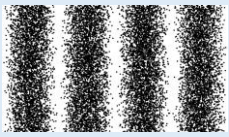
Quantum Weirdness: A Beginner's Guide

Part 3

The Schrödinger Equation
Schrödinger's Cat
Electron Spin and Magnetism

Single Electrons in the Double Slit Experiment

- Firing electrons one at a time through two slits.
- Get a striped pattern.
- A single electron must act like a wave
- It must go through both slits simultaneously



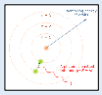
- How can a particle can be in two places at the same time?
- We need a description of a particle in terms of where it is at any given time:
- We need Erwin Schrödinger

Internal Politics in Physics

The Danish and German Schools

- In the 1920s, the physics community generally split into two groups

- The Danish School – lead by Nils Bohr
- Emphasized transitions between discrete states
- Matrix mechanics



- The German School – lead by Albert Einstein
- Emphasized wave particle duality
- Schrödinger's Wave Interpretation

Matrix Mechanics

- Max Born, Werner Heisenberg and Pascual Jordan had been working on their own solution to the quantum jump problem using Matrix Mechanics

Werner Heisenberg

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Pascual Jordan

Max Born

$$R_{90^\circ} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

- Represents a rotation of 90° counterclockwise.

$$\times \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} =$$

Conwy Castle, Conwy, Wales 2018

- Matrices were considered very exotic mathematics by physicists in the 1920s!
- But they had a useful mathematical property:

$$AB - BA \neq 0$$

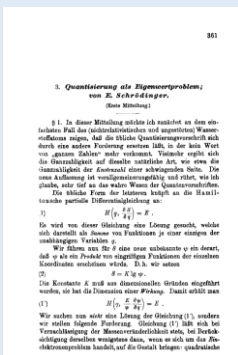
Not commutative!

- Born and Heisenberg did not have a physical interpretation for what their matrices represented in reality

Erwin Schrödinger

- Took a different approach to matrix mechanics
- In 1926 he publishes a revolutionary paper describing particles in terms of waves

https://onlinelibrary.wiley.com/doi/pdf/10.1002/andp.19263840404



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3. *Quantisierung als Eigenwertproblem;*
von *E. Schrödinger.*
(Erste Mitteilung.)

§ 1. In dieser Mitteilung möchte ich zunächst an dem einfachsten Fall das (nichtrelativistische und ungestörte) Wasserstoffatom zeigen, daß die übliche Quantisierungsvorschrift sich durch eine andere Fassung ersetzen läßt, in der kein Wert von „ganzen Zahlen" mehr vorkommt. Vielmehr ergibt sich die Ganzzahligkeit auf direkte natürliche Art, wie etwa die Ganzzahligkeit der *Knotenzahl* einer schwingenden Saite. Die neue Auffassung ist verallgemeinerungsfähig und rührt, wie ich glaube, sehr tief an das wahre Wesen der Quantenvorschriften.

Die übliche Form der letzteren knüpft an die Hamiltonsche partielle Differentialgleichung an:

$$H\left(q, \frac{\partial S}{\partial q}\right) = E \,. \tag{1}$$

Es wird von dieser Gleichung eine Lösung gesucht, welche sich darstellt als *Summe* von Funktionen je einer einzigen der unabhängigen Variablen q.

Wir führen nun für S eine neue unbekannte ψ ein derart, daß ψ als ein *Produkt* von eigentlichen Funktionen der einzelnen Koordinaten erscheinen würde. D. h. wir setzen

$$S = K \lg \psi \,. \tag{2}$$

Die Konstante K muß aus dimensionellen Gründen eingeführt werden, sie hat die Dimension einer *Wirkung*. Damit erhält man

$$H\left(q, \frac{K}{\psi}\frac{\partial \psi}{\partial q}\right) = E \,. \tag{1'}$$

