QUANTUM MECHANICS

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Quantum Mechanics

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TABLE OF CONTENTS

Licensing

1: Introduction to Quantum Mechanics

- 1.1: Black-body radiation
- 1.2: Photo-electric effect
- 1.3: Hydrogen Atom
- 1.4: Wave particle duality
- 1.5: Uncertainty
- 1.6: Tunneling

2: Concepts from Classical Mechanics

- 2.1: Conservative Fields
- 2.2: Energy Function
- 2.3: Simple Example

3: The Schrödinger Equation

- 3.1: The State of a Quantum System
- 3.2: Operators
- 3.3: Analysis of the wave equation

4: Bound states of the Square Well

- 4.1: Bound States
- 4.2: B_2= 0
- 4.3: A_2= 0
- 4.4: Some Consequences
- 4.5: Lessons from the square well
- 4.6: A physical system (approximately) described by a square well

5: Infinite Wells

- 5.1: Zero of Energy is Arbitrary
- 5.2: Solution

6: Scattering from Potential Steps and Square Barriers

- 6.1: Non-normalizable Wavefunctions
- 6.2: Potential step
- 6.3: Square Barrier

7: The Harmonic Oscillator

- 7.1: Prelude to Harmonic Oscillators
- 7.2: Dimensionless Coordinates
- 7.3: Behaviour for large |y|
- 7.4: Taylor Series Solution
- 7.5: A Few Solutions
- 7.6: Quantum-Classical Correspondence

8: The Formalism Underlying Quantum Mechanics

- 8.1: Key Postulates
- 8.2: Expectation Values of x^2 and p^2 for the Harmonic Oscillator
- 8.3: The Measurement Process

9: Ladder operators

- 9.1: Harmonic oscillators
- 9.2: The operators Â and Â†.
- 9.3: Eigenfunctions of H through ladder operations
- 9.4: Normalisation and Hermitean conjugates

10: Time-Dependent Wavefunctions

- 10.1: Correspondence between time-dependent and time-independent solutions
- 10.2: Superposition of time-dependent solutions
- 10.3: Completeness and time-dependence
- 10.4: Simple Example
- 10.5: Wave packets (states of minimal uncertainty)

11: 3D Schrödinger Equation

- 11.1: The momentum operator as a vector
- 11.2: Spherical Coordinates
- 11.3: Solutions independent of angular variables
- 11.4: The hydrogen atom
- 11.5: Now where does the probability peak?
- 11.6: Spherical Harmonics
- 11.7: General solutions

12: Quantum Mechanics of the Hydrogen Atom

- 12.1: The Uncertainty Principle
- 12.2: Bohr Model of the Hydrogen Atom
- 12.3: Schrödinger Theory of the Hydrogen Atom
  - 12.3.1: Schrödinger Theory of Hydrogen
  - 12.3.2: The Spin-Orbit Effect
  - 12.3.3: Kinetic Energy Corrections
- 12.4: Dirac Theory of the Hydrogen Atom
- 12.5: Smaller Effects
  - 12.5.1: Hyperfine Structure
  - 12.5.2: The Lamb Shift
  - 12.5.3: The Zeeman Effect
- 12.6: Conclusion and References

13: Miscellaneous Quantum Mechanics Topics

- 13.1: Bell's Theorem
- 13.2: Black Hole Thermodynamics
- 13.3: Complementarity and Copenhagen Interpretation
- 13.4: Double Slit
- 13.5: Flash Animations for Physics
- 13.6: Locality and Quantum Mechanics

- 13.7: Particle in a 2-dimensional box
- 13.8: Quantum Entanglement
- 13.9: Quantum Interference
- 13.10: Quantum Mechanics- a Poor Person's Guide
- 13.11: Quantum Mechanics- Interpretation
- 13.12: Quantum Teleportation
- 13.13: Schrödinger's Cat
- 13.14: Stern-Gerlach Experiment
- 13.15: The Bohr Model of the Atom
- 13.16: The Development of Quantum Mechanics
- 13.17: Two analogies to Bell's Theorem
- 13.18: Wave-Particle Duality

Index

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CHAPTER OVERVIEW

1: Introduction to Quantum Mechanics

One normally makes a distinction between quantum mechanics and quantum physics. Quantum physics is concerned with those processes that involve discrete energies, and quanta (such as photons). Quantum Mechanics concerns the study of a specific part of quantum physics, those quantum phenomena described by Schrödinger's equation.

Quantum physics plays a rôle on small (atomic and subatomic) scales (say length scales of the order of 1 0− 9 m) and below. You can see whether an expression has a quantum-physical origin as soon as it contains Planck's constant in one of its two guises

$$\begin{aligned} h &= 6.626 \cdot 10^{-34}\,\mathrm{Js} \\ \hbar &= h/2\pi = 1.055 \cdot 10^{-34}\,\mathrm{Js}. \end{aligned} \tag{1.1}$$

Here we shall shortly review some of the standard examples for the break-down classical physics, which can be described by introducing quantum principles.

1.1: Black-body radiation
1.2: Photo-electric effect
1.3: Hydrogen Atom
1.4: Wave particle duality
1.5: Uncertainty
1.6: Tunneling

1.1: Black-body radiation

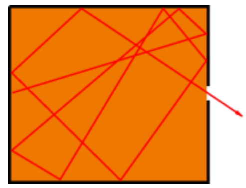

Figure 1.1.1: An oven with a small window

In the 19th century there was a lot of interest in thermodynamics. One of the areas of interest was the rather contrived idea of a black body: a material kept at a constant temperature T, and absorbing any radiation that falls on it. Thus all the light that it emits comes from its thermal energy, non of it is reflected from other sources. A very hot metal is pretty close to this behaviour, since its thermal emission is very much more intense than the environmental radiation. A slightly more realistic device is an oven with a small window, which we need to observe the emitted radiation, see Fig. 1.1.1. The laws of thermal emission have been well tested on such devices. A very different example is the so-called 3 K microwave radiation (Penzias and Wilson, Nobel price 1978). This is a remnant from the genesis of our universe, and conforms extremely well to the black-body picture, as has been shown by the recent COBE experiment, see Fig. 1.1.2

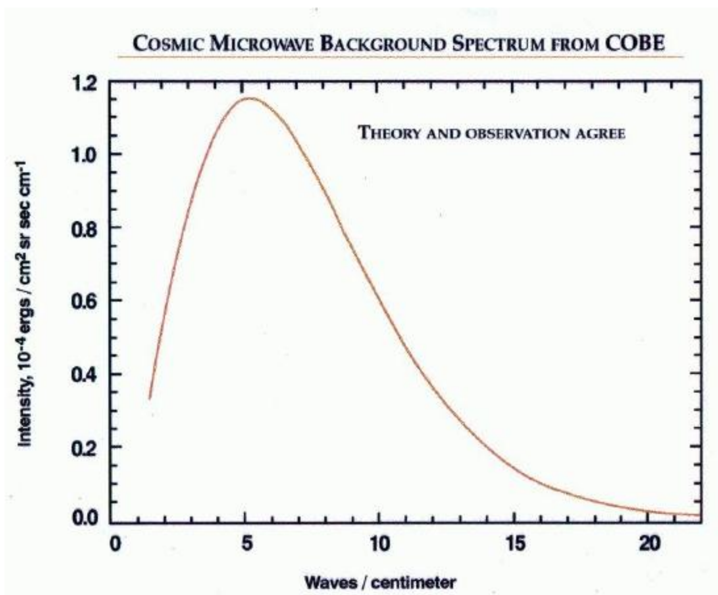

Figure 1.1.2: The black-body spectrum as measured by COBE.

The problem with the classical (Rayleigh-Jeans) law for black-body radiation is that it does suggest emission of infinite amounts of energy, which is clearly nonsensical. Actually it was for the description of this problem Planck invented Planck's constant! Planck's law for the energy density ate frequency v for temperature T is given by

$$\rho(v,T) = \frac{8\pi h}{c^3}\frac{v^3}{e^{hvkT}-1}. \tag{1.1.1}$$

The interpretation of this expression is that light consists of particles called photons, each with energy hv.
If we look at Planck's law for small frequencies $hv \ll kT$, we find an expression that contains no factors h (Taylor series expansion of exponent)

$$\rho(v,T) = \frac{8\pi v^2 kT}{c^3} \tag{1.1.2}$$

This is the Rayleigh-Jeans law as derived from classical physics. If we integrate these laws over all frequencies we find

$$E=\int_0^\infty dv \rho(v,T)=\frac{8\pi^5 k^4}{15c^3h^3}T^4 \tag{1.1.3}$$

for Planck's law, and infinity for the Rayleigh-Jeans law. The T^4 result has been experimentally confirmed, and predates Planck's law.

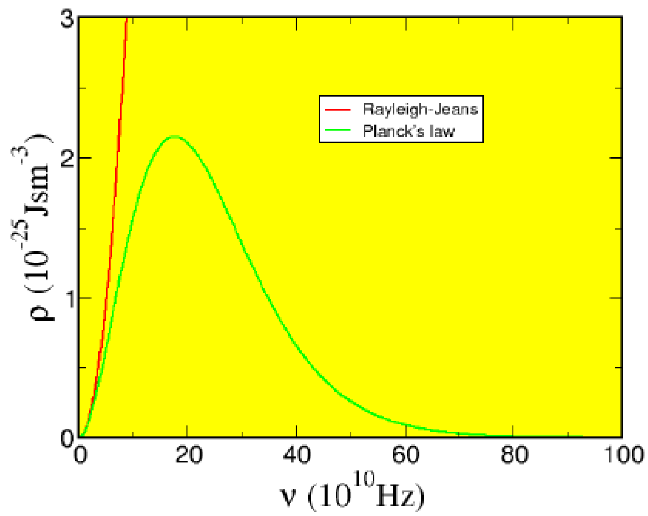

Figure 1.1.3: A comparison between the Rayleigh-Jeans and Planck's law

1.2: Photo-electric effect

When we shine a lamp on a metal surface, electrons escape the surface. This is a simple experimental fact, that can easily be demonstrated. The intreaguing point is that it takes a minimum frequency of light to remove electrons from a metal, and different metals require different minimal frequencies. Intensity plays no rôle in the threshold.

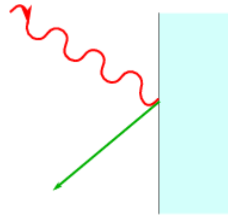

Figure 1.2.1: The photo-electric effect, where a single photon removes an electron from a metal.

Figure 1.4: The photo-electric effect, where a single photon removes an electron from a metal.

The explanation for this effect is due to Einstein (actually he got the Nobel price for this work, since his work on relativity was too controversial). Suppose once again that light is made up from photons. Assume further that the electrons are bound to the metal by an energy E_B. Since they need to absorb light to gain enough energy to escape from the metal, and it is extremely unlikely that they absorb multiple photons, the individual photons must satisfy

$$hv > E_B. \tag{1.2.1}$$

1.3: Hydrogen Atom

The classical picture of the hydrogen atom is planetary in nature: an electron moves in an Kepler orbit around the proton. The problem is that there is a force acting on the electron, and accelerated charges radiate (that is what a radio is based on). This allows the atom to loose energy in a continuous way, slowly spiraling down until the electron lies on the proton. Now experiment show that this is not the case: There are a discrete set of lines in the light emitted by hydrogen, and the electron will never loose all its energy. The first explanation for this fact came from Niels Bohr, in the so-called old quantum theory, where one assumes that motion is quantised, and only certain orbits can occur. In this model the energy of the Balmer series of Hydrogen is given by

$$E_n = -\left[\frac{e^2}{4\pi\epsilon_0}\right]^2 \frac{2\pi^2 me}{h^2}\frac{1}{n^2}. \tag{1.3.1}$$

Clearly this is of quantum origin again.

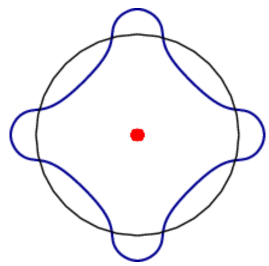

Figure 1.3.1: The Bohr model of the hydrogen atom, where a particle wave fits exactly onto a Keppler orbit.

1.4: Wave particle duality

If waves (light) can be particles (photons), can particles (electrons, etc.) be waves? de Broglie gave a positive answer to this question, and argued that for a particle with energy E and momentum p

$$E = h\nu$$
$$p = h\lambda$$

where v and λ are the frequency and the wavelength, respectively. These are exactly the relations for a photon.

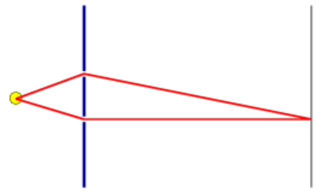

Figure 1.4.1: A double-slit experiment

One way to show that this behaviour is the correct one is to do the standard double slit experiment. For light we know that we have constructive or destructive interference if the difference in the distance traveled between two waves reaching the same point is a integer (integer plus one half) times the wavelength of the light. With particles we would normally expect them to travel through one or the other of each of the slits. If we do the experiment with a lot of particles, we actually see the well known double-slit interference.

1.5: Uncertainty

A wave of sharp frequency has to last infinitely long, and is thus completely delocalised. What does this imply for matter waves? One of the implications is the uncertainty relation between position and momentum

$$\Delta x \Delta p \gtrsim \frac{1}{2}\hbar. \tag{1.5.1}$$

This implies that the combined accuracy of a simultaneous measurement of position and momentum has a minimum. This is not important in problems on standard scales, for the following practical reason. Suppose we measure the velocity of a particle of 1 g to be $1 \pm 10^{-6}\ \mathrm{m/s}$. In that case we can measure its position no more accurate that $5 \cdot 10^{-26}\ \mathrm{m}$, a completely outrageous accuracy (remember, this is 10^{-16} times the atomic scale!)

1.6: Tunneling

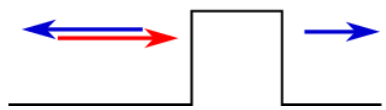

Figure 1.6.1: The tunneling phenomenon, where a particle can sometimes be found at the othee side of a barrier.

The tunneling phenomenon, where a particle can sometimes be found at the othee side of a barrier.

In classical mechanics a billiard ball bounces back when it hits the side of the billiard. In the quantum world it might actually "tunnel" through. Let me make this a little clearer. Classically a particle moving in the following potential would just be bouncing back and fourth between the walls. This can be easily seen from conservation of energy: The kinetic energy can not go negative, and the total energy is conserved. Where the potential is larger than the total energy, the particle cannot go. In quantum mechanics this is different, and particles can penetrate these classically forbidden regions, escaping from their cage.

This is a wave phenomenon, and is related to the behaviour of waves in impenetrable media: rather than oscillatory solutions, we have exponentially damped ones, that allow for some penetration. This also occurs in processes such as total reflection of light from a surface, where the tunneling wave is called "evanescent".

CHAPTER OVERVIEW

2: Concepts from Classical Mechanics

Before we discuss quantum mechanics we need to consider some concepts of classical mechanics, which are fundamental to our understanding of quantum mechanics.

- 2.1: Conservative Fields
- 2.2: Energy Function
- 2.3: Simple Example

2.1: Conservative Fields

In all our discussions I will only consider forces which are conservative, i.e., where the total energy is a constant. This excludes problems with friction. For such systems we can split the total energy in a part related to the movement of the system, called the kinetic energy (Greek κivelv=to move), and a second part called the potential energy, since it describes the potential of a system to produce kinetic energy.

An extremely important property of the potential energy is that we can derive the forces as a derivavtive of the potential energy, typically denoted by $V(r)$, as

$$F=-\left(\frac{\partial}{\partial x}V(r),\frac{\partial}{\partial y}V(r),\frac{\partial}{\partial z}V(r)\right). \tag{2.1.1}$$

A typical example of a potential energy function is the one for a particle of mass m in the earth's gravitationol field, which in the flat-earth limit is written as $V(r)=mgz$. This leads to a gravitational force

$$F=(0,0,-mg) \tag{2.1.2}$$

Of course when total energy is conserved, that doesn't define the zero of energy. The kinetic energy is easily defined to be zero when the particle is not moving, but we can add any constant to the potential energy, and the forces will not change. One typically takes $V(r)=0$ when the length of r goes to ∞.

2.2: Energy Function

Of course the kinetic energy is $\frac{1}{2}mv^2$, with $v = r$

$$E = \frac{1}{2}mv^2 + V(r) \tag{2.2.1}$$

Actually, this form is not very convenient for quantum mechanics. We rather work with the so-called momentum variable $p = mv$. Then the energy functional takes the form

$$E = \frac{1}{2}\frac{p^2}{m} + V(r) \tag{2.2.2}$$

The energy expressed in terms of p and r is often called the (classical) Hamiltonian, and will be shown to have a clear quantum analog.

2.3: Simple Example

We can define all these concepts (velocity, momentum, potential) in one dimensionas well as in three dimensions. Let us look at the example for a barrier

$$V(x)=\left[\begin{array}{ll}0 & |x|>a \\ V_0 & |x|<a\end{array}\right| \tag{2.3.1}$$

We can't find a solution for E less than 0 (no solution for v). For energy less then V_0 the particles can move left or right from the barrier, with constant velocity, but will make a hard bounce at the barrier (sign of v is not determined from energy). For energies higher than V_0 particles can move from one side to the other, but will move slower if they are above the barrier.

CHAPTER OVERVIEW

3: The Schrödinger Equation

3.1: The State of a Quantum System
3.2: Operators
3.3: Analysis of the wave equation

3.1: The State of a Quantum System

Let us first look at how we specify the state for a classical system. Once again, we use the ubiquitous billiard ball. As any player knows, there are three important aspects to its motion:

1. position,
2. velocity and
3. spin (angular momentum around its center).

Knowing these quantities we can in principle (no friction) predict its motion for all times. We have argued before that quantum mechanics involves an element of uncertainty. We cannot predict a state as in classical mechanics, we need to predict a probability. We want to be able to predict the outcome of a measurement of, say, position. Since position is a continuous variable, we cannot just deal with a discrete probability, we need a probability density, To understand this fact look at the probability that we measure x to be between X and $X+\Delta X$. If ΔX is small enough, this probability is directly proportional to the length of the interval

$$P(X<x<X+\Delta X)=P(X)\Delta X \tag{3.1.1}$$

Here $P(X)$ is called the *probability density*. The standard statement that the total probability is one translates to an integral statement,

$$\int_{-\infty}^{\infty} dx\, P(x)=1 \tag{3.1.2}$$

(Here I am lazy and use the lower case x where I have used X before; this a standard practice in QM.) Since probabilities are always positive, we require $P(x)\geq 0$.

Now let us try to look at some aspects of classical waves, and see whether they can help us to guess how to derive a probability density from a wave equation. The standard example of a classical wave is the motion of a string. Typically a string can move up and down, and the standard solution to the wave equation

$$\frac{\partial^2}{\partial x^2}A(x,t)=\frac{1}{c^2}\frac{\partial^2}{\partial x^2}A(x,t) \tag{3.1.3}$$

can be positive as well as negative. Actually the square of the wave function is a possible choice for the probability (this is proportional to the intensity for radiation). Now let us try to argue what wave equation describes the quantum analog of classical mechanics, i.e., quantum mechanics.

The starting point is a propagating wave. In standard wave problems this is given by a plane wave, i.e.,

$$\psi = A\Re\exp(i(kx-\omega t+\phi)). \tag{3.1.4}$$

This describes a wave propagating in the x direction with wavelength $\lambda=2\pi/k$, and frequency $\nu=\omega/(2\pi)$. We interpret this plane wave as a propagating beam of particles. If we define the probability as the square of the wave function, it is not very sensible to take the real part of the exponential: the probability would be an oscillating function of x for given t. If we take the complex function $A\exp(i(kx-\omega t+\phi))$, however, the probability, defined as the absolute value squared, is a constant ($|A|^2$) independent of x and t, which is very sensible for a beam of particles. Thus we conclude that the wavefunction $\psi(x,t)$ is complex, and the probability density is $|\psi(x,t)|^2$.

Using de Broglie's relation

$$p=\hbar/\lambda, \tag{3.1.5}$$

we find

$$p=\hbar k. \tag{3.1.6}$$

The other of de Broglie's relations can be used to give

$$E=h\nu=\hbar\omega. \tag{3.1.7}$$

One of the important goals of quantum mechanics is to generalize classical mechanics. We shall attempt to generalize the relation between momenta and energy,

$$E = 12mv^2 = \frac{p^2}{2m} \tag{3.1.8}$$

to the quantum realm. Notice that

$$p\psi(x,t) = \hbar k\psi(x,t) = \frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x,t) \tag{3.1.9}$$

$$E\psi(x,t) = \hbar\omega\psi(x,t) = \frac{\hbar i\partial}{\partial t}\psi(x,t) \tag{3.1.10}$$

Using this we can guess a wave equation of the form

$$\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x^2}\right)\psi(x,t) = \frac{\hbar i\partial}{\partial t}\psi(x,t). \tag{3.1.11}$$

Actually using the definition of energy when the problem includes a potential,

$$E = \frac{1}{2}mv^2 + V(x) = \frac{p^2}{2m} + V(x) \tag{3.1.12}$$

(when expressed in momenta, this quantity is usually called a ”Hamiltonian”) we find the time-dependent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t) = \frac{\hbar i\partial}{\partial t}\psi(x,t). \tag{3.1.13}$$

We shall only spend limited time on this equation. Initially we are interested in the time-independent Schrödinger equation, where the probability $|\psi(x,t)|^2$ is independent of time. In order to reach this simplification, we find that $\psi(x,t)$ must have the form

$$\psi(x,t) = \phi(x)e^{-iEt/\hbar}. \tag{3.1.14}$$

If we substitute this in the time-dependent equation, we get (using the product rule for differentiation)

$$-e^{-iEt/\hbar}\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x) + e^{-iEt/\hbar}V(x)\phi(x) = Ee^{-iEt/\hbar}\phi(x). \tag{3.1.15}$$

Taking away the common factor $e^{-iEt/\hbar}$ we have an equation for ϕ that no longer contains time, the time-independent Schrödinger equation

$$\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x) + V(x)\phi(x) = E\phi(x). \tag{3.1.16}$$

The corresponding solution to the time-dependent equation is the standing wave (Equation 3.1.14).

