Quantum Mechanics

Physics Olympiad
Wang Jianzhi

"Do you guys just put the word 'quantum' in front of everything?"

--- Scott Lang

"Have any of you guys ever studied Quantum Physics?"
"Only enough to make conversations."

--- Natasha Romanoff

Quantum mechanics is a radical generalisation of classical Physics. Some aspects include quantisation (the restriction of quantities like energy to take on a discrete set of values), wave-particle duality, probability and uncertainty.

Planck's constant $h = 6.63 \times 10^{-34}\ \mathrm{J\ s}$

Well Known Experiments

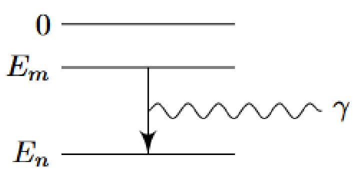
- Bohr's Model of Atom

  When atoms are excited, they emit light at a very specific frequencies. This suggests that the inner structure of an atom is discrete. To resolve this, Bohr proposed *Bohr's quantisation condition* that restricts the angular momentum to take on discrete values:

$$L = mrv = n\hbar$$

  With this result, several other quantities also became discrete:

$$r_n = \frac{4\pi\epsilon_0}{me^2}\hbar^2 n^2$$
$$v_n = \frac{e^2}{4\pi\epsilon_0}\frac{1}{\hbar n}$$
$$E_n = -\frac{1}{2}m\left(\frac{e^2}{4\pi\epsilon_0\hbar}\right)^2\frac{1}{n^2}$$



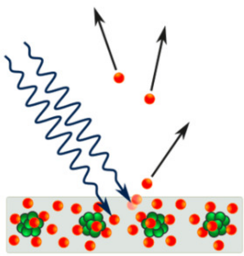
  The emitted frequency can now be solved with $hf = \Delta E = E_m - E_n$.

- Electron Diffraction

  This experiment is usually demonstrated to illustrate the wave-particle duality concept. The De Broglie's wavelength can be calculated via

$$\lambda = \frac{h}{p}$$

- Photoelectric Effect



Einstein proposed the above effect using the concept that light consists of tiny packets of energy called photons (or light quanta). Each packet carries an energy of hf where f is the frequency of the electromagnetic wave.

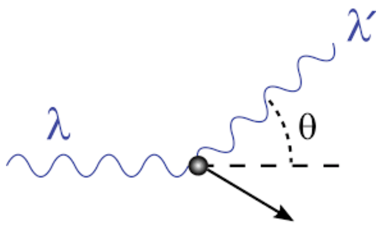
$$E = hf = \frac{hc}{v}$$

The maximum kinetic energy of the electrons that were emitted is given by $KE_{\max}$, where W is the work function of the metal surface.

$$KE_{\max} = hf - W$$

- Compton Scattering

Compton scattering is the scattering of a photon by a charged particle (e.g. electron). It usually results in the decrease in wavelength of the incoming photon. The Compton scattering formula can be proved using 4-vectors.



$$\lambda' - \lambda = \frac{h}{m_0 c}(1 - \cos\theta)$$

Quantum Mechanics

The time evolution of particles in quantum mechanics is governed by the *Schrodinger's equation*.

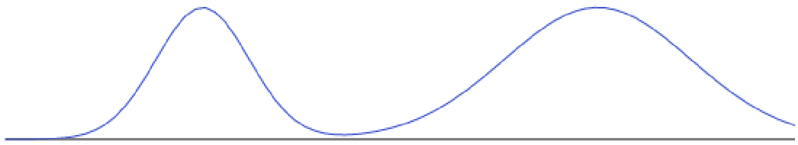
Classically, a point particle in one dimension has a definitive position x and momentum p at each time. But in quantum mechanics, a particle has a *state* at each time, specified by a complex-valued wave function.

Mathematically, you can think of $\psi(x)$ such that $|\psi(x)|^2$ represents the probability density function (recall from Thermodynamics) of finding a particle at position x.

$$P(\text{finding particle in [a, b]}) = \int_a^b |\psi(x)|^2 \, \mathrm{d}x$$

Clearly, $\psi(x)$ must be a normalised function, i.e. it must satisfy the following equation to be a valid probability density function.

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \, \mathrm{d}x = 1$$



For example, if the $|\psi(x)|^2$ function plots out the above graph, we have the highest chance of finding the particle at the peaks and the lowest chance at $x \to \pm\infty$ and the valley in the middle.

Operators

The wavefunction is often called the state of a particle. The nice thing about this wavefunction is that everything that we want to know about the particle can be obtained by doing some operation on the wavefunction. To obtain that information, we apply an *operator* to it.

For those who code, you can assume that the wave function is a blackbox. An operator is like a query to the blackbox and in return you obtain some information.

You: `query_momentum(wave_fn);`

Blackbox: `return momentum_operator(wave_fn);`

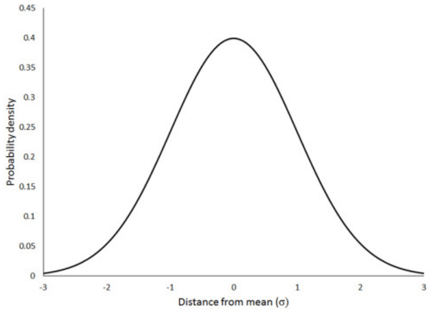
	Operator	Schrodinger's Equation
Position operator	$\hat{x} = x$	$\hat{x}\psi = x\psi(x)$
Momentum operator	$\hat{p} = -i\hbar \frac{\partial}{\partial x}$	$\hat{p}\psi = -i\hbar\, \psi'(x)$
Energy operator	$H = \frac{\hat{p}^2}{2m} + V(\hat{x})$	$H\psi = -\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x)$

The H above is also called the Hamiltonian. The mass of the particle is m and V denotes the potential in space. In general, if we measure an observable, the result is not certain. The values obtained will be randomly distributed over some probability function. However, the result is definite if and only if ψ is an eigenstate of the operator.