Wir suchen nun nicht eine Lösung der Gleichung (1'), sondern wir stellen folgende Forderung: Gleichung (1') läßt sich bei Vernachlässigung der Massenverschiedenheit stets, bei Berücksichtigung derselben wenigstens dann, wenn es sich um das *Wasserstoffelektronenproblem* handelt, auf die Gestalt bringen: quadratische

The Schrödinger Equation

- Schrödinger realised that he could describe the electron in the hydrogen atoms by means of a wave function

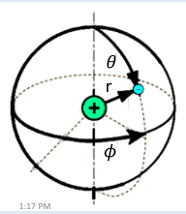
$$\Psi \text{ (Psi)}$$

- His general equation for the energy of a quantum system is

$$\hat{H}\Psi = E_n\Psi$$

He could produce the same results that Bohr had for the hydrogen atom – predicting the same energy levels.

- To describe the electron in three dimensions, Schrödinger needed three quantum numbers
- Bohr's model only had one quantum number, n



To describe the position in three dimensions you need

A distance from the nucleus r

An azimuthal angle ϕ (phi)

A polar angle θ(theta)

http://latitudelongitude.org/ca/ottawa/

$$\Psi(r, \phi, \theta) = R(r)P(\theta)F(\phi)$$

- Schrodinger demonstrated that his wavefunction for hydrogen had three parts, depending on r, ϕ, and ϕ
- Each part had a quantum number associated with it

$$\Psi(r, \phi, \theta) = \boxed{R(r)}P(\theta)F(\phi)$$

Principle Quantum Number n = 1, 2, 3, 4, 5…

The same as Bohr's Quantum number!

$$\Psi(r, \phi, \theta) = R(r)P(\theta)F(\phi)$$

- Orbital quantum number l
- Quantized, but limited by the principle quantum number n

$$l = 0, 1, 2 \ldots n - 1$$

$$if\ n = 1\ then\ l = 0$$

$$if\ n = 2\ then\ l = 0, or\ 1$$

$$\Psi(r, \phi, \theta) = R(r)P(\theta)F(\phi)$$

- The magnetic quantum numbers m_l depend on l.

$$m_l = -l\ to + l, \qquad integer\ steps$$

$$if\ n = 1\ then\ l = 0, m_l = 0$$

$$if\ n = 2\ and\ l = 0, m_l = 0$$

$$if\ n = 2\ and\ l = 1, m_l = -1, 0\ , +1$$

Probability, Position and the Wavefunction

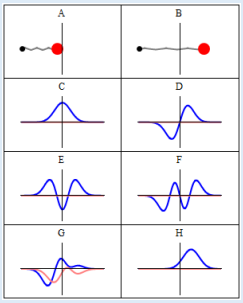
Ψ (Psi)

- Max Born realized that Schrödinger's wave function had a physical meaning
- The wave function squared gave the probability of find the electron at any point in space

Atomic Oscillator

- In a paper the next year, Schrodinger applied his equation to the general problem of a quantum particle oscillating due to its temperature.
- This was the model used by Planck in his black-body analysis

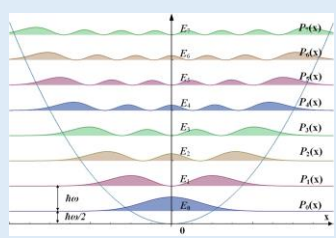
Classical analogue is a mass on a spring



Classical particle oscillating: mass on a spring

Quantum Oscillators

- An exact solution is possible for this problem



The energy levels in the quantum series are equally spaced, just as Planck had hypothesized.

- In his next paper, Schrödinger then proved that his equation was mathematically equivalent to the Matrix Mechanics formulation
- The wave solution approach is the one most often used in teaching quantum mechanics because it is easier to visualize

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Consequences of the Schrödinger Equation

What does the mathematics mean?

Superposition of Two Quantum States

- Any valid wavefunction can **always** be described as some combination of any two other valid wavefunctions
- This helps explain the 3 polarizer experiment
- Any given polarization direction is a sum of two polarization states

Vertical Polarization

Schrödinger's Cat

- A famous thought experiment to describe this quantum superposition.