3.2: Operators

Notice that in deriving the wave equation we replaced the number p or k by a differential acting on the wavefunction. The energy (or rather the Hamiltonian) was replaced by an ”operator”, which when multiplied with the wave function gives a combination of derivatives of the wavefunction and function multiplying the wavefunction, symbolically written as

$$\hat{H}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t). \tag{3.2.1}$$

This appearance of operators (often denoted by hats) where we were used to see numbers is one of the key features of quantum mechanics.

3.3: Analysis of the wave equation

One of the important aspects of the Schrödinger equation(s) is its linearity. For the time independent Schrödinger equation, which is usually called an eigenvalue problem, the only consequence we shall need here, is that if $\phi_i(x)$ is an eigenfunction (a solution for E_i) of the Schrödinger equation, so is $A\phi_i(x)$. This is useful in defining a probability, since we would like

$$\int_{-\infty}^{\infty} |A|^2 |\phi_i(x)|^2 \, dx = 1 \tag{3.3.1}$$

Given $\phi_i(x)$ we can thus use this freedom to ”normalize” the wavefunction! (If the integral over $|\phi(x)|^2$ is finite, i.e., if $\phi(x)$ is “normalizable”; not all functions are).

Example 3.3.1

As an example suppose that we have a Hamiltonian that has the function $\psi_i(x) = e^{-x^2/2}$ as eigenfunction. This function is not normalized since

$$\int_{-\infty}^{\infty} |\phi_i(x)|^2 \, dx = \sqrt{\pi}. \tag{3.3.2}$$

The normalized form of this function is

$$\frac{1}{\pi^{1/4}} e^{-x^2/2}. \tag{3.3.3}$$

We need to know a bit more about the structure of the solution of the Schrödinger equation – boundary conditions and such. Here I shall postulate the boundary conditions, without any derivation.

1. $\phi(x)$ is a continuous function, and is single valued.
2. $$\int_{-\infty}^{\infty} |\phi(x)|^2 \, dx \tag{3.3.4}$$

   must be finite, so that

   $$P(x) = |\phi(x)|^2 \int_{-\infty}^{\infty} |\psi(x)|^2 \, dx \tag{3.3.5}$$

   is a probability density.
3. $\frac{\partial \phi(x)}{\partial x}$ is continuous except where $V(x)$ has an infinite discontinuity.

CHAPTER OVERVIEW

4: Bound states of the Square Well

4.1: Bound States
4.2: B_2= 0
4.3: A_2= 0
4.4: Some Consequences
4.5: Lessons from the square well
4.6: A physical system (approximately) described by a square well

Thumbnail: The barriers outside a one-dimensional box have infinitely large potential, while the interior of the box has a constant, zero potential. (CC-BY 4.0; OpenStax).

4.1: Bound States

One of the simplest potentials to study the properties of is the so-called *square well potential* (Figure 4.1.1),

$$V(x) = \begin{cases} 0 & |x| > a \\ -V_0 & |x| < a \end{cases}$$

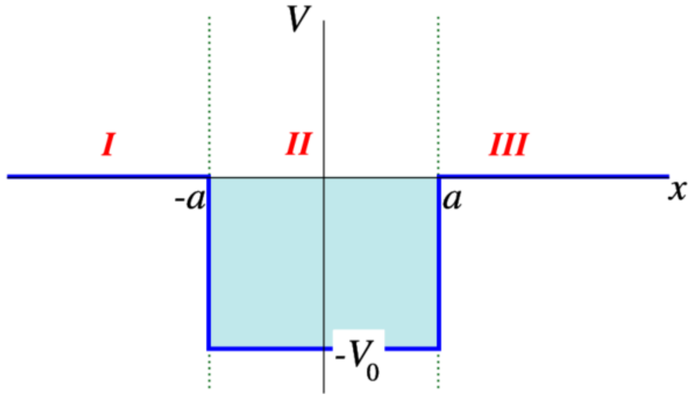

Figure* 4.1.1*: The square well potential

We define three areas, from left to right in Figure 4.1.1: I, II and III. In areas I and III we have the Schrödinger equation for a free particle

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x) \tag{4.1.1}$$

whereas in area II we have the equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = (E+V_0)\psi(x) \tag{4.1.2}$$

Solution to a few Ordinary Differential Equations

In this class we shall quite often encounter the ordinary differential equations

$$\frac{d^2}{dx^2}f(x) = -\alpha^2 f(x) \tag{4.1.3}$$

which has as solution

$$f(x) = A_1\cos(\alpha x) + B_1\sin(\alpha x) \tag{4.1.4}$$

$$= C_1 e^{i\alpha x} + D_1 e^{-i\alpha x}, \tag{4.1.5}$$

and

$$\frac{d^2}{dx^2}g(x) = +\alpha^2 g(x) \tag{4.1.6}$$

which has as solution

$$g(x) = A_2\cosh(\alpha x) + B_2\sinh(\alpha x) \tag{4.1.7}$$

$$= C_2 e^{\alpha x} + D_2 e^{-\alpha x}. \tag{4.1.8}$$

Case 1: E> 0

Let us first look at $E > 0$. In that case the equation in regions I and III can be written as

$$\frac{d^2}{dx^2}\psi(x) = -\frac{2m}{\hbar^2}E\psi(x) = -k^2\psi(x), \tag{4.1.9}$$

where

$$k = \sqrt{\frac{2m}{\hbar^2} E} \tag{4.1.10}$$

The solution to this equation is a sum of sines and cosines of kx, which cannot be normalized: Write

$$\psi_{III}(x) = A\cos(kx) + B\sin(kx) \tag{4.1.11}$$

where (A and B can be complex) and calculate the part of the norm originating in region III,

$$\int_a^\infty |\psi(x)|^2 dx = \int_a^\infty |A|^2 \cos^2 kx + |B|^2 \sin^2 kx + 2\Re(AB^*)\sin(kx)\cos(kx)dx \tag{4.1.12}$$

$$= \lim_{N\to\infty} N \int_a^{2\pi/k} |A|^2 \cos^2(kx) + |B|^2 \sin^2(kx) \tag{4.1.13}$$

$$= \lim_{N\to\infty} N \left(\frac{|A|^2}{2} + \frac{|B|^2}{2} \right) = \infty. \tag{4.1.14}$$

We also find that the energy cannot be less than $-V_0$, since we cannot construct a solution for that value of the energy. We thus restrict ourselves to $-V_0 < E < 0$. We write

$$E = -\frac{\hbar^2}{k^2 2m} \tag{4.1.15}$$

and

$$E + V_0 = \frac{\hbar^2 \kappa^2}{2m}. \tag{4.1.16}$$

The solutions in the areas I and III are of the form ($i = 1, 3$)

$$\psi(x) = A_i e^{kx} + B_i e^{-kx}. \tag{4.1.17}$$

In region II we have the oscillatory solution

$$\psi(x) = A_2\cos(\kappa x) + B_2\sin(\kappa x). \tag{4.1.18}$$

Now we have to impose the conditions on the wave functions we have discussed before, continuity of ψ and its derivatives. Actually we also have to impose normalisability, which means that $B_1 = A_3 = 0$ (exponentially growing functions can not be normalized). As we shall see we only have solutions at certain energies. Continuity implies that

$$A_1 e^{-ka} + B_1 e^{ka} = A_2\cos(\kappa a) - B_2\sin(\kappa a) \tag{4.1.19}$$

$$A_3 e^{ka} + B_3 e^{-ka} = A_2\cos(\kappa a) + B_2\sin(\kappa a) \tag{4.1.20}$$

$$kA_1 e^{ka} - kB_1 e^{ka} = \kappa A_2\sin(\kappa a) + \kappa B_2\cos(\kappa a) \tag{4.1.21}$$

$$kA_3 e^{ka} - kB_3 e^{-ka} = -\kappa A_2\sin(\kappa a) + \kappa B_2\cos(\kappa a) \tag{4.1.22}$$

Tactical Approach

We wish to find a relation between k and κ (why?), removing as maby of the constants A and B. The trick is to first find an equation that only contains A_2 and B_2. To this end we take the ratio of Equations 4.1.19 and 4.1.21 and then the ratio of Equations 4.1.20 and 4.1.22:

$$k = \frac{\kappa[A_2\sin(\kappa a) + B_2\cos(\kappa a)]}{A_2\cos(\kappa a) - B_2\sin(\kappa a)} \tag{4.1.23}$$

$$k = \frac{\kappa[A_2\sin(\kappa a) - B_2\cos(\kappa a)]}{A_2\cos(\kappa a) + B_2\sin(\kappa a)} \tag{4.1.24}$$

We can combine Equations 4.1.23 and \ref4.15B} to a single one by equating the right-hand sides. After deleting the common factor κ, and multiplying with the denominators we find

$$[A_2\cos(\kappa a)+B_2\sin(\kappa a)][A_2\sin(\kappa a)-B_2\cos(\kappa a)]=[A_2\sin(\kappa a)+B_2\cos(\kappa a)][A_2\cos(\kappa a)-B_2\sin(\kappa a)], \tag{4.1.25}$$

which simplifies to

$$A_2B_2=0 \tag{4.1.26}$$

We thus have two families of solutions, those characterized by $B_2=0$ and those that have $A_2=0$.

4.2: B_2= 0

In the first case we read off that $A_1 = B_3$, and we find that k and κ are related by

$$ka = \kappa a \tan \kappa a. \tag{4.2.1}$$

This equation can be solved graphically. Use

$$k = \sqrt{-\kappa^2 + \kappa_0^2} \tag{4.2.2}$$

with $\kappa_0^2 = \frac{2m}{\hbar^2} V_0$, and find that there is always at least one solution of this kind, no matter how small V_0!

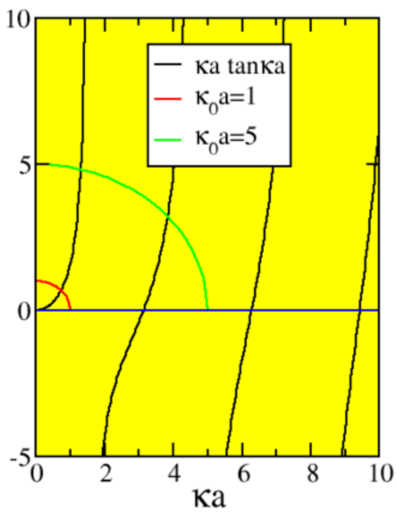

Figure 4.2.1: *The graphical solution for the even states of the square well.*

In the middle region all these solutions behave like sines, and you will be asked to show that the solutions are invariant when x goes to − x. (We say that these functions are even.)

4.3: A₂= 0

In this case $A_1 = -B_3$, and the relation between k and κ is modified to

$$ka = -\kappa a \cot \kappa a. \tag{4.3.1}$$

From the graphical solution, in Figure $4.3.1$ we see that this type of solution only occurs for $\kappa_0 a$ greater than $\pi / 2$.

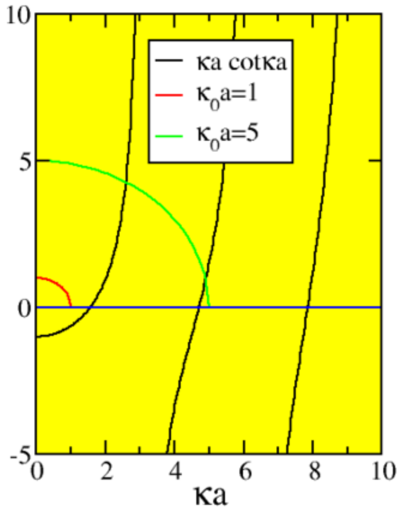

Figure $\mathbf{4.3.1}$ *: The graphical solution for the odd states of the square well.*

In the middle region all these solutions behave like sines, and you will be asked to show that the solutions turn into minus themselves when x goes to $-x$. (We say that these functions are odd.)

4.4: Some Consequences

There are a few good reasons why the dependence in the solution is on ka, κa and $\kappa_0 a$: These are all dimensionless numbers, and mathematical relations can *never* depend on parameters that have a dimension! For the case of the even solutions, the ones with $B_2 = 0$, we find that the number of bound states is determined by how many times we can fit 2π into $\kappa_0 a$. Since κ_0 is proportional to (the square root) of V_0, we find that increasing V_0 increases the number bound states, and the same happens when we increase the width a. Rewriting κ_0 a slightly we find that the governing parameter is

$$\sqrt{\frac{2m}{\hbar^2} V_0 a^2} \tag{4.4.1}$$

so that a factor of two change in a is the same as a factor four change in V_0.

If we put the two sets of solutions on top of one another we see that after every even solution we get an odd solution, and vice versa. There is always at least one solution (the lowest even one), but the first odd solution only occurs when $\kappa_0 a = \pi$.

4.5: Lessons from the square well

The computer demonstration showed the following features:

1. If we drop the requirement of normalisability, we have a solution to the time-indepndent Schrödinger Equation at every energy. Only at a few discrete values of the energy do we have normalisable states.
2. The energy of the lowest state is always higher than the depth of the well (uncertainty principle).
3. Effect of depth and width of well. Making the well deeper gives more eigenfunctions, and decreases the extent of the tail in the classically forbidden region.
4. Wave functions are oscillatory in classically allowed, exponentially decaying in classically forbidden region.
5. The lowest state has no zeroes, the second one has one, etc. Normally we say that the n th state has $n-1$"nodes".
6. Eigenstates (normalisable solutions) for different eigenvalues (energies) are orthogonal.

4.6: A physical system (approximately) described by a square well

After all this tedious algebra, let us look at a possible physical realization of such a system. In order to do that, I shall have to talk a little bit about semi-conductors. A semiconductor is a quantum system where the so-called valence electrons completely fill a valence band, and are separated by a gap from a set of free states in a conduction band. These can both be thought of a continuous set of quantum states. The energy difference between the valence and conduction bands is different for different semi-conductors. This can be used in so-called *quantum-well structures*, where we sandwich a thin layer of, e.g., GaAs between very thick layers of GaAlAs (Figure $4.6.1$).

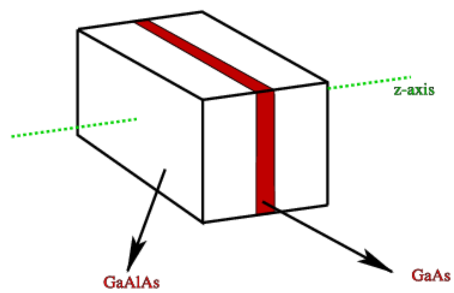

Figure* $4.6.1$*: *A schematic representation of a quantum well*

Since the gap energy is a lot smaller for GaAs than for GaAlAs, we get the effect of a small square well (in both valence and conduction bands). The fact that we can have a few occupied additional levels in the valence, and a few empty levels in the conduction band can be measured.

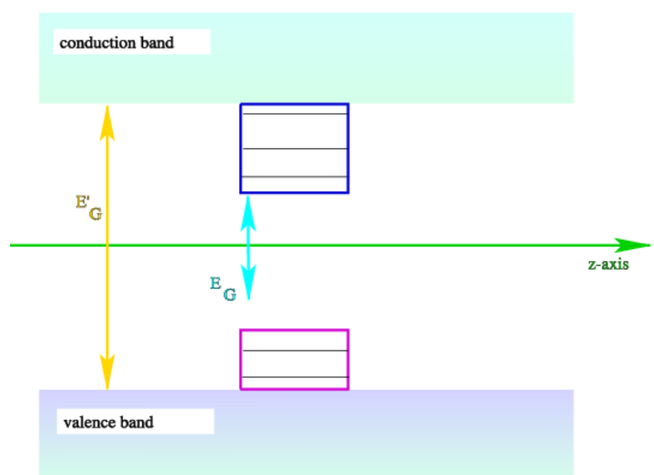

Figure* $4.6.2$*:

The best way to do this, is to shine light on these systems, and see for which frequency we can create a transition (just like in atoms).

CHAPTER OVERVIEW

5: Infinite Wells

5.1: Zero of Energy is Arbitrary
5.2: Solution

5.1: Zero of Energy is Arbitrary

The normal definition of a potential energy is somewhat arbitrary. Consider where a potential comes from: It appears when the total energy (potential plus kinetic) is constant. But if something is constant, we can add a number to it, and it is still constant! Thus whether we define the gravitational potential at the surface of the earth to be 0 or 100 J does not matter. Only differences in potential energies play a rôle. It is customary to define the potential “far away”, as $|x| \rightarrow \infty$ to be zero. That is a very workable definition, except in one case: if we take a square well and make it deeper and deeper, the energy of the lowest state decreases with the bottom of the well. As the well depth goes to infinity, the energy of the lowest bound state reaches $-\infty$, and so does the second, third etc. state. It makes much more physical sense to define the bottom of the well to have zero energy, and the potential outside to have value V_0, which goes to infinity.

5.2: Solution

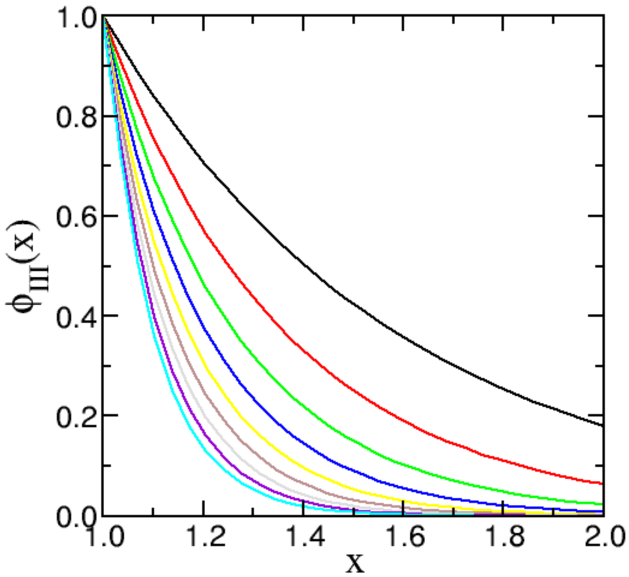

Figure 5.1: The change in the wave function in region III, for the lowest state, as we increase the depth of the potential well. We have used a= 1 0− 1 0 m, and k 0 a= 2, 3, 4, 5, 6, 7, 8, 9 and 1 0.

As stated before the continuity arguments for the derivative of the wave function do not apply for an infinite jump in the potential energy. This is easy to understand as we look at the behaviour of a low energy solution in one of the two outside regions (I or III). In this case the wave function can be approximated as

$$e^{\pm kr}, \quad k = \sqrt{\frac{2m}{\hbar^2} V_0}, \tag{5.2.1}$$

which decreases to zero faster and faster as V 0 becomes larger and larger. In the end the wave function can no longer penetrate the region of infinite potential energy. Continuity of the wave function now implies that ϕ(a)=ϕ(− a)= 0.

Defining

$$\kappa = \sqrt{\frac{2m}{\hbar^2} E}, \tag{5.2.2}$$

we find that there are two types of solutions that satisfy the boundary condition:

$$\phi_{2n+1}(x) = \cos(\kappa_{2n+1} x), \phi_{2n}(x) = \sin(\kappa_{2n} x). \tag{5.2.3}$$

Here

$$\kappa_l = \frac{\pi l}{2a}. \tag{5.2.4}$$

We thus have a series of eigen states $\phi_l(x), l = 1, \cdots, \infty$. The energies are

$$E_l = \frac{\hbar^2 \pi^2 l^2}{8a^2} \tag{5.2.5}$$

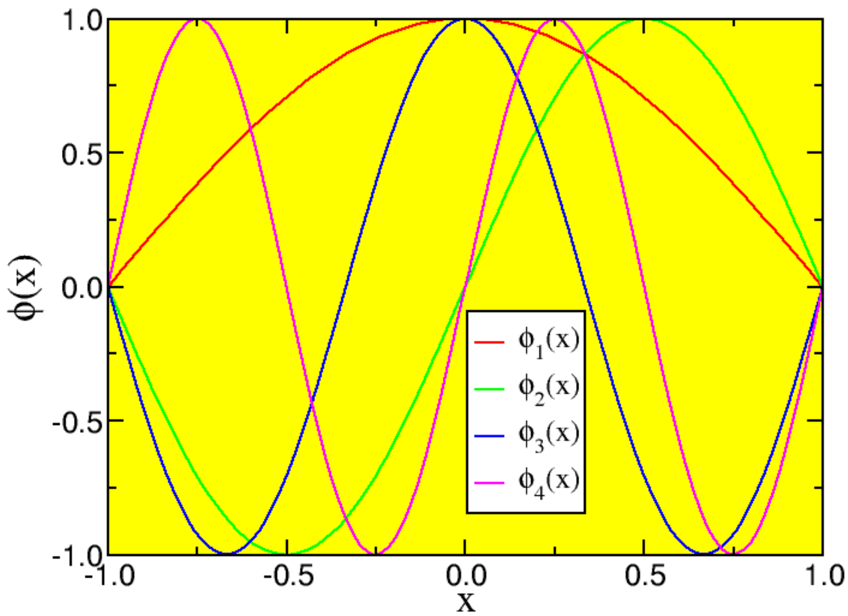

Figure 5.2: A few wave functions of the infinite square well.

