Waves as particles - the Photon

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History of light:

Romer 1676 - light has finite speed, what is moving?
Huygens 1678 - Light is a wave
Newton 1704 - Light is a particle

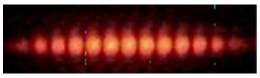
Both theories can explain
- Finite speed
- Shadows
- Reflects
- Refraction

Young double slit experiment

If light is a wave, interferences will be measurable
In experiment, interferences patterns are produced

If one slit is blocked, spread pattern as expected:

With 2 slits interferences occurs



Therefore, Light is a wave

This is caused by constructive and destructive interference

Light patches, phase difference = $0, \lambda, 2\lambda$... Constructive

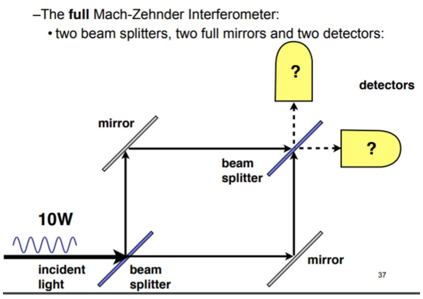
Dark patches, phase difference $= \frac{\lambda}{2}, \frac{3\lambda}{2}$ ... Destructive

Intensity vs amplitude

Amplitude max positive/negative value
Intensity $= amplitude^2$
Interferences is summing of positive/negative amplitudes

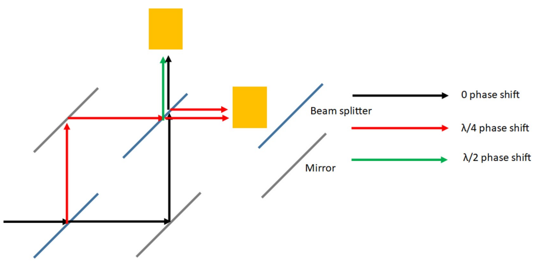
We see the intensity as a result

The Mach-Zehnder interferometer



Beam splitter - 50% of the light reflected, 50% transmitted

Reflected light has phase shift of $\lambda/4$
Transmitted light has no phase shift



In this experiment, no light reaches the top detector because the light interferes destructively.

Energy is still conserved

The light hitting the right detector has constructively interfered

Increased amplitude -> increased intensity -> all the energy

Problems with light as a wave

Couldn't explain black body radiation

Closest was Rayleigh-Jeans law

$$I(\lambda, T) = \frac{2\pi c k T}{\lambda^4}$$

Didn't fit the measured curve for small λ

Ultra violet problem

Planck 1900

Idea! Assumed light could be absorbed and emitted in discrete units

Each unit had E=hf

Derived Planck's law

$$I(\lambda, T) = \frac{2hc^2}{\lambda^5 \left(e^{\frac{hc}{\lambda kT}} - 1\right)}$$

Fit much better

Experimental observation for light as a particle:

Photo-electric effect (Einstein)

Shine light at a metal

Causes electrons to be emitted

Only occurs when shorter wave lengths of light hit

If wave length is too long, no electrons emitted regardless of intensity

But light had solid evidence for travelling as wave, more evidence needed

Photon momentum

Waves have momentum, light has momentum

Photons must have momentum too

Massless particles have momentum $p = E/c$

Photon has energy E=hf

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

This means light must exert pressure

This was already predicted for macroscopic objects (classical electromagnetism)

This isn't true for microscopic particles

Thomson Scattering (1900s)

Developed a theory for how waves should scatter from charged particles

Incoming wave causes charged particles to oscillate

Oscillating particles emit light of same frequency in all directions

But high energy x-ray scattering didn't match Thomson's predictions

Less light scattered backwards (towards incident light)

Angle dependent of frequency

Compton effect (1922)

Compton took Planck and Einstein seriously

Treated incoming x-rays as stream of particles

Scattering -> elastic collision

Momentum and energy conserved

Classically: loss of speed in scattered ball & momentum from recoil of other ball

Model energy and momentum according to Planck-Einstein formula

Treat electron motion using special relativity

Result - scattered photon has longer wave length

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

Wave shift is only dependent on angle

$$\frac{h}{m_e c} \approx 2 \times 10^{-12}\text{m}$$

Only measurable when photon wavelength is large

Hence only seen in x-rays

Verified the effect with variety of conductors

In all cases, his experiments matched his theory and disagreed with Thomson scattering

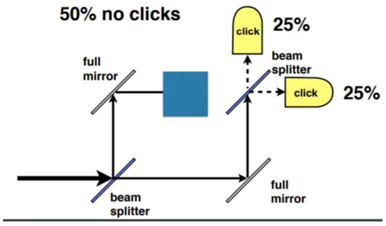
Combination of Planck, Einstein, and Compton meant light had to be a photon!