Inside the box is a cat

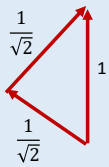
It must be either dead or alive

It is the superposition of two states

- We do not know which state the cat is in, when it is the box
- The act of making a measurement changes the state of the system.
- If we open the box to find out, we have measured the system, and one of the two possibilities must disappear
- This is known as collapsing the wavefunction of that state

Once we have measured it, the cat is either definitely alive or definitely dead

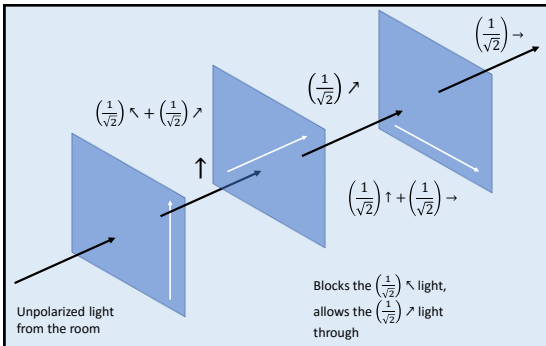
- Vertically polarized light ↑ could be thought of as a combination of two 45°states



$$\uparrow = \left(\frac{1}{\sqrt{2}}\right)\nwarrow + \left(\frac{1}{\sqrt{2}}\right)\nearrow$$

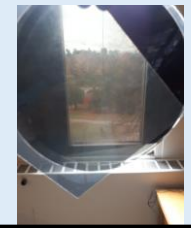
The factors are just there to say there is an equal probability of each of the two slanted positions, and the total probability is 1

The numbers come from Pythagoras theorem on the triangle



- The three film polarizer effect ONLY works if

- Light is a set of quantum particles
- Polarization is a quantum property
- Polarization can be split into two states at each filter



Probability Distributions

What are they?

Schrödinger's Ψ Function and Probability

- The Schrodinger equation assumes that you can never know the exact position of a particle, but you can know the exact energy (the E value).
- The position of the particle has to be represented as the likelihood of finding the particle in a particular place.

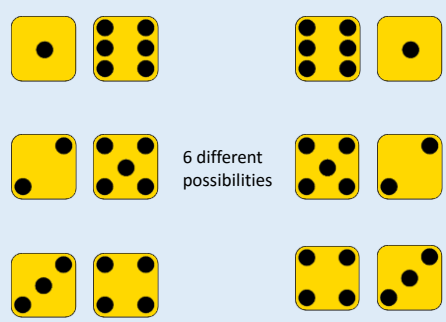
$$\Psi^2 = probability$$

Probability: Dice Rolling for Distribution

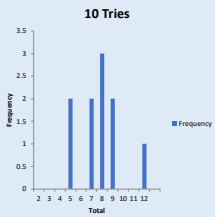
- Roll 2 identical dice, and take the total.
- There are 6 possible values from each dice, so there are 36 possible outcomes
- Some of the outcomes are the same total

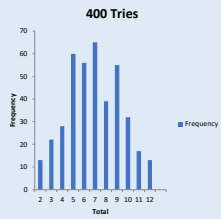
$$P(2) = \frac{1}{6} \times \frac{1}{6} \qquad P(2) = \frac{1}{36}$$

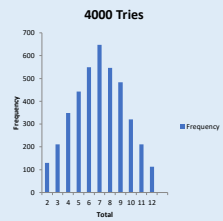
- Probability of getting a total of seven

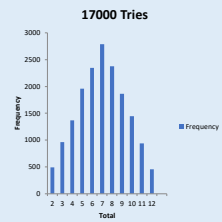


- If we roll the dice many times (trials) we will generate the probability function for the two dice system