For example, if $\hat{p}\psi = p\psi$, then ψ is a state with a definite momentum p. Therefore, quantisation happens in quantum mechanics, because the operators have a distinct set of eigenvalues, resulting in discrete observables.

Consider a Gaussian distribution where $\alpha = \hbar/\sqrt{Km}$

$$\psi(x) = Ce^{-\frac{x^2}{2\alpha}}$$

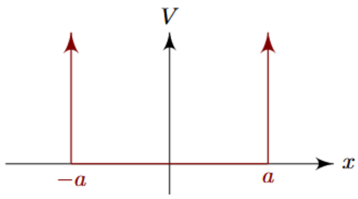


In a harmonic oscillator with potential $V(x) = \frac{1}{2}Kx^2$ and applying the Hamiltonian operator to ψ, we obtain:

$$H\psi = -\frac{\hbar^2}{2m}\psi''(x) + \frac{1}{2}Kx^2\psi(x) = \frac{\hbar}{2}\sqrt{\frac{K}{m}}\psi$$

Hence, the energy is definitely $\frac{\hbar}{2}\sqrt{\frac{K}{m}}$.

Infinite Well



$$V(x) = \begin{cases} 0, & |x| \leq a \\ \infty, & |x| > a \end{cases}$$

For $|x| < a$, the Schrodinger's equation becomes

$$-\frac{\hbar^2}{2m}\psi''(x) = E\psi$$

$$\psi = A\cos\left(\sqrt{\frac{2mE}{\hbar^2}}x\right) + B\sin\left(\sqrt{\frac{2mE}{\hbar^2}}x\right)$$

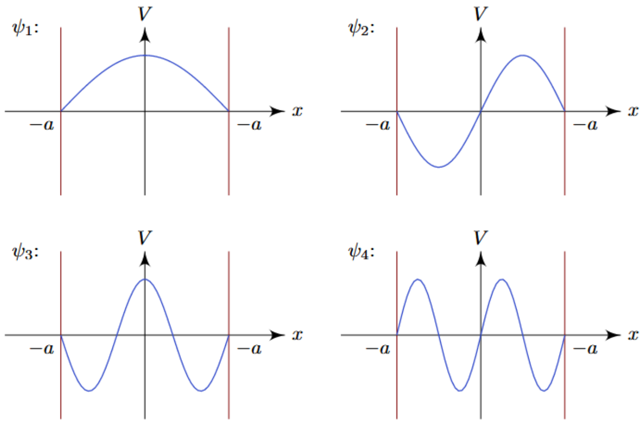
Since ψ needs to satisfy the boundary conditions (i.e. $\psi(\pm a) = 0$),

$$A\cos\left(\sqrt{\frac{2mE}{\hbar^2}}x\right) + B\sin\left(\sqrt{\frac{2mE}{\hbar^2}}x\right) = 0$$

This is only possible when $B = 0$ when $a = \sqrt{\frac{\hbar^2}{2mE}}\frac{n\pi}{2}$ when n is odd and $A = 0$ when $a = \sqrt{\frac{\hbar^2}{2mE}}\frac{n\pi}{2}$ when n is even. Hence, the allowed energy levels are:

$$E_n = \frac{\hbar^2\pi^2}{8ma^2}n^2$$

$$\psi_n(x) = \sqrt{\frac{1}{a}}\begin{cases} \cos\left(\frac{n\pi x}{2a}\right), & n \text{ odd} \\ \sin\left(\frac{n\pi x}{2a}\right), & n \text{ even} \end{cases}$$



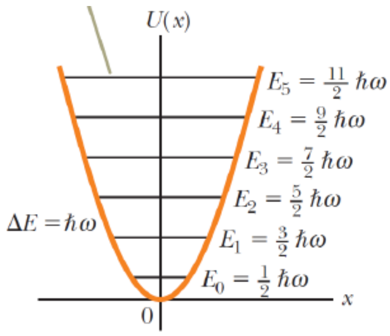
Simple Harmonic Oscillator

A particle subjected to a linear restoring force of $F = -kx$, where k is a constant and x is the displacement relative to equilibrium, undergoes simple harmonic motion. The potential function is $V(x) = \frac{1}{2}m\omega^2x^2$.

$$-\frac{\hbar^2}{2m}\psi''(x) + \frac{1}{2}m\omega^2x^2\psi(x) = E\psi$$

The resulting energy eigenvalues (also called the energy levels) are:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$



The energy levels are quantised. The ground state, represented by $n = 0$, has energy of $E_0 = \frac{1}{2}\hbar\omega$. The separation between the adjacent levels are equal and given by $\Delta E = \hbar\omega$. This was proposed by Max Planck in his explanation of blackbody's radiation, in which he managed to generate all these concepts without the benefit of the Schrodinger's Equation!

Heisenberg's Uncertainty Principle

If ψ is any normalized state (at any fixed time), then

$$(\Delta x)_\psi(\Delta p)_\psi \geq \frac{\hbar}{2}$$

A. Recommended Resources

- Introduction to Quantum Mechanics by David J. Griffiths