Wave-particle duality needed Quantum mechanics to explain

How does the idea of photons work in the experiments used to prove light as a wave?

If incident intensity is turned down, eventually only singular photons are sent, only discrete clicks are measured

- Photo-multiplier tube used to measure single photons
  - Photon hits metal, photoelectron emitted
  - Electron attracted to high PD, releases more electrons
  - Keeps occurring, until large amount of electron hit detector
- Youngs double slit experiment - single photons
  - Interference pattern is still produced, even with nothing to interfere with
- Mach-Zehnder Interferometer
  - Same effect as earlier
    - No interference, yet interference still occurs
    - As soon as one path is blocked, detectors detect equal amount of photons again



    - The photons know that there is a separate path they could travel down, even if there's nothing travel down.
  - Light acts as a wave, until it is measured. Then it acts as a particle

History of Atomic theory

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Old history:
- Democritus 400BC
  - All matter made up of indivisible 'atoms'
  - (no evidence)
- John Dalton 1800
  - All matter composed of atoms
  - Different 'types' of atom, with different mass - elements
  - Atoms that are same element are identical
  - Evidence: mass ratio in chemistry
- J.J. Thomson 1897
  - Discovered electron as a particle
  - Cathode ray - stream of electrons
    - Predicted by electromagnetic theory for negatively charged particles
  - Proposed model for atom - plum pudding model
    - Atoms are neutral, made up of electrons surrounded by positively charged 'liquid'
- Rutherford: 1907
  - Geiger-Marsden experiment
  - Shoot alpha particles at gold foil
  - Plum pudding model predicts slight deflection from positive charge
    - Instead, most pass through unaffected
    - Small amount reflected back
  - Suggested Planetary model
    - Dense positively charged nucleus
    - Electrons orbit
    - Explains reflected alpha particles as small amount would get close to nucleus
  - Contradicted some of the known physics at the time:
    - Orbiting electrons must experience centripetal acceleration
      - EM theory (Maxwell) predicted accelerating charge creates EM radiation
      - This implies electrons would lose energy and spiral into nucleus
    - Atomic spectrometry
      - Elements known to have unique signatures of emitted light
        - Not explained by this model.

Atomic spectrometry:
- Elements release/absorb specific frequencies of light. Each element different
- Hydrogen atom is simplest, so studied most
  - Could find the wavelength of these allowed light bands by Rydberg Formula:

$$\frac{1}{\lambda} = R_H \left(\frac{1}{m^2} - \frac{1}{n^2} \right)$$

  - Rydberg constant

$$R_H = 1.1 \times 10^7 \mathrm{m}^{-1}$$

  - Equation came from experimental values that matched.
  - Rydberg challenged people to derive this formula
    - Rutherford's planetary model fails

Bohr model (1913)
- A new atomic model - half way between Bohr and quantum mechanics
- Starting point - Planetary model for hydrogen
  - Single electron orbiting nucleus
- Extra rules:
  - Only orbits of specific radius allowed
  - Devised quantisation rule based on angular momentum

Producing the model:

- Assume electron orbits don't decay - don't produce light
- Orbits quantised, can only jump between specific orbits
- Quantisation from angular momentum:
  - $L = mvr = \hbar n$
- Consider radius of orbit:
  - Centripetal force and coulombs force:

$$F = \frac{m_e\, v^2}{r} \qquad F = \frac{1}{4\pi\epsilon_0} \times \frac{e^2}{r^2}$$

