Quantum Mechanics of Particles & Fields

Outline :

- Review of Previous Lecture.
- Single Particle Wavefunctions.
- Time−Independent Schrödinger equation.
- Particle in a Box.
- Time−Dependence. Energy Eigenfunctions.
- Particle in a Box Revisited.
- The Hydrogen Atom.
- Quantum Theory of Fields.

Review of Previous Lecture

- Wave−particle duality : all objects display both wave and particle properties
- The De Broglie equation relates wave and particle properties :

$$p = h/\lambda$$

p = momentum
λ = wavelength

- The Uncertainty Principle places fundamental limits on our measurements :

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

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

- Quantum mechanical waves are "probability waves" :

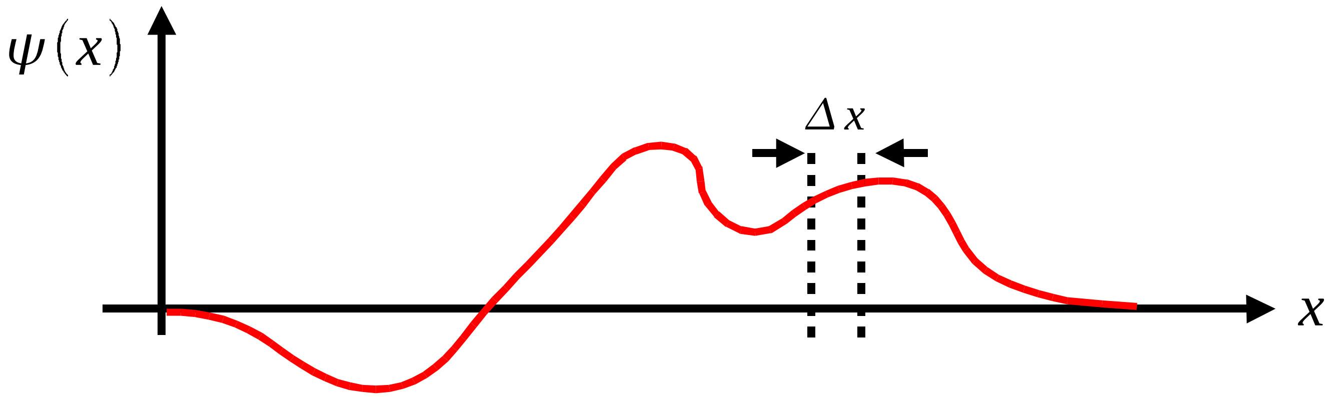
$$\text{Probability} \propto |\psi|^2$$

ψ is generally complex.

- We want to look at the equations governing these quantum mechanical probability waves.

Single Particle Wavefunctions

- In 1−dimension :



- Probability for the particle to be found in the small interval Δx is :

$$|\psi(x)|^2 \times \Delta x$$

- Given that the probability to find the particle anywhere must be exactly 1, we have the condition :

$$\int |\psi(x)|^2 \, dx = 1$$

Wavefunction normalisation

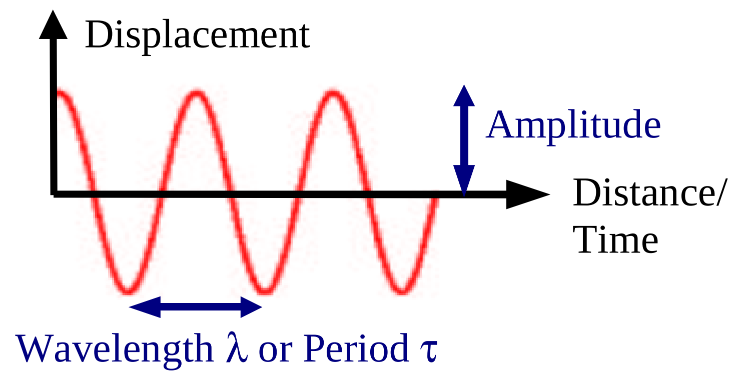
Schrödinger Equation

- We have already seen that :

$$\cos(kx - \omega t) = \mathrm{Re}\left(e^{i(kx - \omega t)}\right)$$

$$\boxed{k = 2\pi/\lambda \qquad \omega = 2\pi/\tau}$$

is a suitable representation of a plane wave.



- The quantum mechanical equivalent of the plane wave is simply :

$$\psi(x, t) = A\, e^{i(kx - \omega t)}$$

- This has the property that :

$$\left|\psi(x, t)\right|^2 = A^2$$

- This is completely independent of *x*
  - ➡ This wavefunction contains no information about the location of the particle.
- But if Δ*x* is infinite, then by the uncertainty relationship, the momentum is known perfectly.

Schrödinger Equation

- So, the following wavefunction describes a particle of unique momentum :

$$\psi(x, t) = A\, e^{i(kx - \omega t)}$$

- This means that I expect the following two relations to be relevant :

De Broglie :

$$p = \hbar k$$

Kinetic energy :

$$E = \frac{p^2}{2m}$$

- These are both satisfied if the above wavefunction is inserted into :

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

(spatial part of the wavefunction only)

- A slight generalisation takes into account the possibility that the particle has energy by virtue of being in a potential ***V*** as well as kinetic energy :

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

Time−independent Schrödinger equation.

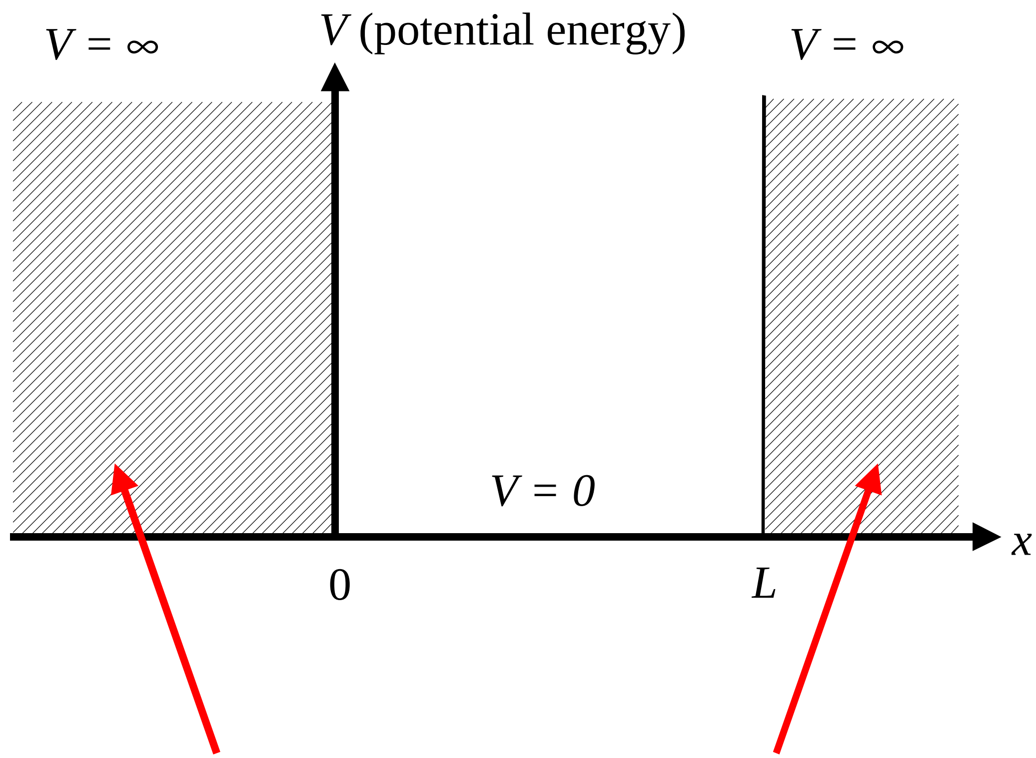
Schrödinger Equation

- A lot of quantum mechanics consists in simply solving this equation for different potentials ***V*** **:**

Potential :	Physical significance :
$\frac{1}{2}Kx^2$	Simple harmonic oscillator
$\frac{q_1 q_2}{4\pi\epsilon_0 r}$	Coulomb potential : atoms
Complicated crystal lattice	Solid state physics

Particle in a Box

- We're going to start with something much simpler − a particle in a one dimensional box. The box is represented by an infinite potential well.



Wavefunction must be 0 in these regions, otherwise there would be a finite probability to find the particle with infinite energy.

Particle in a Box

- For the region $0 \leq x \leq L$:

$$\frac{-\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi \qquad (1)$$

$$\Rightarrow \quad \psi = A\cos kx + B\sin kx$$

- Since $\psi(0) = \psi(L) = 0$ this leaves :

$$\psi = N\sin(\frac{n\pi x}{L}) \qquad n = 1, 2, 3, \ldots$$

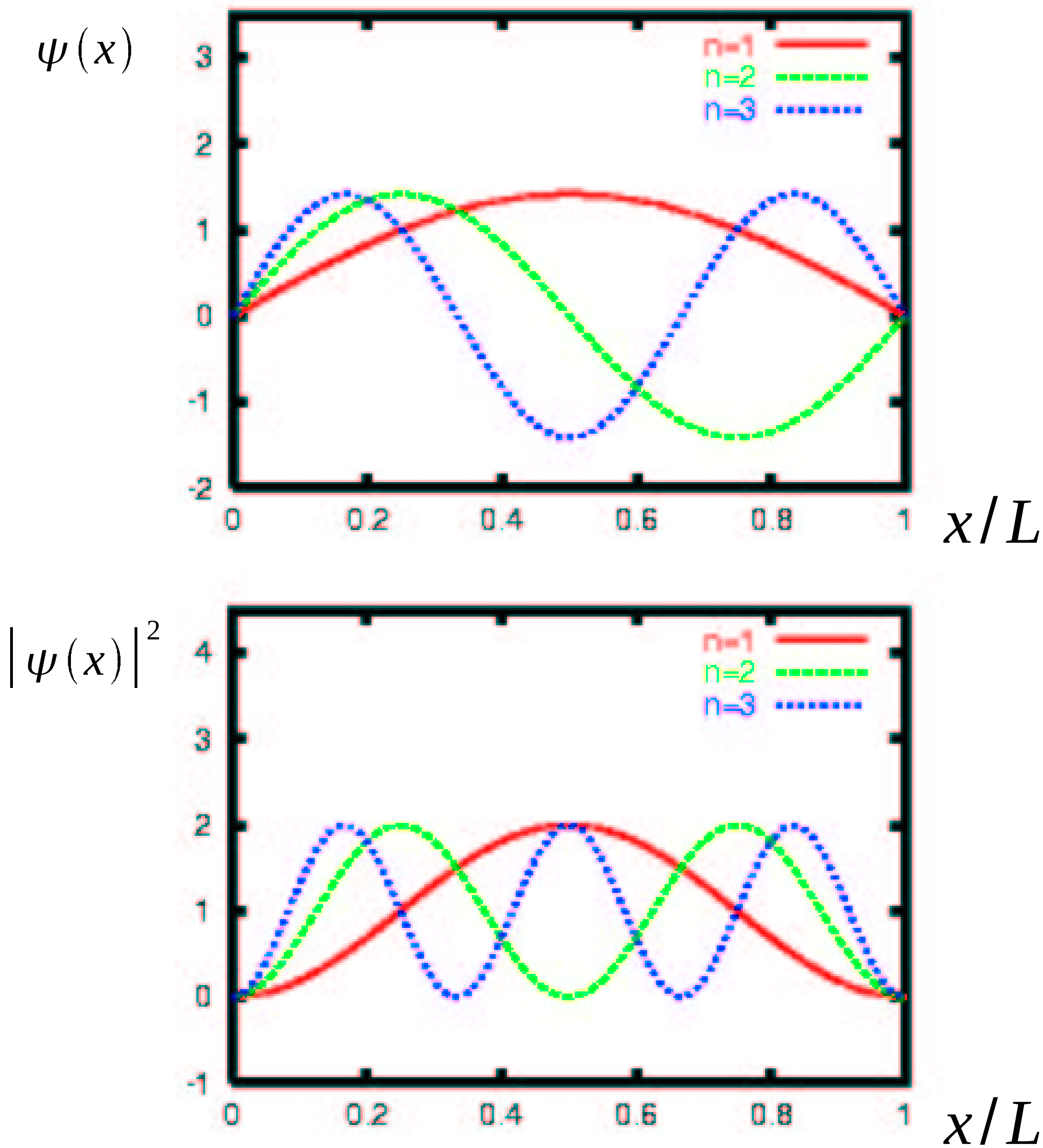
Normalisation factor

- Substituting in (1) gives :

