Introduction to Quantum Mechanics

ICME Fall 2012

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Greek philosophers – Early 20th century scientists: Evolution of wave-particle duality

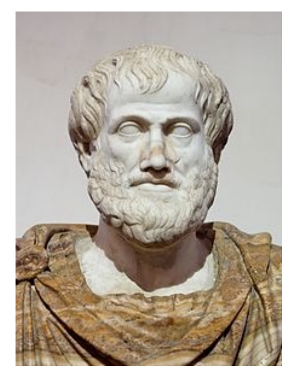
HISTORICAL PERSPECTIVE

Earlier thoughts

- Democritus (460 BC –370 BC)
  - Atoms and void
  - All phenomena – dynamics of atoms

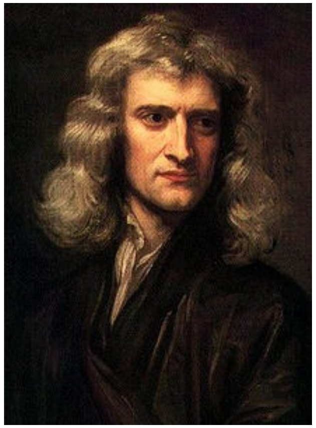
Democritus

- Aristotle (384 BC – 322 BC)– continuous substance
  - no voids – all made from fire, earth, air, water
  - “Nature abhors vacuum”


Aristotle

17th Century

- Basic nature of light
  - Newton
    - stream of corpuscles – different colors corresponds to different corpuscles – intensity of light is the no. of corpuscles
    - light's ability to travel in straight lines and reflect off surfaces.
  - Huygens
    – continuous wave – like sound waves – different colors corresponds to different frequency – intensity is strength of vibrations.

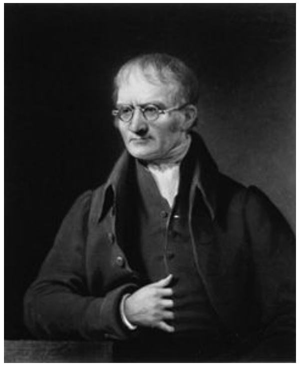


Newton

Huygen

The 19th Century

- Matter is discrete, made of atoms
  - John Dalton – periodic table – chemical recipes
    - Structure of crystals – due to periodic arrangement of atoms
  - Maxwell & Boltzmann
    - Properties of gas explained through atoms
    - Heat energy is the random motion of atoms
    - Heat – result of microscopic motion



John Dalton

Maxwell

Boltzmann

The 19th century

- Light is continuous
  - Maxwell
    - Light is an electromagnetic wave
    - Theory of light unified with electromagnetism
  - Thomas Young
    - Showed light is a wave – Young’s double-slit experiment
    - Particle theory of light (Newton) out the door.

$$\nabla \cdot \mathbf{E} = \frac{\rho_v}{\varepsilon} \qquad \text{(Gauss' Law)}$$

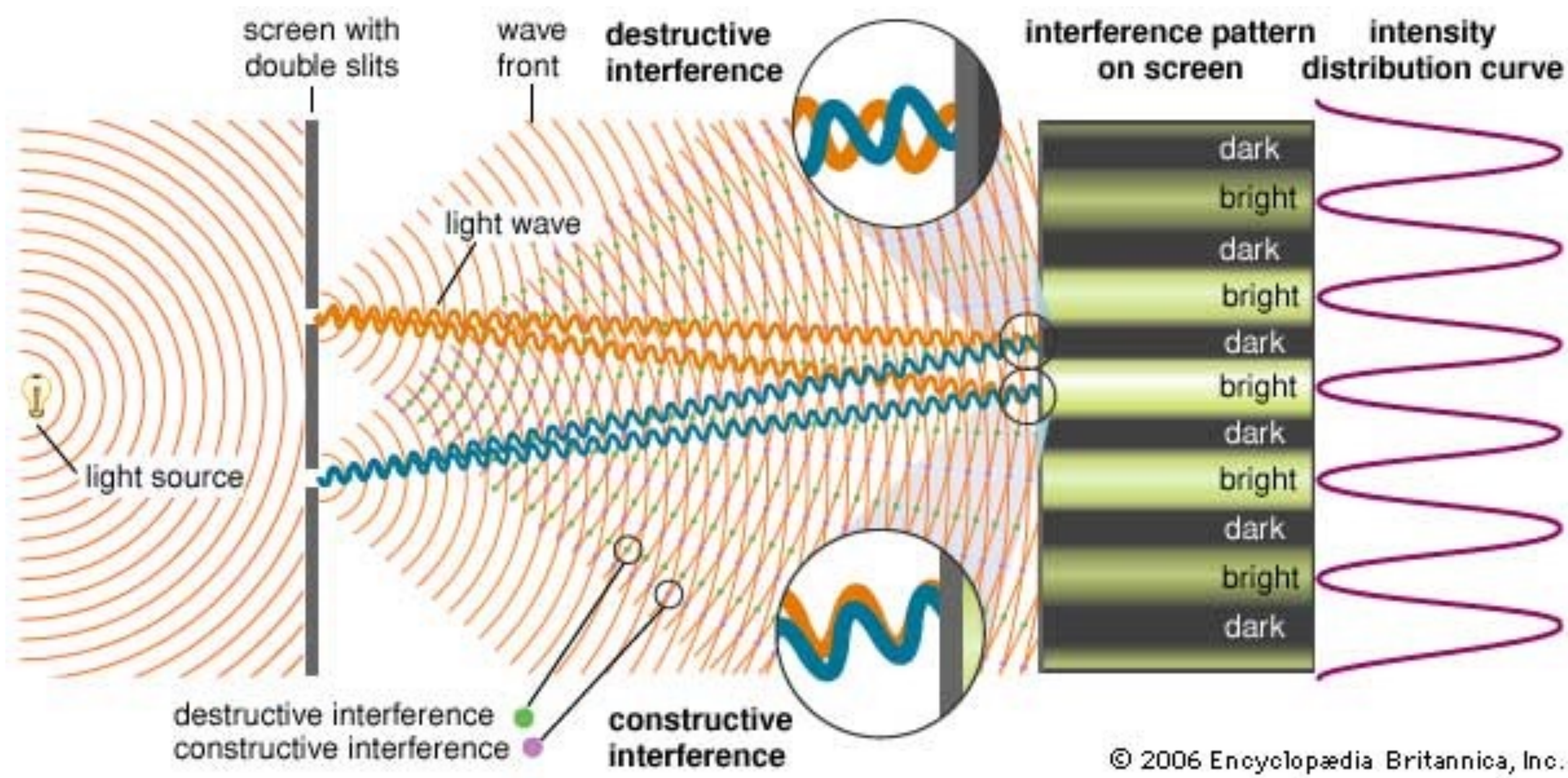
$$\nabla \cdot \mathbf{H} = 0 \qquad \text{(Gauss' Law for Magnetism)}$$

