \frac{\partial}{\partial t} \psi(x, t) = \sum_j i \hbar \frac{d}{dt} c_j(t) \varphi_j(x) \text{ and } \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t) \right) \psi(x, t) = \sum_j E_j c_j(t) \varphi_j(x)$$

or,

$$i \hbar \frac{d}{dt} c_j(t) = E_j c_j(t) \text{ which means } c_j(t) = e^{-\frac{i}{\hbar} E_j t} c_j(0)$$

If we assume that $c_j(0) = 0$ for all j except one special $j = n$ where $c_n(0) = 1$ then we obtain a stationary state.

$$\psi(x, t) = e^{-\frac{i}{\hbar} E_n t} \varphi_n(x)$$

This has the property that the probability density $|\psi(x, t)|^2$ is independent of time. It also means all expectation values are independent of time.

$$\langle A \rangle = \int dx \psi^*(x, t) A \psi(x, t) = \int dx \varphi_n^*(x) A \varphi_n(x)$$

Practical Quantum Mechanics

Q. A stationary state of a quantum particle has an eigen function described by,

$$\varphi_0(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right) ; & 0 < x < L \\ 0 ; & \text{otherwise} \end{cases}$$

a) Find the expectation value of the position.

$$\langle x \rangle = \int_0^L \varphi_0(x) x \varphi_0(x) dx = \frac{L}{2}$$

b) Find the expectation value of the momentum.

$$\langle p \rangle = \int_0^L \varphi_0(x) \left(-i \hbar \frac{\partial}{\partial x}\right) \varphi_0(x) dx = 0$$

This is because the waves are moving in both directions.

c) Find the expectation value of the kinetic energy.

$$\langle KE \rangle = \frac{1}{2m} \int_0^L \varphi_0(x) \left(-i \hbar \frac{\partial}{\partial x} \right)^2 \varphi_0(x) dx = \frac{\hbar^2 \pi^2}{2m L^2}$$

d) Find the probability that the particle is between 0 and L/4

$$\text{probability} = \int_0^{L/4} \varphi_0(x) \varphi_0(x) dx = \frac{\pi - 2}{(4\pi)} = 0.09$$

e) Estimate the size of the deviation of the position of the particle from its expected value.

$$\text{Deviation from expected value} = x - \frac{L}{2}$$

But is as likely for the particle to be to the left of $x = \frac{L}{2}$ as it is to the right of this value.

We want to know how far in absolute terms it can be found far away from $x = \frac{L}{2}$. For this we can do one of two things. We could calculate the average of $|x - \frac{L}{2}|$. This means we could say,

$$\Delta x = \int_0^L \varphi_0(x) \left| x - \frac{L}{2} \right| \varphi_0(x) dx$$

which is possible but the absolute value is a mathematically clumsy operation since we have to take into account the cases $x > \frac{L}{2}$ and $x < \frac{L}{2}$ separately while performing the above integral [do it as a homework]. What is usually done is to find the average of the square of $x - \frac{L}{2}$ and then we get a quantity whose units is $[\text{length}]^2$ but represents the deviation from the average value. To get a quantity with units of length we simply take the square root at the end. This is called RMS value.

$$(\Delta x)^2 = \int_0^L \varphi_0(x) \left(x - \frac{L}{2} \right)^2 \varphi_0(x) dx$$

In the present example we may evaluate this to get, $\Delta x = \mathbf{0.18 L}$. Hence the quantum particle is most likely to be found between $0.5 L - 0.18 L$ and $0.5 L + 0.18 L$.

Next natural question is how likely is most likely? The probability that the particle is found between $0.5 L - 0.18 L$ and $0.5 L + 0.18 L$ is,

$$\text{probability} = \int_{0.5 L - 0.18 L}^{0.5 L + 0.18 L} \varphi_0(x) \varphi_0(x) dx = 0.65$$

or 65% probability. If you want a higher probability choose, the interval to be $\frac{L}{2} - 2 \Delta x$ and $\frac{L}{2} + 2 \Delta x$. The probability that the particle is in this interval now is much higher.

$$\text{probability} = \int_{0.5 L - 0.36 L}^{0.5 L + 0.36 L} \varphi_0(x) \varphi_0(x) dx = 0.97$$

or 97% probability.

e) Estimate the size of the deviation of the momentum of the particle from its expected value.

This is easier to do since the expected value of momentum is zero.

$$(\Delta p)^2 = \int_0^L \varphi_0(x) \left(-i \hbar \frac{\partial}{\partial x} - 0 \right)^2 \varphi_0(x) dx = \langle p^2 \rangle = 2m \langle KE \rangle = \frac{\hbar^2 \pi^2}{L^2}$$

or $\Delta p = \frac{\hbar \pi}{L}$ Combining with the earlier result namely, $\Delta x = \mathbf{0.18 L}$ we conclude that

$$\Delta x \Delta p = \mathbf{0.565 \hbar} > \hbar/2$$

which is consistent with **Heisenberg's uncertainty principle**.