  - We can equate them:

$$v^2 = \frac{1}{4\pi\epsilon_0} \times \frac{e^2}{m_e r}$$

  - Next, take angular momentum and rearrange:

$$mvr = L = \hbar n \rightarrow v^2 = \frac{\hbar^2 n^2}{m^2 r^2}$$

  - Equate with the forces and rearrange for r

$$\frac{\hbar^2 n^2}{m_e^2 r^2} = \frac{1}{4\pi\epsilon_0} \times \frac{e^2}{m_e r} \rightarrow r = \frac{4\pi\epsilon_0 \hbar^2}{m_e e^2} n^2 = a_0 n^2$$

    Where a_0 is the Bohr radius $\approx 5.3 * 10^{-11} m$
- Next consider energy:

$$E = Ke + PE = \frac{1}{2} mv^2 - \frac{1}{4\pi\epsilon_0} \times \frac{e^2}{r}$$

  - We know what v^2 from the above, so

$$E = \frac{1}{2} m \left(\frac{1}{4\pi\epsilon_0} \frac{e^2}{m_e r}\right) - \frac{1}{4\pi\epsilon_0} \frac{e^2}{r} \rightarrow E = -\frac{1}{2}\left(\frac{1}{4\pi\epsilon_0} \frac{e^2}{r}\right)$$

  - But we know r in terms of the Bohr radius, and so can substitute:

$$r = a_0 n^2 \rightarrow E = -\frac{1}{2}\left(\frac{e a^0}{4\pi\epsilon_0} \times \frac{1}{n^2}\right) \rightarrow E = \frac{13.6eV}{n^2}$$

The Bohr model has multiple successes

- Atoms are stable (but only because we've defined them to be)
- Rydberg formula can be fully derived
- Rydberg constant expressed in terms of fundamental constants
- Bohr radius gives size scale of atoms
- Gives intuition to quantum atomic models

Failures:

- Only works for Hydrogen
- No justification for energy related to $\hbar$
- Not fully experimentally accurate:
  - Finer features in atomic spectra seen in modern experiments
  - Angular momentum of H in ground state = 0
  - Electron is not a classical partial

To do better than Bohr, we need quantum mechanics

Particles as waves

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The Bohr model was the best attempt at an atomic model, but it had flaws
A better model was required
- After the Bohr model, wave-particle duality of photons was growing in acceptance
- De Broglie said other particles should satisfy wave-particle duality

De Broglie waves
- Momentum of massless particles could be found based off their wavelength
- So the wavelength of a particle could be found by its momentum:
  - $\lambda = \frac{h}{p}$
  - This suggestion was quickly confirmed experimentally:
  - Davisson and Germer scattered an electron beam from Nickel
    - They thought the electrons would act as particles, allowing them to image the crystals surface
    - Instead, the electrons produced an interference pattern, just as with the double slit experiment
    - The distance between peaks was consistent with the De Broglie wave length

Scattering can be done with quite large particles, but the de Droglie wave length is too insignificant to see on a day to day basis.
- Just like with light, when observed particle like behaviour occurs. When unobserved, they have wave like behaviour
  - If buckminsterfullerene(BMF) is shot at a diffraction grating, interference occurs.
  - Hot BMF emits light.
  - If hot BMF is shot at a diffraction grating, no interference occurs
    - We can detect the light, meaning the particle's path can be detected
    - The probability breaks down, and it acts as a particle.

QM I - The wave function

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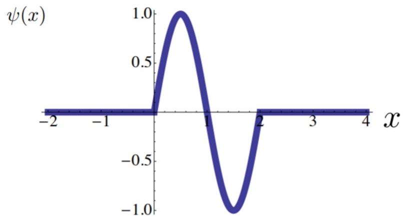
Wave-particle duality cannot be fully explained by classical methods
Quantum mechanics provides
- A new way to describe properties of a system
- To calculate physical quantities, such as energy
- Compute the evolution of systems over time
- Predict outcomes of experiments

In the double slit experiment, trying to measure which slit the photon is passing through stops an interference pattern from occurring
Buckminsterfullerene(BMF) gives a good example
- If BMF is shot at a diffraction grating, interference occurs.
- Hot BMF emits light.
- If hot BMF is shot at a diffraction grating, no interference occurs
  - We can detect the light, meaning the particle's path can be detected
  - The probability breaks down, and it acts as a particle.