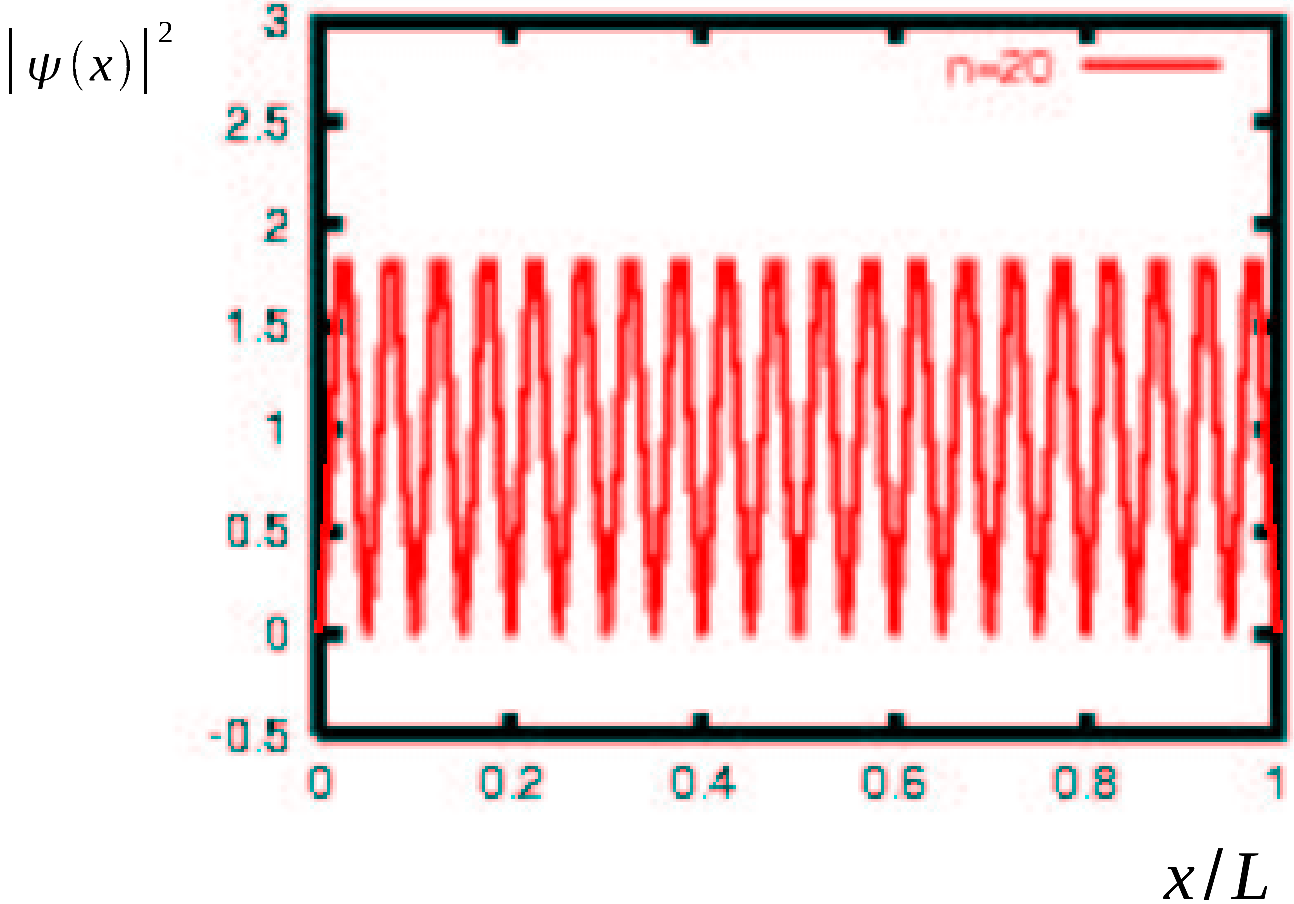
$$E = \frac{\hbar^2\pi^2 n^2}{2mL^2}$$

A discrete set of allowed energy levels : **quantisation** of energy.

Particle in a Box



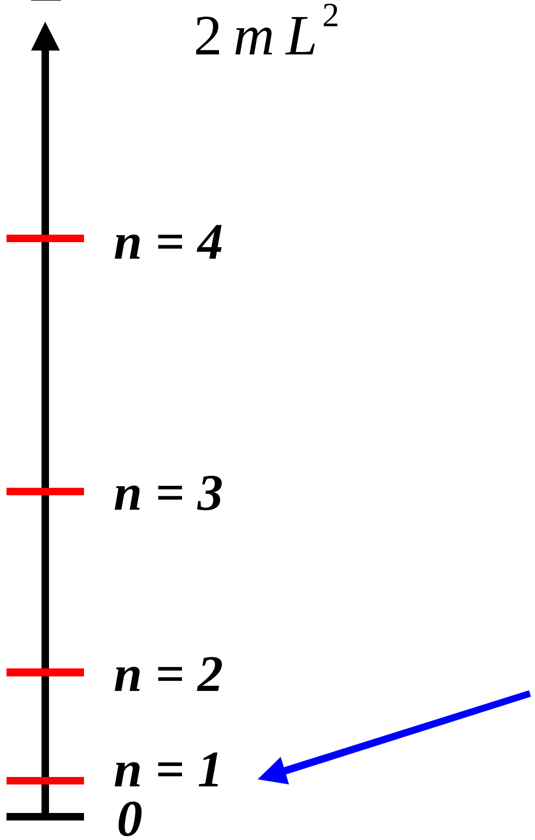
Particle in a Box



- As ***n*** increases, the probability distribution approaches the classical expectation : uniformly distributed across the width of the box $\Rightarrow$ correspondence principle.

Particle in a Box

$$E = \frac{\hbar^2 n^2 \pi^2}{2 m L^2}$$



Energy Level Diagrams :

- Represent allowed energy levels ("energy eigenvalues").
- Labelled by quantum numbers (in this case just ***n***).
- Interactions can be represented as transitions between energy states.
- Similar diagrams for other observables, for example angular momentum.

Lowest energy state (ground state) is not zero. This is a common feature of quantum mechanical systems that is not generally the case classically.

Time Dependence

- Going back to the wavefunction describing free particles of fixed momentum :

$$\psi(x,t) = A\, e^{i(kx - \omega t)}$$

- We also expect particles described by this wavefunction to satisfy the second De Broglie relation :

$$E = \hbar\,\omega$$

- This suggests the equation :

$$i\hbar \frac{\mathrm{d}\,\psi(t)}{\mathrm{d}\,t} = E\,\psi(t)$$ (temporal wavefunction only)

- Solutions to this are simply :

$$\psi(t) = A\, e^{-i E t/\hbar}$$

Time Dependence

- Then the product wavefunction :

$$\psi(x, t) = \psi(x) \times \psi(t)$$

satisfies :

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

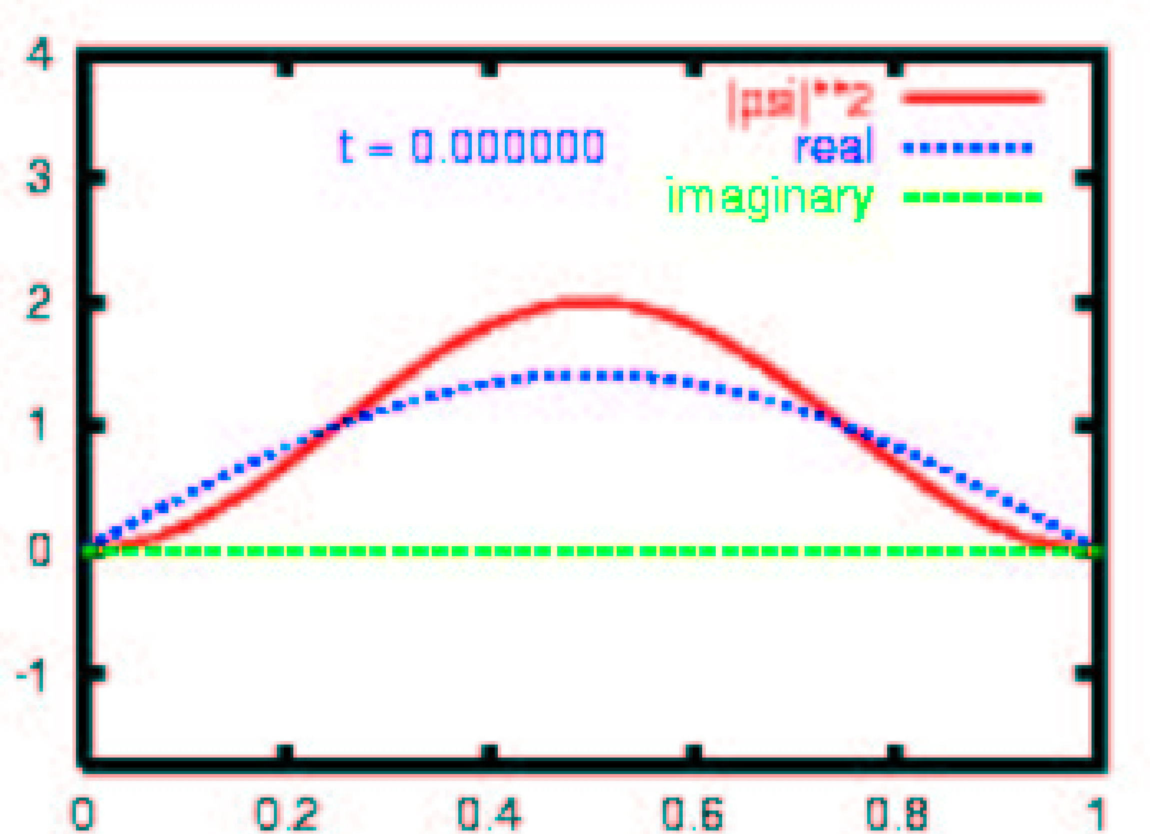
Schrödinger equation.