These wave functions are very good to illustrate the idea of normalisation. Let me look at the normalisation of the ground state (the lowest state), which is

We need to require

$$\int_{-\infty}^{\infty} |\phi_0(x)|^2 dx = 1 \tag{5.2.6}$$

where we need to consider the absolute value since A_1 can be complex. We only have to integrate from $-a$ to a, since the rest of the integral is zero, and we have

$$\begin{aligned} \int_{-\infty}^{\infty} |\phi_0(x)|^2 dx \\ &= |A|^2 \int_{-a}^{a} \cos^2\left[\frac{\pi x}{2a}\right] dx \\ &= |A|^2 \frac{2a}{\pi} \int_{-\pi 2}^{\pi 2} \cos^2[y] dy \\ &= |A|^2 \frac{2a}{\pi} \int_{-\pi 2}^{\pi 2} \frac{1}{2}(1+\cos[2y[]) dy \\ &= |A|^2 \frac{2a}{\pi} \pi \end{aligned}$$

Here we have changed variables from x to $y = \frac{\pi x}{2a}$. We thus conclude that the choice

$$A = \sqrt{\frac{1}{2a}} \tag{5.2.7}$$

leads to a normalised wave function.

CHAPTER OVERVIEW

6: Scattering from Potential Steps and Square Barriers

6.1: Non-normalizable Wavefunctions
6.2: Potential step
6.3: Square Barrier

6.1: Non-normalizable Wavefunctions

I have argued that solutions to the time-independent Schrödinger equation must be normalized, in order to have a the total probability for finding a particle of one. This makes sense if we think about describing a single Hydrogen atom, where only a single electron can be found. But if we use an accelerator to send a beam of electrons at a metal surface, this is no longer a requirement: What we wish to describe is the flux of electrons, the number of electrons coming through a given volume element in a given time.

Let me first consider solutions to the "free" Schrödinger equation, i.e., without potential, as discussed before. They take the form

$$\phi(x) = Ae^{ikx} + Be^{-ikx}. \tag{6.1.1}$$

Let us investigate the two functions. Remembering that

$$\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x} \tag{6.1.2}$$

we find that $\phi(x)$ (Equation 6.1.1) represents the sum of two states, one with momentum $\hbar k$, and the other with momentum $-\hbar k$. The first one describes a beam of particles going to the right, and the other term a beam of particles traveling to the left. A standing wavefunction associated with a bound state is when $A = B$ (Figure $6.1.1$).

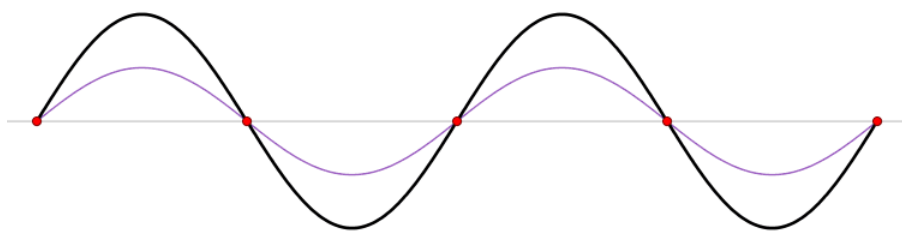

***Figure 6.1.1**: A standing wave. The blue wave moves toward right while the red wave moves in the opposite direction. The combined wave (black) does not propagate*

Let me concentrate on the first term, that describes a beam of particles going to the right. We need to define a probability current density. Since current is the number of particles times their velocity, a sensible definition is the probability density times the velocity,

$$|\phi(x)|^2 \frac{\hbar k}{m} = |A|^2 \frac{\hbar k}{m}. \tag{6.1.3}$$

This concept only makes sense for states that are not bound, and thus behave totally different from those I discussed previously.

6.2: Potential step

Consider a potential step

$$V(x)=\begin{cases} V_0 & x<a \\ V_1 & x>a \end{cases}$$

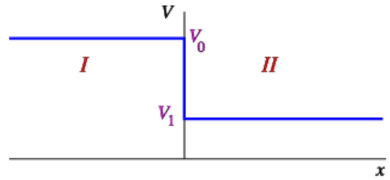

Figure* $6.2.1$*: The step potential discussed in the text

Let me define

$$k_0=\sqrt{\frac{2m}{\hbar^2}(E-V_0)}, \tag{6.2.1}$$

$$k_1=\sqrt{\frac{2m}{\hbar^2}(E-V_1)}. \tag{6.2.2}$$

I assume a beam of particles comes in from the left,

$$\phi(x)=A_0 e^{ik_0x} \text{ for } x<0. \tag{6.2.3}$$

At the potential step the particles either get reflected back to region I, or are transmitted to region II. There can thus only be a wave moving to the right in region II, but in region I we have both the *incoming* and a *reflected* wave,

$$\phi_I(x)=A0e^{ik_0x}+B_0e^{-ik_0x}, \tag{6.2.4}$$

$$\phi_{II}(x)=A_1e^{ik_1x}. \tag{6.2.5}$$

We define a *transmission (T)* and *reflection (R) coefficient* as the ratio of currents between reflected or transmitted wave and the incoming wave, where we have canceled a common factor

$$R=\frac{|B_0|^2}{|A_0|^2} \tag{6.2.6}$$

$$T=\frac{k_1|A_1|^2}{k_0|A_0|^2}. \tag{6.2.7}$$

Even though we have given up normalisability, we still have the two continuity conditions. At $x=0$ these imply, using continuity of ϕ and $\frac{d}{dx}\phi$,

$$A_0+B_0=A_1, \tag{6.2.8}$$

$$ik_0(A_0-B_0)=ik_1A_1. \tag{6.2.9}$$

We thus find

$$A_1=\frac{2k_0}{k_0+k_1A_0} \tag{6.2.10}$$

$$B_0=\frac{k_0-k_1}{k_0+k_1A_0}, \tag{6.2.11}$$

and the reflection and transmission coefficients can thus be expressed as

$$R=\left(\frac{k_0-k_1}{k_0+k_1}\right)^2, \tag{6.2.12}$$

$$T=\frac{4k_1k_0}{(k_0+k_1)^2}. \tag{6.2.13}$$

Notice that $R+T=1$!

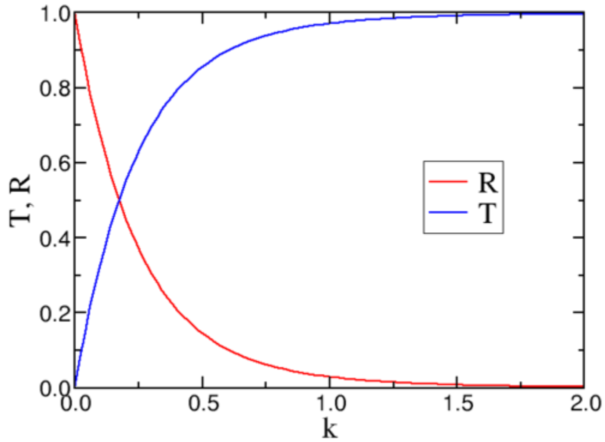

***Figure $6.2.2$:** The transmission and reflection coefficients for a square barrier.*

In Figure $6.2.2$ we have plotted the behaviour of the transmission and reflection of a beam of Hydrogen atoms impinging on a barrier of height 2 meV.

6.3: Square Barrier

A slightly more involved example is the square potential barrier, an inverted square well, see Figure $6.3.1$.

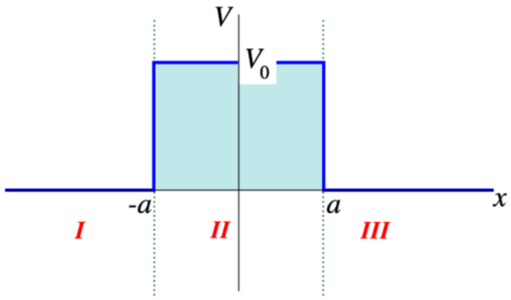

Figure $\mathbf{6.3.1}$***:*** *The square barrier.*

We are interested in the case that the energy is below the barrier height, $0 < E < V_0$. If we once again assume an incoming beam of particles from the right, it is clear that the solutions in the three regions are

$$\phi_I(x) = A_1 e^{ikx} + B_1 e^{-ikx} \tag{6.3.1}$$

$$\phi_{II}(x) = A_2 \cosh(\kappa x) + B_2 \sinh(\kappa x) \tag{6.3.2}$$

$$\phi_{III}(x) = A_3 e^{ikx}. \tag{6.3.3}$$

Here

$$k = \sqrt{\frac{2m}{\hbar^2} E} \tag{6.3.4}$$

and

$$\kappa = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}. \tag{6.3.5}$$

Matching ϕ_I and ϕ_{II} at $x = -a$ and ϕ_{II} and ϕ_{III} at $x = a$ gives (use $\sinh(-x) = -\sinh x$ and $\cosh(-x) = \cosh x$).

$$A_1 e^{-ika} + B_1 e^{ika} = A_2 \cosh \kappa a - B_2 \sinh \kappa a \tag{6.3.6}$$

$$ik(A_1 e^{-ika} - B_1 e^{ika}) = \kappa(-A_2 \sinh \kappa a + B_2 \cosh \kappa a) \tag{6.3.7}$$

$$A_3 e^{ika} = A_2 \cosh \kappa a + B_2 \sinh \kappa a \tag{6.3.8}$$

$$ik(A_3 e^{ika}) = \kappa(A_2 \sinh \kappa a + B_2 \cosh \kappa a) \tag{6.3.9}$$

These are four equations with five unknowns. We can thus express for of the unknown quantities in one other. Let us choose that one to be A_1, since that describes the intensity of the incoming beam. We are not interested in A_2 and B_2, which describe the wave function in the middle. We can combine the equation above so that they either have A_2 or B_2 on the right hand side, which allows us to eliminate these two variables, leading to two equations with the three interesting unknowns A_3, B_1 and A_1. These can then be solved for A_3 and B_1 in terms of A_1:

The way we proceed is to add Equations 6.3.6 and 6.3.8, subtract Equations 6.3.7 from 6.3.9, subtract 6.3.8 from 6.3.6, and add 6.3.7 and 6.3.9. We find

$$A_1 e^{-ika} + B_1 e^{ika} + A_3 e^{ika} = 2A_2 \cosh \kappa a \tag{6.3.10}$$

$$ik(-A_1 e^{-ika} + B_1 e^{ika} + A_3 e^{ika}) = 2\kappa A_2 \sinh \kappa a \tag{6.3.11}$$

$$A_1 e^{-ika} + B_1 e^{ika} - A_3 e^{ika} = -2B_2 \sinh \kappa a \tag{6.3.12}$$

$$ik(A_1 e^{-ika} - B_1 e^{ika} + A_3 e^{ika}) = 2\kappa B_2 \cosh \kappa a \tag{6.3.13}$$

We now take the ratio of equations 6.3.10 and 6.3.11 and of 6.3.12 and 6.3.13, and find (i.e., we take ratios of left- and right hand sides, and equate those)

$$\frac{A_1 e^{-ika} + B_1 e^{ika} + A_3 e^{ika}}{ik(-A_1 e^{-ika} + B_1 e^{ika} + A_3 e^{ika})} = \frac{1}{\kappa \tanh \kappa a} \tag{6.3.14}$$

$$\frac{A_1 e^{-ika} + B_1 e^{ika} - A_3 e^{ika}}{ik(-A_1 e^{-ika} + B_1 e^{ika} + A_3 e^{ika})} = -\frac{\tanh \kappa a}{\kappa} \tag{6.3.15}$$

These equations can be rewritten as (multiplying out the denominators, and collecting terms with A_1, B_3 and A_3)

$$A_1 e^{-ika}(\kappa \tanh \kappa a + ik) + B_1 e^{ika}(\kappa \tanh \kappa a - ik) + A_3 e^{ika}(\kappa \tanh \kappa a - ik) = 0 \tag{6.3.16}$$

$$A_1 e^{-ika}(\kappa - ik \tanh \kappa a) + B_1 e^{ika}(\kappa + ik \tanh \kappa a) + A_3 e^{ika}(-\kappa + ik \tanh \kappa a) = 0 \tag{6.3.17}$$

Now eliminate A_3, add Equations 6.3.16 and 6.3.17 to find

$$\begin{aligned}&A_1e^{-ika}[(\kappa-ik\tanh\kappa a)(\kappa\tanh\kappa a+ik)+\\&(\kappa\tanh\kappa a-ik)(\kappa-ik\tanh\kappa a)]\\&+B_1e^{ika}[(\kappa-ik\tanh\kappa a)(\kappa\tanh\kappa a-ik)+\\&(\kappa\tanh\kappa a-ik)(\kappa+ik\tanh\kappa a)]=0\end{aligned} \tag{6.3.18}$$

Thus we find

$$B_1=-A_1e^{-2ika}\frac{\tanh\kappa a(k^2+\kappa^2)}{(\kappa-ik\tanh\kappa a)(\kappa\tanh\kappa a-ik)} \tag{6.3.19}$$

and we find, after using some of the angle-doubling formulas for hyperbolic functions, that the absolute value squared, i.e., the reflection coefficient, is

$$R=\frac{\sinh^2 2\kappa a\left(\kappa^2+k^2\right)^2}{4\kappa^2k^2+\left(\kappa^2-k^2\right)^2\sinh^2 2\kappa a} \tag{6.3.20}$$

In a similar way we can express A_3 in terms of A_1 (add Equations 6.3.16 and Equation 6.3.17, or use

$$T=1-R! \tag{6.3.21}$$

Alternative approach

The equation can be given in matrix form as

$$\begin{pmatrix} e^{-ika} & e^{ika} \\ ike^{-ika} & -ike^{ika}\end{pmatrix}\begin{pmatrix}A_1\\B_1\end{pmatrix}\begin{pmatrix} cosh\,\kappa a & -sinh\,\kappa a \\ -\kappa\,sinh\,\kappa a & \kappa\,cosh\,\kappa a\end{pmatrix}\begin{pmatrix}A_2\\B_2\end{pmatrix}\begin{pmatrix} e^{ika} & e^{-ika} \\ ike^{-ika} & -ike^{ika}\end{pmatrix}\begin{pmatrix} cosh\,\kappa a & sinh\,\kappa a \\ \kappa\,sinh\,\kappa a & \kappa\,cosh\,\kappa a\end{pmatrix}\begin{pmatrix}A_2\\B_2\end{pmatrix} \tag{6.3.22}$$

Question: Can you invert the matrices and find the same answer as before?

Example 6.3.1: Hydrogen Atom Scattering

We now consider a particle of the mass of a hydrogen atom, $m=1.67\times10^{-27}kg$, and use a barrier of height 4 meV and of width $10^{-10}m$. The picture for reflection and transmission coefficients can seen in Figure 6.3.1; $left$. We have also evaluated R and T for energies larger than the height of the barrier (the evaluation is straightforward).

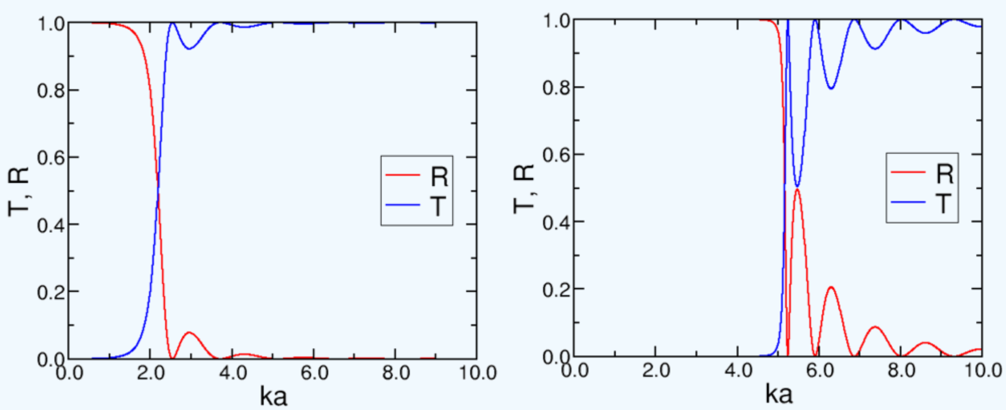

***Figure 6.3.2**: The reflection and transmission coefficients for a square barrier of height 4 meV (left) amd 50 meV (right) and width 1 0− 1 0 m.*

If we heighten the barrier to 50 meV, we find a slightly different picture (Figure 6.3.1; $right$).

Notice the oscillations (resonances) in the reflection. These are related to an integer number of oscillations fitting exactly in the width of the barrier, $\sin^2\kappa a=0$.

CHAPTER OVERVIEW

7: The Harmonic Oscillator

7.1: Prelude to Harmonic Oscillators

7.2: Dimensionless Coordinates

7.3: Behaviour for large |y|

7.4: Taylor Series Solution

7.5: A Few Solutions

7.6: Quantum-Classical Correspondence

7.1: Prelude to Harmonic Oscillators

You may be familiar with several examples of harmonic oscillators form classical mechanics, such as particles on a spring or the pendulum for small deviation from equilibrium, etc.

Figure 7.1.1: The mass on the spring and its equilibrium position

Let me look at the characteristics of one such example, a particle of mass m on a spring. When the particle moves a distance x away from the equilibrium position x_0, there will be a restoring force $-kx$ pushing the particle back ($x > 0$ right of equilibrium, and $x < 0$ on the left). This can be derived from a potential

$$V(x) = \frac{1}{2} k x^2. \tag{7.1.1}$$

Actually we shall write $k = m\omega^2$. The equation of motion

$$m\bar{x} = -m\omega^2 x \tag{7.1.2}$$

has the solution

$$x(t) = A\cos(\omega t) + B\sin(\omega t). \tag{7.1.3}$$

7.2: Dimensionless Coordinates

The classical energy (Hamiltonian) is

$$E=\frac{1}{2} m \bar{x}^2+\frac{1}{2} m \omega^2 x^2=\frac{1}{2 m} p^2+\frac{1}{2} m \omega^2 x^2 \tag{7.2.1}$$

The quantum Hamiltonian operator is thus

$$\widehat{H}=\frac{1}{2 m} \frac{1}{2 m} \hat{p}^2+\frac{1}{2} m \omega^2 x^2=-\frac{\hbar^2}{2 m} \frac{d^2}{d x^2}+\frac{1}{2} m \omega^2 x^2. \tag{7.2.2}$$

And we thus have to solve Schrödinger's equation

$$-\frac{\hbar^2}{2 m} \frac{d^2}{d x^2} \phi(x)+\frac{1}{2} m \omega^2 x^2 \phi(x)=E \phi(x) \tag{7.2.3}$$

In order to treat this equation it is better to remove all the physical constants, and go over to dimensionless coordinates

$$y=\sqrt{\frac{m \omega}{\hbar}} x, \quad \epsilon=\frac{E}{\hbar \omega}. \tag{7.2.4}$$

When we substitute these new variables into the Schrödinger equation we get, using

$$\frac{d}{d x} f(y)=\frac{d y}{d x} \frac{d}{d y} f(y)=\sqrt{\frac{m \omega}{\hbar}} \frac{d}{d y} f(y), \tag{7.2.5}$$

that $(\phi(x)=u(y))$

$$-\frac{\hbar^2}{2 m} \frac{m \omega}{\hbar} \frac{d^2}{d y^2} u(y)+\frac{1}{2} m \omega^2 \frac{\hbar}{m \omega} y^2 u(y)=\epsilon \hbar \omega u(y) \tag{7.2.6}$$

Cancelling the common factor

$$\hbar \omega \text{ we find } \\ \frac{d^2}{d y^2} u(y)+\left(2 \epsilon-y^2\right) u(y)=0 \tag{7.2.7}$$

7.3: Behaviour for large |y|

Before solving the equation we are going to see how the solutions behave at large $|y|$ (and also large $|x|$, since these variable are proportional!). For $|y|$ very large, whatever the value of ϵ, $\epsilon \ll y^2$, and thus we have to solve

$$\frac{d^2u}{dy^2} = y^2 u(y) \tag{7.3.1}$$

This has two type of solutions, one proportional to $e^{y^2/2}$ and one to $e^{-y^2/2}$. We reject the first one as being not normalisable.
Question: Check that these are the solutions. Why doesn't it matter that they don't exactly solve the equations?
Substitute $u(y) = H(y)e^{-y^2/2}$. We find

$$\frac{d^2u}{dy^2} = \left[H''(y) - 2yH'(y) + y^2H(y)]e^{-y^2/2}\right]. \tag{7.3.2}$$

so we can obtain a differential equation for $H(y)$ in the form

$$H''(y) - 2yH'(y) + (2\epsilon - 1)H(y) = 0. \tag{7.3.3}$$

This equation will be solved by a substitution and infinite series (Taylor series!), and showing that it will have to terminates somewhere, i.e., $H(y)$ is a polynomial!

7.4: Taylor Series Solution

Let us substitute a Taylor series for $H(y)$,

$$H(y)=\sum_{p=0}^{\infty} a_p y^p. \tag{7.4.1}$$

This leads to

$$\begin{aligned}H'(y) &=\sum_{p=0}^{\infty} p a_p y^{p-1}=\sum_{q=0}^{\infty}(q+1)a_{q+1}y^q \\ H''(y) &=\sum_{p=0}^{\infty} p(p-1)a_p y^{p-2}=\sum_{r=0}^{\infty}(r+1)(r+2)a_{r+2}y^r\end{aligned}$$

How to deal with equations involving polynomials.

If I ask you when is $a+by+cy^2=0$ for all y, I hope you will answer when $a=b=c=0$. In other words a polynomial is zero when all its coefficients are zero. In the same vein two polynomials are equal when all their coefficients are equal. So what happens for infinite polynomials? They are zero when all coefficients are zero, and they are equal when all coefficients are equal.