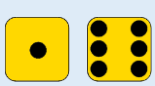


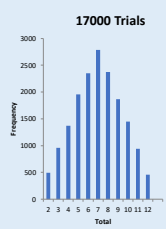






- We can use the probability distribution to predict what we will roll on the dice
- The total probability of all outcomes = 1
- There are 36 possible outcomes from the two dice
- We must get a result
- Probability of rolling a total of 7, from any combination is 1/6

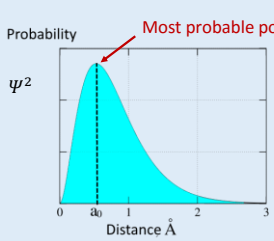




Total of 2 dice	Predicted Probability	Probability from 17000 trials
2	1/36	1.0/36
3	2/36	2.0/36
4	3/36	2.9/36
5	4/36	4.1/36
6	5/36	5.0/36
7	6/36	5.9/36
8	5/36	5.0/36
9	4/36	4.0/36
10	3/36	3.1/36
11	2/36	2.0/36
12	1/36	1.0/36

Probability and the Wavefunction

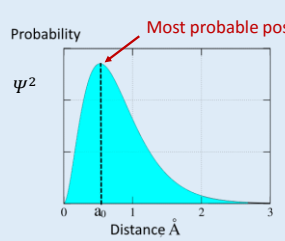
- The square of Schrodinger's wavefunction Ψ gives the probability of finding the particle at a particular place

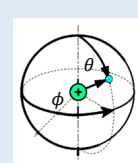


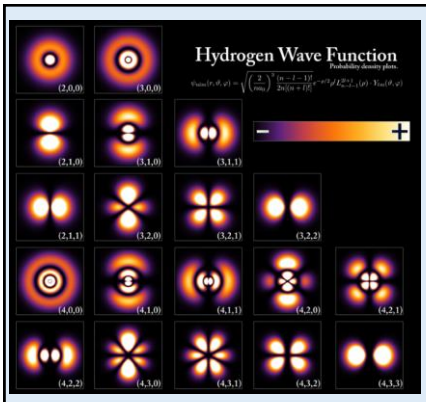
Total area = 1 (Particle must be somewhere)

Quantum numbers
n = 0, l = 0, m_l = 0

- The most probable distance of the electron from the nucleus, a_0 (known as the Bohr radius) agrees exactly with Bohr's calculation using his simpler model
- It does not depend on angles θ and ϕ.





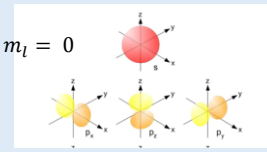


Some of the probabilities for higher quantum numbers are angle dependent

The lowest energy state for various quantum number combinations of Hydrogen look like this

These shapes represent the probability of 90% of finding the electron somewhere inside the shape

$n = 1\,, l = 0, m_l = 0$

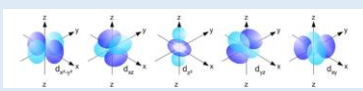


s -orbital

p - orbitals

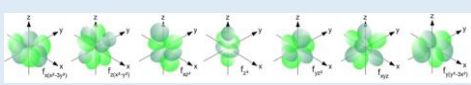
$n = 2\,, l = 1, m_l = -1, 0\,, +1$

$n = 3\,, l = 2, m_l = -2, -1, 0\,, +1, +2$

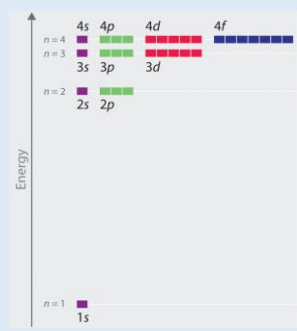


d -orbital

$n = 4\,, l = 3, m_l = -3, -2, -1, 0\,, +1, +2, +3$



f - orbitals



Schrodinger's Equation produced energy levels identical to those of Bohr

The mathematical solutions are naturally quantized

They explain the observed spectroscopic measurements

Spin and Magnetism

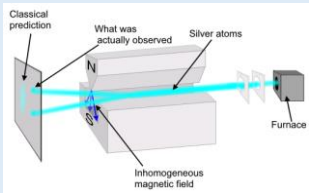
A Purely Quantum Effect

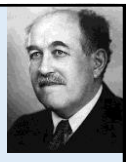
Electron Spin

- Schrodinger's solution has three quantum numbers.
- But there is an additional quantum property of the electron, which also needs a quantum number
- This property is known as the Spin
- It has two states: "Up" or "Down"
- The spin property gives rise to the magnetic properties of materials