- For the energy states we have been considering, the time−dependent factor $e^{-iEt/\hbar}$ does not change $|\psi(x)|^2$, so it was safe to treat them in a time−independent way.

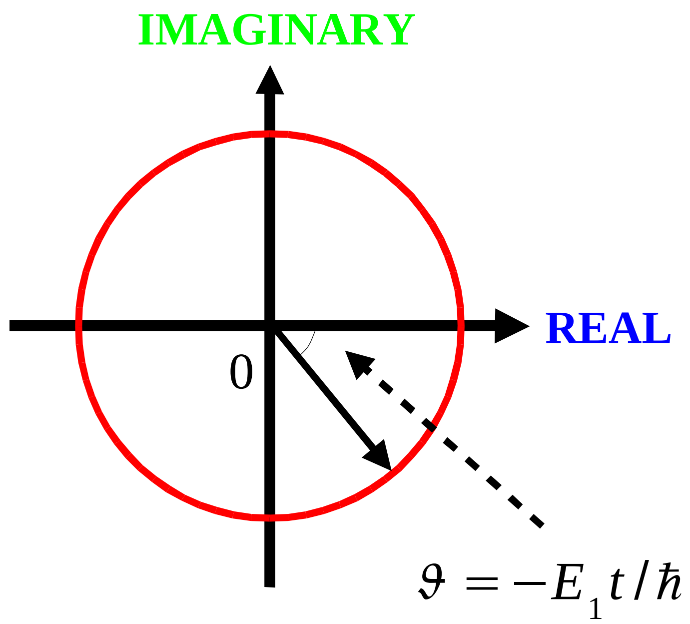
Time Dependence

Particle in a box : $n = 1$

$$\hbar = m = L = 1 \quad \Rightarrow \quad E_1 = \frac{\pi^2}{2}$$



x/L

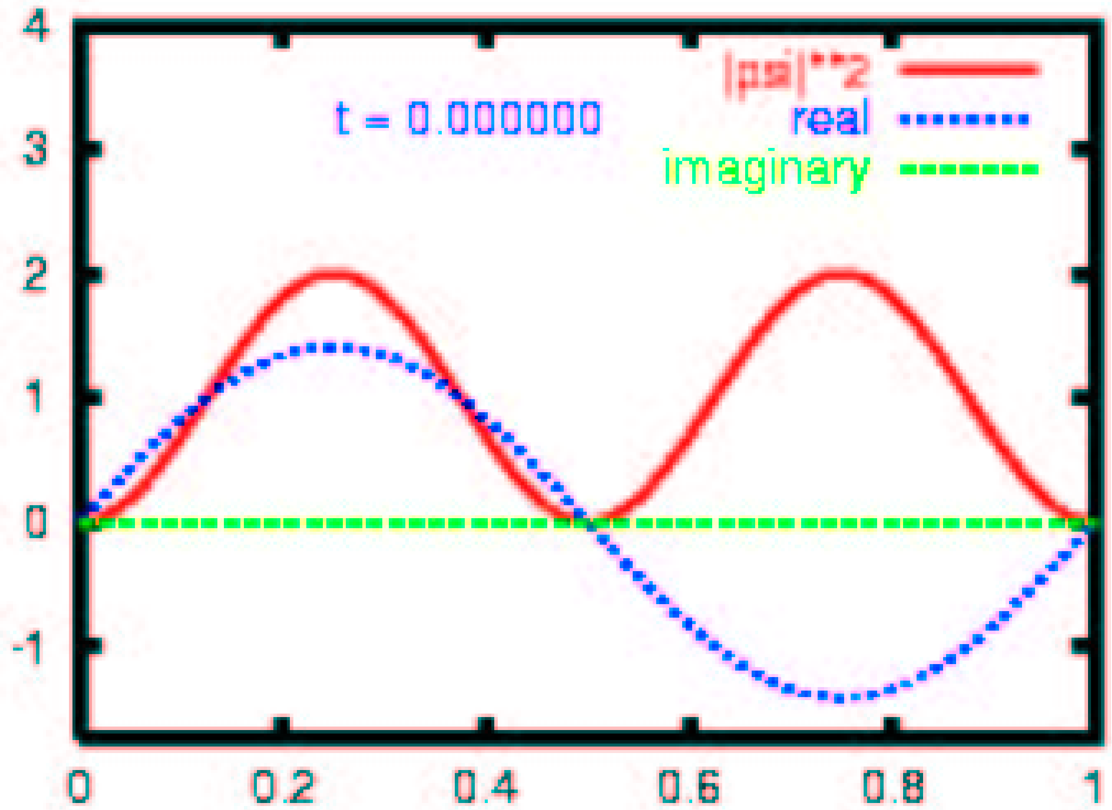


Animation

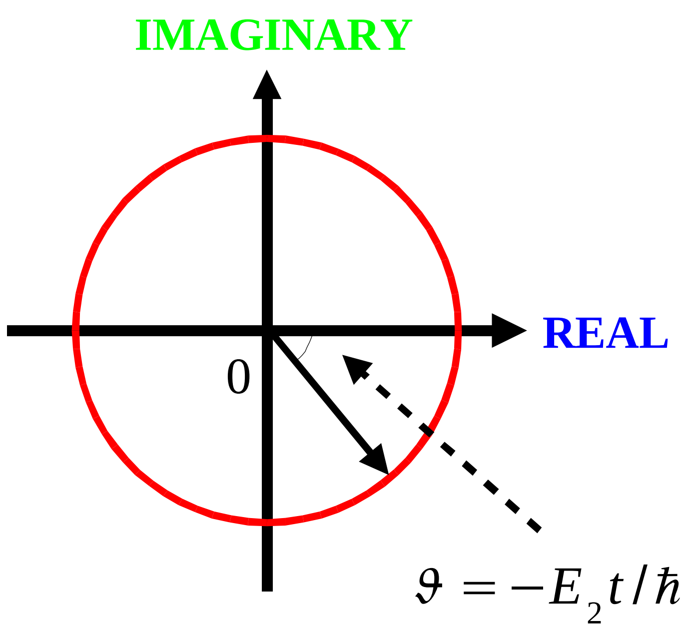
Time Dependence

Particle in a box : $n = 2$

$$\hbar = m = L = 1 \quad \Rightarrow \quad E_2 = \frac{4\pi^2}{2}$$



x/L



Animation

Quantum Superposition

- If ψ_1 and ψ_2 are both solutions to the Schrödinger equation, then so is :

$$\psi \propto A\psi_1 + B\psi_2$$

- The wavefunction must still be correctly ***normalised*** to give unit probability :

$$\psi = \frac{1}{\sqrt{A^2 + B^2}} \left(A\psi_1 + B\psi_2 \right)$$

- ψ_1 and ψ_2 are solutions corresponding to energies $\boldsymbol{E_1}$ and $\boldsymbol{E_2}$. What energy does a particle described by ψ have ?
  - It does ***not*** have a well defined energy.
  - An energy measurement could yield $\boldsymbol{E_1}$ with probability $\propto \boldsymbol{A^2}$ or energy $\boldsymbol{E_2}$ with probability $\propto \boldsymbol{B^2}$.

Note : to show that this is the correct way to normalise the combined wavefunction, you will need to know that when both wavefunctions are real :

$$\int \psi_1 \times \psi_2 \, \mathrm{d}x = 0$$

This is fairly easy to show for the wavefunctions describing a particle in a box that we have already seen.

Quantum Superposition

- The <u>average</u> energy obtained in an energy measurement is still well defined :

$$\langle E \rangle = \frac{1}{(A^2 + B^2)} (A^2 E_1 + B^2 E_2)$$

- One could also define the spread or standard deviation of a series of energy measurements on the same state ψ .
  - This is how one formally derives the quantum mechanical uncertainty relations.

Quantum Superposition

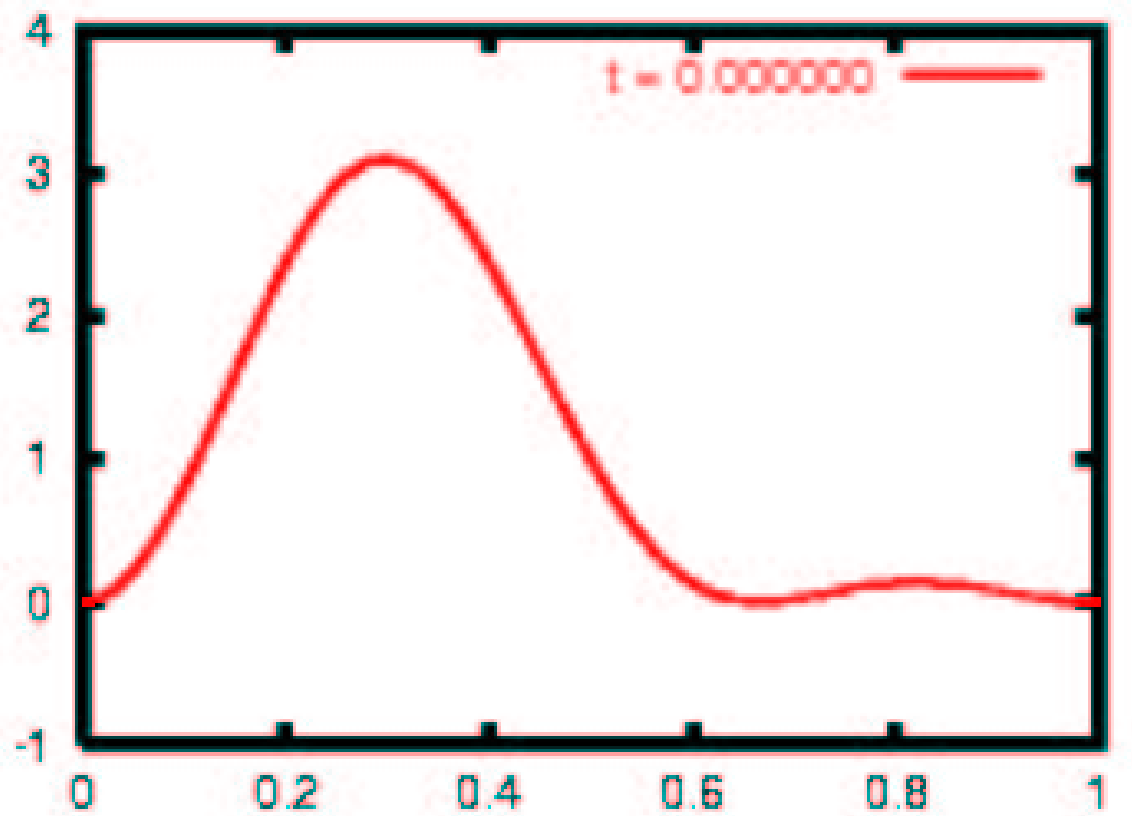
Particle in a box :