$$\nabla \times \mathbf{E} = -\mu \frac{\partial \mathbf{H}}{\partial t} \qquad \text{(Faraday's Law)}$$

$$\nabla \times \mathbf{H} = \mathbf{J} + \varepsilon \frac{\partial \mathbf{E}}{\partial t} \qquad \text{(Ampere's Law)}$$

Thomas Young

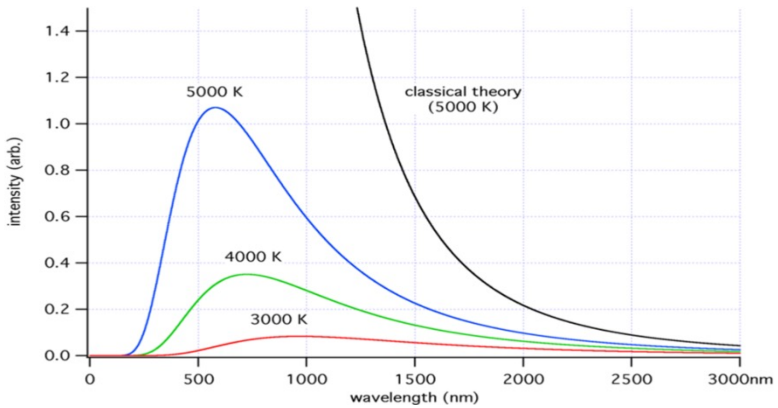
Young's double slit experiment



$$V = \lambda \times f$$

1900

- Two dark clouds of physics
  - Ether
    - Light is an EM wave that passes through ‘ether’.
    - Michelson and Morley experiment fails to detect the ether
  - Thermal radiation – warm objects give off EM radiation e.g. light bulb
    - Classical physics fails to explain this.
    - Black body radiation
    - Classical theory predict too much UV light
    - Ultraviolet catastrophe



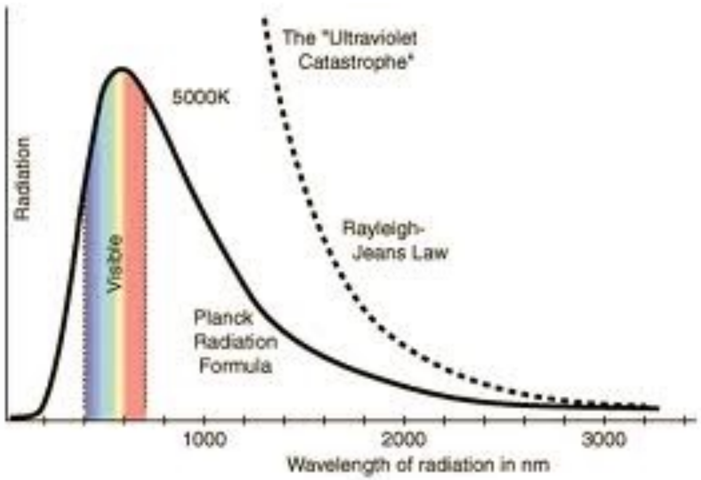
Max Planck

- Hypothesis
  - Radiation is emitted in discrete quantities – 'light quanta' – packets of energy

$$E = hf \qquad \begin{array}{c} \text{E}-\text{energy} \\ \text{h}-\text{Plank's constant} \\ \text{f}-\text{frequency} \end{array}$$

$$h \approx 6.63\times 10^{-34}\ J\cdot s$$

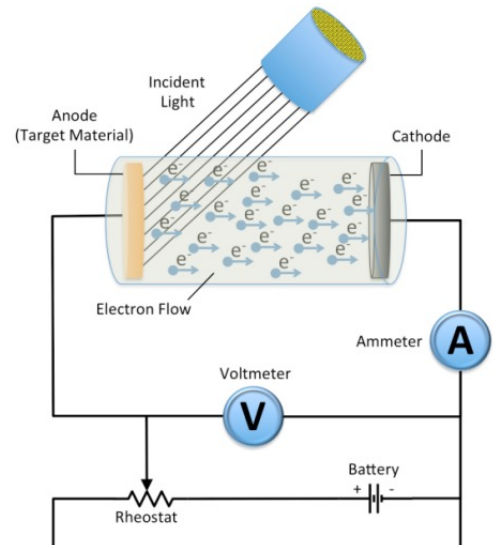
- *h* is small – E is small - light appears continuous (f of light is very large (order of 10^{15} s^{-1}))