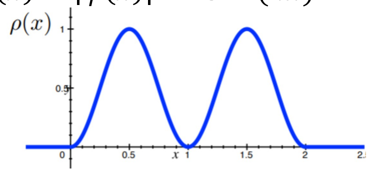
Any physical process which leaves a record of a physical property can be considered a measurement

Quantum particles are not particles
- They travel as waves, so can interfere
- Measurements are probabilistic
- Measurement changes evolution of the system

The wave function of a particle represents its position
- It can be positive, negative, or complex
- We use the Greek letter ψ
- We only study 1 dimensional waves
- To find the probability of the position:
  - $\mathrm{P}(a \leq x \leq b) = \int_a^b |\psi(x)|^2 dx$
- For example:
  - $\psi(x) = \sin(\pi x)\ \ for\ 0 \leq x \leq 2$
  - $\psi(x) = 0 \qquad elsewhere$



So, $\rho(x) = |\psi(x)|^2 = \sin^2(\pi x)$



From this we can see that there is a 100% chance of finding the particle between 0 and 2
What is the probability $0.5 \leq x \leq 1$
- Logically, it's 1/4, but we can do it mathematically and prove the same

Sometimes, the total area under the curve isn't equal to 1, which it needs to be for probabilities.
So we must normalise:

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

If this is true, then the wave function is 'normalised'

This means we must divide the wave function by something:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = N \neq 1 \rightarrow \int_{-\infty}^{\infty} \left|\frac{\psi(x)}{\sqrt{N}}\right|^2 dx = 1$$

Properties a wave-function must satisfy:

- It must be continuous
- Their first derivatives must be continuous
    - This means the second derivative is finite
- Is normalised

We sometimes need to find the expectation value:

This is the expected value of a probability function

$$< x > = \int_{-\infty}^{\infty} \rho(x) x \, dx$$

De Broglie waves arise in wave-functions

$$\psi(x) = e^{\frac{ipx}{\hbar}}$$

This is a complex wave-function so we don't study it this year

Instead we look at a simpler version:

$$\psi(x) = \sin\left(\frac{px}{\hbar}\right)$$

This however cannot be solved for, as it cannot be normalised

This is due to the Heisenberg uncertainty principle

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

This means that particles can't have an exact momentum, and why particles can behave like waves... (iI think...)

The Time independent Schrodinger Equation (TISE):

When not being measured, wave-functions evolve in time:

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

- This is similar to classical waves like water
    - However can be complex
- This means wave-function evolves like a wave

QM II - Energy in QM

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Towards a Quantum model

We want a quantum model for an atom

We need a wave-function for the electron

This will replace the orbits of the Bohr model

Atomic spectra give us some clues:

Discrete frequencies imply discrete energy in atom

In Bohr model this was forced in via angular momentum.

We need to look at the Time Independent Schrodinger equation:

In 1 dimension:

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

This is a second order differential equation.

When solved, we can find the allowed energies and their corresponding wave functions

The TISE contains a term for potential, this is very useful

Potential can be used to describe any conservative force, such as Coulomb's law

Overall, the TISE can be used to study any potential energy problem

If there is no potential, $V(x) = 0$, the partical is free and the TISE becomes:

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

This is a form of SHM, and can be solved the same way:

Assume $\psi(x) = Asin\left(\frac{2\pi(x-\phi)}{\lambda}\right)$

$$\frac{d\phi}{dx} = \frac{2\pi}{\lambda}\cos\left(\frac{2\pi(x-\phi)}{\lambda}\right)$$

$$\frac{d^2\phi}{dx^2} = -\left(\frac{2\pi}{\lambda}\right)^2 Asin\left(\frac{2\pi(x-\phi)}{\lambda}\right) \rightarrow \frac{d^2\phi}{dx^2} = -\left(\frac{2\pi}{\lambda}\right)^2 \psi(x)$$

Looking back at the TISE with no potential:

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2mE\psi(x)}{\hbar^2} = -\left(\frac{2\pi}{\lambda}\right)^2 \psi(x)$$

$$\rightarrow \frac{2mE}{\hbar^2} = \left(\frac{2\pi}{\lambda}\right)^2 \rightarrow \sqrt{2mE} = \frac{2\pi\hbar}{\lambda} = \frac{h}{\lambda} = p\ (from\ de\ Broglie) \rightarrow E = \frac{p^2}{2m}$$

$$\frac{2\pi}{\lambda} = \frac{p}{\hbar} \rightarrow \psi(x) = Asin\left(\frac{2\pi x}{\lambda} - \frac{2\pi\phi}{\lambda}\right) = Asin\left(\frac{px}{\hbar} + C\right)$$