$\hbar = m = L = 1$

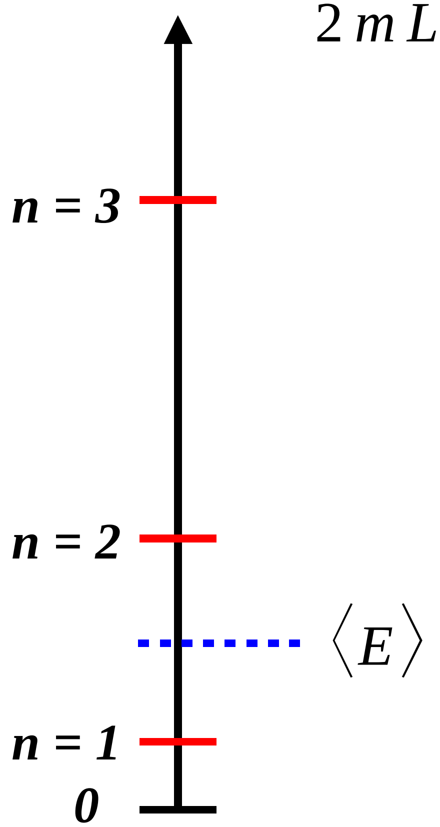
$$\psi = \frac{1}{\sqrt{2}}(\psi_1 + \psi_2)$$

$$E = \frac{\hbar^2 n^2 \pi^2}{2 m L^2}$$

$|\psi(x)|^2$



x/L



Animation

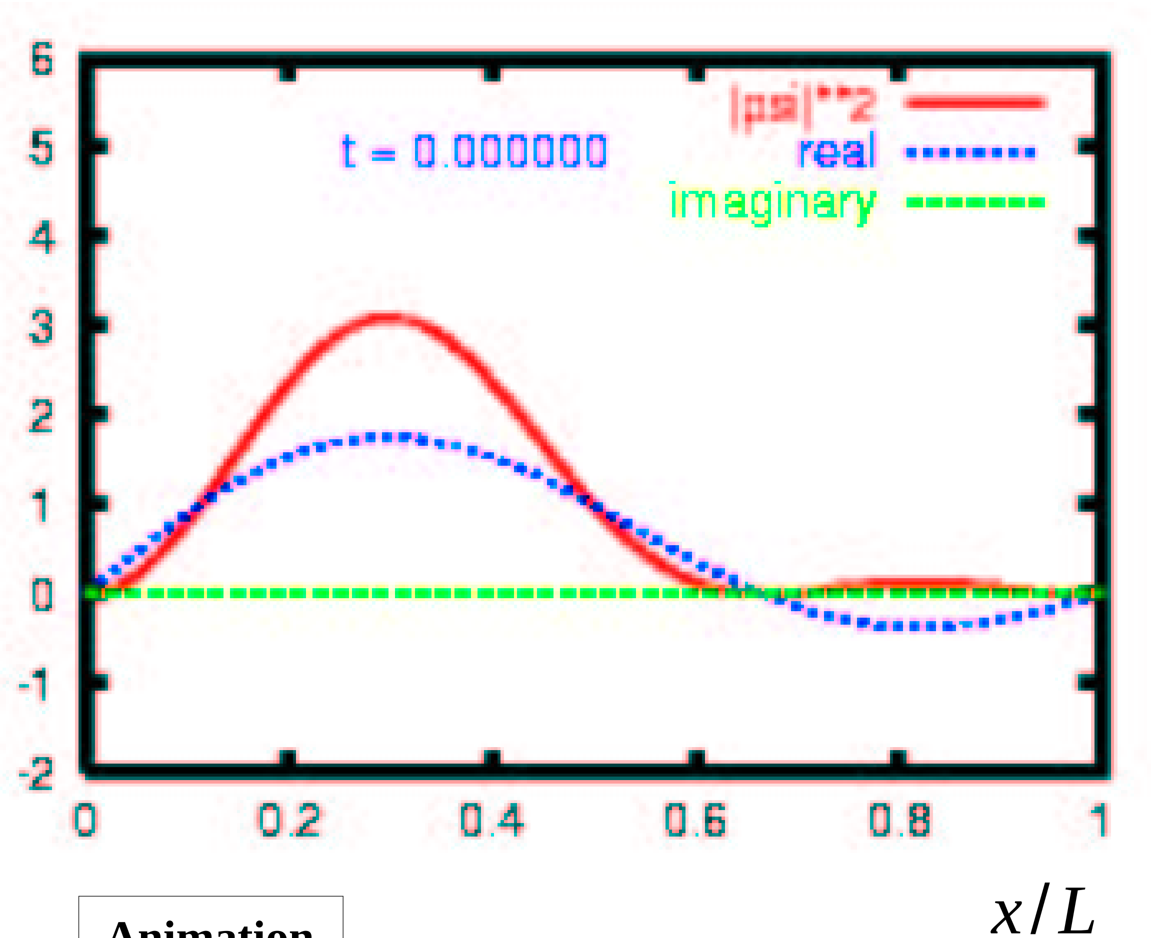
Quantum Superposition

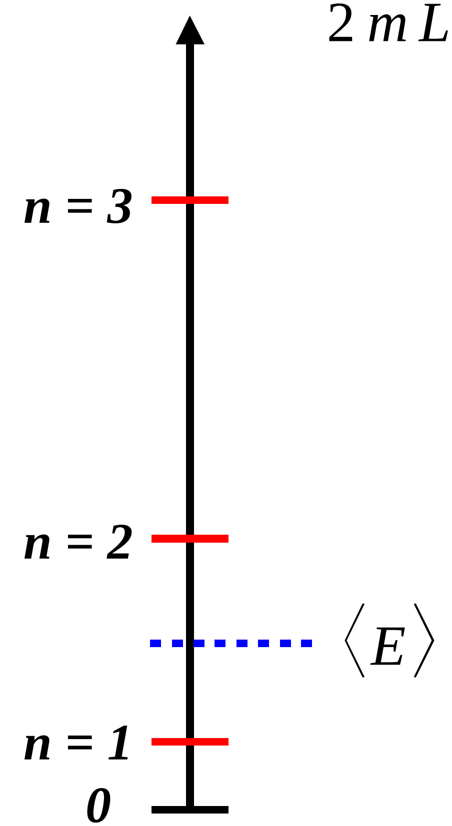
Particle in a box :

$\hbar = m = L = 1$

$$\psi = \frac{1}{\sqrt{2}}(\psi_1 + \psi_2)$$

$$E = \frac{\hbar^2 n^2 \pi^2}{2 m L^2}$$





Animation

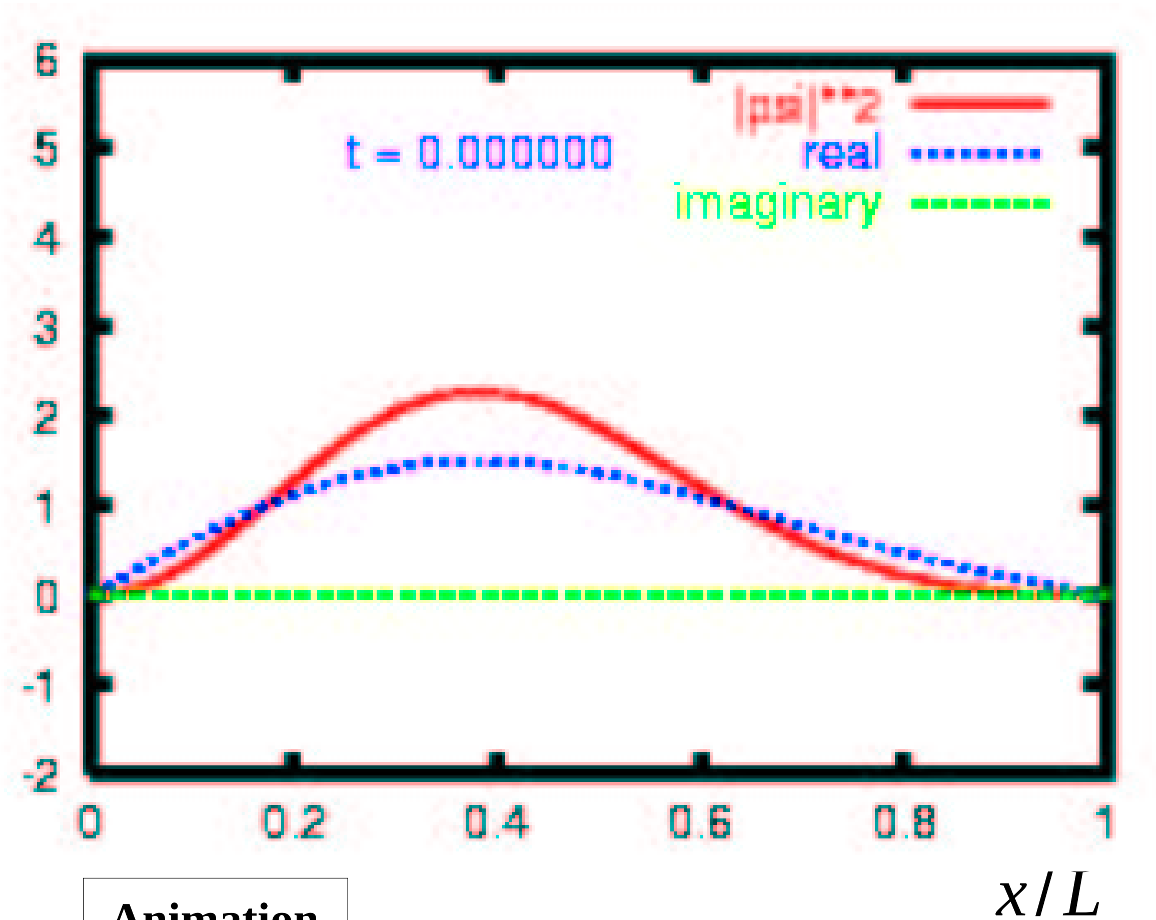
Quantum Superposition

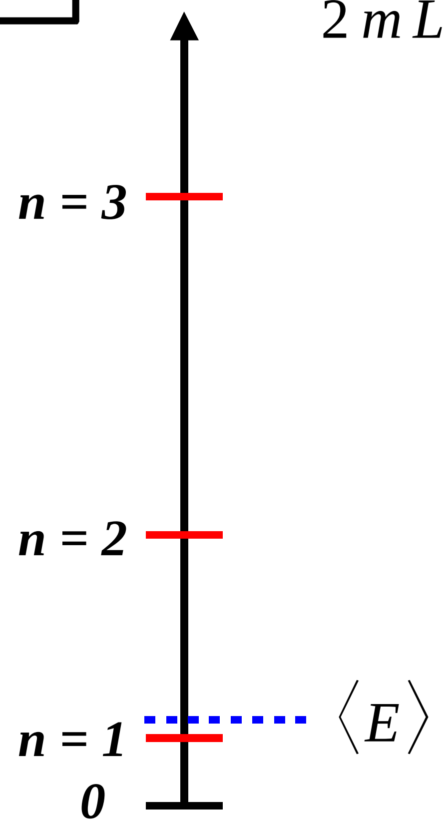
Particle in a box :