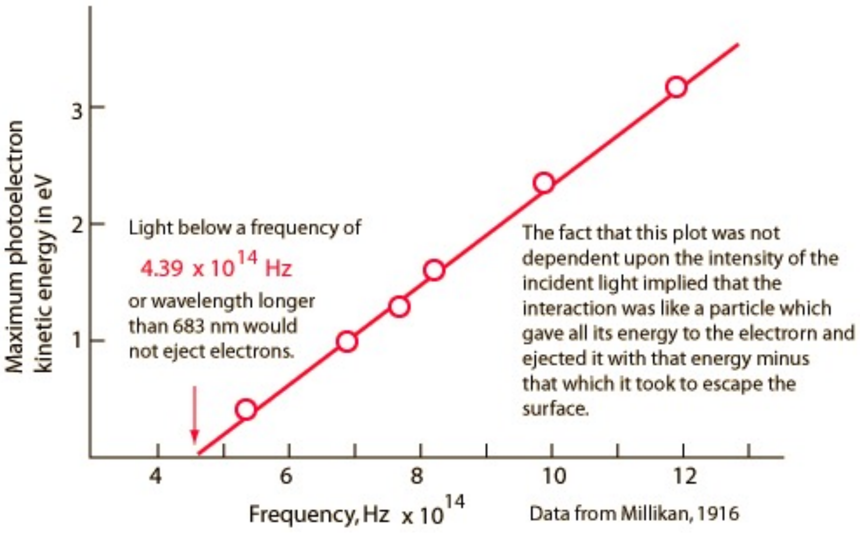
- Higher frequency light has quanta that has higher E
  - Therefore harder to emit UV photon
  - No UV catastrophe

Photoelectric effect

- Energy of the electrons do not depend on the intensity of the light



- E ∞ f
- Threshold frequency –
  - minimum frequency of incident radiation below which no photoelectrons are emitted



1905 – Einstein's Miracle year

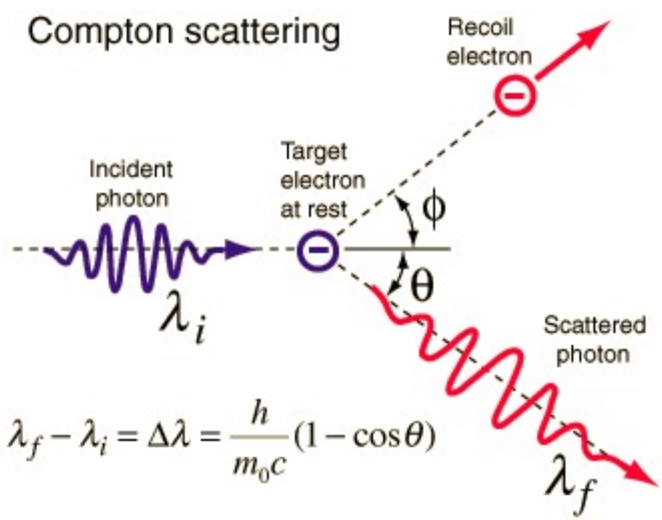
"According to the assumption to be contemplated here, when a light ray is spreading from a point, the energy is not distributed continuously over ever-increasing spaces, but consists of a finite number of energy quanta that are localized in points in space, move without dividing, and can be absorbed or generated only as a whole."

$$E = hf$$

- Each photo electron gets the energy from a single photon
- Energy of electrons are same for brighter and dimer light

Compton effect (1923)

- When x-rays are scattered by atoms their λ increase.
- Incoming photon scatters off an electron that is initially at rest
- Collision between two particles
  - Energy-momentum must both be conserved simultaneously



$$\lambda_f - \lambda_i = \frac{h}{m_e c^2}(1 - \cos\theta)$$

Light consist of particles called photons

Wave-Particle Duality

- Light travels as an EM wave
- Light is emitted and absorbed as a stream of particles
- 1924 – Louis de Broglie
  - Particles have wave like properties
  - Confirmed through expt .
    - Electrons shot through crystals form interference pattern
  - 1999 – Anton Zeilenger – Two – slit expt. with C_{60}

Dust particles

$$\lambda \sim 6.6\times10^{-6}\text{Å}$$

$$\underset{\text{momentum}}{P} = \frac{h}{\lambda} = mv\ ; \quad k = \frac{2\pi}{\lambda}$$

$$P = \frac{hk}{2\pi} = \hbar k$$

Born rule (1926) – probability interpretation

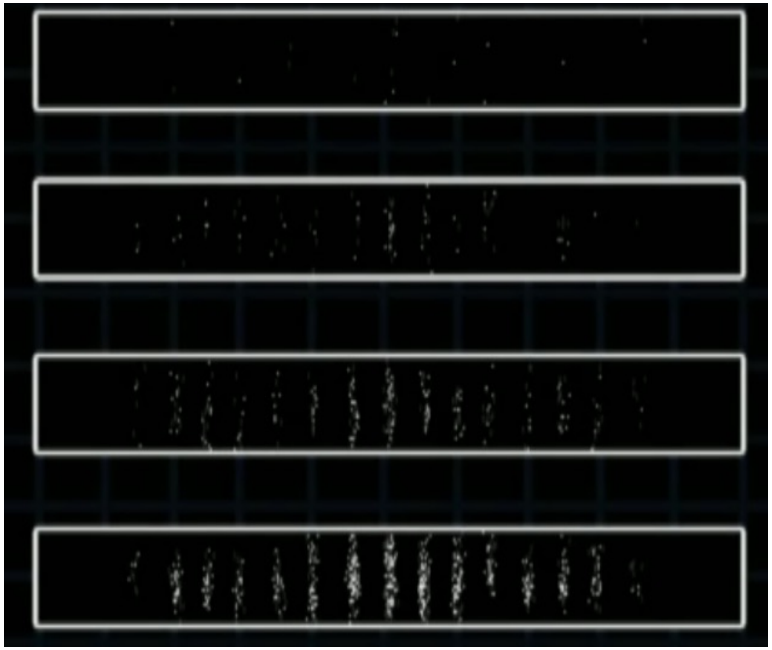
- In matter waves what is waving?
  - Particle has definite position
  - Wave is spread out over space
- The intensity of quantum wave at a point- probability of finding the particle at that point

Intensity ∞ amplitude^2

- QM only tells us the probability
- De Broglie waves are probability waves

Two – slit experiment with Electrons

- 10 particles – no pattern
- Many particles – statistical pattern emerge
- Billions of particles – Interference pattern

