PHYS2003 Quantum Physics

Introduction to Some Basics

In classical mechanics, it is easy for us to unambiguously know the position of a particle $x(t)$ and its velocity $v(t)$ at a particular point in time. We know these from Newton's Laws of motion and other classical laws. For example, from Newton's 2nd Law and the definition of potential $V(x)$, we can write the equation:

$$m\frac{d^2x}{dt^2} = -\frac{dV}{dx}$$

Notice that this has a derivative of time on one side and a derivative of space on the other.

However, this type of analysis is not possible with Quantum Mechanics. Here, we get a very different equation of motion:

$$\boxed{i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi}$$

This is the Schrodinger Equation where $\hbar = \frac{h}{2}$ and ψ is the wave function.

What is this wavefunction ψ?

We define this such that the probability of finding a particle between $x=a$ and $x=b$ at a time t is:

$$\boxed{P([a,b]) = \int_a^b |\psi(x,t)|^2\,dx}$$

So we see that $|\psi|^2$ gives us a probability density function.

It is important to realise that ψ is complex by definition so $|\psi|^2 = \psi^*\psi$ where ψ^* is the complex conjugate.

It's a bit weird to get your head round but in Quantum Mechanics, we cannot predict unambiguosly, we can only predict probabilistically.

Since we can only predict probabilistically, do repeat measurements of, say, position of a particle at a particular time yield results drawn from a probability distribution?

No! Surprisingly repeat measurements yield the same value. This indicates the measurement has already changed (collapsed) the wave function.

Probability Distributions

Let's first consider discrete variables. Imagine a room with 14 students where age is distributed as $N(j)$ where N is the number of students with age j:

Total number of students: $N = \sum_{j=0}^{\infty} N(j)$

Probability of student being age k: $P(k) = \frac{N(k)}{N}$

Probability of being any age: $\sum_{j=0}^{\infty} P(j) = 1$

This is important to remember: probabilities are normalised to 1

Mean age, expectation value: $\langle j \rangle = \frac{1}{N} \sum_{j=0}^{\infty} j N(j) = \sum_{j=0}^{\infty} j P(j)$

expectation value of age^2: $\langle j^2 \rangle = \sum_{j=0}^{\infty} j^2 P(j)$

NB:// $\langle j \rangle^2 \neq \langle j^2 \rangle$

variance: $\sigma^2 = \langle j^2 \rangle - \langle j \rangle^2$

standard deviation: $\sigma = \sqrt{\langle j^2 \rangle - \langle j \rangle^2}$

We can now easily extend this for continuous variables. Now, we will have a continuous probability density function ρ instead of the discrete function N.

Probability between $[a, b]$: $P([a,b]) = \int_a^b \rho(x)\,dx$

Normalisation: we require that $\boxed{\int_{-\infty}^{\infty} \rho(x)\,dx = 1}$

expection value: $\boxed{\langle x \rangle = \int_{-\infty}^{\infty} x\,\rho(x)\,dx}$

We can also find the expectation value of a function:

$$\boxed{\langle f(x) \rangle = \int_{-\infty}^{\infty} f(x)\,\rho(x)\,dx}$$

Normalisation

As mentioned earlier, we define the wave function $\Psi(x,t)$ such that its norm-square $|\Psi(x,t)|^2$ is a probability density function. We know that $\int_{-\infty}^{\infty} \rho(x)\,dx = 1$ so we require the same for $|\Psi(x,t)|^2$.

The norm-square may not be 1 initially so we define a constant:

$$\boxed{|A|^2 \int_{-\infty}^{\infty} |\Psi(x,t)|^2\,dx}$$

It may not be possible to normalise a function. In general, we say that:

- Only normaliseable solutions are physical (although later we will see how to construct a normaliseable function out of non-normaliseable ones
- To normalise, they must be square integrable.
  ↳ i.e $\Psi(x,t)$ decays faster that $\frac{1}{\sqrt{x}}$ as $x \to \infty$

An important property of normalisation in the context of the Schrodinger Equation is that once a function is normalised, it remains normalised throughout time. This is because the SE is independent of time.
To show this, we start with:

$$\underbrace{\frac{d}{dt}\int_{-\infty}^{\infty} |\psi(x,t)|^2 \, dx}_{} = \int_{-\infty}^{\infty} \frac{\partial}{\partial t} |\psi(x,t)|^2 \, dx \qquad (*)$$

we are trying to show this $= 0$ to show normalisation does not change with time.

$$\frac{\partial}{\partial t}|\psi|^2 = \frac{\partial}{\partial t}(\psi^* \psi) = \psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t} \qquad (**)$$

We can now make substitutions with the schrodinger equation: $i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi$

$$\left.\begin{aligned} &\Rightarrow \frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2 \psi}{\partial x^2} - \frac{i}{\hbar} V\psi \\ &\Rightarrow \frac{\partial \psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2 \psi^*}{\partial x^2} + \frac{i}{\hbar} V\psi^* \end{aligned}\right\}$$

Note that the potential V is real so $V^* = V$

Subbing these into $(**)$ gives us:

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

$$= \frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right)\right] \qquad \text{sub into } (*)$$

$$\frac{d}{dt}\int_{-\infty}^{\infty} |\psi(x,t)|^2 \, dx = \underbrace{\frac{i\hbar}{2m}\left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right]_{-\infty}^{+\infty}}_{=0 \text{ since we require } \psi \to 0 \text{ as } x \to \infty} = \underline{\underline{0}}$$

Therefore, normalisation is <u>independent of time</u>.