So lets deal with the equation, and collect terms of the same order in y.

$$\begin{array}{ll} y^0: & 2a_2+(2\epsilon-1)a_0=0 \\ y^1: & 6a_3-2a_1+(2\epsilon-1)a_1=0 \\ y^s: & (s+1)(s+2)a_{s+2}-(2s+1-2\epsilon)a_s=0 \end{array} \tag{7.4.2}$$

These equations can be used to determine a_{s+2} if we know a_s. The only thing we do not want of our solutions is that they diverge at infinity. Notice that if there is an integer such that

$$2\epsilon=2n+1, \tag{7.4.3}$$

that $a_{n+2}=0$, and $a_{n+4}=0$, etc. These solutions are normalisable, and will be investigated later. If the series does not terminates, we just look at the behaviour of the coefficients for large s, using the following

Theorem 7.4.1

The behaviour of the coefficients a_s of a Taylor series $u(y)=\sum_s a_s y^s$ for large index s describes the behaviour of the function $u(y)$ for large value of y.

Now for large s,

$$a_{s+2}=\frac{2}{s}a_s, \tag{7.4.4}$$

which behaves the same as the Taylor coefficients of e^{y^2} :

$$e^{y^2}=\sum_{s\text{ even}} b_s y^s=\sum_{s\text{ even}}\frac{1}{\frac{s}{2}!}y^s, \tag{7.4.5}$$

and we find

$$b_{s+2}=\frac{2}{s+2}b_s, \tag{7.4.6}$$

which for large s is the same as the relation for a_s. Now $e^{y^2}e^{-y^2/2}=e^{y^2/2}$, and this diverges....

7.5: A Few Solutions

The polynomial solutions occur for

$$\epsilon_n = \left(n + \frac{1}{2}\right). \tag{7.5.1}$$

The terminating solutions are the ones that contains only even coefficients for even n and odd coefficients for odd n. Let me construct a few, using the relation (7.16). For n even I start with $a_0 = 1, a_1 = 0$, and for n odd I start with $a_0 = 0, a_1 = 1$,

$$\begin{aligned} H_0(y) &= 1 \\ H_1(y) &= y \\ H_2(y) &= 1 - 2y^2, \\ H_3(y) &= y - \tfrac{2}{3}y^3. \end{aligned} \tag{7.5.2}$$

Question: Can you reproduce these results? What happens if I start with $a_0 = 0, a_1 = 1$ for, e.g., H_0 ?

In summary: The solutions of the Schrödinger equation occur for energies $\left(n + \frac{1}{2}\right)\hbar\omega$, an the wavefunctions are

$$\phi_n(x) \propto H_n \sqrt{\frac{m\omega}{\hbar}} x \exp\left(-\frac{m\omega}{\hbar} x^2\right) \tag{7.5.3}$$

(In analogy with matrix diagonalisation one often speaks of eigenvalues or eigenenergies for E, and eigenfunctions for ϕ.)
Once again it is relatively straightforward to show how to normalise these solutions. This can be done explicitly for the first few polynomials, and we can also show that

$$\int_{-\infty}^{\infty} \phi_{n_1}(x)\phi_{n_2}(x)dx = 0 \quad \text{if} \quad n_1 \neq n_2. \tag{7.5.4}$$

This defines the orthogonality of the wave functions. From a more formal theory of the polynomials $H_n(y)$ it can be shown that the normalised form of $\phi_n(x)$ is

$$\phi_n(x) = 2^{-m2}(n!)^{-12}\left[\frac{m\omega}{\hbar\pi}\right]^{1/4} \exp\left(-\frac{m\omega}{2\hbar}x^2\right) H_n\left[\frac{m\omega}{\hbar}x\right]. \tag{7.5.5}$$

7.6: Quantum-Classical Correspondence

One of the interesting questions raised by the fact that we can solve both the quantum and the classical problem exactly for the harmonic oscillator, is “Can we compare the Classical and Quantum Solutions?”

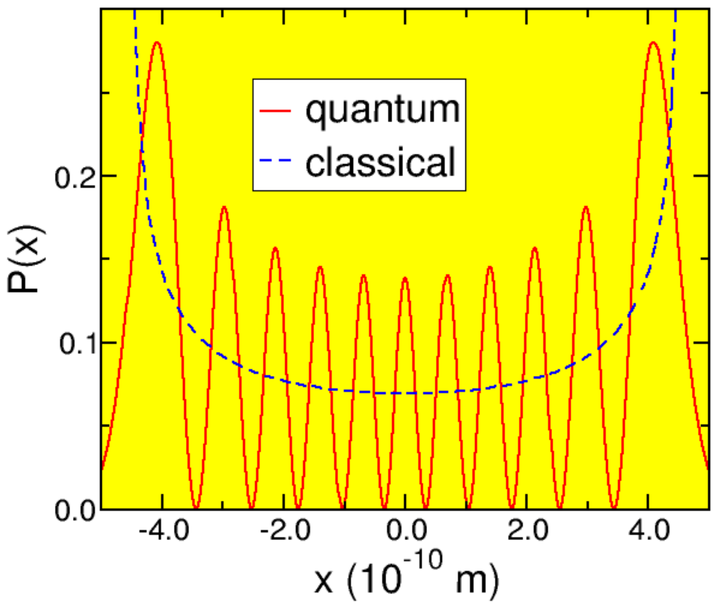

Figure 7.6.1:The correspondence between quantum and classical probabilities

In order to do that we have to construct a probability for the classical solution. The variable over which we must average to get such a distribution must be time, the only one that remains in the solution. For simplicity look at a cosine solution, a sum of sine and cosines behaves exactly the same (check!). We thus have, classically,

$$x = A\cos(\omega t), \quad v = -A\omega\sin(\omega t) \tag{7.6.1}$$

If we substitute this in the energy expression, $E = \frac{1}{2}mv^2 + \frac{1}{2}m\omega^2x^2$, we find that the energy depends on the amplitude A and ω,

$$E(A) = \frac{1}{2}mA^2\omega^2\sin^2(\omega t) + \frac{1}{2}m\omega^2A^2\cos^2(\omega t) = \frac{1}{2}m\omega^2A^2 \tag{7.6.2}$$

Now the probability to find the particle at position x, where $-A < x < A$ is proportional to the time spent in an area dx around x. The time spent in its turn is inversely proportional to the velocity v

$$P_{\text{class}}(x)dx \propto \frac{1}{|v(x)|}dx \tag{7.6.3}$$

Solving v in terms of x we find

$$|v(x)| = \omega\sqrt{A^2 - x^2} \tag{7.6.4}$$

Doing the integration of $1/v(x)$ over x from $-A$ to A we find that the normalised probability is

$$P_{\text{class}}(x)dx = \frac{1}{\pi\sqrt{A^2 - x^2}}dx. \tag{7.6.5}$$

We now would like to compare this to the quantum solution. In order to do that we should consider the probabilities at the same energy,

$$\frac{1}{2}m\omega^2 A^2 = \hbar\omega\left(n + \frac{1}{2}\right), \tag{7.6.6}$$

which tells us what A to use for each n,

$$A(n) = \sqrt{\frac{\hbar}{m\omega}(2n+1)}. \tag{7.6.7}$$

So let us look at an example for $n = 10$. Suppose we choose m and ω such that $\frac{\hbar}{m\omega} = 10^{-10}\ \mathrm{m}$. We then get the results shown in Fig. $7.6.1$, where we see the correspondence between the two functions.

CHAPTER OVERVIEW

8: The Formalism Underlying Quantum Mechanics

Now we have worked a bit with wave functions, we do have to consider some of the underlying interpretation. This can be most easily captured in some formal statements. Note, however, that even though there is no problem with calculations of quantum processes, the interpretation of QM and the measurement process is a complicated and partially unsolved problem. The problem is probably more philosophical than physical!

- 8.1: Key Postulates
- 8.2: Expectation Values of x^2 and p^2 for the Harmonic Oscillator
- 8.3: The Measurement Process

8.1: Key Postulates

1. Every single system has a wave function $\psi(x, t)$.
2. Every observable is represented by a Hermitean operator $\widehat{O}$.
3. The expectation value (average outcome of a measurement) is given by $\int \phi(x)^* \widehat{O} \phi(x) dx$
4. The outcome of an individual experiment can be any of the eigenvalues of $\widehat{O}$.

Let me take each of these in turn.

Wavefunction

The detailed statement is that: for every physical system there exists a wave function, a function of the parameters of the system (coordinates and such) and time, from which the outcome of any experiment can be predicted.

In these lectures I will not touch on systems that depend on other parameters than coordinates, but examples are known, such as the spin of an electron, which can be up or down, and is not like a coordinate at all.

Observables

In classical mechanics "observables" (the technical term for anything that can be measured) are represented by numbers. Think e.g., of $x, y, z, p_x, p_y, p_z, E$, In quantum mechanics "observables" are often quantised, they cannot take on all possible values: how to represent such quantities?

We have already seen that energy and momentum are represented by operators,

$$\hat{p} = -i\hbar\nabla = -i\hbar\left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right). \tag{8.1.1}$$

and

$$\widehat{H} = -\frac{\hbar^2 d^2}{2mdx^2} + V(x) \tag{8.1.2}$$

Let me look at the Hamiltonian, the energy operator. We know that its normalisable solutions (eigenvalues) are discrete.

$$\widehat{H}\phi_n(x) = E_n\phi_n(x). \tag{8.1.3}$$

The numbers E_n are called the eigenvalues, and the functions $\phi_n(x)$ the eigenfunctions of the operator $\overset{\square}{H}$. Our postulate says that the only possible outcomes of any experiment where we measure energy are the values E_n !

Hermitean operators

Hermitean operators are those where the outcome of any measurement is always real, as they should be (complex position?). This means that both its eigenvalues are real, and that the average outcome of any experiment is real. The mathematical definition of a Hermitean operator can be given as

```
\int_{\text {all space }} \psi_1^*(x) \widehat{ O } \psi _ { 2 } ( x ) d x=\int_{\text {all space }} \widehat{O} \psi_1(x)\right]^* \psi_2(x) d x.
```

Quiz show that $\widehat{x}$ and $\hat{p}$ (in 1 dimension) are Hermitean.

Eigenvalues of Hermitean operators

Eigenvalues and eigen vectors of Hermitean operators are defined as for matrices, i.e., where there is a matrix-vector product we get an operator acting on a function, and the eigenvalue/function equation becomes

$$\widehat{O} f(x) = o_n f(x), \tag{8.1.4}$$

where o_n is a number (the "eigenvalue") and $f(x)$ is the "eigenfunction".

A list of important properties of the eigenvalue-eigenfunction pairs for Hermitean operators are:

1. The eigenvalues of an Hermitean operator are all real.
2. The eigenfunctions for different eigenvalues are orthogonal.
3. The set of all eigenfunction is complete.

- Ad 1. Let $\phi_n(x)$ be an eigenfunction of $\widehat{O}$. Use

$$o_n = \int dx \phi_n(x)^* \widehat{O} \phi_n(x) = \int dx \widehat{O} \phi_n(x)^* \phi_n(x) = o_n^* \tag{8.1.5}$$

- Ad 2. Let $\phi_n(x)$ and $\phi_m(x)$ be eigenfunctions of $\widehat{O}$. Use

This leads to

$$(o_n - o_m) \int dx \phi_n(x)^* \phi_n(x) = 0, \tag{8.1.6}$$

and if $o_n \neq o_m \int dx \phi_n(x)^* \phi_n(x) = 0$, which is the definition of two orthogonal functions.

- Ad 3. This is more complex, and no proof will be given. It means that any function can be written as a sum of eigenfunctions of $\widehat{O}$,

$$f(x) = \sum_{n=0}^{\infty} c_n \phi_n(x) \tag{8.1.7}$$

- Ad 3. This is more complex, and no proof will be given. It means that any function can be written as a sum of eigenfunctions of O,

$$f(x) = \sum_{n=0}^{\infty} c_n \phi_n(x) \tag{8.1.8}$$

(A good example of such a sum is the Fourier series.)

Outcome of a single experiment

The outcome of a measurement of any quantity can only be the set of natural values of such a quantity. These are just the eigenvalues of $\widehat{O}$

$$\widehat{O} f_n(x) = o_n f_n(x) \tag{8.1.9}$$

Is this immediately obvious from the formalism? The short answer is no, but suppose we measure the value of the obervable for a wave function known to be an eigenstate. The outcome of a measurement better be this eigenvalue and nothing else. This leads us to surmise that this rule holds for any wave function, and we get the answer we are looking for. This also agrees with the experimentally observed quantisation of observables such as energy.

Eigenfunctions of $\widehat{x}$

The operator $\widehat{x}$ multiplies with x. Solving the equation

$$\widehat{x}^{\square} \phi(x) = x_0 \phi(x) \tag{8.1.10}$$

we find that the solution must be exactly localised at $x = x_0$. The function that does that is called a Dirac δ function $\delta(x - x_0)$. This is defined through integration,

$$\int_{-\infty}^{\infty} \delta(x - x_0) g(x) dx = g(x_0) \tag{8.1.11}$$

and is not normalisable,

$$\int \delta(x - x_0)^2 dx = \infty \tag{8.1.12}$$

Eigenfunctions of $\hat{p}$

The operator $\hat{p}$ is $-i\hbar\frac{\partial}{\partial x}$. Solving the equation

$$-i\hbar\frac{d}{dx}\phi(x)=p_0\phi(x) \tag{8.1.13}$$

we get

$$\frac{d}{dx}\phi(x)=ip_0\hbar\phi(x) \tag{8.1.14}$$

with solution

$$\phi(x)=e^{ip_0xh} \tag{8.1.15}$$

a "plane wave". As we have seen before these states aren't normalised either!

8.2: Expectation Values of x² and p² for the Harmonic Oscillator

As an example of all we have discussed let us look at the harmonic oscillator. Suppose we measure the average deviation from equilibrium for a harmonic oscillator in its ground state. This corresponds to measuring $\bar{x}$. Using

1. $$\phi_0(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar}x^2\right). \tag{8.2.1}$$

we find that

$$\langle x\rangle = \int_{-\infty}^{\infty} \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} x \exp\left(-\frac{m\omega}{\hbar}x^2\right) dx = 0. \tag{8.2.2}$$

Qn Why is it 0 ? Similarly, using $\hat{p} = -i\hbar\frac{d}{dx}$ and

$$\hat{p}\left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar}x^2\right) = im\ \omega x \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar}x^2\right) \tag{8.2.3}$$

we find

$$\langle p\rangle = 0 \tag{8.2.4}$$

More challenging are the expectation values of x^2 and p^2. Let me look at the first one first:

$$\begin{aligned} \langle x^2\rangle &= \int_{-\infty}^{\infty} \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} x^2 exp\left(-\frac{m\omega}{\hbar\pi}x^2\right) dx \\ &= \left(\frac{\hbar}{m\omega}\right) \pi^{-1/2} \int_{-\infty}^{\infty} exp\left(-y^2\right) dy \\ &= \left(\frac{\hbar}{m\omega}\right) \frac{1}{2} \end{aligned} \tag{8.2.5}$$

Now for $\hat{p}^2$,

$$\hat{p}^2 \exp\left(-\frac{m\omega}{2\hbar}x^2\right) = \left(-(m\omega x)^2 + \hbar m\omega\right) \exp\left(-\frac{m\omega}{2\hbar}x^2\right). \tag{8.2.6}$$

Thus,

$$\begin{aligned} \left\langle \hat{p}^2\right\rangle &= \int_{-\infty}^{\infty} \left(\frac{m\omega}{\hbar\pi}\right)^{1/2} \left(-(m\omega x)^2 + \hbar m\omega\right) \exp\left(-\frac{m\omega}{\hbar}x^2\right) dx \\ &= \hbar m\omega\pi^{-1/2} \int_{-\infty}^{\infty} \left(1-y^2\right) \exp\left(-y^2\right) dy \\ &= \hbar m\omega\frac{1}{2}. \end{aligned} \tag{8.2.7}$$

This is actually a form of the uncertainity relation, and shows that

$$\Delta x\Delta p \geq \frac{1}{2}\hbar! \tag{8.2.8}$$

8.3: The Measurement Process

Suppose I know my wave function at time $t = 0$ is the sum of the two lowest-energy harmonic oscillator wave functions,

$$\psi(x,0) = \frac{1}{\sqrt{2}}[\phi_0(x) + \phi_1(x)]\,. \tag{8.3.1}$$

The introduction of the time independent wave function was through the separation $\psi_n(x,t) = e^{-iE_n/\hbar t}\phi_n(x)$. Together with the superposition for time-dependent wave functions, we find

$$\psi(x,t) = \frac{1}{\sqrt{2}}\left[\phi_0(x)e^{-i\frac{1}{2}\omega t} + \phi_1(x)e^{-i\frac{3}{2}\omega t}\right]. \tag{8.3.2}$$

The expectation value of $\hat{H}$, i.e., the expectation value of the energy is

$$\langle\hat{H}\rangle = \frac{1}{2}(E_0 + E_1) = \hbar\omega. \tag{8.3.3}$$

The interpretation of probilities now gets more complicated. If we measure the energy, we don't expect an outcome E_3, since there is no ϕ_3 component in the wave functon. We do expect $E_0 = \frac{1}{2}\hbar\omega$ or $E_1 = \frac{3}{2}\hbar\omega$ with 50% propability, which leads to the right average. Actually simple mathematics shows that the result for the expectation value was just that, $\langle E\rangle = \frac{1}{2}E_0 + \frac{1}{2}E_1$.

We can generalise this result to stating that if

$$\psi(x,t) = \sum_{n=0}^{\infty} c_n(t)\phi_n(x), \tag{8.3.4}$$

where $\phi_n(x)$ are the eigenfunctions of an (Hermitean) operator $\hat{O}$,

$$\hat{O}\phi_n(x) = o_n\phi_n(x), \tag{8.3.5}$$

then

$$\langle\hat{O}\rangle = \sum_{n=0}^{\infty} |c_n(t)|^2, \tag{8.3.6}$$

and the probability that the outcome of a measurement of $\hat{O}$ at time t_0 is o_n is $|c_n(t)|^2$. Here we use orthogonality and completeness of the eigenfunctions of Hermitean operators.

Repeated measurements

If we measure E once and we find E_i as outcome we know that the system is in the i th eigenstate of the Hamiltonian. That certainty means that if we measure the energy again we must find E_i again. This is called the "collapse of the wave function": before the first measurement we couldn't predict the outcome of the experiment, but the first measurements prepares the wave function of the system in one particuliar state, and there is only one component left!

Now what happens if we measure two different observables? Say, at 12 o'clock we measure the position of a particle, and a little later its momentum. How do these measurements relate? Measuring $\hat{x}$ to be x_0 makes the wavefunction collapse to $\delta\left(x - x_0\right)$, whatever it was before. Now mathematically it can be shown that

$$\delta\left(x - x_0\right) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ik(x-x_0)}\,dk \tag{8.3.7}$$

Incompatible operators

The reason is that $\hat{x}$ and $\hat{p}$ are so-called incompatible operators, where

$$\hat{p}\hat{x} \neq \hat{x}\hat{p}! \tag{8.3.8}$$

The way to show this is to calculate

$$(\hat{p}\hat{x} - \hat{x}\hat{p})f(x) \equiv [\hat{p},\hat{x}]f(x) \tag{8.3.9}$$

for arbitrary $f(x)$. A little algebra shows that

$$\begin{aligned}[\hat{p},\hat{x}]f(x) &= \frac{\hbar}{i}\left(\frac{d}{dx}x\right)f(x)\\ &= \frac{\hbar}{i}f(x)\end{aligned}$$

In operatorial notation,

$$[\hat{p},\hat{x}] = \frac{\hbar}{i}\hat{1}, \tag{8.3.10}$$

where the operator $\hat{1}$, which multiplies by 1 , i.e., changes $f(x)$ into itself, is usually not written.

The reason these are now called "incompatible operators" is that an eigenfunction of one operator is not one of the other: if $\hat{x}\phi(x) = x_0\phi(x)$, then

$$\hat{x}\hat{p}\phi(x) = x_0\hat{p}\phi(x) - \frac{\hbar}{i}\phi(x) \tag{8.3.11}$$

If $\phi(x)$ was also an eigenstate of $\hat{p}$ with eigenvalue p_0 we find the contradiction $x_0p_0 = x_0p_0 - \frac{\hbar}{i}$.

Now what happens if we initially measure $\hat{x} = x_0$ with finite acuracy Δx ? This means that the wave function collapses to a Gaussian form,

$$\phi(x) \propto \exp\left(-(x-x_0)^2/\Delta x^2\right) \tag{8.3.12}$$

It can be shown that

$$\exp\left(-(x-x_0)^2/\Delta x^2\right) = \int_{-\infty}^{\infty} dk e^{ikx} e^{-ikx_0} \exp\left(-1/4k^2\Delta x^2\right) \tag{8.3.13}$$

from which we read off that $\Delta p = \hbar/(2\Delta x)$, and thus we conclude that at best

$$\Delta x \Delta p = \hbar/2 \tag{8.3.14}$$

which is the celeberated Heisenberg uncertainty relation.

CHAPTER OVERVIEW

9: Ladder operators

9.1: Harmonic oscillators
9.2: The operators Â and Â†.
9.3: Eigenfunctions of H through ladder operations
9.4: Normalisation and Hermitean conjugates

9.1: Harmonic oscillators

One of the major playing fields for operatorial methods is the harmonic oscillator. Even though they look very artificial, harmonic potentials play an extremely important role in many areas of physics. This is due to the fact that around an equilibrium point, where the forces vanish, any potential behaves as an harmonic one (plus small corrections). This can best be seen by making a Taylor series expansion about such a point,

$$V(x)=V_0+\frac{1}{2}m\omega^2x^2+O(x^3). \tag{9.1.1}$$

Question

Why is there no linear term in Equation 9.1.1?