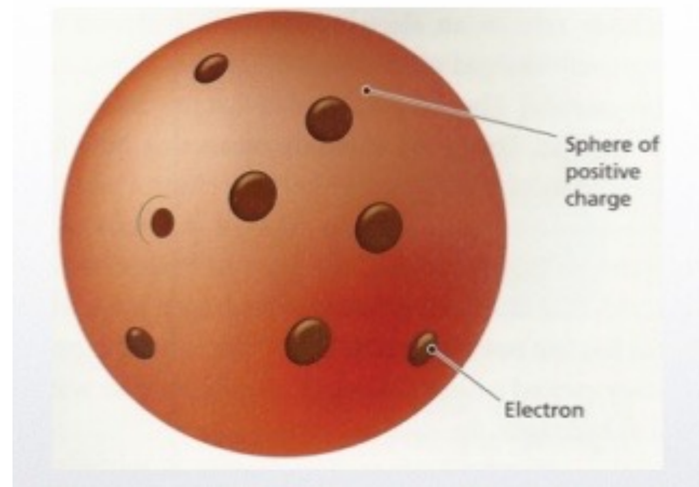


- QM individual events are random

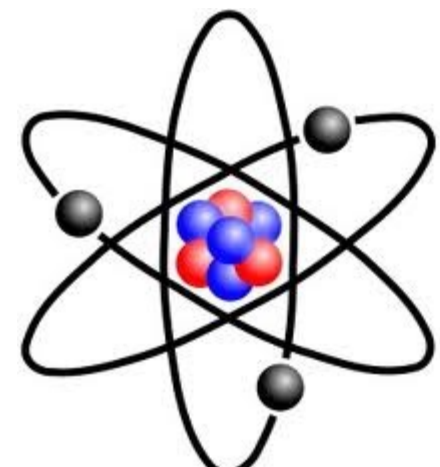
- Particles – discrete
- Probability waves - continuous

Evolution of the Model of the atom

- Thompson (1898) – plum pudding model

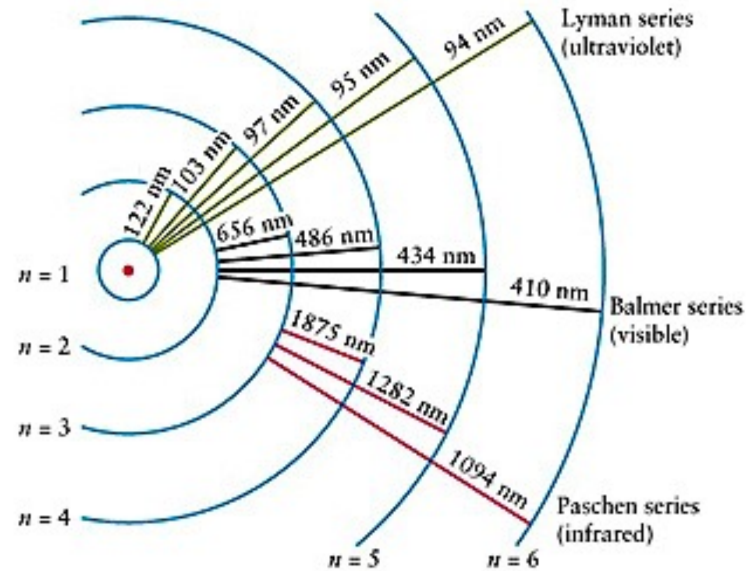


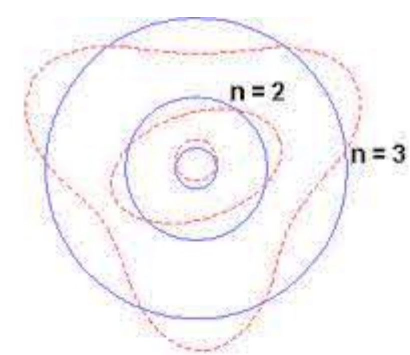
- Rutherford (1911) – solar system model
  - Orbiting electrons will emit radiation
  - Therefore they will lose energy and collapse on the nucleus
  - Atoms should implode on themselves



Evolution of the Model of the atom

- Bohr's model (1913)
  - Electron's orbits are stationary states
  - If electron jumps from high energy orbit to lower energy orbit it emits photons.
- De Broglie (1924)
  - Bohr orbits explained by standing electron waves
  - Only certain wave patterns allowed
    - Only certain frequencies
    - Only certain energies
  - Standing waves are Bohr's orbits





The standing de Broglie waves set up in the first three Bohr orbits.

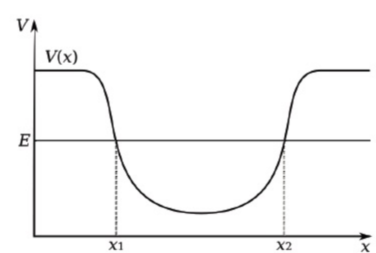
Schrödinger equation

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

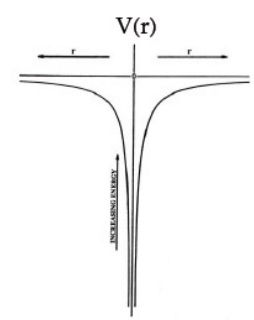
$$KE + PE = E_{Total}$$

- 1926 – Erwin Schrödinger develops wave mechanics
- Energy equation
- Ψ - Wave function
  - Mathematical object that corresponds to de Broglie's wave
- There are NO physical assumptions available to "derive" the Schrödinger Equation

- V(x,t) is the Potential Energy experienced by the quantum object at all points in space and time



Arbitrary 1-D "Potential Well"