Momentum

We previously defined $\langle x \rangle = \int_{-\infty}^{\infty} x \rho(x) dx$. If x is the position of a particle, then:

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\Psi(x,t)|^2 dx$$

We can observe how this changes over time:

$$\frac{d\langle x \rangle}{dt} = \int_{-\infty}^{\infty} x \frac{\partial}{\partial t} |\Psi|^2 dx = \frac{i\hbar}{2m} \int_{-\infty}^{\infty} x \frac{\partial}{\partial x} \left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right) dx$$

integrating by parts $= -\frac{i\hbar}{2m} \int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} dx + \frac{i\hbar}{2m} \frac{\partial}{\partial x} \int_{-\infty}^{\infty} x \left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right) dx$

$$\frac{d\langle x \rangle}{dt} = -\frac{i\hbar}{2m} \int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} dx + \frac{i\hbar}{2m} \left[\underbrace{x \left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right)}_{=0 \text{ since } \Psi = 0 \text{ as } x \to \infty} \right]_{-\infty}^{\infty}$$

$$\therefore \frac{d\langle x \rangle}{dt} = -\frac{i\hbar}{2m} \int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} dx$$

integrating by parts $= -\frac{i\hbar}{2m} \int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial x} + \Psi^* \frac{\partial \Psi}{\partial x} dx - [\Psi^* \Psi]_{-\infty}^{\infty}$

$$\frac{d\langle x \rangle}{dt} = -\frac{i\hbar}{m} \int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial x} dx$$

This is the "velocity of the expectation value"

This is a very important result. A good interpretation of this is that this is the probability of getting a particular value for velocity.

- $\langle v \rangle = \frac{d\langle x \rangle}{dt} = -\frac{i\hbar}{m} \int \Psi^* \frac{\partial \Psi}{\partial x} dx$
- $\langle p \rangle = m \frac{d\langle x \rangle}{dt} = m \langle v \rangle$

Can this be true? We postulate these two statements using our knowledge of classical mechanics but can they work in quantum mechanics? Yes! This is <u>Ehrenfest's</u> Theorem: The expectation values of quantum mechanical quantities behave according to classical laws.

Operators

We now introduce the concept of operators:

$$\boxed{\hat{x} = x} \quad \text{such that} \quad \langle x \rangle = \int_{-\infty}^{\infty} \hat{x} |\Psi|^2 \, dx = \int_{-\infty}^{\infty} \Psi^* x \Psi \, dx$$

$$\boxed{\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x} = -i\hbar \frac{\partial}{\partial x}} \qquad \langle p \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{p} \Psi \, dx = -i\hbar \int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial x} \, dx$$

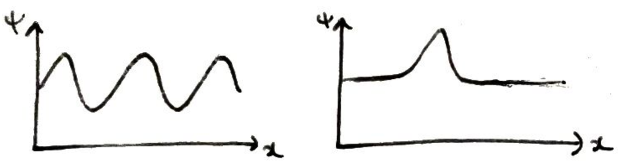
In general, a function $Q(x, p)$ has expection value:

$$\langle Q(x, p) \rangle = \int \Psi(x,t)^* \hat{Q}\left(\hat{x}, \frac{\hbar}{i}\frac{\partial}{\partial x}\right) \Psi(x,t) \, dx$$

So we can define one for kinetic energy. Classically we see $K = \frac{p^2}{2m}$ so:

$$\langle K \rangle = \frac{\langle p^2 \rangle}{2m} \quad \text{so} \quad \boxed{\hat{K} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}}$$

Uncertainty Principle



Consider these two wave functions. On the left, we see that the position of the particle is not clear but the wavelength is. On the right, the position of the particle is clear but the wavelength is not. Since the de Broglie relation relates momentum to wavelength: $p = \frac{\hbar}{\lambda}$, wavelength is analogous to momentum in this thought experiment.

So we see, if a particle's position is known precisely, its momentum is not known precisely. If a particle's momentum is known precisely, its position is not known precisely:

$$\boxed{\sigma_x \sigma_p \geq \frac{\hbar}{2}}$$

This is the Heisenberg Uncertainty Principle.