For small enough x the quadratic term dominates, and we can ignore other terms. Such situations occur in many physical problems, and make the harmonic oscillator such an important problem.

As explained in our first discussion of harmonic oscillators, we scale to dimensionless variables ("pure numbers")

$$y=\sqrt{\frac{m\omega}{\hbar}}x \tag{9.1.2}$$

with $\epsilon=E/\hbar\omega$.

In these new variables the Schrödinger equation becomes

$$\frac{1}{2}\left(\frac{-d^2}{dy^2}+y^2\right)u(y)=\epsilon u(y). \tag{9.1.3}$$

9.2: The operators Â and Â†.

In a previous chapter I have discussed a solution by a power series expansion. Here I shall look at a different technique, and define two operators $\hat{a}$ and $\hat{a}^{\dagger}$,

$$\hat{a}=\frac{1}{\sqrt{2}}\left(y+\frac{d}{dy}\right), \quad \hat{a}^{\dagger}=\frac{1}{\sqrt{2}}\left(y-\frac{d}{dy}\right). \tag{9.2.1}$$

Since

$$\frac{d}{dy}(yf(y))=y\frac{d}{dy}f(y)+f(y) \tag{9.2.2}$$

or in operator notation

$$\frac{d}{dy}\hat{y}=\hat{y}\frac{d}{dy}+\hat{1} \tag{9.2.3}$$

(the last term is usually written as just 1) we find

$$\begin{aligned}\hat{a}\hat{a}^{\dagger}&=\tfrac{1}{2}\left(\hat{y}^{2}-\tfrac{d^{2}}{dy^{2}}+\hat{1}\right)\\ \hat{a}^{\dagger}\hat{a}&=\tfrac{1}{2}\left(\hat{y}^{2}-\tfrac{d^{2}}{dy^{2}}-\hat{1}\right)\end{aligned} \tag{9.2.4}$$

If we define the commutator

$$[\hat{f},\hat{g}]=\hat{f}\hat{g}-\hat{g}\hat{f} \tag{9.2.5}$$

we have

$$\left[\hat{a},\hat{a}^{\dagger}\right]=\hat{1} \tag{9.2.6}$$

Now we see that we can replace the eigenvalue problem for the scaled Hamiltonian by either of

$$\begin{aligned}\left(\hat{a}^{\dagger}\hat{a}+\frac{1}{2}\right)u(y)&=\epsilon u(y)\\ \left(\hat{a}\hat{a}^{\dagger}-\frac{1}{2}\right)u(y)&=\epsilon u(y)\end{aligned}$$

By multiplying the first of these equations by $\hat{a}$ we get

$$\left(\hat{a}\hat{a}^{\dagger}\hat{a}+\frac{1}{2}\hat{a}\right)u(y)=\epsilon\hat{a}u(y). \tag{9.2.7}$$

If we just rearrange some brackets, we find

$$\left(\hat{a}\hat{a}^{\dagger}+\frac{1}{2}\right)\hat{a}u(y)=\epsilon\hat{a}u(y). \tag{9.2.8}$$

If we now use

$$\hat{a}\hat{a}^{+}=\hat{a}^{\dagger}\hat{a}-\hat{1}, \tag{9.2.9}$$

we see that

$$\left(\hat{a}^{\dagger}\hat{a}+\frac{1}{2}\right)\hat{a}u(y)=(\epsilon-1)\hat{a}u(y). \tag{9.2.10}$$

Question: Show that

$$\left(\hat{a}^{\dagger}\hat{a}+\frac{1}{2}\right)\hat{a}^{\dagger}u(y)=(\epsilon+1)\hat{a}^{\dagger}u(y). \tag{9.2.11}$$

We thus conclude that (we use the notation $u_n(y)$ for the eigenfunction corresponding to the eigenvalue ϵ_n)

$$\begin{aligned} \hat{a} u_n(y) &\propto u_{n-1}(y), \\ \hat{a}^\dagger u_n(y) &\propto u_{n+1}(y). \end{aligned}$$

So using $\hat{a}$ we can go down in eigenvalues, using $a^\dagger$ we can go up. This leads to the name lowering and raising operators (guess which is which?).

We also see from $9.2.12$ that the eigenvalues differ by integers only!

9.3: Eigenfunctions of H through ladder operations

If we start with the ground state we would expect that we can't go any lower,

$$\hat{a} u_0(y) = 0. \tag{9.3.1}$$

This can of course be checked explicitly,

$$\begin{aligned} \hat{a} e^{-y^2/2} &= \frac{1}{\sqrt{2}}\left(\hat{y} + \frac{d}{dy}\right) e^{-y^2/2} \\ &= \frac{1}{\sqrt{2}}\left(y e^{-y^2/2} - y e^{-y^2/2}\right) \\ &= 0 \end{aligned}$$

Quiz Can you show that $\boldsymbol{\epsilon_0 = 1/2}$ using the operators $\hat{\boldsymbol{a}}$?

Once we know that $\epsilon_0 = 1/2$, repeated application of

$$(a^\dagger a^+ 12) a^\dagger u(y) = (\epsilon + 1) a^\dagger u(y) \tag{9.3.2}$$

from the previous page shows that $\epsilon_n = n + 1/2$, which we know to be correct from our previous treatment.

Actually, once we know the ground state, we can now easily determine all the Hermite polynomials up to a normalisation constant:

$$\begin{aligned} u_1(y) &\propto a^\dagger e^{-y^2/2} \\ &= \frac{1}{\sqrt{2}}\left(\hat{y} - \frac{d}{dy}\right) e^{-y^2/2} \\ &= \frac{1}{\sqrt{2}}\left(y e^{-y^2/2} + y e^{-y^2/2}\right) \\ &= \sqrt{2} y e^{-y^2/2} \end{aligned}$$

Indeed $H_1(y) \propto y$.

From math books we can learn that the standard definition of the Hermite polynomials corresponds to

$$H_n(y) e^{-y^2/2} = (\sqrt{2})^n \left(\hat{a}^\dagger\right)^n e^{-y^2/2} \tag{9.3.3}$$

We thus learn $H_1(y) = 2y$ and $H_2(y) = \left(4y^2 - 2\right)$.

Question: Prove this last relation.

9.4: Normalisation and Hermitean conjugates

If you look at the expression $\int_{-\infty}^{\infty} f(y)^* \hat{a}^\dagger g(y) dy$ and use the explicit form $\hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(y - \frac{d}{dy}\right)$, you may guess that we can use partial integration to get the operator acting on f,

$$\begin{aligned} &\int_{-\infty}^{\infty} f(y)^* \hat{a}^\dagger g(y) dy \\ &\quad = \int_{-\infty}^{\infty} f(y)^* \frac{1}{\sqrt{2}}\left(y - \frac{d}{dy}\right) g(y) dy \\ &\quad = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2}}\left(y + \frac{d}{dy}\right) f(y)^* g(y) dy \\ &\quad = \int_{-\infty}^{\infty} [\hat{a} f(y)]^* g(y) dy \end{aligned}$$

This is the first example of an operator that is clearly not Hermitean, but we see that $\hat{a}$ and $\hat{a}^\dagger$ are related by "Hermitean conjugation". We can actually use this to normalise the wave function! Let us look at

$$\begin{aligned} O_n &= \int_{-\infty}^{\infty} \left[\left(\hat{a}^\dagger\right)^n e^{-y^2/2}\right]^* \left(\hat{a}^\dagger\right)^n e^{-y^2/2} dy \\ &= \int_{-\infty}^{\infty} \left[\hat{a}\left(\hat{a}^\dagger\right)^n e^{-y^2/2}\right]^* \left(\hat{a}^\dagger\right)^{n-1} e^{-y^2/2} dy \end{aligned}$$

If we now use $\hat{a}\hat{a}^\dagger = \hat{a}^\dagger \hat{a} + \hat{1}$ repeatedly until the operator $\hat{a}$ acts on $u_0(y)$, we find

$$O_n = n O_{n-1} \tag{9.4.1}$$

Since $O_0 = \sqrt{\pi}$, we find that

$$u_n(y) = \frac{1}{\sqrt{n!\sqrt{\pi}}} \left(\hat{a}^+\right)^n e^{-y^2/2} \tag{9.4.2}$$

Question: Show that this agrees with the normalisation proposed in the previous study of the harmonic oscillator!

Question: Show that the states u_n for different n are orthogonal, using the techniques sketched above.

CHAPTER OVERVIEW

10: Time-Dependent Wavefunctions

Up till now I have ignored time dependence. I cannot always do that, which is what these notes are about!

- 10.1: Correspondence between time-dependent and time-independent solutions
- 10.2: Superposition of time-dependent solutions
- 10.3: Completeness and time-dependence
- 10.4: Simple Example
- 10.5: Wave packets (states of minimal uncertainty)

10.1: Correspondence between time-dependent and time-independent solutions

The time dependent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t)+V(x)\psi(x,t)=\frac{\hbar i\partial}{\partial t}\psi(x,t). \tag{10.1.1}$$

As we remember, a solution of the form

$$\psi(x,t)=\phi(x)e^{-iEt/\hbar} \tag{10.1.2}$$

leads to a solution of the time-independent Schrödinger equation of the form

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi(x)+V(x)\phi(x)=E\phi(x) \tag{10.1.3}$$

10.2: Superposition of time-dependent solutions

There has been an example problem, where I asked you to show "that if $\psi_1(x,t)$ and $\psi_2(x,t)$ are both solutions of the time-dependent Schrödinger equation, than $\psi_1(x,t)+\psi_2(x,t)$ is a solution as well." Let me review this problem

$$\begin{aligned}
-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_1(x,t)+V(x)\psi_1(x,t) &= \frac{\hbar i\partial}{\partial t}\psi_1(x,t)\\
-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_2(x,t)+V(x)\psi_2(x,t) &= \frac{\hbar i\partial}{\partial t}\psi_2(x,t)\\
-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}[\psi_1(x,t)+\psi_2(x,t)]+V(x)\,[\psi_1(x,t)+\psi_2(x,t)] &= \frac{\hbar i\partial}{\partial t}[\psi_1(x,t)+\psi_2(x,t)]
\end{aligned}$$

where in the last line I have use the sum rule for derivatives. This is called the superposition of solutions, and holds for any two solutions to the same Schrödinger equation!

Question: Why doesn't it work for the time-independent Schrödinger equation?

10.3: Completeness and time-dependence

In the discussion on formal aspects of quantum mechanics I have shown that the eigenfunctions to the Hamiltonian are complete, i.e., for any $\psi(x,t)$

$$\psi(x,t)=\sum_{n=1}^{\infty} c_n(t)\phi_n(x) \tag{10.3.1}$$

where

$$\hat{H}\phi_n(x)=E_n\phi_n(x). \tag{10.3.2}$$

We know, from the superposition principle, that

$$\psi(x,t)=\sum_{n=1}^{\infty} c_n(0)e^{-iEt/\hbar}\phi_n(x), \tag{10.3.3}$$

so that the time dependence is completely fixed by knowing $c(0)$ at time $t=0$ only! In other words if we know how the wave function at time $t=0$ can be written as a sum over eigenfunctions of the Hamiltonian, we can then determibe the wave function for all times.

10.4: Simple Example

The best way to clarify this abstract discussion is to consider the quantum mechanics of the Harmonic oscillator of mass m and frequency ω,

$$\hat{H}=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega^2x^2 \tag{10.4.1}$$

If we assume that the wave function at time $t=0$ is a linear superposition of the first two eigenfunctions,

$$\begin{aligned}\psi(x,t=0) &=\sqrt{\frac{1}{2}}\phi_0(x)-\sqrt{\frac{1}{2}}\phi_1(x)\\ \phi_0(x) &=\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\\ \phi_1(x) &=\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\sqrt{\frac{m\omega}{\hbar}}x\end{aligned}$$

(The functions ϕ_0 and ϕ_1 are the normalised first and second states of the harmonic oscillator, with energies $E_0=\frac{1}{2}\hbar\omega$ and $E_1=\frac{3}{2}\hbar\omega$.) Thus we now kow the wave function for all time:

$$\psi(x,t)=\sqrt{\frac{1}{2}}\phi_0(x)e^{-\frac{1}{2}i\omega t}-\sqrt{\frac{1}{2}}\phi_1(x)e^{-\frac{3}{2}i\omega t}. \tag{10.4.2}$$

In figure $10.4.1$ we plot this quantity for a few times.

The best way to visualize what is happening is to look at the probability density,

$$\begin{aligned}\mathcal{P}(x,t) &=\psi(x,t)^*\psi(x,t)\\ &=\frac{1}{2}\left(\phi_0(x)^2+\phi_1(x)^2-2\phi_0(x)\phi_1(x)\cos\omega t\right)\end{aligned}$$

This clearly oscillates with frequency ω.

Question: Show that $\int_{-\infty}^{\infty}\mathcal{P}(x,t)dx=1$.

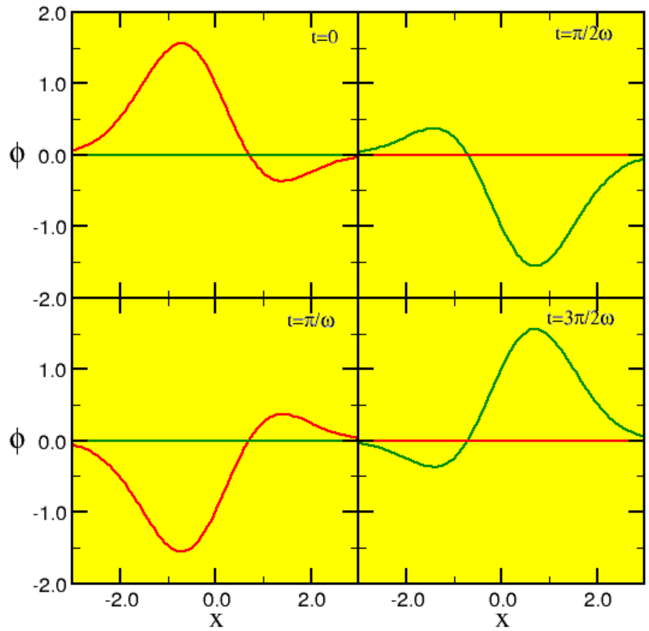

Figure 10.4.1: The wave function (10.10) for a few values of the time t. The solid line is the real part, and the dashed line the imaginary part.

Another way to look at that is to calculate the expectation value of $\hat{x}$:

$$\begin{aligned}
\langle\hat{x}\rangle &= \int_{-\infty}^{\infty} \mathcal{P}(x,t) dx \\
&= \underbrace{\frac{1}{2}\int_{-\infty}^{\infty} \phi_0(x)^2 x dx}_{=0} + \underbrace{\frac{1}{2}\int_{-\infty}^{\infty} \phi_1(x)^2 x dx}_{=0} - \cos\omega t \int_{-\infty}^{\infty} \phi_0(x)\phi_1(x) x dx \\
&= -\cos\omega t \sqrt{\frac{\hbar}{m\omega}} \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} y^2 e^{-y^2} \\
&= -\frac{1}{2}\sqrt{\frac{\hbar}{m\omega}} \cos\omega t.
\end{aligned}$$

This once again exhibits oscillatory behaviour!

10.5: Wave packets (states of minimal uncertainty)

One of the questions of some physical interest is "how can we create a qunatum-mechanical state that behaves as much as a classical particle as possible?" From the uncertainty principle,

$$\Delta x \Delta p \geq \frac{1}{2}\hbar \tag{10.5.1}$$

this must be a state where Δx and Δp are both as small as possible. Such a state is known as a "wavepacket". We shall see below (and by using a computer demo) that its behavior depends on the Hamiltonian governing the system that we are studying!

Let us start with the uncertainty in x. A state with width $\Delta x = \sigma$ should probably be a Gaussian, of the form

$$\psi(x,t) = \exp\left(-\frac{(x-x_0)^2}{2\sigma^2}\right) A(x). \tag{10.5.2}$$

In order for ψ to be normalised, we need to require

$$|A(x)|^2 = \sqrt{\frac{1}{\sigma^2\pi}}. \tag{10.5.3}$$

Actually, I shall show below that with

$$A(x) = \sqrt[4]{\frac{1}{\sigma^2\pi}} e^{ip_0 x/\hbar} \tag{10.5.4}$$

we have

$$\langle \hat{x} \rangle = x_0, \quad \langle \hat{p} \rangle = p_0, \quad \Delta x = \sigma, \quad \Delta p = \hbar/\sigma \tag{10.5.5}$$

The algebra behind this is relatively straightforward, but I shall just assume the first two, and only do the last two in all gory details.

$$\hat{p} \exp\left(-\frac{(x-x_0)^2}{2\sigma^2}\right) A(x) = \left(p_0 + i\hbar\frac{(x-x_0)}{\sigma^2}\right) \exp\left(-\frac{(x-x_0)^2}{2\sigma^2}\right) A(x) \tag{10.5.6}$$

Thus

$$\langle p \rangle = \sqrt{\frac{1}{\sigma^2\pi}} \int_{-\infty}^{\infty} \left(p_0 + i\hbar\frac{(x-x_0)}{\sigma^2}\right) \exp\left(-\frac{(x-x_0)^2}{2\sigma^2}\right) = p_0. \tag{10.5.7}$$

Let $\hat{p}$ act twice,

$$\hat{p}^2 \exp\left(-\frac{(x-x_0)^2}{2\sigma^2}\right) A(x) = \left(p_0^2 + 2i\hbar p_0 \frac{(x-x_0)}{\sigma^2} - \hbar^2 \left[\frac{(x-x_0)^2}{\sigma^4} - \frac{1}{\sigma^2}\right]\right) \times$$

$$\exp\left(-\frac{(x-x_0)^2}{2\sigma^2}\right) A(x).$$

Doing all the integrals we conclude that

$$\langle p^2 \rangle = p_0^2 + \frac{\hbar^2}{2\sigma^2} \tag{10.5.8}$$

Thus, finally,

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \frac{\hbar}{\sigma} \tag{10.5.9}$$

This is just the initial state, which clearly has minimal uncertainty. We shall now investigate how the state evolves in time by usin a numerical simulation. What we need to do is to decompose our state of minimal uncertainty in a sum over eigenstates of the Hamiltonian which describes our system!

CHAPTER OVERVIEW

11: 3D Schrödinger Equation

Up till now we have been studying (very(artificial systems, where space is one dimensional. Of course the real world is three dimensional, and even the Schrödinger equation will have to take this into account. So how do we go about doing this?

11.1: The momentum operator as a vector

11.2: Spherical Coordinates

11.3: Solutions independent of angular variables

11.4: The hydrogen atom

11.5: Now where does the probability peak?

11.6: Spherical Harmonics

11.7: General solutions

11.1: The momentum operator as a vector

First of all we know from classical mechanics that velocity and momentum, as well as position, are represented by vectors. Thus we need to represent the momentum operator by a vector of operators as well,

$$\hat{p}=\left(\frac{\hbar}{i}\frac{\partial}{\partial x},\frac{\hbar}{i}\frac{\partial}{\partial y},\frac{\hbar}{i}\frac{\partial}{\partial z}\right). \tag{11.1.1}$$

There exists a special notation for the vector of partial derivatives, which is usually called the gradient, and one writes

$$\hat{p}=\frac{\hbar}{i}\nabla. \tag{11.1.2}$$

We now that the energy, and Hamiltonian, can be written in classical mechanics as

$$E=\frac{1}{2}mv^2+V(x)=\frac{1}{2m}p^2+V(x), \tag{11.1.3}$$

where the square of a vector is defined as the sum of the squares of the components,

$$(v_1,v_2,v_3)^2=v_1^2+v_2^2+v_3^2. \tag{11.1.4}$$

The Hamiltonian operator in quantum mechanics can now be read of from the classical one,

$$\hat{H}=\frac{1}{2m}\hat{p}^2+V(x)=-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V(x). \tag{11.1.5}$$

Let me introduce one more piece of notation: the square of the gradient operator is called the Laplacian, and is denoted by Δ.

11.2: Spherical Coordinates

The solution to Schrödinger's equation in three dimensions is quite complicated in general. Fortunately, nature lends us a hand, since most physical systems are "rotationally invariant", i.e., $V(x)$ depends on the size of x, but not its direction! In that case it helps to introduce spherical coordinates, as denoted in Fig. 11.2.1.

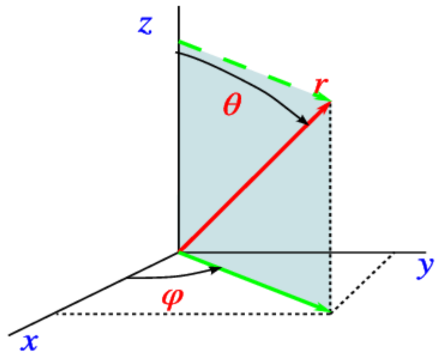

Figure 11.2.1: The spherical coordinates r, θ, φ .

The coordinates r, θ and ϕ are related to the standard ones by

$$\begin{aligned} x &= r\cos\varphi\sin\theta \\ y &= r\sin\varphi\sin\theta \\ &= r\cos\theta \end{aligned}$$

where $0 < r < \infty, 0 < \theta < \pi$ and $0 < \phi < 2\pi$. In these new coordinates we have

$$\Delta f(r,\theta,\varphi) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}f(r,\theta,\varphi)\right) - \frac{1}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}f(r,\theta,\varphi)\right) + \frac{\partial^2}{\partial\varphi^2}f(r,\theta,\varphi)\right]. \tag{11.2.1}$$

11.3: Solutions independent of angular variables

Initially we shall just restrict ourselves to those cases where the wave function is independent of θ and φ, i.e.,

$$\phi(r,\theta,\varphi) = R(r). \tag{11.3.1}$$

In that case the Schrödinger equation becomes (why?)

