

Introducton to Quantum Mechanics

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1 Describing Motion

1.1 The Schrödinger Equation

In quantum mechanics, the wave function $\Psi(x, t)$ of a particle describes the position of that particle. It is given as the solution to the Schrödinger equation

$$\imath\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi$$

for some potential $V(x, t)$ and the initial condition $\Psi(x, 0)$. Here, $\hbar = \frac{h}{2\pi}$ is known as the reduced Planck constant and $\imath = \sqrt{-1}$.

But wait! If Ψ describes the motion of a particle, why does it depend on x ? Well, the wave function of a particle doesn't describe exactly where the particle is at a given time t , but rather related to the **probability** that the particle will be found at position x and time t . To put it more formally, the probability of finding the particle at time t between positions $x = a$ and $x = b$ is given by

$$\int_a^b |\Psi(x, t)|^2 dx.$$

Since $|\Psi(x, t)|^2$ is a probability, it must be true that

$$\int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx = 1.$$

If this integral diverges or is equal to zero, the particle described by the wave function cannot exist. If this is not the case and the integral exists but is not equal to one, we can simply normalize $\Psi(x, t)$ by multiplying by a factor A such that

$$\int_{-\infty}^{\infty} |A\Psi(x, t)|^2 dx = 1.$$

1.2 Taking Measurements and Expectation Values

Before a particle is observed, its position is not known and can only be described by the wave function of the particle. But physicists can take measurements of the position of the particle if they want to! Conducting such a measurement will result in what is known as the collapse of the wave function. Suppose the measurement taken returned a position D . The graph of $|\Psi|^2$ will have a large spike at $x = D$ and will be practically zero everywhere else - this make sense, because it is known where the particle is. However, as time after the measurement increases, Ψ transforms as directed by the Schrödinger equation and spreads

out.

If physicists were to set up a number of particles with the same wave function Ψ and measure their position at exactly the same time, they would most likely get a different answer each time. If the physicists did this enough times, though, they could average their results and obtain the expectation value of x , $\langle x \rangle$, given by

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

In general, given any continuous probability density $P(x)$ on the interval $(-\infty, \infty)$ and a function $f(x)$, the expectation value of $f(x)$ is given by

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} f(t) P(t) dt.$$

Going back to our wave function, $\langle x \rangle$ depends on time... so lets find the expectation value of the velocity. It can be shown that

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

where Ψ^* denotes the complex conjugate of Ψ . Since $p = mv$,

$$\langle p \rangle = -i\hbar \int_{-\infty}^{\infty} \left(\Psi^* \frac{\partial \Psi}{\partial x} \right) dx.$$

We can rewrite $\langle x \rangle$ and $\langle p \rangle$ to find something interesting:

$$\langle x \rangle = \int_{-\infty}^{\infty} \Psi^*(x) \Psi dx$$

$$\langle p \rangle = \int_{-\infty}^{\infty} \Psi^* \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right) \Psi dx$$

This suggests that the operator x is related to position, and the operator $\frac{\hbar}{i} \frac{\partial}{\partial x}$ is related to momentum. As it turns out, the expectation value of any quantity that can be represented through position and momentum can be found using the expectation values of x and p . For some quantity $Q(x, p)$,

$$\langle Q(x, p) \rangle = \int_{-\infty}^{\infty} \Psi^* Q \left(x, \frac{\hbar}{i} \frac{\partial}{\partial x} \right) \Psi dx.$$

1.3 Heisenberg's Uncertainty Principle

Earlier we mentioned that a physicist taking measurements on a set of particles with identical wave functions would produce different results each time. Some wave functions will produce a very small spread of values when these measurements are taken, but it turns out that as some quantities become more precise others become less precise and there exists an absolute minimum precision when measuring two different quantities of a particle. This is known as Heisenberg's uncertainty principle, and is described by

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

where σ_j is the standard deviation of j , defined as

$$\sigma_j^2 = \langle (j - \langle j \rangle)^2 \rangle = \langle j^2 \rangle - \langle j \rangle^2.$$

1.4 Problems

1. Consider the wave function

$$\Psi(x, t) = Ae^{-\lambda|x|}e^{-i\omega t}.$$

- (a) Normalize $\Psi(x, t)$ and find A .
(b) Find $\langle x \rangle$, $\langle x^2 \rangle$, and σ_x .