$\hbar = m = L = 1$

$$\psi = \frac{1}{\sqrt{0.68}}\left(0.8\,\psi_1 + 0.2\,\psi_2\right)$$

$$E = \frac{\hbar^2 n^2 \pi^2}{2\,m\,L^2}$$





Animation

Quantum Superposition

Particle in a box :

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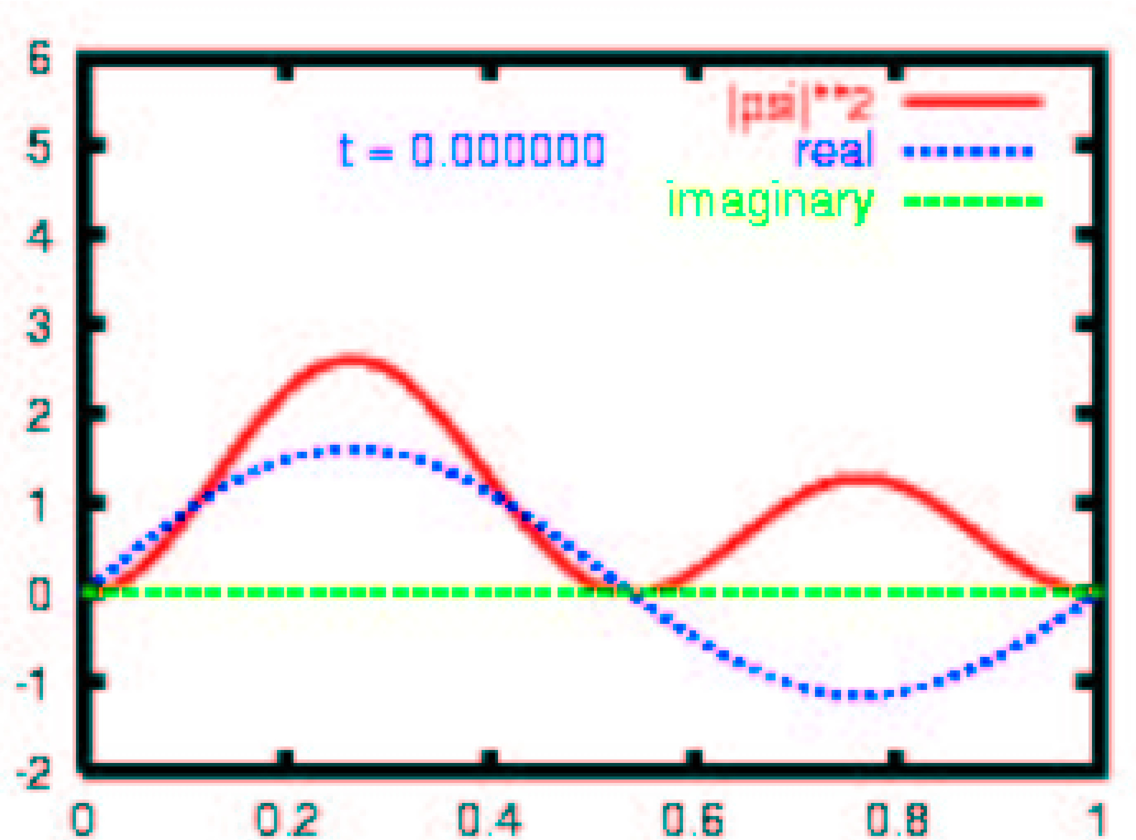
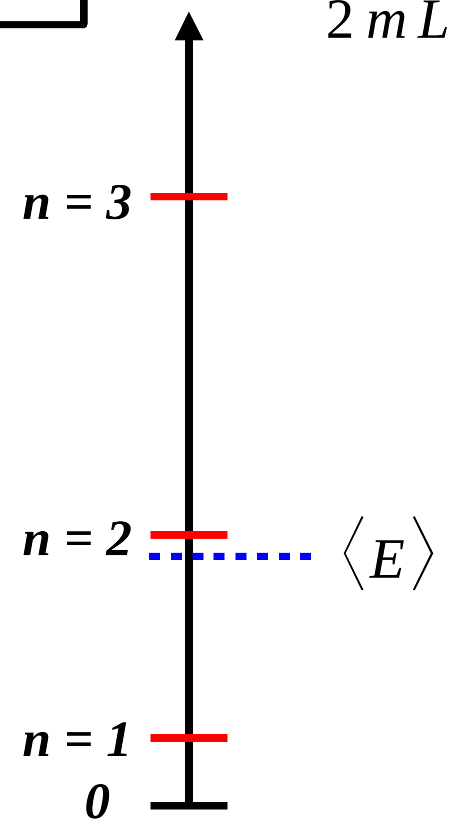
$$\psi = \frac{1}{\sqrt{0.68}}\left(0.2\,\psi_1 + 0.8\,\psi_2 \right)$$

$$E = \frac{\hbar^2 n^2 \pi^2}{2\,m\,L^2}$$



x/L



Animation

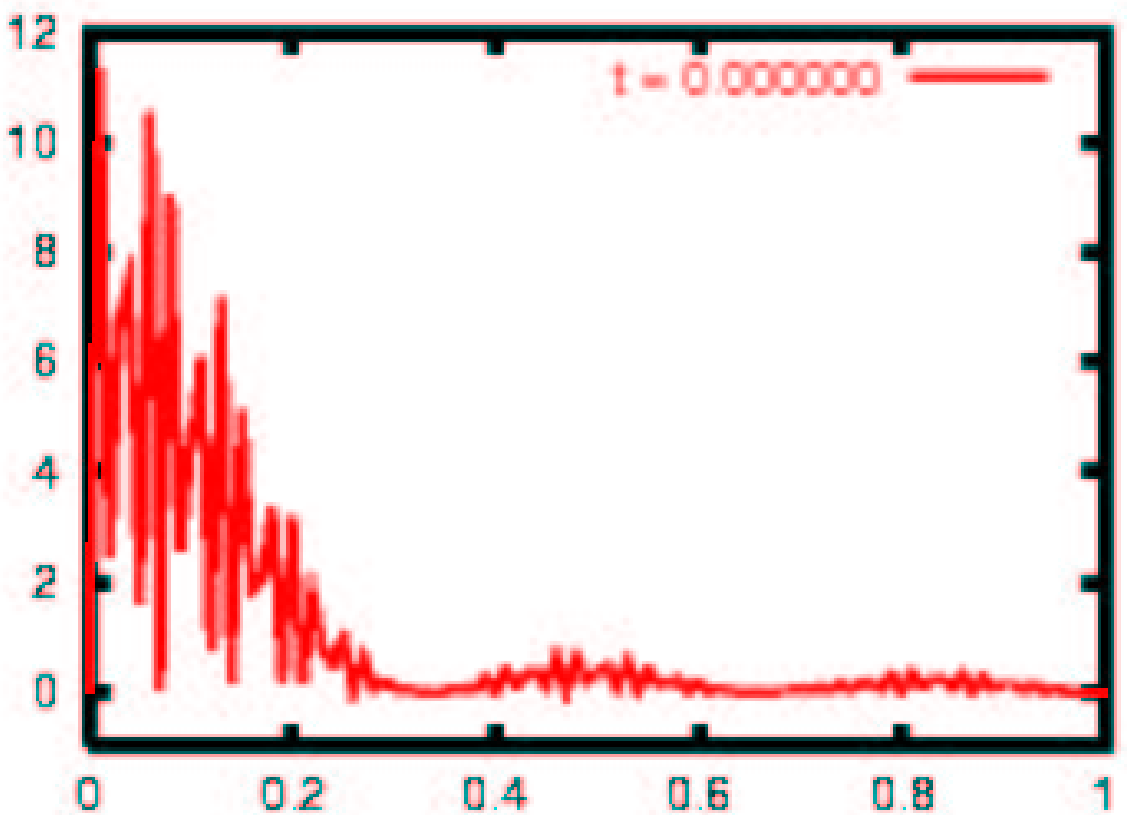
Quantum Superposition

Particle in a box :

$\hbar = m = L = 1$

$$\psi = \frac{1}{\sqrt{6}}\left(\psi_{40} + \psi_{41} + \psi_{42} + \psi_{43} + \psi_{44} + \psi_{45}\right)$$

$|\psi(x)|^2$



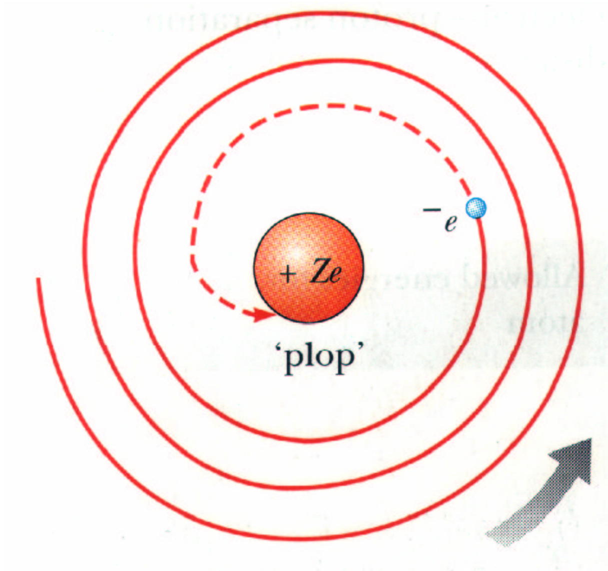
Animation

x/L

- Motion begins to look classical.
- Time averaged probability is uniform in ***x***, as would be expected for a classical particle rattling around in a box.

The Hydrogen Atom

- Classical electromagnetism does not predict a stable atom :



  - Electron suffers centripetal acceleration and radiates energy in the form of electromagnetic waves.
  - Eventually the electron would spiral into the nucleus.

- In general, quantum mechanical systems do not have a ground state corresponding to the classical energy minimum (e.g. particle in a box).
- In the case of the hydrogen atom, the quantum mechanical ground state corresponds to an electron at a radius of :

$$a_0 \approx 0.529 \times 10^{-10} \text{ m} \quad (\text{Bohr radius})$$

- Since there are no lower energy states to occupy, the electron ***cannot*** lose more energy through radiation $\Rightarrow$ the hydrogen atom is stable !