This is all consistent with classical mechanics

The TISE tells us these sinusoidal waves represent energy $E = \frac{p^2}{2m}$

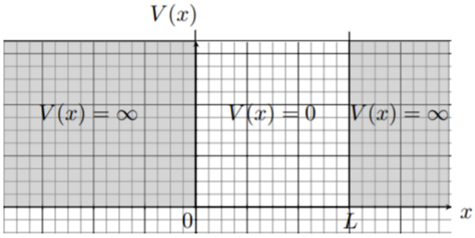
Infinite Square well:

We look at an example with the TISE were potential is taken into account

The infinite square well:

$V(x) = 0$ for $0 \leq x \leq L$

$V(x) = \infty \quad \text{elsewhere}$



In the area with infinite potential energy, the wave function must equal 0, as a particle can't have infinite energy. ($\psi_A(x) = 0$)

In the area with 0 potential energy the wave equation takes the form we calculated above:

$$\psi_B(x) = Asin\left(\frac{px}{\hbar} + C\right)$$

The overall wave equation must be continuous. This means that:

$$\psi_A(0) = 0 \ = \psi_B(0) \quad \& \ \psi_A(L) = 0 = \ \psi_B(L)$$

$$Asin(C) = 0 \therefore C = n\pi, Asin\left(\frac{pL}{\hbar} + n\pi\right) = 0 \therefore \frac{pL}{\hbar} + n\pi = m\pi$$

$$\frac{pL}{\hbar} = n\pi \rightarrow \frac{p}{\hbar} = \frac{n\pi}{L} \rightarrow \psi_B(x) = Asin\left(\frac{n\pi x}{L}\right)$$

We can then find the energy:

$$\psi_B(x) = Asin\left(\frac{n\pi x}{L}\right) \rightarrow \frac{d\psi_B^2(x)}{dx^2} = -\left(\frac{n\pi}{L}\right)^2 \psi_B(x)$$

$$\frac{2mE}{\hbar^2} = \left(\frac{n\pi}{L}\right)^2 \rightarrow E = \frac{\hbar^2\pi^2 n^2}{2mL^2} = \frac{h^2}{8mL^2}n^2$$

The energy takes discrete values. This isn't forced like the Bohr model, it comes as a requirement of the continuous nature of the wave function.

The only step left is to normalise the function:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = 1 \rightarrow \int_0^L A^2 \sin^2\left(\frac{n\pi x}{L}\right) dx = N$$

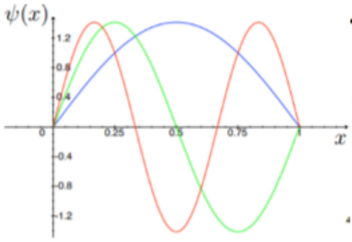
$$N = A^2 \left[\frac{x}{2} - \frac{L}{4\pi n}\sin\left(\frac{2\pi n x}{L}\right)\right]_0^L = \frac{A^2 L}{2}$$

The normalised function is therefore:

$$\frac{\psi(x)}{\sqrt{N}} = \sqrt{\frac{2}{L}} sin\left(\frac{n\pi x}{L}\right)$$

We can plot this for different values of n and L, and their corresponding probabilities :

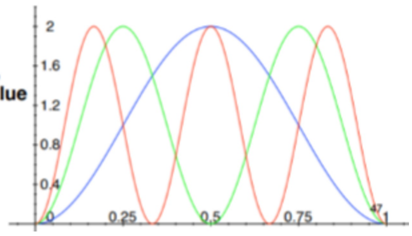
E.g. n=1,2,3
L=1



• E.g. n=1,2,3
L=1,

For all values of n, the expectation value of x is:

$$\langle x \rangle = \frac{L}{2}$$



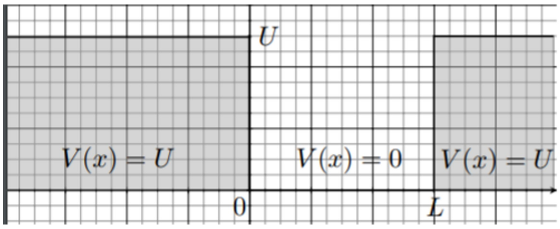
We have shown quantised energy states and the associated probability of a simple wave function

Finite square well:

In nature, there is no such thing as an infinite potential, so instead we can study the finite square well:

$V(x) = 0$ for $0 \leq x \leq L$

$V(x) = U$ elsewhere (U>0)



We know a wave function must be continuous, but we also need the first derivative to be continuous (means no part of the TISE is infinite). This adds a second boundary condition.

