Quantum Weirdness: A Beginner’s Guide

Part 3

The Schrödinger Equation
Schrödinger’s Cat
Electron Spin and Magnetism

Electrons in the Double Slit Experiment

• Repeat of Young’s experiment, but firing streams electrons through double slits.
• They show the striped diffraction patterns – acting like a wave

https://www.youtube.com/watch?v=M4_0oblwQ_U
https://www.youtube.com/watch?v=A9tKncAdlHQ (9 minute video)

• How can a particle 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

Internal Politics

• 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 fit with their viewpoint nicely
  • The German School – lead by Albert Einstein
  • Emphasized wave particle duality
  • Schrödinger’s Wave Interpretation

Matrix Mechanics

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

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

- Represents a rotation of $90^\circ$ counterclockwise.

Conway 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


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

The wavefunction $\Psi$ (Psi)

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

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

The Schrödinger Equation

- $\hat{H}$ is known as the Hamiltonian operator
- Contains details about the type of energy interactions acting on the particle
- $E$ is the energy of the particle

Sir William Rowan Hamilton — Irish Mathematician and Physicist

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 $\phi$ (phi)
- A polar angle $\theta$ (theta)

http://latitudelongitude.org/ca/ottawa/
Schrodinger demonstrated that his wavefunction for hydrogen had three parts, depending on $r$, $\phi$, and $\theta$.

Each part had a quantum number associated with it.

\[ \Psi(r, \phi, \theta) = \frac{R(r)}{P(\theta)}F(\phi) \]

- **Principle Quantum Number** $n = 1, 2, 3, 4, 5\ldots$
  - The same as Bohr’s Quantum number!

- **Orbital quantum number** $l$
  - Quantized, but limited by the principle quantum number $n$
  \[ l = 0, 1, 2 \ldots n - 1 \]
  - \[ if \ n = 1 \ then \ l = 0 \]
  - \[ if \ n = 2 \ then \ l = 0, or 1 \]

- **Magnetic quantum numbers** $m_l$
  - depend on $l$.
  \[ m_l = -l \ to + l, \ \text{integer steps} \]
  - \[ if \ n = 1 \ then \ l = 0, m_l = 0 \]
  - \[ if \ n = 2 \ and \ l = 0, m_l = 0 \]
  - \[ if \ n = 2 \ and \ l = 1, m_l = -1, 0, +1 \]

- **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.

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.

Consequences of the Schrödinger Equation
What does the mathematics mean?

Superposition of Two Quantum States
• One result of the Schrödinger equation is that any valid wavefunction can always be described as some combination of any two other valid wavefunctions

$$\hat{H}\psi = E\psi$$

• This helps explain the 3 polarizer experiment

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
• 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 $\uparrow$ could be thought of as a combination of two 45° states

$$\uparrow = \left(\frac{1}{\sqrt{2}}\right) \wedge + \left(\frac{1}{\sqrt{2}}\right) \vee$$

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
Unpolarized light from the room

\[ \left( \frac{1}{2} \right) \uparrow \left( \frac{1}{\sqrt{2}} \right) \left( \frac{1}{\sqrt{2}} \right) \left( \frac{1}{2} \right) \left( \frac{1}{\sqrt{2}} \right) \left( \frac{1}{\sqrt{2}} \right) \uparrow \]

Blocks the $\left( \frac{1}{\sqrt{2}} \right) \uparrow$ light, allows the $\left( \frac{1}{\sqrt{2}} \right) \left( \frac{1}{\sqrt{2}} \right) \left( \frac{1}{2} \right) \uparrow$ light through

- 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 $\Psi$ 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.

\[ \Psi^2 = \text{probability} \]

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

\[ P(2) = \frac{1}{6} \times \frac{1}{6} \quad P(2) = \frac{1}{36} \]

- Probability of getting a total of seven

6 different possibilities
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

Probability and the Wavefunction
The square of Schrodinger’s wavefunction $\Psi$ 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 $\theta$ and $\phi$.
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.

- \( n = 1, l = 0, m_l = 0 \)
- \( n = 2, l = 1, m_l = -1, 0, +1 \)

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.

- 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".

- Stern got the Nobel prize in Physics for 1943, but not for this experiment!

Electron Spin

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

- 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!

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.

- The 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

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

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)

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

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 charged particles hit an oxygen molecule (O₂), they can excite an electron to a higher quantum state.

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

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