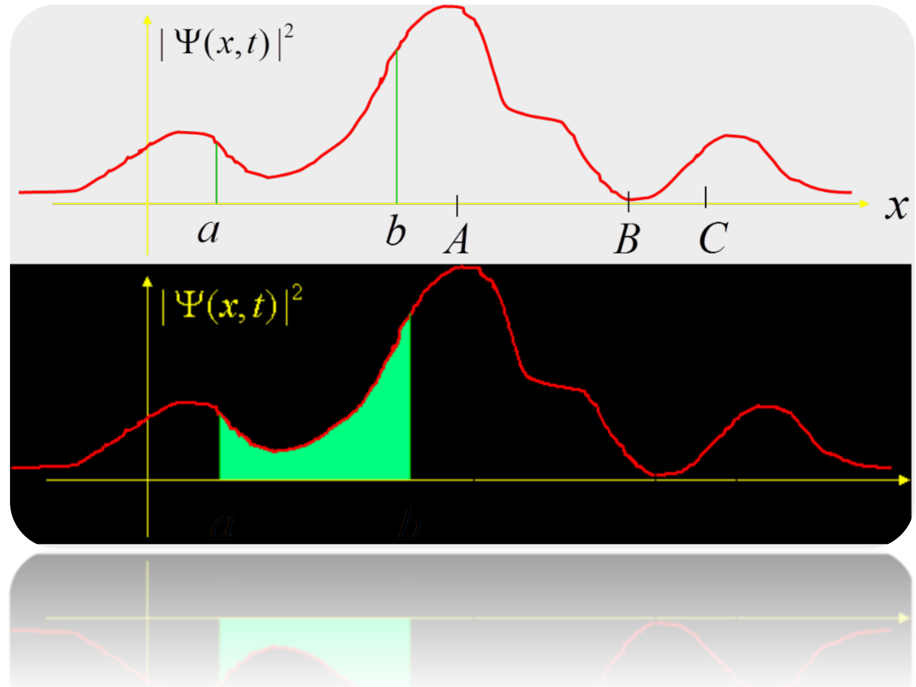
Potential an electron in a Hydrogen atom sees due to the Coulomb attraction of the Proton.

Interpretation of Ψ

- Max Born's (1926) statistical interpretation

- $|\Psi(x,t)|^2$

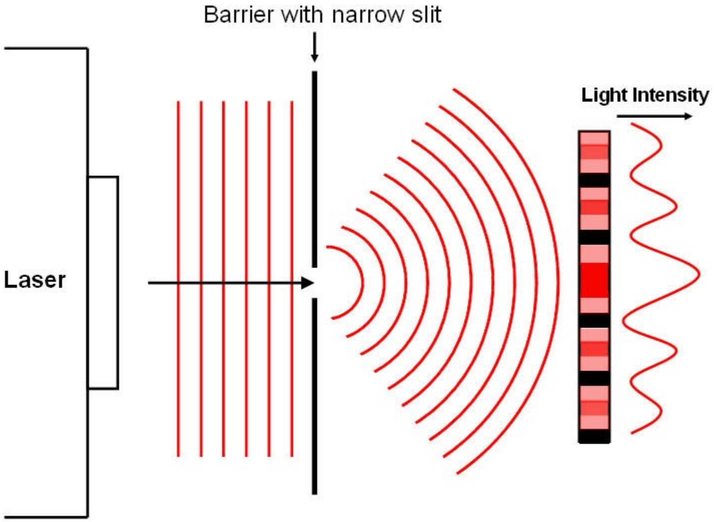
  - gives the probability of finding the particle at point x, at time t

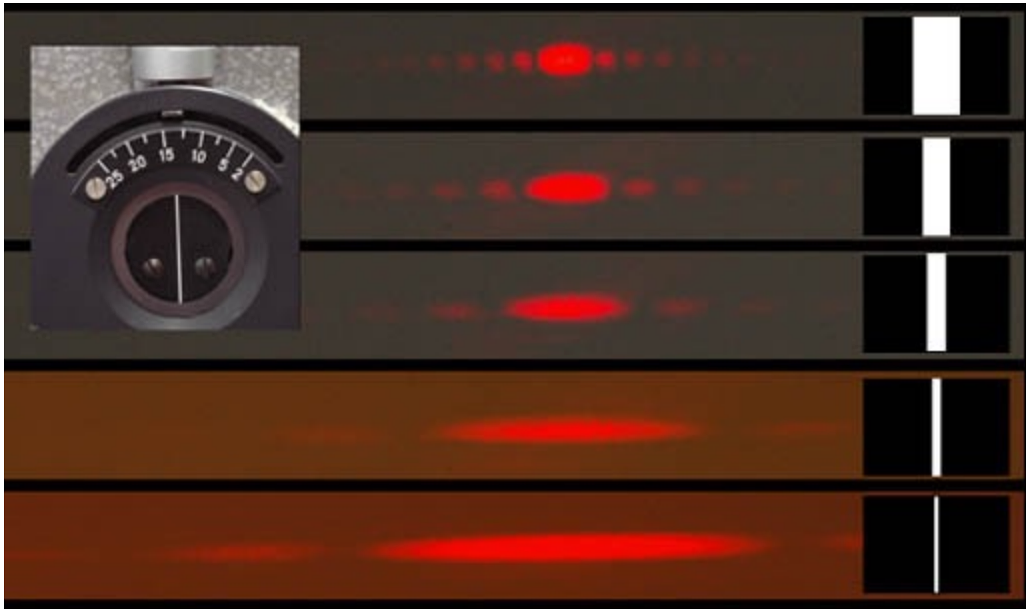


- $\int_a^b |\Psi(x,t)|^2 \, dx$
  - Probability of finding the particle between a and b, at time t.

- $\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \, dx = 1$
  - Probability of finding particle in the universe should be 1.

Single slit diffraction





- When slit width is large – uncertainty in position is large – uncertainty in lateral momentum small

Heisenberg's Uncertainty Principle

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

- Position and momentum of a particle cannot be known with infinite precision at the same time.
- Also same for energy and time

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

Postulates and Interpretations

PRINCIPLES OF QUANTUM MECHANICS

Postulates of QM

1. The state of QM system is completely specified by $\Psi(x,t)$.

   – $|\Psi(x,t)|^2\, dx$ is the probability of finding the particle between x and $x + dx$

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

   – $\Psi(x,t)$ and $\frac{\partial\Psi(x,t)}{\partial x}$ are continuous. $\Psi(x,t)$ is finite and single valued.

Ψ^*: Complex conjugate

Postulates of QM

2. For every observable (dynamic variable) in classical mechanics – Position, momentum, energy etc. there exists a linear operator in QM.