We already know $\psi_B(x) = Asin\left(\frac{px}{\hbar} + C\right)$ for the zone with 0 potential

We must now solve the differential equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U\psi(x) = E\psi(x)$$

There are two possibilities: U>E, or E>U

Consider U>E

Try solution $\psi(x) = ae^{bx+c}$

$$\frac{d\psi(x)}{dx} = abe^{bx+c}, \qquad \frac{d^2\psi(x)}{dx^2} = ab^2e^{bx+c} = b^2\psi(x)$$

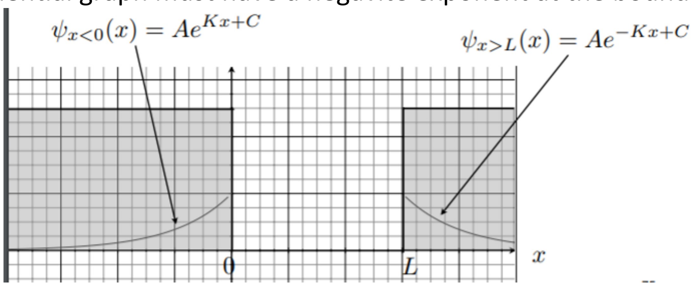
$-\frac{\hbar^2}{2m}b^2 = (E-U)$ U>E, therefore (E-U) = -(U-E) therefore…

$$b = \pm\frac{\sqrt{2m(U-E)}}{\hbar} = \pm k \rightarrow \psi_A(x) = ae^{\pm kx+c} \rightarrow De^{\pm kx}$$

Now consider boundary conditions:

$$\psi_A(0) = \psi_B(0), \psi_A(L) = \psi_B(L), \frac{d\psi_A(0)}{dx} = \frac{d\psi_B(0)}{dx}, \frac{d\psi_A(L)}{dx} = \frac{d\psi_B(L)}{dx}$$

For $V(x) = U$, the line must tend towards 0, as the graph must have a finite area, so the exponential graph must have a negavite exponent at the boundary points:



With some re-arranging, the boundary conditions can be found through graphical methods, but there is no analytical solution for this problem.

The solutions take the form of sinusoidal within the well and exponentially decay outside of it.

If E>U:

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2m(E-U)}{\hbar^2}\psi(x) \rightarrow \psi(x) = Asin\left(\frac{p'x}{\hbar} + C\right)$$

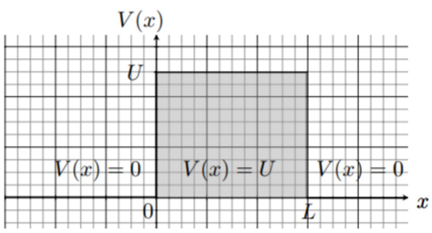
$$p' = \sqrt{2m(E-U)}, \rightarrow E = \frac{p'^2}{2m} + U$$

-> Solution for a classical particle.

Quantum tunnelling

As we can see from the finite square well, there is a non 0 chance of finding the particle in a potential it does not have energy to achieve (E<U). This allows for quantum tunnelling to occur:

We can study a quantum potential barrier using TISE:



$V(x) = U$ for $0 \le x \le L$
$V(x) = 0$ elsewhere
We don't need to solve it, but we can again know that the wavefunction will be sinusoidal in the regions of $V(x) = 0$, and exponential within the potential.

This means a particle can overcome a potential even if it doesn't have enough energy to. For radioactive decay to occur, an alpha particle tunnels through a potential barrier. This is why radioactive decay has a probabilistic nature.
It also occurs in the sun, with particles overcoming the coulomb potential to bind.
We also use quantum tunnelling in a scanning tunnelling microscope, which detects the current required for a potential to be overcome. This allows us to generate images at an atomic scale.