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}R(r)\right) + V(r)R(r) = ER(r) \tag{11.3.2}$$

One often simplifies life even further by substituting $u(r)/r = R(r)$, and multiplying the equation by r at the same time,

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2}u(r) + V(r)u(r) = Eu(r) \tag{11.3.3}$$

Of course we shall need to normalise solutions of this type. Even though the solution are independent of θ and φ, we shall have to integrate over these variables. Here a geometric picture comes in handy. For each value of r, the allowed values of x range over the surface of a sphere of radius r. The area of such a sphere is $4\pi r^2$. Thus the integration over r, θ, φ can be reduced to

$$\int_{\text{all space}} f(r)\,dx\,dy\,dz = \int_0^\infty f(r) 4\pi r^2\,dr. \tag{11.3.4}$$

Especially, the normalisation condition translates to

$$\int_0^\infty |R(r)|^2 4\pi r^2\,dr = \int_0^\infty |u(r)|^2 4\pi\,dr = 1 \tag{11.3.5}$$

11.4: The hydrogen atom

For the hydrogen atom we have a Coulomb force exerted by the proton forcing the electron to orbit around it. Since the proton is 1837 heavier than the electron, we can ignore the reverse action. The potential is thus

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r} \tag{11.4.1}$$

If we substitute this in the Schrödinger equation for $u(r)$, we find

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2}u(r) - \frac{e^2}{4\pi\epsilon_0 r}u(r) = Eu(r). \tag{11.4.2}$$

The way to attack this problem is once again to combine physical quantities to set the scale of length, and see what emerges. From a dimensional analysis we find that the length scale is set by the Bohr radius a_0,

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2} = 0.53 \times 10^{-10}\text{ m} \tag{11.4.3}$$

The scale of energy is set by these same parameters to be

$$\frac{e^2}{4\pi\epsilon_0 a_0} = 2\text{Ry} \tag{11.4.4}$$

and one Ry (Rydberg) is 13.6 eV . Solutions can be found by a complicated argument similar to the one for the Harmonic oscillator, but (without proof) we have

$$E_n = -\frac{1}{2}\Box\frac{e^2}{4\pi\epsilon_0 a_0}\Bigg\lceil\frac{1}{n^2} = -13.6\frac{1}{n^2}\text{eV} \tag{11.4.5}$$

and

$$R_n = e^{-r(na_0)}\left(c_0 + c_1 r + \ldots + c_{n-1}r^{n-1}\right) \tag{11.4.6}$$

The explicit, and normalised, forms of a few of these states are

$$\begin{aligned} R_1(r) &= \tfrac{1}{\sqrt{4\pi}}2a_0^{-3/2}e^{-r/a_0}, \\ R_2(r) &= \tfrac{1}{\sqrt{4\pi}}2(2a_0)^{-32}\left[1 - \tfrac{r}{2a_0}\Box e^{-r(2a_0)}.\right. \end{aligned} \tag{11.4.7}$$

Remember these are normalised to

$$\int_0^\infty R_n(r)^* R_m(r)dr = \delta_{nm} \tag{11.4.8}$$

Notice that there are solution that do depend on θ and φ as well, and that we have not looked at such solutions here!

11.5: Now where does the probability peak?

Clearly the probability density to find an electron at point x is

$$P(x) = R(r)^* R(r), \tag{11.5.1}$$

but what is the probability to find the electron at a distance r from the proton? The key point to realise is that for each value of r the electron can be anywhere on the surface of a sphere of radius r, so that for larger r more points contribute than for smaller r. This is exactly the source of the factor $4\pi r^2$ in the normalisation integral. The probability to find a certain value of r is thus

$$P(r) = 4\pi r^2 R(r)^* R(r) \tag{11.5.2}$$

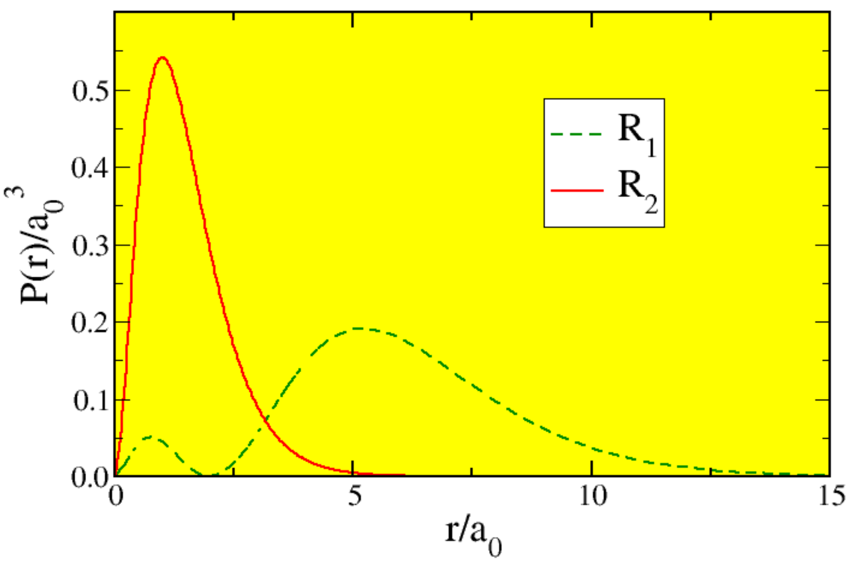

Figure 11.5.1: The probability to find a certain value of r for the first two Harmonic oscillator wave functions.

These probabilities are sketched in Fig. 11.5.1. The peaks are of some interest, since they show where the electrons are most likely to be found. Let's investigate this mathematically:

$$P_1 = 4r^2/a_0^3 e^{-2r/a_0}. \tag{11.5.3}$$

if we differentiate with respect to r, we get

$$\frac{d}{dr} P_1 = \frac{4}{a_0^3}\left(2re^{-2r/a_0} - 2r^2/a_0 e^{-2r/a_0}\right) \tag{11.5.4}$$

This is zero at $r = a_0$. For the first excited state this gets a little more complicated, and we will have to work harder to find the answer.

11.6: Spherical Harmonics

The key issue about three-dimensional motion in a spherical potential is angular momentum. This is true classically as well as in quantum theories. The angular momentum in classical mechanics is defined as the vector (outer) product of r and p,

$$L = r \times p. \tag{11.6.1}$$

This has an easy quantum analog that can be written as

$$\hat{L} = \hat{r} \times \hat{p} \tag{11.6.2}$$

After exapnsion we find

$$\hat{L} = -i\hbar \left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}, z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}, x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \right) \tag{11.6.3}$$

This operator has some very interesting properties:

$$[\hat{L}, \hat{r}] = 0. \tag{11.6.4}$$

Thus

$$[\hat{\boldsymbol{L}}, \hat{H}] = 0! \tag{11.6.5}$$

And even more surprising,

And even more surprising,

$$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar\hat{L}_z. \tag{11.6.6}$$

Thus the different components of L are not compatible (i.e., can't be determined at the same time). Since L commutes with H we can diagonalise one of the components of L at the same time as H. Actually, we diagonalsie $\hat{L}^2$, $\hat{L}_z$ and H at the same time!

The solutions to the equation

$$\hat{L}^2 Y_{LM}(\theta, \phi) = \hbar^2 L(L+1) Y_{LM}(\theta, \phi) \tag{11.6.7}$$

are called the spherical harmonics.

Question: check that $\hat{\boldsymbol{L}}^2$ is independent of $\boldsymbol{r}$!

The label M corresponds to the operator $\hat{L}_z$,

$$\hat{L}_z Y_{LM}(\theta, \phi) = \hbar M Y_{LM}(\theta, \phi). \tag{11.6.8}$$

11.7: General solutions

One of the reasons for playing such game is that we can rewrite the kinetic energy as

$$-\frac{\hbar^2}{2m}\hat{p}^2 f(\boldsymbol{r}) = -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}f(\boldsymbol{r})\right) + \frac{1}{r^2}\hat{L}^2 f(\boldsymbol{r}) \tag{11.7.1}$$

CHAPTER OVERVIEW

12: Quantum Mechanics of the Hydrogen Atom

A thorough review of the structure of the hydrogen atom will be presented with emphasis on the quantum-mechanical principles involved rather than calculational detail, which will be minimized. First, the relationship of the Heisenberg uncertainty principle to the hydrogen atom will be discussed briefly. This is followed by a discussion of the energy level structure of the hydrogen atom, including fine structure, in the context of the quantum-mechanical theories of Bohr, Schrödinger, and Dirac. Finally, smaller-order corrections to these theories will be discussed, including the Lamb shift, hyperfine structure, and the Zeeman effect.

- 12.1: The Uncertainty Principle
- 12.2: Bohr Model of the Hydrogen Atom
- 12.3: Schrödinger Theory of the Hydrogen Atom
  - 12.3.1: Schrödinger Theory of Hydrogen
  - 12.3.2: The Spin-Orbit Effect
  - 12.3.3: Kinetic Energy Corrections
- 12.4: Dirac Theory of the Hydrogen Atom
- 12.5: Smaller Effects
  - 12.5.1: Hyperfine Structure
  - 12.5.2: The Lamb Shift
  - 12.5.3: The Zeeman Effect
- 12.6: Conclusion and References

Contributors and Attributions

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12.1: The Uncertainty Principle

Before discussing specifics about the structure of the hydrogen atom, it is interesting to note what information about the hydrogen atom can be derived just from the Heisenberg uncertainty principle. A familiar form of the uncertainty principle looks like the following:

$$\Delta x \Delta p_x \sim \hbar \tag{12.1.1}$$

where Δx and Δp_x are the uncertainty in the x-component of the position and momentum of a particle, respectively. Consider an electron in a classical circular orbit in the xy-plane. It is then reasonable to write $\Delta x \sim r$, where r is the radius of the orbit. Assuming a state of minimum uncertainty, Δp_x is then known from the uncertainty principle, and it should be roughly equal

to the magnitude of the momentum for the circular orbit being considered. That is,

$$p \sim \Delta p_x \sim \frac{\hbar}{r}. \tag{12.1.2}$$

Classically, the energy is simply [1]

$$E = \frac{p^2}{2m} - \frac{e^2}{r} = \frac{\hbar^2}{2mr^2} - \frac{e^2}{r}, \tag{12.1.3}$$

where m is the electron mass and e the electron charge. The last step results from the substitution of p from equation 2 . The value of r is unknown, but one would expect it to have a value that minimizes the energy, as Nature likes to do. Differentiating equation 3 with respect to r and setting equal to zero gives

$$\frac{dE}{dr} = -\frac{\hbar^2}{mr^3} + \frac{e^2}{r^2} = 0. \tag{12.1.4}$$

This yields

$$r = \frac{\hbar^2}{me^2} \equiv a_0 = 0.529\text{Å}, \tag{12.1.5}$$

where a_0 is the Bohr radius. Substituting into equation 3 gives

$$E = -13.6\text{eV} \tag{12.1.6}$$

The Bohr radius is exactly the radius of the circular orbit in the ground state of the electron in Bohr theory, and it holds up as representative of the extent of the orbit in Schrödinger theory. The energy -13.6 eV is the known ground state energy of the hydrogen atom. So, starting with only a very rough view of the structure of the atom and the uncertainty principle, one can make some reasonable assumptions and derive two extremely important fundamental results - the "size" if the hydrogen atom in its ground state and its ionization energy. Of course, to get precisely the right results one needs to make the right assumptions, and so this calculation is certainly not rigorously accurate. It merely illustrates the relation of the fundamental physical structure of the hydrogen atom to the uncertainty principle. The fact that these results were derived assuming minimum uncertainty leads to a rather important conclusion-the hydrogen atom in its ground state is essentially in a state of minimum uncertainty. This explains why the electron in its ground state cannot radiate, as one expects classically, and get drawn in towards the nucleus - to do so would violate the uncertainty principle. If the electron were confined closer to the nucleus, so that Δx were much smaller, then Δp_x would be much larger and so it would not be possible to consider the electron as necessarily bound to the nucleus.

1. To achieve consistency and avoid confusion all equations are written in Gaussian units

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12.2: Bohr Model of the Hydrogen Atom

With the use of spectroscopy in the late 19th century, it was found that the radiation from hydrogen, as well as other atoms, was emitted at specific quantized frequencies. It was the effort to explain this radiation that led to the first successful quantum theory of atomic structure, developed by Niels Bohr in 1913. He developed his theory of the hydrogenic (one-electron) atom from four postulates:

1. *An electron in an atom moves in a circular orbit about the nucleus under the influence of the Coulomb attraction between the electron and the nucleus, obeying the laws of classical mechanics.*
2. *Instead of the infinity of orbits which would be possible in classical mechanics, it is only possible for an electron to move in an orbit for which its orbital angular momentum L is and integral multiple of $\hbar$.*
3. *Despite the fact that it is constantly accelerating, an electron moving in such an allowed orbit does not radiate electromagnetic energy. Thus, its total energy \(E\) remains constant.*
4. *Electromagnetic radiation is emitted if an electron, initially moving in an orbit of total energy E_i, discontinuously changes its motion so that it moves in an orbit of total energy \(E_f\). The frequency of the emitted radiation ν is equal to the quantity \(E_i-E_f\) divided by \(h\).* [1]

The third postulate can be written mathematically

$$L = n\hbar$$
$$n = 1, 2, 3, \dots$$

For an electron moving in a stable circular orbit around a nucleus, Newton's second law reads

$$\frac{Ze^2}{r^2} = m\frac{v^2}{r} \tag{12.2.1}$$

where v is the electron speed, and r the radius of the orbit. Since the force is central, angular momentum should be conserved and is given by $L = |\mathbf{r} \times \mathbf{p}| = mvr$. Hence from the quantization condition of of the third postulate

$$mvr = n\hbar. \tag{12.2.2}$$

Equations 12.2.1 and 12.2.2 therefore give two equations in the two unknowns r and v. These are easily solved to yield

$$r = \frac{n^2\hbar^2}{mZe^2} = \frac{n^2}{Z}a_0$$
$$v = \frac{Ze^2}{n\hbar} = \frac{Z}{n}\alpha c$$

where

$$\alpha \equiv \frac{e^2}{\hbar c} \approx \frac{1}{137} \tag{12.2.3}$$

is a dimensionless number known as the fine-structure constant for reasons to be discussed later. Hence αc is the speed of the electron in the Bohr model for the hydrogen atom $(Z = 1)$ in the ground state $(n = 1)$. Since this is the maximum speed for the electron in the hydrogen atom, and hence $v \ll c$ for all n, the use of the classical kinetic energy seems appropriate. From equation 8, one can then write the kinetic energy,

$$K = \frac{1}{2}mv^2 = \frac{Ze^2}{2r}, \tag{12.2.4}$$

and hence the total energy, [2]

$$E = K + V = \frac{Ze^2}{2r} - \frac{Ze^2}{r} = -\frac{Ze^2}{2r}. \tag{12.2.5}$$

Having solved for r as equation 10, one can then write

$$E = -\frac{mZ^2e^4}{2\hbar^2}\frac{1}{n^2} = -\frac{mc^2}{2}(Z\alpha)^2\frac{1}{n^2}. \tag{12.2.6}$$

Numerically, the energy levels for a hydrogenic atom are

$$E = -13.6\text{eV}\frac{Z^2}{n^2} \tag{12.2.7}$$

One correction to this analysis is easy to implement, that of the finite mass of the nucleus. The implicit assumption previously was that the electron moved around the nucleus, which remained stationary due to being infinitely more massive than the electron. In reality, however, the nucleus has some finite mass M, and hence the electron and nucleus both move, orbiting about the center of mass of the system. It is a relatively simple exercise in classical mechanics to show one can transform into the rest frame of the nucleus, in which frame the physics remains the same except for the fact that the electron acts as though it has a mass

$$\mu = \frac{mM}{m+M}, \tag{12.2.8}$$

which is less than m and is therefore called the reduced mass. One can therefore use μ in all equations where m appears in this analysis and get more accurate results. With this correction to the hydrogen energy levels, along with the fourth Bohr postulate which gives the radiative frequencies in terms of the energy levels, the Bohr model correctly predicts the observed spectrum of hydrogen to within three parts in 10^5.

Along with this excellent agreement with observation, the Bohr theory has an appealing aesthetic feature. One can write the angular momentum quantization condition as

$$L = pr = n\frac{h}{2\pi}, \tag{12.2.9}$$

where p is the linear momentum of the electron. Louis de Broglie's theory of matter waves predicts the relationship $p = h/\lambda$ between momentum and wavelength, so

$$2\pi r = n\lambda. \tag{12.2.10}$$

That is, the circumference of the circular Bohr orbit is an integral number of de Broglie wavelengths. This provided the Bohr theory with a solid physical connection to previously developed quantum mechanics.

Unfortunately, in the long run the Bohr theory, which is part of what is generally referred to as the old quantum theory, is unsatisfying. Looking at the postulates upon which the theory is based, the first postulate seems reasonable on its own, acknowledging the existence of the atomic nucleus, established by the scattering experiments of Ernest Rutherford in 1911, and assuming classical mechanics. However, the other three postulates introduce quantum-mechanical effects, making the theory an uncomfortable union of classical and quantum-mechanical ideas. The second and third postulates seem particularly ad hoc. The electron travels in a classical orbit, and yet

its angular momentum is quantized, contrary to classical mechanics. The electron obeys Coulomb's law of classical electromagnetic theory, and yet it is assumed to not radiate, as it would classically. These postulates may result in good predictions for the hydrogen atom, but they lack a solid fundamental basis.

The Bohr theory is also fatally incomplete. For example, the WilsonSommerfeld quantization rule, of which the second Bohr postulate is a special case, can only be applied to periodic systems. The old theory has no way of approaching non-periodic quantum-mechanical phenomena, like scattering. Next, although the Bohr theory does a good job of predicting energy levels, it predicts nothing about transition rates between levels. Finally, the theory is really only successful for one-electron atoms, and fails even for helium. To correct these faults, one needs to apply a more completely quantum-mechanical treatment of atomic structure, and such an approach is used in Schrödinger theory.

Footnote

[1] The reader may notice that $E = -K$, as a natural consequence of the virial theorem of classical mechanics.

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SECTION OVERVIEW

12.3: Schrödinger Theory of the Hydrogen Atom

12.3.1: Schrödinger Theory of Hydrogen

12.3.2: The Spin-Orbit Effect

12.3.3: Kinetic Energy Corrections

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12.3.1: Schrödinger Theory of Hydrogen

The Schrödinger theory of quantum mechanics extends the de Broglie concept of matter waves by providing a formal method of treating the dynamics of physical particles in terms of associated waves. One expects the behavior of this wavefunction, generally called tex2html_wrap_inline1306 , to be governed by a wave equation, which can be written

$$\left(\frac{p^2}{2m}+V(\mathbf{x},t)\right)\Psi(\mathbf{x},t)=H\Psi(\mathbf{x},t) \tag{12.3.1.1}$$

where the first term of the left represents the particle's kinetic energy, the second the particle's potential energy, and H is called the Hamiltonian of the system. Making the assertion that p and H are associated with differential operators,

$$p=-i\hbar\nabla \tag{12.3.1.2}$$

$$H=i\hbar\frac{\partial}{\partial t}, \tag{12.3.1.3}$$

this becomes

$$\left(-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{x},t)\right)\Psi(\mathbf{x},t)=i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x},t) \tag{12.3.1.4}$$

which is known as the *time-dependent Schrödinger equation*. For the specific case of a hydrogenic atom, the electron moves in a simple Coulomb potential, and hence the Schrödinger equation is

$$\left(-\frac{\hbar^2}{2m}\nabla^2-\frac{Ze^2}{r}\right)\Psi(\mathbf{x},t)=i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x},t). \tag{12.3.1.5}$$

The solution proceeds by the method of separation of variables. First one writes the wavefunction as a product of a space component and a time component, for which the solution for the time part is easy and yields

$$\Psi(\mathbf{x},t)=\psi(\mathbf{x})e^{-iEt/\hbar} \tag{12.3.1.6}$$

Here E is the constant of the separation and is equal to the energy of the electron. The remaining equation for the spatial component is

$$\left(-\frac{\hbar^2}{2m}\nabla^2-\frac{Ze^2}{r}\right)\psi(\mathbf{x})=E\psi(\mathbf{x}) \tag{12.3.1.7}$$

and is called the *time-independent Schrödinger equation*. Due to the spherical symmetry of the potential, this equation is best solved in spherical polar coordinates, and hence one separates the spatial wavefunction as

$$\psi(r,\theta,\phi)=R(r)\Theta(\theta)\Phi(\phi). \tag{12.3.1.8}$$

The equations are more difficult but possible to solve and yield

$$\Theta(\theta)\Phi(\phi)=Y_l^{m_l}(\theta,\phi) \tag{12.3.1.9}$$

$$R(r)=e^{-Zr/na_0}\left(\frac{Zr}{a_0}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2Zr}{na_0}\right), \tag{12.3.1.10}$$

where L is an associated Laguerre polynomial, and for convenience the product of the angular solutions are written together in terms of a single function, the spherical harmonic Y. With foresight the separation constants $-m_l^2$ and and $l(l+1)$ were used. The meaning of the numbers n, l, and m_l will now be discussed.