– For position X, momentum $\frac{\hbar}{i}\frac{\partial}{\partial x}$

– Ensemble average (expectation value) of $\hat{A}$ are real

- $\langle \hat{A} \rangle = \langle \hat{A} \rangle^*$
- $\langle \hat{A} \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\hat{A}\Psi(x,t)dx$
- All QM operators are “Hermitian”

$< f|Ag > = < Af|g >$ always iff A is Hermitian

Postulates of QM

3. I. Measurement of $\hat{A}$ will only yield the values a which satisfy the equation.

$$\hat{A}\Psi = a\Psi$$

- Eigenvalue equation
- Eigenvalues a are real numbers
- Central point of QM – dynamic variables are quantized
- Only Hermitian operators will yield real eigenvalues.

Postulates of QM

3. II. Each eigenvalue has an "eigenstate" associated with it
   – Initial state of system can be arbitrary.
   – Can be expanded in the complete set of eigenstates.

$$\hat{A}\psi_i = a_i\psi_i$$

$$\Psi = \sum_i^n c_i\psi_i$$

   – $\hat{A}$ will yield one of the eigenvalues a_i
   – Probability that a_i will occur is $|c_i|^2$

Postulates of QM

4. State of system (wave function) evolves according to *Time dependent Schrödinger equation* (TDSE).

$$\boxed{\hat{\mathrm{H}}\Psi(x,t) = i\hbar\frac{\partial\Psi}{\partial t}}$$

– Where $\hat{\mathrm{H}} = \frac{\hbar^2}{2m}\frac{\partial^2}{\partial^2 x} + V$

Uncertainty

- Expectation value of $\hat{A}$

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

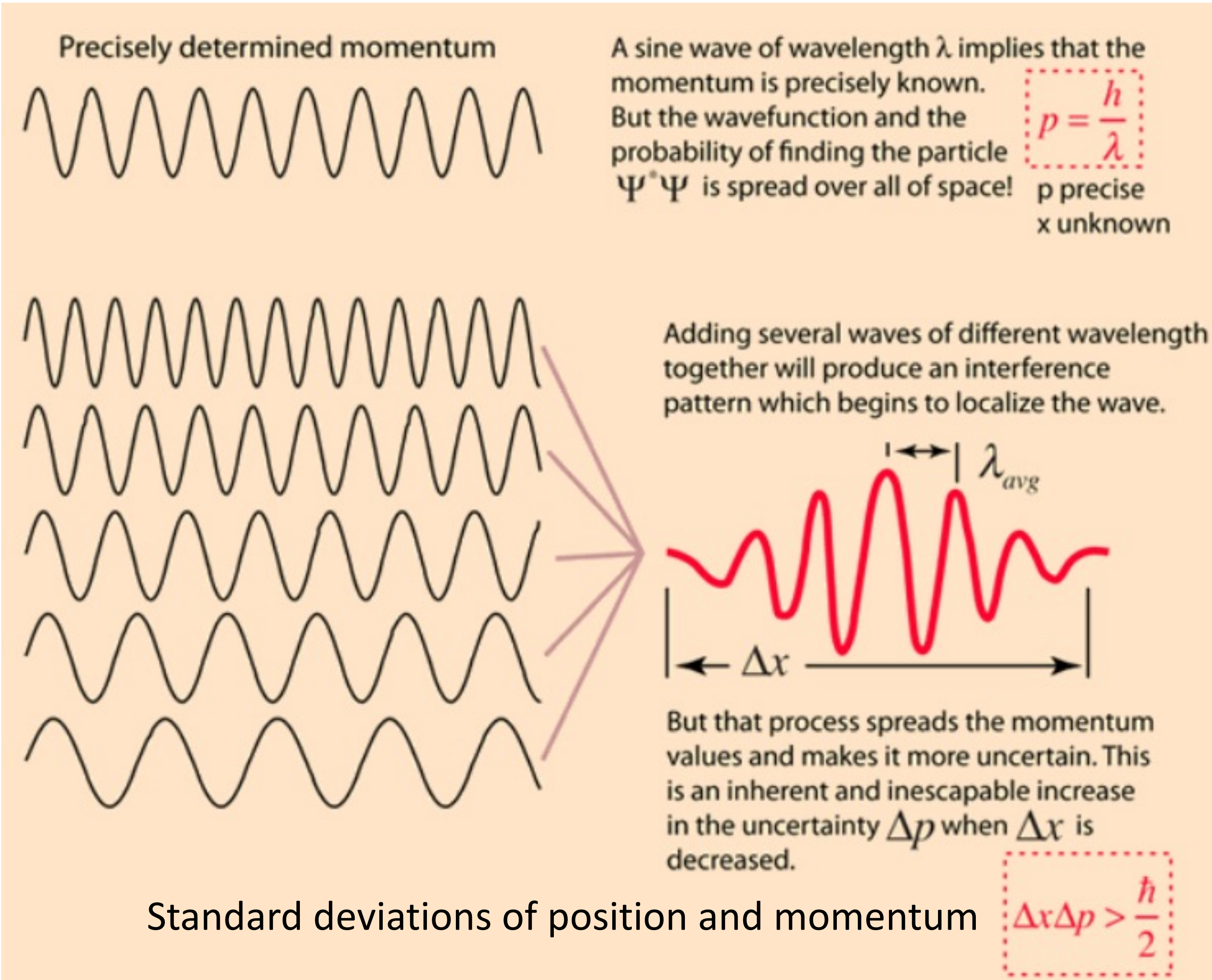
$$\langle \hat{A} \rangle = \langle \Psi | \hat{A} | \Psi \rangle$$

- Uncertainity in $\Delta\hat{A}$

$$\Delta\hat{A} = \langle \Psi | (\hat{A} - \langle \hat{A} \rangle)^2 | \Psi \rangle$$

- Expectation value and uncertainty provide a good description of the system
  - e.g.) If for a particle $\langle X \rangle = a$ and $\Delta X = \Delta$ then we know it can be spotted at $x = a$ with deviation of order Δ