2. Consider the distribution

$$\rho(x) = Ae^{-\lambda(x-a)^2}.$$

- (a) Normalize $\rho(x)$ and find A .
(b) Determine $\langle x \rangle$, $\langle x^2 \rangle$, and σ_x .

3. A particle is represented at time $t = 0$ by the wave function

$$\Psi(x) = \begin{cases} A(a^2 - x^2) & \text{if } -a \leq x \leq a, \\ 0 & \text{otherwise.} \end{cases}$$

- (a) Normalize $\Psi(x, 0)$ and find A .
(b) Find $\langle x \rangle$ and $\langle p \rangle$.
(c) Find $\langle x^2 \rangle$ and $\langle p^2 \rangle$.
(d) Find σ_x and σ_p . Does Heisenberg's uncertainty principle hold?

2 Finding the Wave Function

2.1 The Time-Independent Schrödinger Equation

So now that we know all this, how do we go about solving the Schrödinger equation for $\Psi(x, t)$ for a given potential $V(x, t)$? If we let V be time-independent, then solutions to the wave function are of the form $\Psi(x, t) = \psi(x)\phi(t)$. The Schrödinger equation becomes

$$i\hbar\psi \frac{d\phi}{dt} = -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} \phi + V\psi\phi,$$

or,

$$i\hbar \frac{1}{\phi} \frac{d\phi}{dt} = -\frac{\hbar^2}{2m} \frac{1}{\psi} \frac{d^2\psi}{dx^2} + V.$$

c Note that the left side is only a function of t , and the right side in only a function of x . As such, they both must be constant. Call the constant they are both equal to E . Then,

$$\frac{d\phi}{dt} = -\frac{iE}{\hbar}\phi \Rightarrow \phi = e^{-iEt/\hbar}$$

and

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi = E\psi.$$

These equations don't look so bad! They're both ordinary differential equations (think back to last lecture). The equation involving t is trivially solvable, and the equation involving x is known as the time-independent Schrödinger equation and cannot be solved until we know what $V(x)$ is.

Now, what's truly remarkable is that solving the time-independent Schrödinger equation yields an infinite number of solutions (ψ_1, ψ_2, \dots) with an infinite number of corresponding values of E (which turns out to be energy). As it turns out, every solution to the Schrödinger equation $\Psi(x, t)$ can be expressed as a linear combination of the solutions to the time-independent equation. That is,

$$\Psi(x, t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}$$

where (c_1, c_2, \dots) satisfy

$$\Psi(x, 0) = \sum_{n=1}^{\infty} c_n \psi_n(x).$$

2.2 The Hamiltonian

In non-quantum mechanics, the Hamiltonian is the total energy of a system, or

$$H(x, p) = T + V = \frac{p^2}{2m} + V(x).$$

We previously learned that classical quantities can be represented by operators, so the Hamiltonian operator is

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

Conveniently, the time-independent Schrödinger equation can now be written as

$$\hat{H}\psi = E\psi.$$

Since $\langle H \rangle = E$, $\langle H^2 \rangle = E^2$, and $\sigma_H = 0$, we can conclude that for a separable solution, any measurement of the total energy of the particle will be E .

2.3 Big Problems

1. Consider the potential

$$V(x) = \begin{cases} 0 & \text{if } 0 \leq x \leq a, \\ \infty & \text{otherwise.} \end{cases}$$

Determine the wave function $\Psi(x, t)$ given an arbitrary initial function $\Psi(x, 0)$.

2. Consider the potential of the harmonic oscillator

$$V(x) = \frac{1}{2} m \omega^2 x^2.$$

Determine $\psi_0(x)$, where $\psi_0(x)$ is the solution to the time-independent Schrödinger equation with the lowest corresponding energy.