The physics of the Schrödinger theory relies on the interpretation of the wave function in terms of probabilities. Specifically, the absolute square of the wavefunction, $|\Psi(\mathbf{x},t)|^2$, is interpreted as the probability density for finding the associated particle in the vicinity of $\mathbf{x}$ at time t. For this to make physical sense, the wavefunction needs to be a well-behaved function of $\mathbf{x}$ and t; that is, Ψ should be a finite, single-valued, and continuous function. Inorder to satisfy these conditions, the separation constants that appear while solving the Schrödinger equation can only take on certain discrete values. The upshot is, with the solution written as it is here, that the numbers n, l, and m_l, called quantum numbers of the electron, can only take on particular integer values, and each of these corresponds to the quantization of some physical quantity. The allowed values of the energy turn out to be exactly as predicted by the Bohr theory,

$$E=-\frac{mc^2}{2}(Z\alpha)^2\frac{1}{n^2} \tag{12.3.1.11}$$

The quantum number n is therefore called the principle quantum number. To understand the significance of l and m_l, one needs to consider the orbital angular momentum of the electron. This is defined as $\mathbf{L}=\mathbf{r}\times\mathbf{p}$, or as an operator, $\mathbf{L}=-i\hbar\mathbf{r}\times\nabla$. With proper coordinate transformations, one can write the operators L^2 and the z-component of angular momentum L_z in spherical coordinates as

$$L^2=-\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \tag{12.3.1.12}$$

$$L_z=-i\hbar\frac{\partial}{\partial\phi}. \tag{12.3.1.13}$$

It can be shown that when these operators act on the solution Ψ, the result is

$$L^2\Psi=l(l+1)\hbar^2\Psi \tag{12.3.1.14}$$

$$L_z\Psi=m_l\hbar\Psi \tag{12.3.1.15}$$

It can also be shown that this means that an electron in a particular state has orbital angular momentum of constant magnitude $\sqrt{l(l+1)}\,\hbar$ and constant projection onto the z-axis of $m_l\hbar$. Since the electron obeys the timeindependent Schrödinger equation $H\Psi=E\Psi$, and hence has constant energy, one says that the wavefunction Ψ is a simultaneous eigenstate of the operators H, L^2, and L_z. Table 1 summarizes this information and gives the allowed values for each quantum number. It is worth repeating that these numbers can have only these specific values because of the demand that Ψ be a well-behaved function.

It is common to identify a state by its principle quantum number n and a letter which corresponds to its orbital angular momentum quantum number l, as shown in table 2. This is called spectroscopic notation. The first four designated letters are of historical origin. They stand for sharp, primary, diffuse, and fundamental, and refer to the nature of the spectroscopic lines when these states were first studied.

Table 12.3.1.1: Some quantum numbers for the electron in the hydrogen atom.

Quantum number	Integer values	Quantized quantity
n	$n\geq 1$	Energy
l	\(0 \leq *l*<n\)	Magnitude of orbital angular momentum
m_l	\(-l \leq m_*l* \leq *l* \)	z-component of orbital angular momentum

Table 12.3.1.2: Spectroscopic notation

Quantum Number *l*	0 1 2 3 4 . . .
Letter	s p d f g . . .

Figure 12.3.1.1shows radial probability distributions for some different states, labelled by spectroscopic notation.

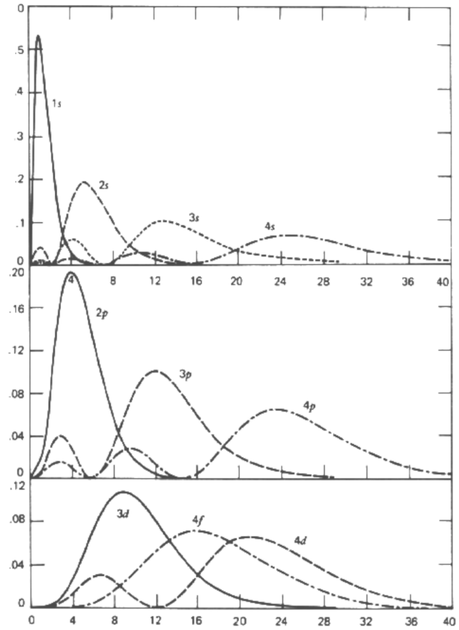

Figure 12.3.1.1: Radial probability distribution for an electron in some low-energy levels of hydrogen. The abscissa is the radius in units of a_0.

The radial probability density P_{nl} is defined such that

$$P_{nl}(r)dr = |R_{nl}(r)|^2 4\pi r^2 dr \tag{12.3.1.16}$$

is the probability of finding the electron with radial coordinate between r and $r+dr$. The functions are normalized so that the total probability of finding the electron at some location is unity. It is interesting to note that each state has $n-l-1$ nodes, or points where the probability goes to zero. This is sometimes called the radial node quantum number and appears in other aspects of quantum theory. It is also interesting that for each n, the state with $l=n-1$ has maximum probability of being found at $r=n^2a_0$, the radius of the orbit predicted by Bohr theory. This indicates that the Bohr model, though known to be incorrect, is at least similar to physical reality in some respects, and it is often helpful to use the Bohr model when trying to visualize certain effects, for example the spin-orbit effect, to be discussed in the next section. The angular probability distributions will not be explored here [1], except to say that they have the property that if the solutions with all possible values of l and m_l for a particular n are summed together, the result is a distribution with spherical symmetry, a feature which helps to greatly simplify applications to multielectron atoms

Footnote

[1] See Eisberg and Resnick, chapter 7, for a more thorough discussion.

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12.3.2: The Spin-Orbit Effect

In order to further explain the structure of the hydrogen atom, one needs to consider that the electron not only has orbital angular momentum $\mathbf{L}$, but also intrinsic angular momentum $\mathbf{S}$, called spin. There is an associated spin operator $\mathbf{S}$, as well as operators S^2 and S_z, just as with $\mathbf{L}$. Usually written in matrix form, these operators yield results analogous to L^2 and L_z when acting on the wavefunction Ψ,

$$S^2\Psi = s(s+1)\hbar^2\Psi$$
$$S_z\Psi = m_s\hbar\Psi$$

where s and m_s are quantum numbers defining the magnitude of the spin angular momentum and its projection onto the z-axis, respectively. For an electron $s = 1/2$ always, and hence the electron can have $m_s = +1/2, -1/2$.

Associated with this angular momentum is an intrinsic magnetic dipole moment

$$\mu_{\mathrm{S}} = -g_s\mu_b\frac{\mathbf{S}}{\hbar} \tag{12.3.2.1}$$

where

$$\mu_b \equiv \frac{e\hbar}{2mc} \tag{12.3.2.2}$$

is a fundamental unit of magnetic moment called the Bohr magneton. The number g_s is called the spin gyromagnetic ratio of the electron, expected from Dirac theory to be exactly 2 but known experimentally to be $g_s = 2.00232$. This is to be compared to the magnetic dipole moment associated with the orbit of the electron,

$$\mu_{\mathrm{l}} = -g_l\mu_b\frac{\mathbf{L}}{\hbar} \tag{12.3.2.3}$$

where $g_l = 1$ is the orbital gyromagnetic ratio of the electron. That is, the electron creates essentially twice as much dipole moment per unit spin angular momentum as it does per unit orbital angular momentum. One expects these magnetic dipoles to interact, and this interaction constitutes the spin-orbit effect.

The interaction is most easily analyzed in the rest frame of the electron, as shown in figure 2. The electron sees the nucleus moving around it with speed v in a circular orbit of radius r, producing a magnetic field

$$B = \frac{Zev}{cr^2}. \tag{12.3.2.4}$$

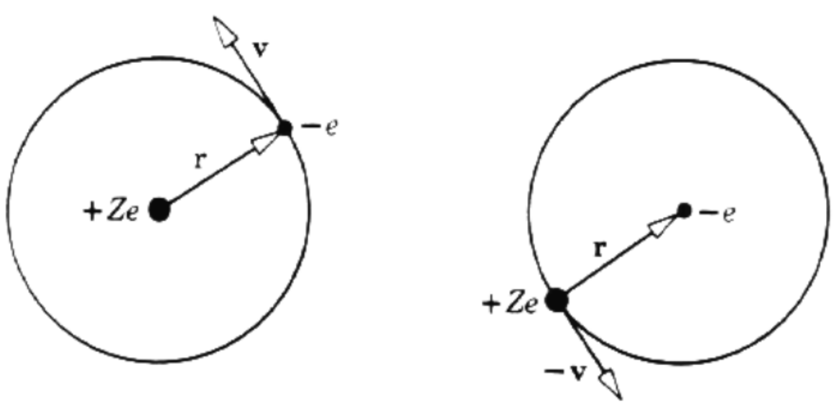

Figure 12.3.2.1:On the left an electron moves around the nucleus in a Bohr orbit. On the right as seen by the electron the nucleus is in a circular orbit.

In terms of the electron orbital angular momentum $L = mrv$, the field may be written

$$\mathbf{B} = \frac{Ze}{mcr^3}\mathbf{L} \tag{12.3.2.5}$$

The spin dipole of the electron has potential energy of orientation in this magnetic field given by

$$\Delta E_{so} = -\mu_S \cdot \mathbf{B}. \tag{12.3.2.6}$$

However, the electron is not in an inertial frame of reference. In transforming back into an inertial frame, a relativistic effect known as Thomas precession is introduced, resulting in a factor of $1/2$ in the interaction energy. With this, the Hamiltonian of the spin-orbit interaction is written

$$\Delta H_{so} = \frac{Ze^2}{2m^2c^2r^3}\mathbf{L}\cdot\mathbf{S} \tag{12.3.2.7}$$

With this term added to the Hamiltonian, the operators L_z and S_z no longer commute with the Hamiltonian, and hence the projections of $\mathbf{L}$ and $\mathbf{S}$ onto the z-axis are not conserved quantities. However, one can define the total angular momentum operator

$$\mathbf{J} = \mathbf{L} + \mathbf{S} \tag{12.3.2.8}$$

It can be shown that the corresponding operators J^2 and J_z do commute with this new Hamiltonian. Physically what happens is that the dipoles associated with the angular momentum vectors $\mathbf{S}$ and $\mathbf{L}$ exert equal and opposite torques on each other, and hence they couple together and precess uniformly around their sum $\mathbf{J}$ in such a way that the projection of $\mathbf{J}$ on z-axis remains fixed. The operators J^2 and J_z acting on Ψ yield

$$\begin{aligned} J^2\Psi &= j(j+1)\hbar^2\Psi \\ J_z\Psi &= m_j\hbar\Psi \end{aligned}$$

where j has possible values

$$j = |l-s|, |l-s|+1, \ldots, l+s-1, l+s. \tag{12.3.2.9}$$

For a hydrogenic atom $s = 1/2$, and hence the only allowed values are $j = l-1/2, l+1/2$, except for $l = 0$, where only $j = 1/2$ is possible. Figure 3 illustrates spin-orbit coupling for particular values of l, j, and m_j.

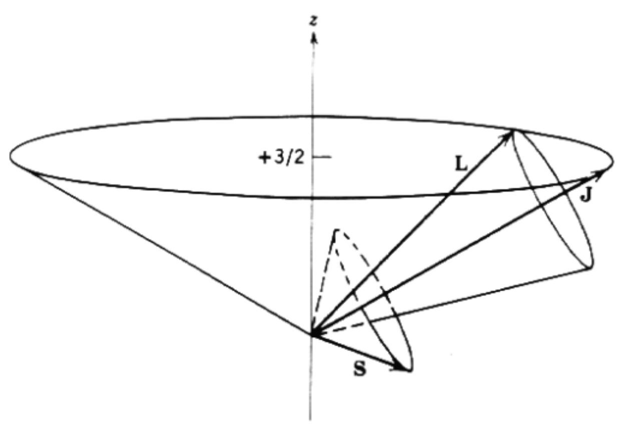

Figure 12.3.2.2: Spin-orbit coupling for a typical case of $s = 1/2, l = 2, j = 5/2$, $m_j = 3/2$, showing how $\mathbf{L}$ and $\mathbf{S}$ precess about $\mathbf{J}$.

Since the coupling is weak and hence the interaction energy is small relative to the principle energy splittings, it is sufficient to calculate the energy correction by first-order perturbation theory using the previously found wavefunctions. The energy correction is then

$$\Delta E_{so} = \langle \Delta H_{so} \rangle = \int \Psi^* \Delta H_{so} \Psi d^3x. \tag{12.3.2.10}$$

The value of $\mathbf{L}\cdot\mathbf{S}$ is easily found by calculating

$$J^2 = \mathbf{J}\cdot\mathbf{J} = L^2 + S^2 + 2\mathbf{L}\cdot\mathbf{S} \tag{12.3.2.11}$$

and hence when acting on Ψ,

$$\mathbf{L}\cdot\mathbf{S}\Psi = \frac{1}{2}\hbar^2[j(j+1)-l(l+1)-s(s+1)]\Psi. \tag{12.3.2.12}$$

One then needs to calulate the expectation of r^{-3}, which is more complicated. The answer is

$$\Delta E_{so} = \left(Z\alpha^4\right) mc^2 \frac{\left[j(j+1)-l(l+1)-\frac{3}{4}\right]}{4n^3 l\left(l+\frac{1}{2}\right)(l+1)}, \tag{12.3.2.13}$$

where the value $s=1/2$ has been included.

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12.3.3: Kinetic Energy Corrections

Before claiming that this formula explains the fine structure of the hydrogen atom, however, one needs to be careful. The correction is of the order α^4, which means it of the order v^4, where v is the electron speed. The kinetic energy used in the Hamiltonian when solving the Schrödinger equation was just $p^2/2m$, which contributed to order α^2. However, the next term in the expansion of the true relativistic kinetic energy is of order p^4 and hence will contribute to order α^4. So if one wishes to quote the energy splittings of the hydrogen atom accurate to order α^4, one had better include the contribution from this further correction.

The relativistic kinetic energy of the electron can be expanded in terms of momentum as

$$T=\frac{p^2}{2m}-\frac{p^4}{8m^3c^2}+\ldots \tag{12.3.3.1}$$

Therefore, the correction to the Hamiltonian is

$$\Delta H_{rel}=-\frac{1}{8m^3c^2}p^4. \tag{12.3.3.2}$$

At first sight, this looks quite complicated, since it involves the operator $p^4=\hbar^4\nabla^4$. However, one can make use of the fact that

$$\frac{p^2}{2m}=E_n-V \tag{12.3.3.3}$$

to get

$$\Delta H_{rel}=-\frac{1}{2mc^2}\left(E_n^2-2E_nV+V^2\right). \tag{12.3.3.4}$$

With $V=-Ze^2/r$, applying first-order perturbation theory to this Hamiltonian reduces to the problem of finding the expectation values of r^{-1} and r^{-2}. This can be done with some effort, and the result is

$$\Delta E_{\text{rel}}=-(Z\alpha)^4mc^2\frac{1}{2n}\left[\frac{1}{\left(l+\frac{1}{2}\right)}-\frac{3}{4n}\right]. \tag{12.3.3.5}$$

Combining this equation with

$$\Delta E_{so}=\left(Z\alpha^4\right)mc^2\frac{\left[j(j+1)-l(l+1)-\frac{3}{4}\right]}{4n^3l\left(l+\frac{1}{2}\right)(l+1)}, \tag{12.3.3.6}$$

from the previous page and using the fact that $j=l-1/2, l+1/2$, the complete energy correction to order $(Z\alpha)^4$ may be written

$$\Delta E_{fs}=\Delta E_{rel}+\Delta E_{so}=-(Z\alpha)^4mc^2\frac{1}{2n}\left[\frac{1}{\left(j+\frac{1}{2}\right)}-\frac{3}{4n}\right]. \tag{12.3.3.7}$$

This energy correction depends only on j and is called the fine structure of the hydrogen atom, since it is of order $\alpha^2\sim10^{-4}$ times smaller than the principle energy splittings. This is why α is known as the fine-structure constant. The fine structure of the hydrogen atom is illustrated in figure 4. Note that all levels are shifted down from the Bohr energies, and that for every n and l there are two states corresponding to $j=l-1/2$ and $j=l+1/2$, except for s states. Also note that states with the same n and j but different l have the same energies, though this will be shown later not to be true due an effect know as the Lamb shift. As an aside, these fine structure splittings were derived by Sommerfeld by modifying the Bohr theory to allow elliptical orbits and then calculating the energy differences between the different states due to differences in the average velocity of the electron. By using the wrong method he got exactly the right answer, a coincidence which caused much confusion at the time.

Strictly speaking, the last equation has only been shown to be correct for $l\neq0$ states, although it turns out to be correct for all l. To do the calculation correctly for $l=0$, one needs to include the effect of an additional term in the Hamiltonian known as the Darwin term, which is purely an effect of relativistic quantum mechanics and can only be understood in the context of the Dirac theory. It is therefore appropriate to discuss the Dirac theory to achieve a more complete understanding of the fine structure of the hydrogen atom.

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12.4: Dirac Theory of the Hydrogen Atom

The theory of Paul Dirac represents an attempt to unify the theories of quantum mechanics and special relativity. That is, one seeks a formulation of quantum mechanics which is Lorentz invariant, and hence consistent with special relativity. For a free particle, relativity states that the energy is given by

$$E+p^2c^2+m^2c^4 \tag{12.4.1}$$

Associating E with a Hamiltonian in quantum mechanics, one has

$$H^2=p^2c^2+m^2c^4 \tag{12.4.2}$$

If H and p are associated with the same operators as in Schrödinger theory, then one expects the wave equation

$$-\hbar\frac{\partial^2}{\partial t^2}\Psi=(-\hbar^2\nabla^2c^2+m^2c^4)\Psi \tag{12.4.3}$$

This is known as the *Klein-Gordan Equation*. Unfortunately, attempts to utilize this equation are not successful, since that which one would wish to interpret as a probability distribution turns out to be not **positive definite**. To alleviate this problem, the square root may be taken to get

$$H=\sqrt{p^2c^2+m^2c^4} \tag{12.4.4}$$

However, this creates a new problem. What is meant by the square root of an operator? The approach is to guess the form of the answer, and the correct guess turns out to be

$$H=c\alpha\cdot p+\beta mc^2 \tag{12.4.5}$$

With this form of the Hamiltonian, the wave equation can be written

$$i\hbar\frac{\partial\chi}{\partial t}=(c\alpha\cdot p+\beta mc^2)\chi \tag{12.4.6}$$

In order for this to be valid, one hopes that when it is squared the **Klein-Gordan equation** is recovered. For this to be true, Equation 12.4.6 must be interpreted as a matrix equation, where α and β are at least 4×4 matrices and the wavefunction χ is a four-component column matrix.

It turns out that Equation 12.4.6 describes only a particle with spin 1/2. This is fine for application to the hydrogen atom, since the electron has spin 1/2, but why should it be so? The answer is that the linearization of the Klein-Gordan equation is not unique. The particular linearization used here is the simplest one, and happens to describe a particle of spin 1/2, but other more complicated Hamiltonians may be constructed to describe particles of spin 0,1,5/2 and so on. The fact that the relativistic Dirac theory automatically includes the effects of spin leads to an interesting conclusion - spin is a relativistic effect. It can be added by hand to the non-relativistic Schödinger theory with satisfactory results, but spin is a natural consequence of treating quantum mechanics in a completely relativistic fashion.

> *Spin is a relativistic effect*

Including the potential now in the Hamiltonian, Equation 12.4.6 becomes

$$i\hbar\frac{\partial\chi}{\partial t}=\left(c\alpha\cdot\mathbf{p}+\beta mc^2-\frac{Ze^2}{r}\right)\chi. \tag{12.4.7}$$

When the square root was taken to linearize the Klein-Gordan equation, both a positive and a negative energy solution was introduced. One can write the wavefunction

$$\chi=\begin{pmatrix}\Psi_+\\ \Psi_-\end{pmatrix}, \tag{12.4.8}$$

where Ψ_+ represents the two components of χ associated with the positive energy solution and Ψ_- represents the components associated with the negative energy solution. The physical interpretation is that Ψ_+ is the particle solution, and Ψ_- represents an anti-particle. Anti-particles are thus predicted by Dirac theory, and the discovery of anti-particles obviously represents a huge triumph for the theory. In hydrogen, however, the contribution of Ψ_- is small compared to Ψ_+. With enough effort, the equations for Ψ_+ and Ψ_- can be decoupled to whatever order is desired. When this is done, the Hamiltonian to order v^2/c^2 can be written

$$H + H_s + \Delta H_{rel} + \Delta H_{so} + \Delta H_d \tag{12.4.9}$$

where

- H_s is the original Schrödinger Hamiltonian,
- ΔH_{rel} is the relativistic correction to the kinetic energy,
- ΔH_{so} is the spin-orbit term, and
- ΔH_d is the previously mentioned Darwin term.

The Darwin Term

The physical origin of the Darwin term is a phenomenon in Dirac theory called *zitterbewegung*, whereby the electron does not move smoothly, but instead undergoes extremely rapid small-scale fluctuations, causing the electron to see a smeared-out Coulomb potential of the nucleus.

The Darwin term may be written

$$\Delta H_d = -\frac{e\hbar^2}{8m^2c^2}\nabla^2\Psi \tag{12.4.10}$$

For the hydrogenic-atom potential $V = \dfrac{Ze}{r}$, Equation 12.4.10is

$$H_d = -\frac{Ze^2\pi\hbar^2}{2m^2c^2}\delta^3(r) \tag{12.4.11}$$

When first-order perturbation theory is applied, the energy correction depends on $|\Psi(0)|^2$. This term will only contribute for *s* states (i.e., (*l*=0)), since only these wavefunctions have **non-zero probability** for finding the electron at the origin. The energy correction for $l = 0$ can be calculated to be

$$\Delta E_d = (Z\alpha)^4 mc^2 \frac{1}{2n^3} \tag{12.4.12}$$

Including this term, the fine-structure splitting can be reproduced for all *l*. All the effects that go into fine structure are thus a natural consequence of the Dirac theory.