The Hydrogen Atom

- The quantum mechanical prescription for understanding the hydrogen atom is simple. We just find the solutions to the Schrödinger equation with the relevant potential :

$$\frac{-\hbar^2}{2m}\left(\frac{d^2\psi}{dx^2}+\frac{d^2\psi}{dy^2}+\frac{d^2\psi}{dz^2}\right)-\frac{e^2}{4\pi\epsilon_0 r}\psi = E\psi$$

Coulomb potential

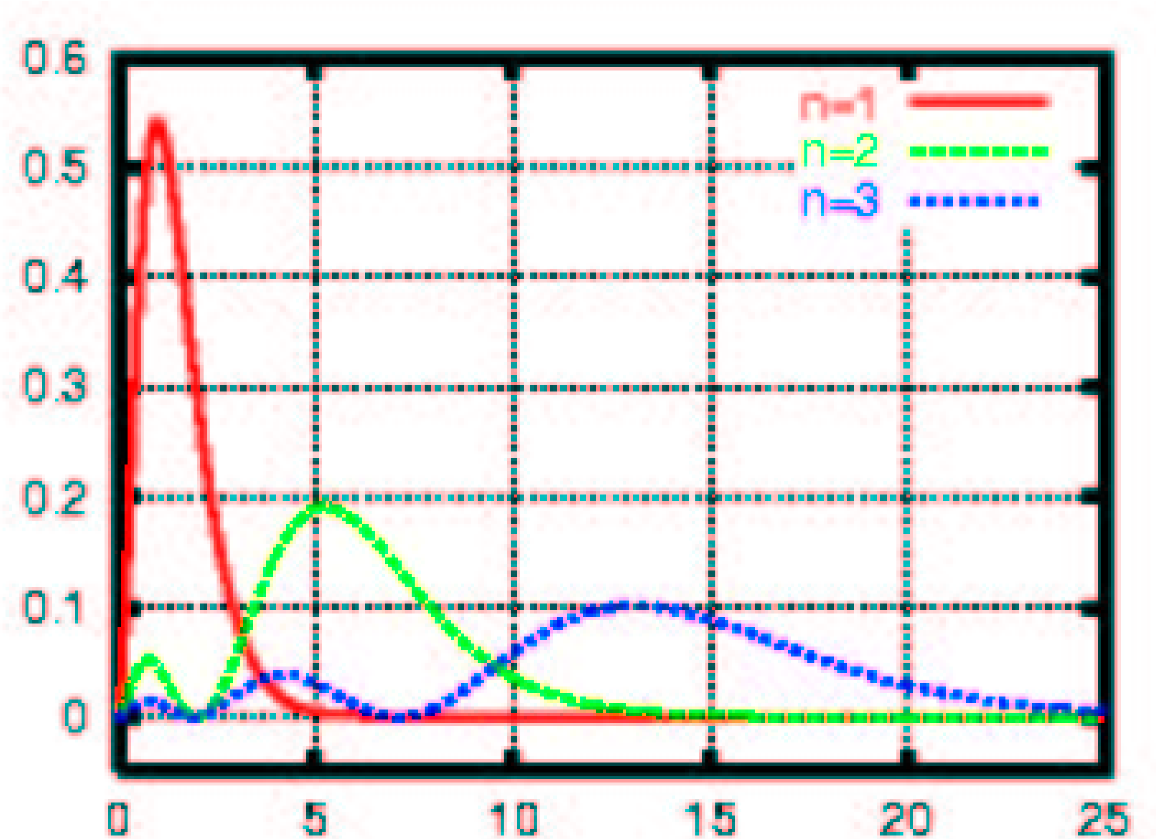
$$r = \sqrt{x^2+y^2+z^2}$$

$$\psi = \psi(x, y, z)$$

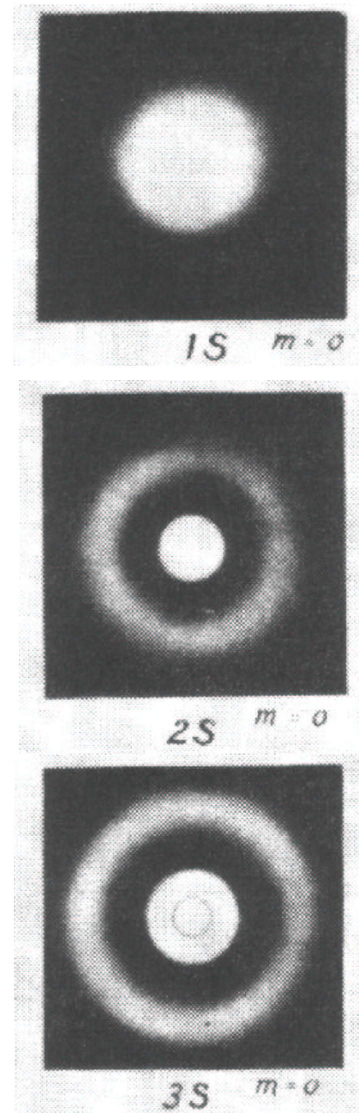
- The approach is exactly the same as for a simple 1−dimensional problem such as a particle in a box, but the algebra is a bit more complicated.
- Energy of electron defined by principal quantum number ***n* = 1, 2, 3, ...** (for a free atom in the absence of external magnetic fields etc.)

The Hydrogen Atom

Probability

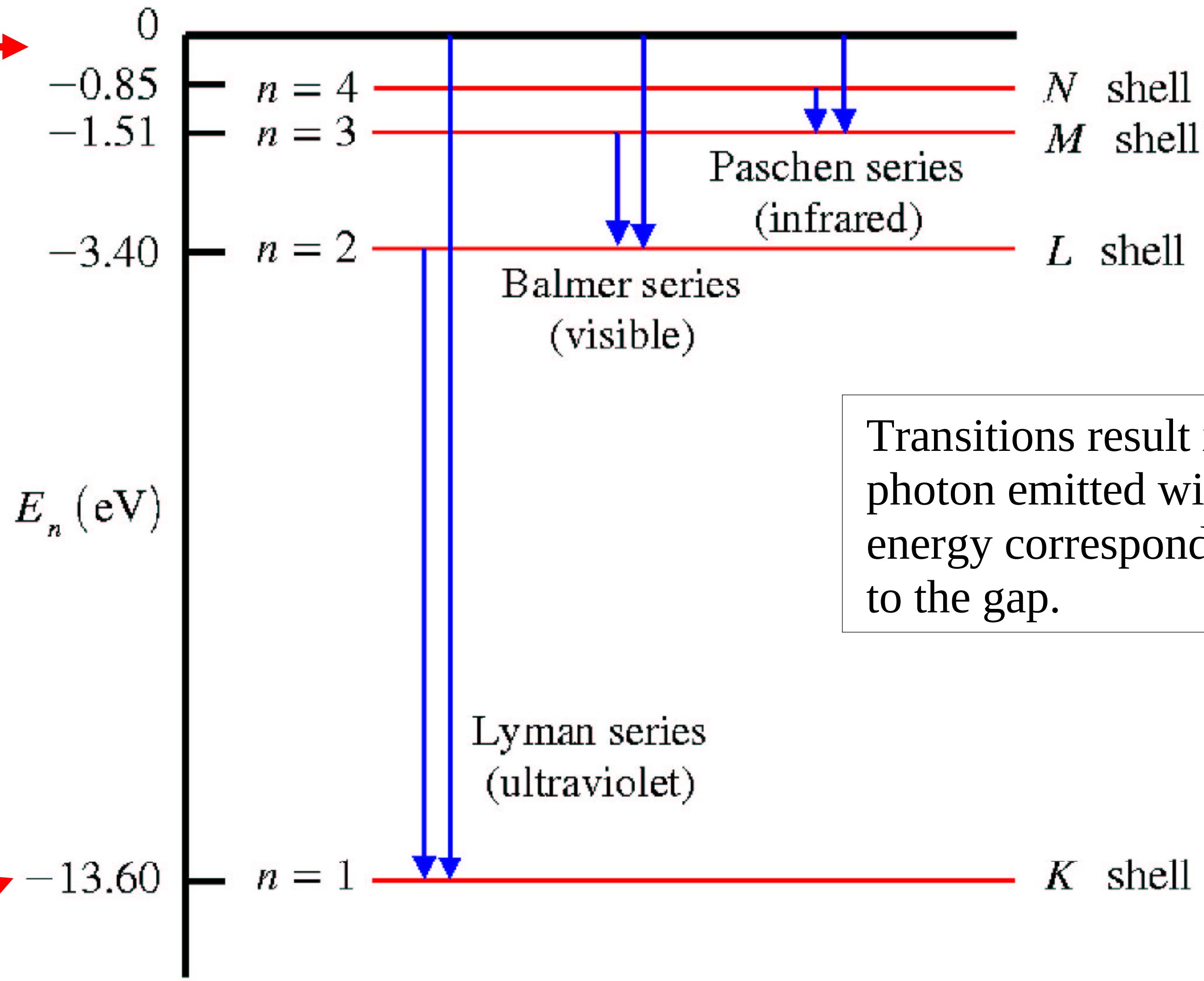


r / a_0



The Hydrogen Atom

Free electron has zero energy



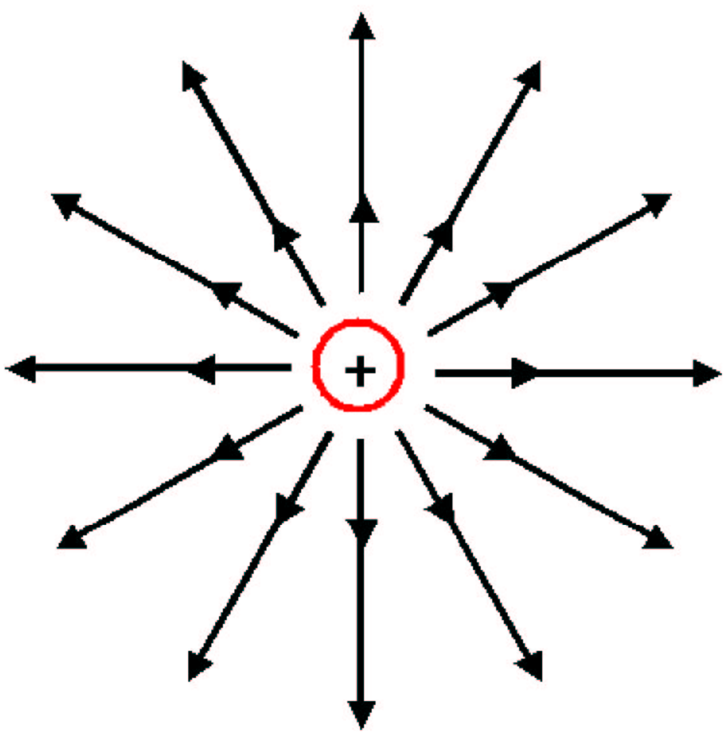
Ground State

Transitions result in a photon emitted with energy corresponding to the gap.

Fields

- So far we have been treating particles quantum mechanically but the fields and potentials classically $\Rightarrow$ continuous and not subject to uncertainty.