Uncertainty Principle (Heisenberg): due to duality of particle-wave, precise momentum and position of the particle cannot be simultaneously determined. More precise momentum (related to wavelength after de Broglie), less the position. More precise position, less the momentum.



de Broglie

Standard deviations of position and momentum

QM – Interpretation of Motion

- Quantum mechanics does not predict precise trajectories
- Quantum mechanics does not predict the exact position of a particle.
  - Instead **it predicts the probability of finding a particle in different locations.**
- The electron exists in an undetermined state until measurement.
  - This interaction causes the electron to materialize at some position in space, determined randomly but weighted by the probability distribution of the wave function.
- The predictions of quantum mechanics coincide with those of classical mechanics for heavy particles

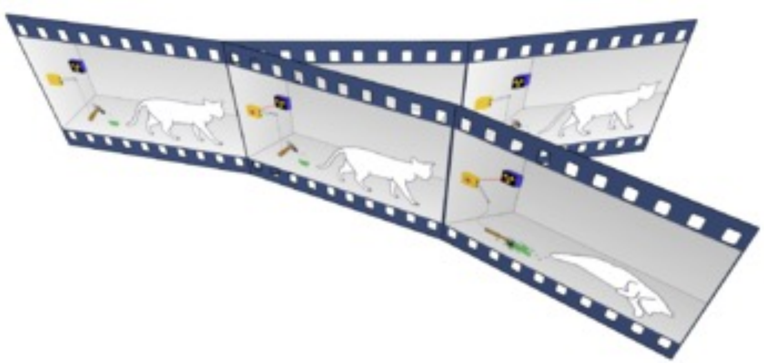
Einstein’s quotes on QM

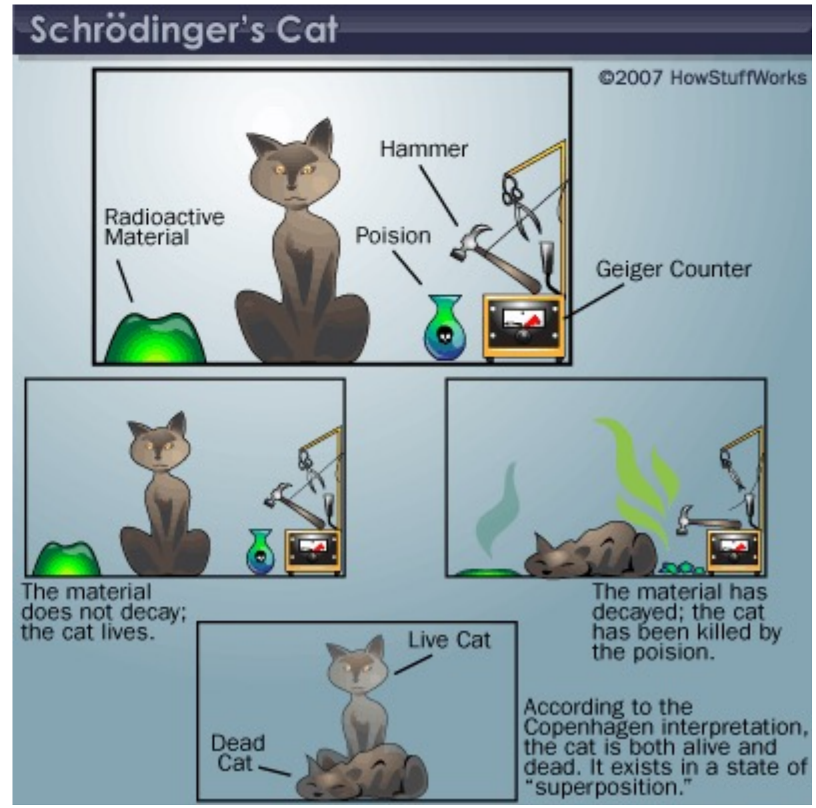
- The theory says a lot, but does not really bring us any closer to the secret of the “Old One." I, at any rate, am convinced that He does not throw dice.

- Whether you can observe a thing or not depends on the theory which you use. It is the theory which decides what can be observed.

Schrödinger's Cat

- Different interpretations of QM
  - Copenhagen interpretation
  - Many-worlds interpretation
  - Ensemble interpretation
  - and many more.





"….one cannot get around the assumption of reality, if only one is honest. … " – Einstein (1950)

Free particle

- Consider free particle $V = 0$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} = i\hbar\frac{\partial\Psi}{\partial t}$$

$$\Psi(x,t) = Ae^{i(kx-\omega t)}$$

$$k = \frac{2\pi}{\lambda}$$

$$E = \hbar\omega = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

$$|\Psi(x,t)|^2 = A^2$$

- Plane wave solution
  - de Broglie relations connect particle and wave properties
  - Impossible to normalize
  - Unphysical
  - Solution – superposition of plane waves

Wave packets

- Definition (when restricted to t=0)

Superpose components of different wave number (Fourier expansion)

$$\Psi(x,0) = \frac{1}{(2\pi)^{3/2}} \int_{-\infty}^{\infty} dk \psi(k) e^{ikx}$$

Fourier elements are set by

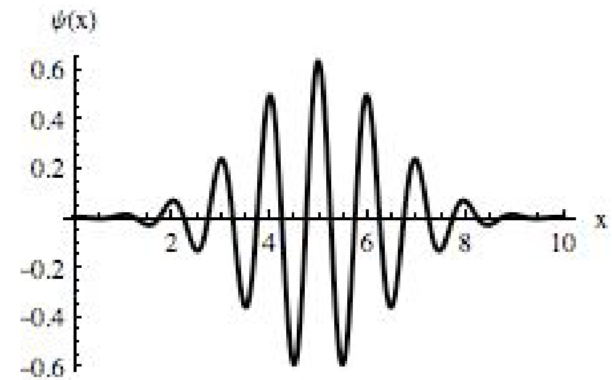
$$\psi(k) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} dx \Psi(x,0) e^{-ikx}$$