Stern-Gerlach Experiment

- Stern and Gerlach fired silver atoms through a magnetic field, and measured the scattering





Otto Stern
Walter Gerlach

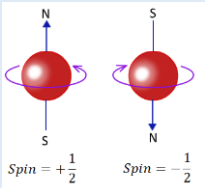
- The silver atoms act like magnets
- But not classical magnets, where orientation of the north-south axis is random, and should produce random scattering
- Atoms have an intrinsic magnetic orientation, but it is in only two "orientations".

https://commons.wikimedia.org/wiki/File:Quantum_spin_and_the_Stern-Gerlach_experiment.ogv

Stern got the Nobel prize in Physics for 1943, but not for this experiment!
https://www.nobelprize.org/prizes/physics/1943/summary/

Electron Spin

- Quantum particles have quantum property called "Spin"
- Electrons can be either
  - Spin Up
  - Spin Down



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- Proposed by Samuel Goudsmit (NL/USA) and George Uhlenbeck (NL/USA)
- The Spin property has no classical analog.
- Spin is not really a good name for it!

Samuel Goudsmit

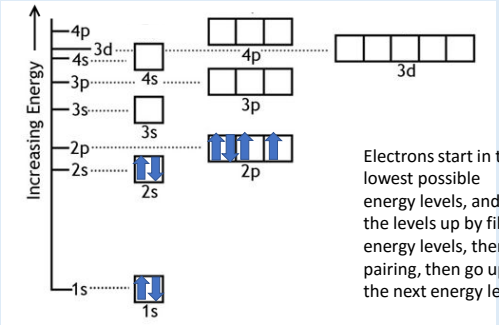
George Uhlenbeck

Pauli Exclusion Principle

- Wolfgang Pauli proposed that each electron in an atom must have a unique set of quantum numbers
- 3 From the Schrödinger equation
- 1 from the Spin
- Two electrons could exist in a single energy level, but only if they had opposite spin

https://www.nobelprize.org/prizes/physics/1945/summary/

Austria/USA/Switzerland



Electrons start in the lowest possible energy levels, and fill the levels up by filling energy levels, then pairing, then go up to the next energy level*

*Some exceptions apply. This is what makes chemistry interesting and complex

Natural Permanent Magnets

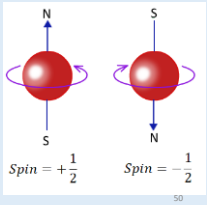
- Known for at least 2500 years
- Lodestone (magnetite) mined in Turkey, at Magnesia - some of the pieces of this mineral were permanent magnets

- The quantum property electron spin is responsible for magnetism in materials

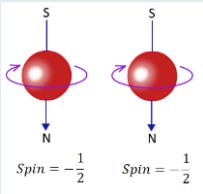
https://www.youtube.com/watch?v=Mp0Bu75MSj8

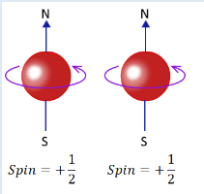
Non-Magnetic Materials

- The electrons are paired up
- The spin up cancels with the spin down in the pair
- There is no overall magnetic field generated



- To create a material which is a permanent magnet, some of the electrons must either be unpaired,
- Or arranged with spins in parallel