Reminder of Classical Fields :



- The direction of the electric field is parallel to the field lines at any point in space.
- The relative strength is given by the spacing of the field lines :

$$\vec{E}_1 = \frac{q_1}{4\pi\epsilon_0 r^2}\vec{\hat{r}}$$

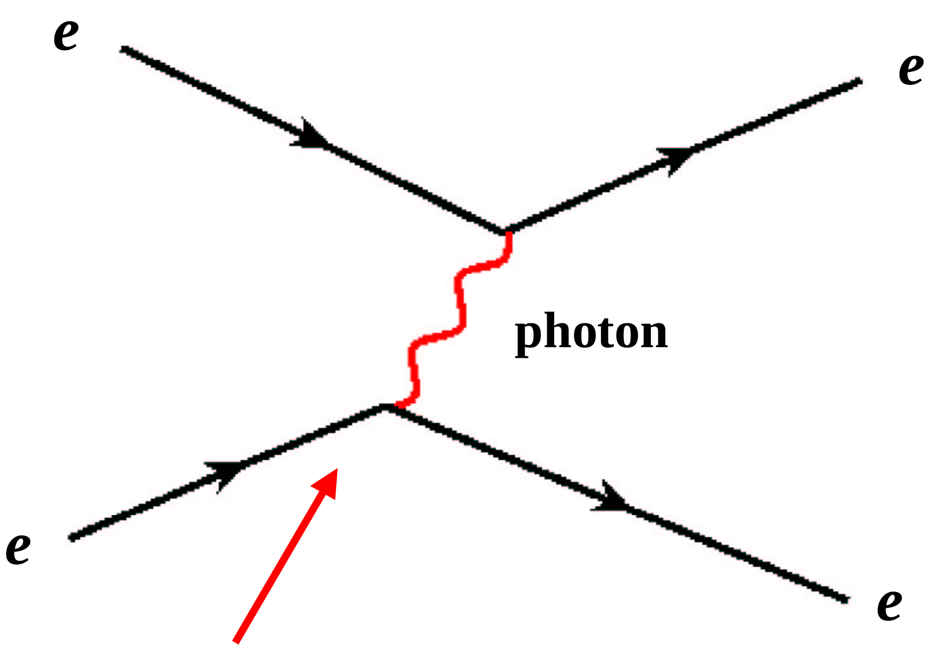
$$\vec{F}_{12} = q_2 \vec{E}_1$$

force between charges 1 and 2

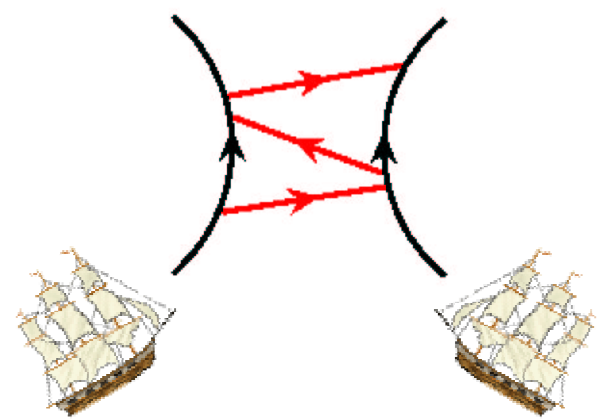
unit vector in radial direction

Quantum Fields

- We know from the photoelectric effect that the electromagnetic field is ***quantised*** : the energy in the field is "lumped" into photons, which are subject to the same quantum uncertainty as particles.
- A full quantum mechanical treatment of particles and fields needs to treat the interaction of field ***quanta*** with particles :



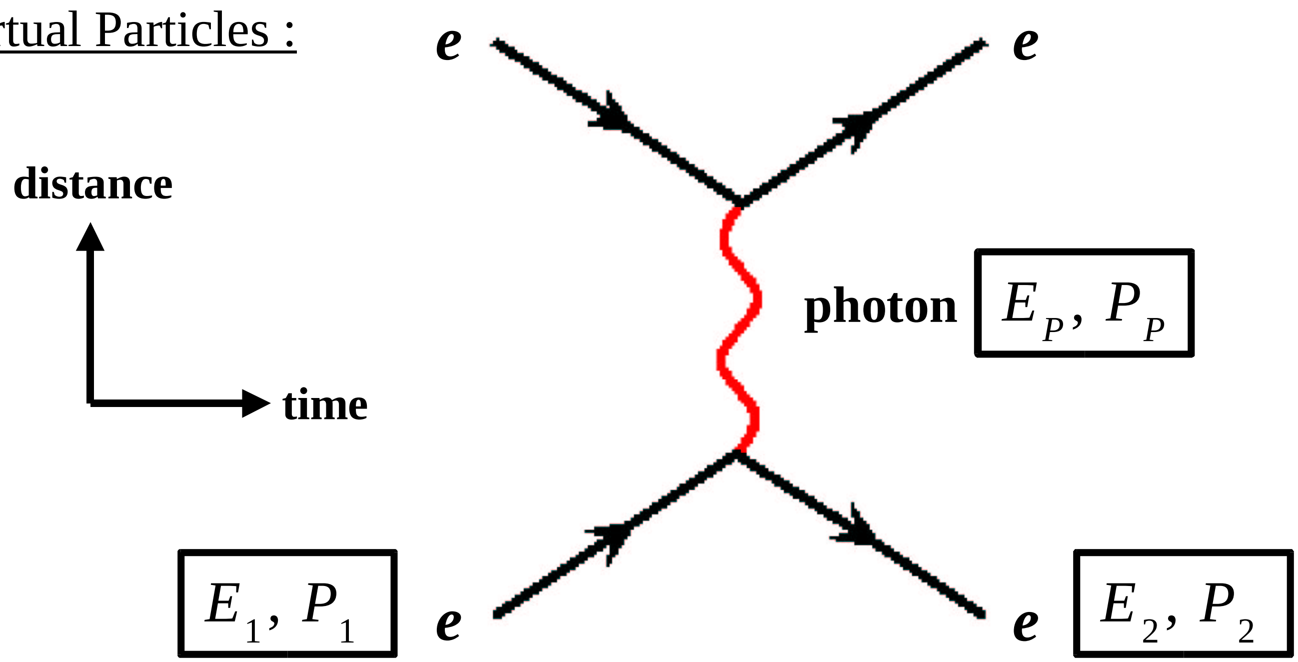
Electromagnetic interaction between two electrons.



Electrons deflected due to the momentum of the exchanged photon.
Analogy with ships exchanging cannon balls ⇒

Quantum Fields

Virtual Particles :



- Suppose the collision is head−on and the electrons are scattered at 180°:

$$E_P = E_1 - E_2 = 0 \qquad \text{(same speed)}$$

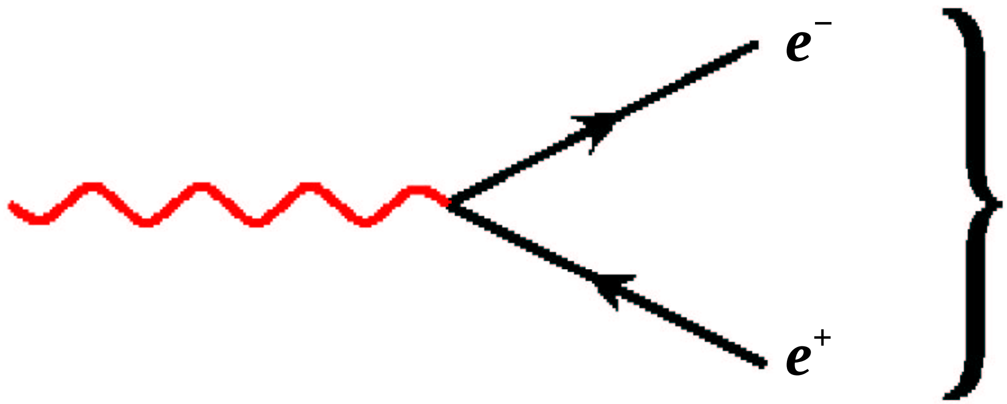
$$P_P = P_1 - P_2 = 2 \times P_1 \qquad \text{(change of direction)}$$

- But for a "**real**" photon : $E_P = P_P\, c$

➡ Photon does not have the right relationship between energy & momentum ⇒"**virtual**"

Quantum Fields

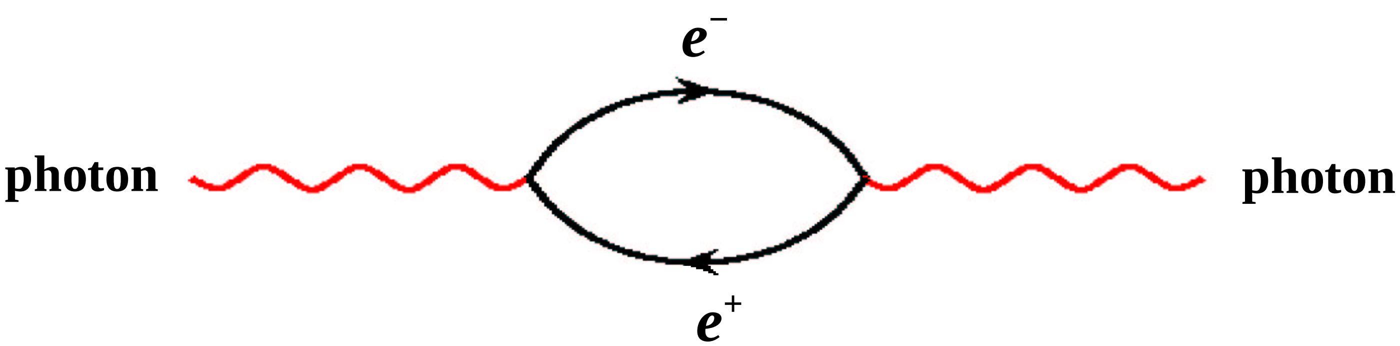
- In fact, even particles can be considered to be ***quanta*** of their corresponding matter fields. Photons can excite these matter fields :



An electron and an anti-electron (**positron**) are created from the vacuum.