Gaussian wave packet

- Gaussian form for elements

$$\psi(k) = \left(\frac{2\alpha}{\pi}\right)^{1/4} e^{-\alpha(k-k_0)^2}$$

$$\Psi(x,0) = \left(\frac{1}{2\pi\alpha}\right)^{1/4} e^{ik_0x} e^{-\frac{x^2}{4\alpha}}$$



- We can localize a wave packet to a region of space
  - At the expense of having some width in *k*
  - Gaussian wave packet has minimum uncertainty.

$$\boxed{\Delta p \, \Delta x = \frac{\hbar}{2}}$$

Time Independent Schrödinger Equation

- For particle in a time independent potential

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

$$\left[\frac{\hbar^2}{2m}\frac{\partial^2}{\partial^2 x} + V\right]\psi(x) = \mathrm{E}\psi(x)$$

$$H\psi_n(x) = En\psi_n(x)$$

$$\Psi_n(x,t) = \psi_n(x)e^{-iEnt}$$

Many electron wave function

- Each electron moves, to a first approximation, independently of the others
- For the He-atom(2 electron system), we can approximate

$$\psi(x_1, y_1, z_1, x_2, y_2, z_2) = \psi_{1s}(\mathrm{x}_1, \mathrm{y}_1, \mathrm{z}_1).\,\psi_{1s}(\mathrm{x}_2, \mathrm{y}_2, \mathrm{z}_2)$$

- When single-electron wave functions are used as part of a many-electron wave function those single-electron wave functions are called orbitals, thus
- The two electrons of He are in 1s orbitals

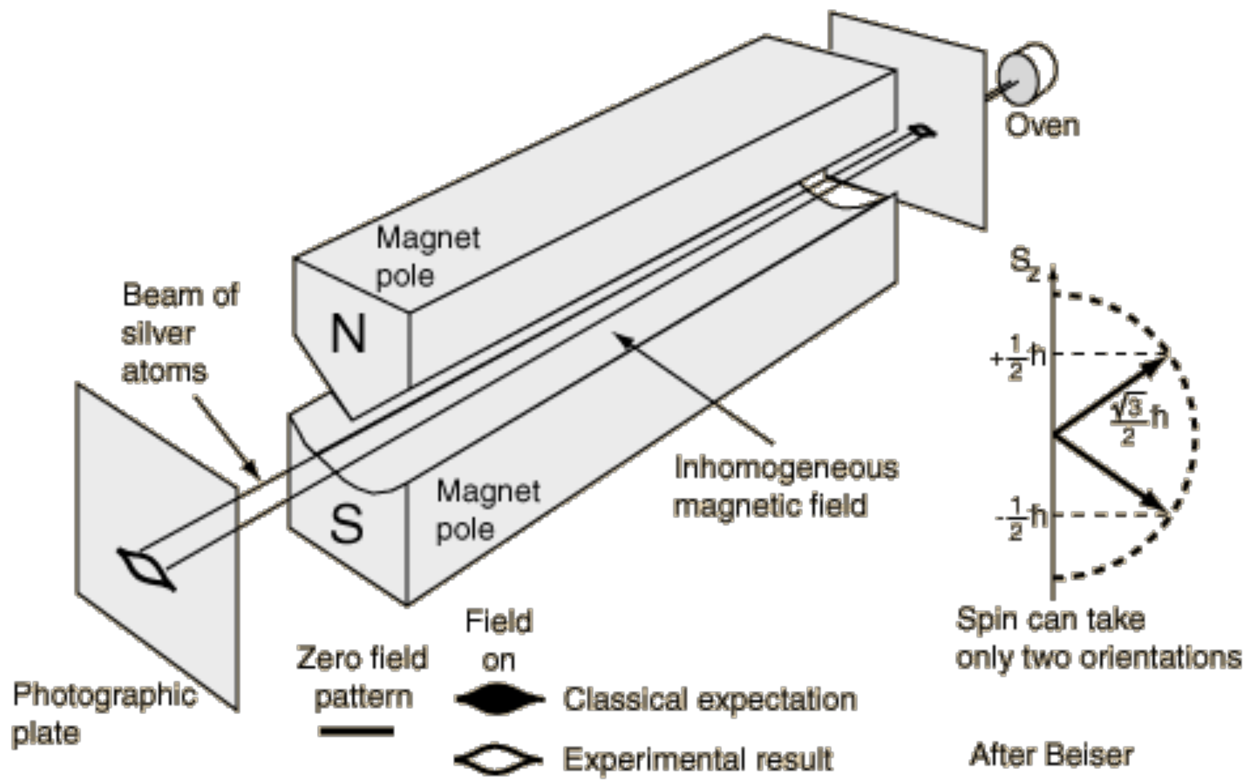
Pauli exclusion principle

- The Pauli principle requires that electrons use different wave functions
- For He we need to distinguish the electrons

$$\psi(x_1, y_1, z_1, x_2, y_2, z_2) = \psi_{1s,ms=\frac{1}{2}}(\mathrm{x}_1, \mathrm{y}_1, \mathrm{z}_1).\,\psi_{1s,ms=-\frac{1}{2}}(\mathrm{x}_2, \mathrm{y}_2, \mathrm{z}_2)$$

- Where m_s is the spin of the electron

Stern-Gerlach experiment (1922)



Electron spin

- In *classical mechanics* a rigid body has
  - Orbital angular momentum ($\mathbf{L} = \boldsymbol{r} \times \boldsymbol{p}$)
  - Spin ($\boldsymbol{S} = \boldsymbol{I}\omega$)
  - For Earth $\boldsymbol{S}$ is nothing but sum of $\boldsymbol{L_i}$of all particles that make up Earth
- The electron is a structureless point particle
  - Therefore $\boldsymbol{S}$ cannot be decomposed in to $\boldsymbol{L_i}$ of constituent parts.
  - We say it carries an "intrinsic" angular momentum ($\boldsymbol{S}$) in addition to the extrinsic orbital momentum ($\boldsymbol{L}$)
- Spin is a property of all elementary particles
- Spin gives rise to magnetic properties

Reference texts

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