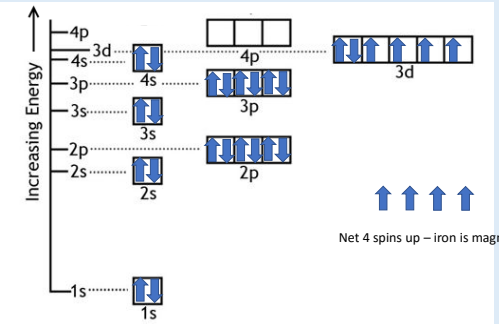


Ferromagnetic Materials

- Substances which experience a substantial magnetic force when near a magnet
  - Iron, nickel, cobalt, chromium dioxide
- Materials which may be permanent magnets require the electrons to be distributed in a certain way (with unpaired spins)

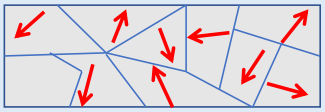
https://www.youtube.com/watch?v=6wEWbX_FruY

Fe = $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$



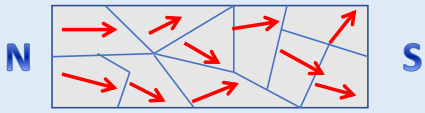
Unmagnetized Ferromagnet

- The domains in the material have random orientation, so there is no net magnetic interaction with an external magnet

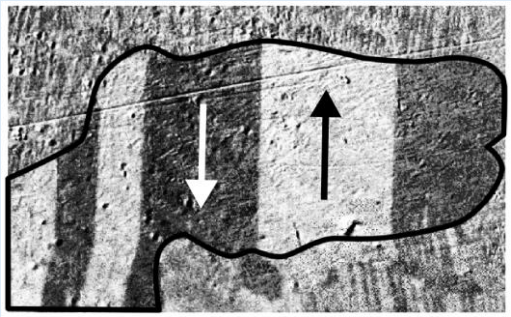


Magnetized Ferromagnet

- If the domains are aligned with each other, then there is an overall magnetic moment



- Magnetising a ferromagnetic material is possible by exposing it to a large magnetic field - changing the magnetic orientation of the domains

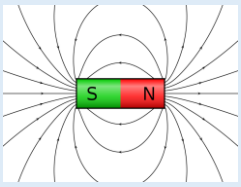


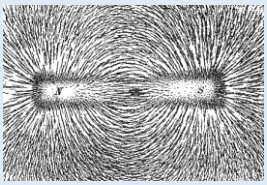
Non-magnetic steel

http://commons.wikimedia.org/wiki/File:Magnetic_domain_by_Zureks.png

Magnetic Field

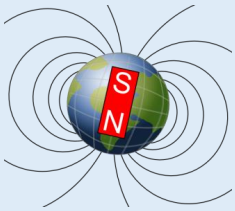
- Iron filings placed in a magnetic field align themselves with the field, indicating the orientations of the magnetic field





The Earth's Magnetic Field

- The earth generates a magnetic field, which is approximated by a bar magnet (dipole) near the surface of the earth



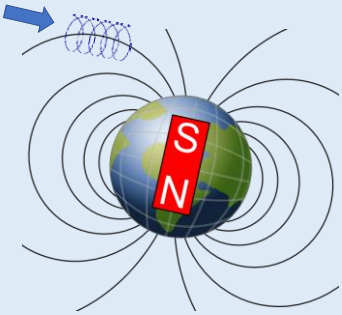
What we call the magnetic north pole is actually the south pole of the dipole magnet model!

Aurora

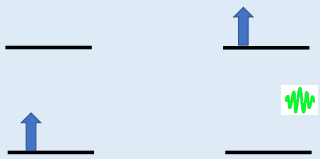
- The Aurora is caused by charged particles from the sun trapped in the Earth's magnetic field and spiralling towards the North or South Poles.

Green colours most common
Blue and Pink rarer

- Charged particles from the sun are trapped in the magnetic field and spiral towards the poles



- If q charged particles hit an oxygen molecule (O_2) they can excite an electron to a higher quantum state



"Collisional pumping"

Emits a photon with a wavelength of 577 nm (green)

- Double quantum phenomena (magnetism and spectroscopy)
- Aurora viewed from the International Space Station