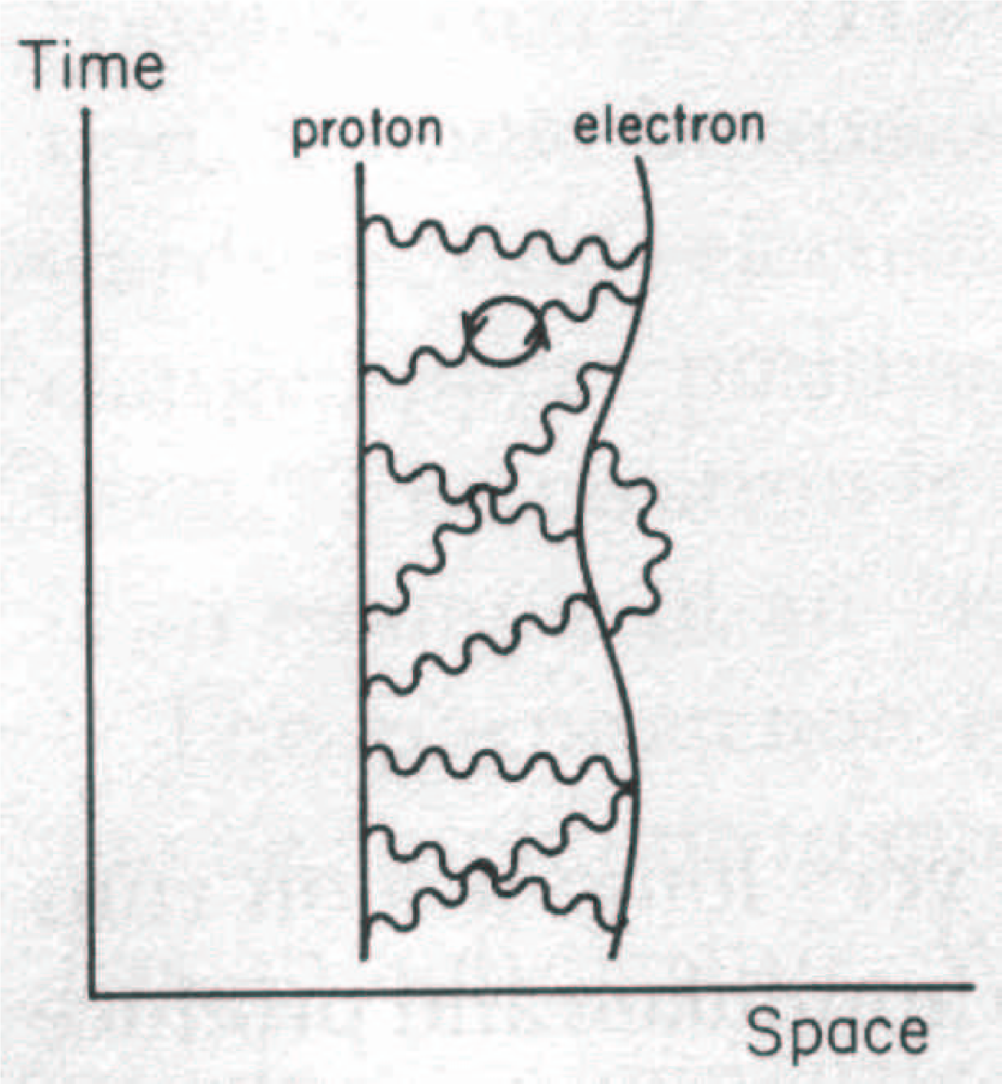
More about anti−matter in forthcoming lectures.

- Even a photon then becomes a complex object since it can spend part of its time as electrons and positrons :



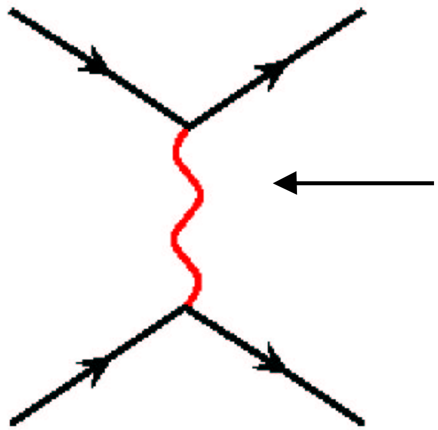
Quantum Fields

- Quantum field picture of hydrogen :



Quantum Fields

- Fluctuations in quantum fields are governed by the same uncertainty relationships we saw earlier for particles.
- For example, we can calculate the range of force mediated by virtual particles of different masses.



Exchange particle has rest mass M_0

Energy that must be "borrowed" :

$$\Delta E = M_0 c^2$$

- The energy can be "borrowed" for a time dictated by the uncertainty principle :

$$\Delta E \, \Delta t \approx \hbar \quad \Rightarrow \quad \Delta t \approx \frac{\hbar}{\Delta E}$$

- Since the particle cannot travel faster than the speed of light, the maximum range is :

$$\text{Range} = c\,\Delta t \approx \frac{\hbar c}{M_0 c^2}$$

Quantum Fields

- For example, the weak nuclear force is mediated by particles with mass :

$$M_W, M_Z \approx 100 \ \ \mathrm{GeV/c^2}$$

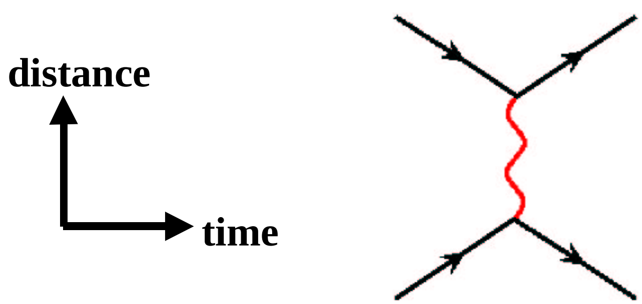
- Range of weak force :

$$\mathrm{R_{WEAK}} \approx \frac{\hbar c}{M_{W,Z} c^2} = \frac{197 \ \mathrm{MeV\,fm}}{100 \ \mathrm{GeV}} \approx 10^{-3} \ \mathrm{fm} \approx 10^{-18} \ \mathrm{m}$$

- This is short even compared to the radius of the proton (10^{-15} m) !

Summary

- We have looked at some of the laws that dictate the behaviour of quantum mechanical "probability waves".
- Most non−relativistic quantum mechanical systems can be understood just by solving the Schrödinger equation for the relevant potential.
- It always emerges that bound states (e.g. a particle in a box or an electron in an atom) have a discrete energy spectrum $\rightarrow$ energy is quantised. Loosely speaking, this is because we have to fit a certain number of De Broglie wavelengths into the space available (like standing waves on a violin string).
- Different quantum states can be superposed on top of one another. In that case the energy of the system might not even be well defined.
- Our quantum mechanical picture of forces involves drawing diagrams, which represent the exchange of force carrying particles :



$\Rightarrow$ **Feynman diagam**

- These diagrams will help us make sense of elementary particle physics next term.

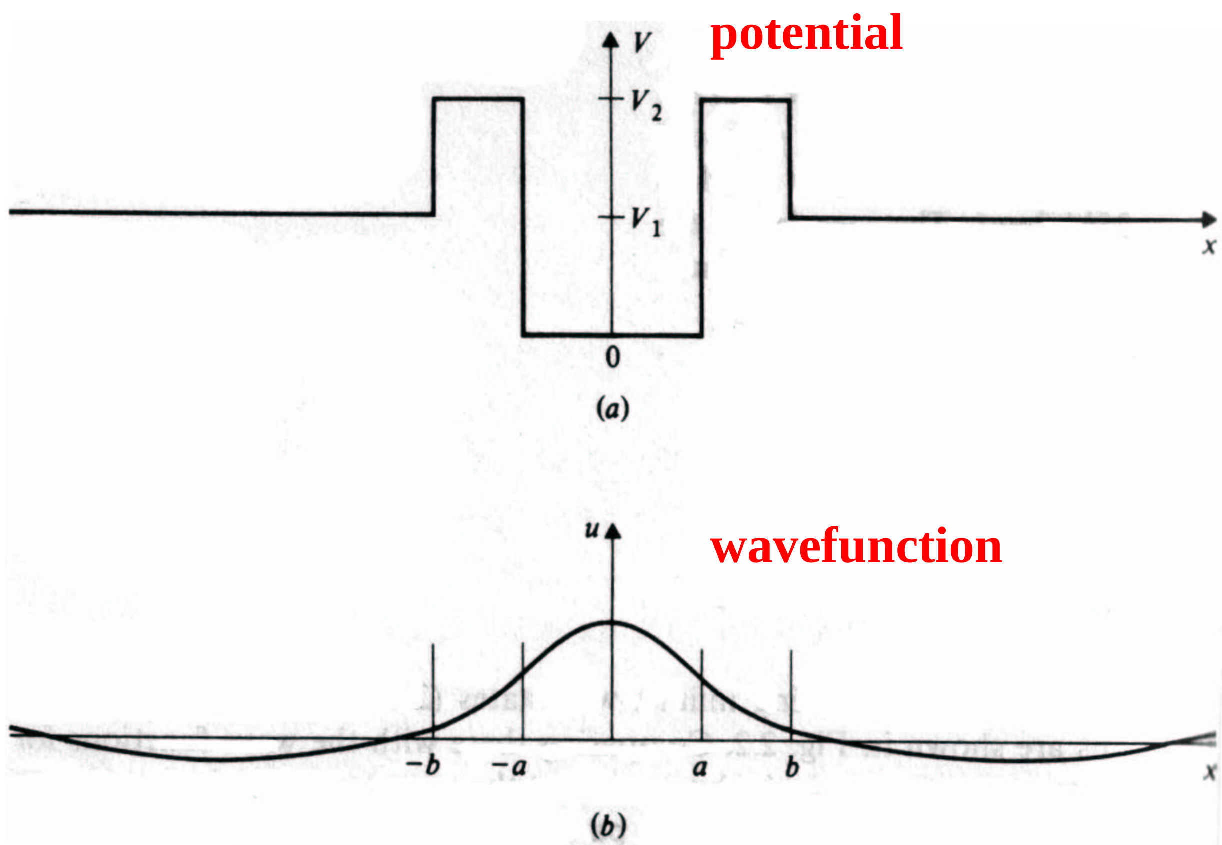
Exercises

1) The figure below shows the wavefunction for a particle in a finite potential well, with energy between V_1 and V_2 :

   i. Can the particle escape from the potential well classically ?

   ii. Can the particle escape from the potential well quantum mechanically ?

   iii. What physical situations might such a potential represent ?



Exercises

2) One way in which the strong nuclear force manifests itself is through the exchange of particles called pions, with masses around 140 MeV/c^2. What is the approximate range of the force mediated by pion exchange ?

3) Photons have zero rest−mass. What does the formula predict for the range of the electromagnetic interaction ?

The Hydrogen Atom (*advanced*)

Degeneracy :

- Hidden in the energy level diagram for hydrogen is a high level of ***degeneracy*** : different quantum states that happen to have the same energy.
- For the hydrogen atom (in fact, for any quantum mechanical system with a central potential), each energy level has a well defined angular momentum.

Quantum Numbers →

Principal	Total Angular Momentum	z−component of Angular Momentum
$n = 1$	$l = 0$	
$n = 2$	$l = 0$ $l = 1$	 → $m = -1, 0, 1$
$n = 3$	$l = 0$ $l = 1$ $l = 2$	 → $m = -1, 0, 1$ → $m = -2, -1, 0, 1, 2$

↑

$$\text{Angular Momentum} = \sqrt{l(l+1)}\,\hbar$$

Complex Atoms (*advanced*)

Two more key principles are needed to understand atoms containing >1 electron :

- **<u>Pauli Exclusion Principle</u>** : no two fermions (e.g. electrons) can be in the same state.
- Electrons have half a unit of spin or intrinsic angular momentum :

$$s = \sqrt{\frac{1}{2}\times\frac{3}{2}}\ \hbar \quad ; \quad m_s = -\frac{1}{2}\ ,\ \frac{1}{2}$$

2 different orientations :
"up" & "down"

- This means that 2 electrons can occupy states identified by unique combinations of quantum numbers ***n***, ***l*** and ***m***.

This material will be revisited in the fourth lecture on the structure of matter

Complex Atoms (*advanced*)

Energy−level diagram for a complex atom :