The hydrogen atom can be solved exactly in Dirac theory, where the states found are simultaneous eigenstates of H, J^2, and J_z, since these operators can be shown to mutually commute. The exact energy levels in Dirac theory are

$$E_{nj} = mc^2\left[1+\left(\frac{Z\alpha}{n-(j+\frac{1}{2})+\sqrt{(j+\frac{1}{2})^2-(Z\alpha)^2}}\right)^2\right]^{-1/2}. \tag{12.4.13}$$

This can be expanded in powers of $Z\alpha$, yielding

$$E_{nj} = mc^2\left\{1-\frac{1}{2}\frac{(Z\alpha)^2}{n^2}\left[1+\frac{(Z\alpha)^2}{n}\left(\frac{1}{j+\frac{1}{2}}-\frac{3}{4n}\right)\right]+\dots\right\} \tag{12.4.14}$$

This includes an amount mc^2 due to the relativistic energy associated with the rest mass of the electron, along with the principle energy levels and fine structure, in exact agreement to order $(Z\alpha)^4$ with what was previously calculated. However, even this exact solution in Dirac theory is not a complete description of the hydrogen atom, and so the the next section describes further effects not yet discussed.

Footnote

See Bjorken and Drell Chapter 4 for a thorough discussion of the transfer

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SECTION OVERVIEW

12.5: Smaller Effects

One correction to the Dirac theory involves the use of the reduced electron mass, which was previously discussed. Another involves considering that the proton has some finite size and is not exactly a point charge. Instead of having a $V = -Ze^2/r$ potential energy, one might imagine something like

$$V = \begin{cases} -\frac{Ze^2}{r} & r > r_0 \\ -V_0 & r \leq r_0, \end{cases} \tag{12.5.1}$$

where r_0 is some representative size of the proton $\sim 10^{-13}$ cm. Like the Darwin term, this will only affect s states, since only in these states can the electron be found at the origin. However, even for s states this correction turns out to be of the order $\Delta E \sim 10^{-10}$eV, and hence it is not very important. Other effects will now be discussed which are more important, not only because the energy shifts are larger but because they split the energy levels of states that would otherwise be degenerate

From this point on, effects will only be discussed only in terms of the hydrogen atom, although they can be extended to other one-electron atoms.

Thumbnail: Pieter Zeeman

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12.5.1: Hyperfine Structure

To this point, the nucleus has been assumed to interact with the electron only through its electric field. However, like the electron, the proton has spin angular momentum with $s=1/2$, and associated with this angular momentum is an intrinsic dipole moment

$$\mu_{\mathrm{p}}=\gamma_{p}\frac{e}{Mc}\mathbf{S}_{\mathrm{p}}, \tag{12.5.1.1}$$

where M is the proton mass and γ_p is a numerical factor known experimentally to be $\gamma_p=2.7928$. Note that the proton dipole moment is weaker than the electron dipole moment by roughly a factor of $M/m\sim 2000$, and hence one expects the associated effects to be small, even in comparison to fine structure, so again treating the corrections as a perturbation is justified. The proton dipole moment will interact with both the spin dipole moment of the electron and the orbital dipole moment of the electron, and so there are two new contributions to the Hamiltonian, the nuclear spin-orbit interaction and the spin-spin interaction. The derivation for the nuclear spin-orbit Hamiltonian is the same as for the electron spin-orbit Hamiltonian, except that the calculation is done in the frame of the proton and hence there is no factor of $1/2$ from the Thomas precession. The nuclear spin-orbit Hamiltonian is

$$\Delta H_{pso}=\frac{\gamma_{p}e^{2}}{mMc^{2}r^{3}}\mathbf{L}\cdot\mathbf{S}_{\mathrm{p}} \tag{12.5.1.2}$$

The spin-spin Hamiltonian can be derived by considering the field produced by the proton spin dipole, which can be written

$$\mathbf{B}(\mathbf{r})=\frac{1}{r^{3}}\left[3\frac{(\mu_{\mathrm{p}}\cdot\mathbf{r})\,\mathbf{r}}{r^{2}}-\mu_{\mathrm{p}}\right]+\frac{8\pi}{3}\mu_{\mathrm{p}}\delta^{3}(\mathbf{r}). \tag{12.5.1.3}$$

The first term is just the usual field associated with a magnetic dipole, but the second term requires special explanation. Normally, when one considers a dipole field, it is implicit that one is interested in the field far from the dipole-that is, at distances far from the source compared to the size of the current loop producing the dipole. However, every field line outside the loop must return inside the loop, as shown in figure 6. If the size of the current loop goes to zero, then the field will be infinite at the origin, and this contribution is what is reflected by the second term in equation 77. The electron has additional energy

$$\Delta E_{ss}=-\mu_{\mathrm{e}}\cdot\mathbf{B} \tag{12.5.1.4}$$

due to the interaction of its spin dipole with this field, and hence the spinspin Hamiltonian is

$$\Delta H_{ss}=\frac{\gamma_{p}e^{2}}{mMc^{2}}\left\{\frac{1}{r^{3}}\left[3\left(\mathbf{S}_{\mathrm{p}}\cdot\hat{r}\right)\left(\mathbf{S}_{\mathrm{e}}\cdot\hat{r}\right)-\left(\mathbf{S}_{\mathrm{p}}\cdot\mathbf{S}_{\mathrm{e}}\right)\right]+\frac{8\pi}{3}\left(\mathbf{S}_{\mathrm{p}}\cdot\mathbf{S}_{\mathrm{e}}\right)\delta^{3}(\mathbf{r})\right\}. \tag{12.5.1.5}$$

The operator J_z does not commute with this Hamiltonian. However, one can define the total angular momentum

$$\mathbf{F}=\mathbf{L}+\mathbf{S}_{\mathrm{e}}+\mathbf{S}_{\mathrm{p}}=\mathbf{J}+\mathbf{S}_{\mathrm{p}} \tag{12.5.1.6}$$

The corresponding operators F^2 and F_z commute with the Hamiltonian, and they introduce new quantum numbers f and m_f through the relations

$$F^{2}\Psi=f(f+1)\hbar^{2}\Psi$$

$$F_{z}\Psi=m_{f}\hbar\Psi$$

The quantum number f has possible values $f=j+1/2, j-1/2$ since the proton is spin $1/2$, and hence every energy level associated with a particular set of quantum numbers n, l, and j will be split into two levels of slightly different energy, depending on the relative orientation of the proton magnetic dipole with the electron state.

Consider first the case $l=0$, since the hyperfine splitting of the hydrogen atom ground state is of the most interest. Since the electron has no orbital angular momentum, there is no nuclear spin-orbit effect. It can be shown that because the wavefunction has spherical symmetry, only the delta function term contributes from the spin-spin Hamiltonian. First order perturbation theory yields

$$\Delta E_{hf}=\frac{8\pi\gamma_{p}e^{2}}{3mMc^{2}}\left(\mathbf{S}_{\mathrm{p}}\cdot\mathbf{S}_{\mathrm{e}}\right)|\Psi(0)|^{2} \tag{12.5.1.7}$$

Like the Darwin term, this depends on the probability of finding the electron at the origin. The value of $\mathbf{S}_{\mathrm{p}}\cdot\mathbf{S}_{\mathrm{e}}$ can be found by squaring $\mathbf{F}$, which with $l=0$ gives

$$F^2 = S_e^2 + S_p^2 + 2\mathbf{S}_\mathrm{e} \cdot \mathbf{S}_\mathrm{p} \tag{12.5.1.8}$$

Hence

$$\mathbf{S}_\mathrm{p} \cdot \mathbf{S}_\mathrm{e} = \frac{\hbar^2}{2}\left[f(f+1) - s_p\left(s_p+1\right) - s_e\left(s_e+1\right)\right] = \frac{\hbar^2}{2}\left[f(f+1) - \frac{3}{2}\right], \tag{12.5.1.9}$$

where the last step includes the values $s_e = s_p = 1/2$. The hyperfine energy shift for $l = 0$ is then

$$\Delta E_{hf} = \left(\frac{m}{M}\right)\alpha^4 mc^2 \frac{4\gamma_p}{3n^3}\left[f(f+1) - \frac{3}{2}\right]. \tag{12.5.1.10}$$

It is easy to see from this expression that the hyperfine splittings are smaller than fine structure by a factor of M/m. For the specific case of the ground state of the hydrogen atom $(n = 1)$, the energy separation between the states of $f = 1$ and $f = 0$ is

$$\Delta E_{hf}(f=1) - \Delta E_{hf}(f=0) = 5.9 \times 10^{-6}\,\mathrm{eV} \tag{12.5.1.11}$$

The photon corresponding to the transition between these two states has frequency and wavelength

$$\begin{aligned} \nu &= 1420.4057517667(10)\,\mathrm{MHz} \\ \lambda &= 21.1\ \mathrm{cm}. \end{aligned}$$

This is the source of the famous " 21 cm line," which is extremely useful to radio astronomers for tracking hydrogen in the interstellar medium of galaxies. The transition is exceedingly slow, but the huge amounts of interstellar hydrogen make it readily observable. It is too slow to be seen in a terrestrial laboratory by spontaneous emission, but the frequency can be measured to very high accuracy by using stimulated emission, and this frequency is in fact one of the best-known numbers in all of physics.

For $l \neq 0$, the δ term does not contribute but the other terms in the spin-spin Hamiltonian as well as the nuclear spin-orbit Hamiltonian do contribute. The calculation is much harder but yields

$$\Delta E_{hf} = \left(\frac{m}{M}\right)\alpha^4 mc^2 \frac{\gamma_p}{2n^3} \frac{\pm 1}{\left(f+\frac{1}{2}\right)\left(l+\frac{1}{2}\right)} \tag{12.5.1.12}$$

for $f = j \pm 1/2$.

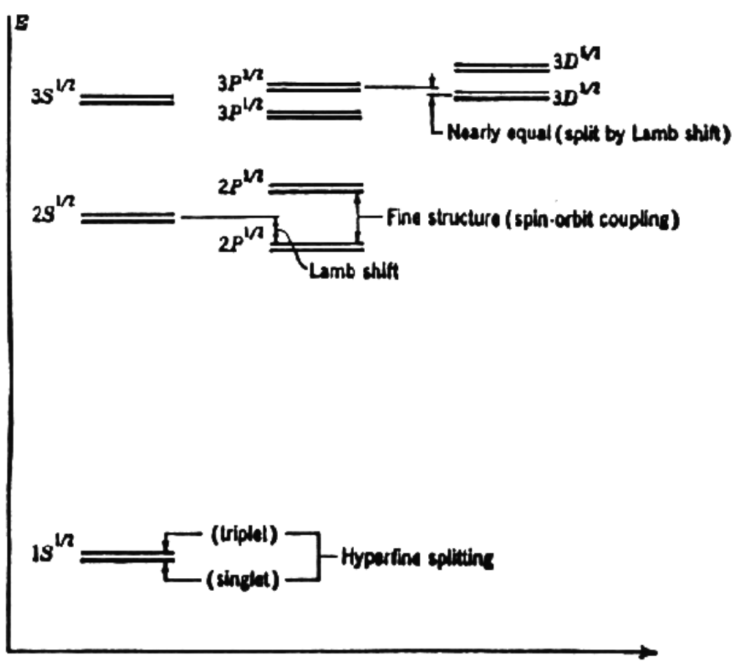

Figure 12.5.1.1: Some lowenergy states of the hydrogen atom including ne struc ture hyperne structure and the Lamb shift

Figure $12.5.1.1$ shows a revised version of the structure of the hydrogen atom, including the Lamb shift and hyperfine structure. Note that each hyperfine state still has a $2f+1$ degeneracy associated with the different possible values of m_f which correspond to different orientations of the total angular momentum with respect to the z-axis. For example, in the ground state, the higher-energy state $f=1$ is actually a triplet, consisting of three degenerate states, and the $f=0$ state is a singlet. This degeneracy can be broken by the presence of an external magnetic field.

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12.5.2: The Lamb Shift

According to Dirac and Schrödinger theory, states with the same n and j quantum numbers but different l quantum numbers ought to be degenerate. However, a famous experiment by Lamb and Retherford in 1947 showed that the $2s_{1/2}(n=2, l=0, j=1/2)$ and $2p_{1/2}(n=2, l=1, j=1/2)$ states of the hydrogen atom were not degenerate, but that the s state had slightly higher energy by an amount now known to be $E/h = 1057.864\text{MHz}$. The effect is explained by the theory of quantum electrodynamics, in which the electromagnetic interaction itself is quantized. Some of the effects of this theory which cause the Lamb shift are shown in the Feynman diagrams of figure 5. Table 3 shows how much each of these contribute to the splitting of $2s_{1/2}$ and $2p_{1/2}$. The most important effect is illustrated by the center diagram, which is a result of the fact that the ground state of the electromagnetic field is not zero, but rather the field undergoes "vacuum fluctuations" that interact with the electron. Any discussion of the calculation is beyond the scope of this paper, so the answers will merely be given. For $l=0$,

$$\Delta E_{Lamb} = \alpha^5 mc^2 \frac{1}{4n^3}\{k(n,0)\} \tag{12.5.2.1}$$

where $k(n,0)$ is a numerical factor which varies slightly with n from 12.7 to 13.2. For $l \neq 0$,

$$\Delta E_{Lamb} = \alpha^5 mc^2 \frac{1}{4n^3}\left\{k(n,l) \pm \frac{1}{\pi\left(j+\frac{1}{2}\right)\left(l+\frac{1}{2}\right)}\right\} \tag{12.5.2.2}$$

for $j = l \pm 1/2$, where $k(n,l)$ is a small numerical factor < 0.05 which varies slightly with n and l. Notice that the Lamb shift is very small except for $l=0$.

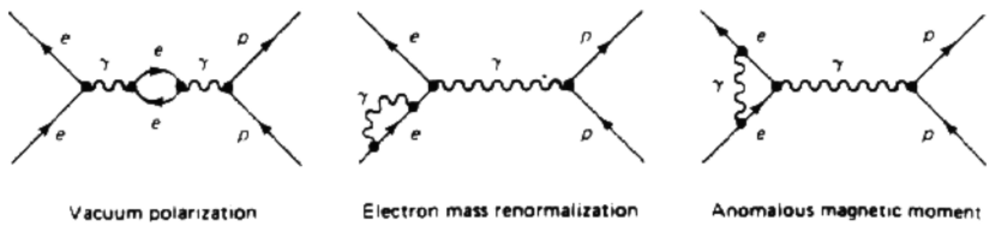

Figure 12.5.2.1:Feynman loop diagrams showing some effects that contribute to the Lamb shift

Table 12.5.2.1: Contribution of different effects to the energy splitting of $2s_{1/2}$ and $2p_{1/2}$ in hydrogen. Numbers are given in units of frequency $\nu = E/h$.

Effect	Energy contribution
Vacuum polarization	-27 MHz
Electron mass renormalization	+1017 MHz
Anomalous magnetic moment	+68 MHz
Total	+1058 MHz

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12.5.3: The Zeeman Effect

When considering the Zeeman effect, it is easiest first to consider the hydrogen atom without hyperfine structure. Then m_j is a good quantum number, and the atom has a $2j+1$ degeneracy associated with the different possible values of m_j. In the presence of an external magnetic field, these different states will have different energies due to having different orientations of the magnetic dipoles in the external field. The splitting of these energy levels is called the Zeeman effect.

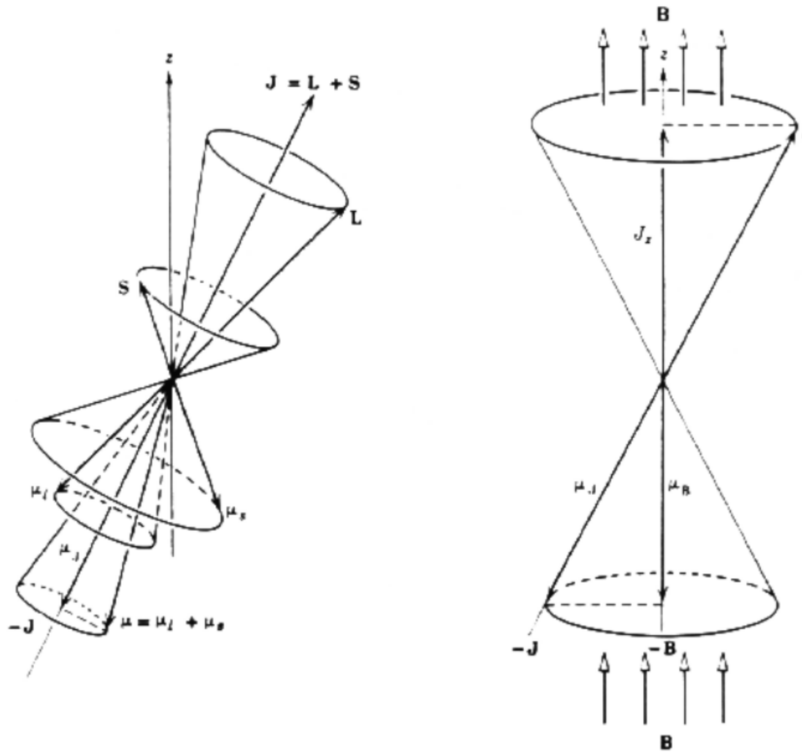

Figure 12.5.3.1:Geometry of the Zeeman effect. On the left, the total dipole moment μ precesses around the total angular momentum J. On the right, $\mathbf{J}$ precesses much more slowly about the magnetic field.

Figure 12.5.3.1 illustrates the geometry of the Zeeman effect. The total magnetic dipole moment of the electron is

$$\mu=\mu_{\mathrm{l}}+\mu_{\mathrm{S}}=-\frac{\mu_b}{\hbar}(\mathbf{L}+2\mathbf{S}) \tag{12.5.3.1}$$

where $g_l=1$ and $g_s=2$ have been used. Because of the difference in the orbital and spin gyromagnetic ratios of the electron, this is not in general parallel to

$$\mathbf{J}=\mathbf{L}+\mathbf{S} \tag{12.5.3.2}$$

So, as $\mathbf{L}$ and $\mathbf{S}$ precess about $\mathbf{J}$, the total dipole moment μ also precesses about J. Assuming the external field to be in the z direction, this field causes $\mathbf{J}$ to precess about the z-axis. Typical internal magnetic fields in the hydrogen atom can be shown to be of the order 1 Tesla. If the external field is much weaker than 1 Tesla, which it is for almost all practical purposes, then the precession of $\mathbf{J}$ around the z-axis will take place much more slowly than the precession of μ around $\mathbf{J}$. The Hamiltonian of the Zeeman effect is

$$\Delta H_z=-\mu\cdot\mathbf{B}=-\mu_B B, \tag{12.5.3.3}$$

where μ_B is the projection of the dipole moment onto the direction of the field, the z-axis. Because of the difference in the precession rates, it is reasonable to evaluate μ_b by first evaluating the projection of μ onto $\mathbf{J}$, called μ_J, and then evaluating the projection of this onto $\mathbf{B}$, thus giving some average projection of μ onto $\mathbf{B}$. First, the projection of μ onto $\mathbf{J}$ is

$$\mu_J=\frac{\mu\cdot\mathbf{J}}{J}=-\frac{\mu_b}{\hbar}\frac{(\mathbf{L}+2\mathbf{S})\cdot(\mathbf{L}+\mathbf{S})}{J}. \tag{12.5.3.4}$$

Then

$$\mu_B = \mu_J \frac{\mathbf{J}\cdot\mathbf{B}}{JB} = \mu_J \frac{J_z}{J} = -\frac{\mu_b}{\hbar}\frac{(\mathbf{L}+2\mathbf{S})\cdot(\mathbf{L}+\mathbf{S})J_z}{J^2}. \tag{12.5.3.5}$$

Evaluating the dot product using again that $J^2 = L^2 + S^2 + 2\mathbf{L}\cdot\mathbf{S}$, this becomes

$$\mu_B = -\frac{\mu_b}{\hbar}\frac{\left(3J^2 + S^2 - L^2\right)}{2J^2} J_z. \tag{12.5.3.6}$$

So when first order perturbation theory is applied, the energy shift is

$$\Delta E_z = \mu_b B g m_j, \tag{12.5.3.7}$$

where

$$g = 1 + \frac{j(j+1) + s(s+1) - l(l+1)}{2j(j+1)} \tag{12.5.3.8}$$

is called the Landé g factor for the particular state being considered. Note that if $s=0$, then $j=l$ so $g=1$, and if $l=0, j=s$ so $g=2$. The Landé g factor thus gives some effective gyromagnetic ratio for the electron when the total dipole moment is partially from orbital angular momentum and partially from spin. From equation 97 , it can be seen that the energy shift caused by the Zeeman effect is linear in B and m_j, so for a set of states with particular values of n, l, and j, the individual states with different m_j will be equally spaced in energy, separated by $\mu_b B g$. However, the spacing will in general be different for a set of states with different n, l, and j due to the difference in the Landé g factor.

Including hyperfine structure with the Zeeman effect is more difficult, since the field associated with the proton magnetic dipole moment is weak, and hence it does not take a particularly strong external field to make the Zeeman effect comparable in magnitude to the strength of the hyperfine interactions. The approximation of small external field is thus not practical when discussing the Zeeman splitting of hyperfine structure. However, it can be treated, and the result for the most important case of the Zeeman splitting of the hyperfine levels in the ground state of hydrogen [1] is shown in Figure 12.5.3.2 The degeneracy of the triplet state is lifted, the three states of $m_f = -1, 0, +1$ having different energies in the external field. Notice how the splitting is linear for small external field, but then deviates as the field gets larger. The " 21 cm " transitions shown on the right will have slightly different energies, and measuring the amount of this splitting is a good tool for radio astronomers to measure magnetic fields in the interstellar medium.

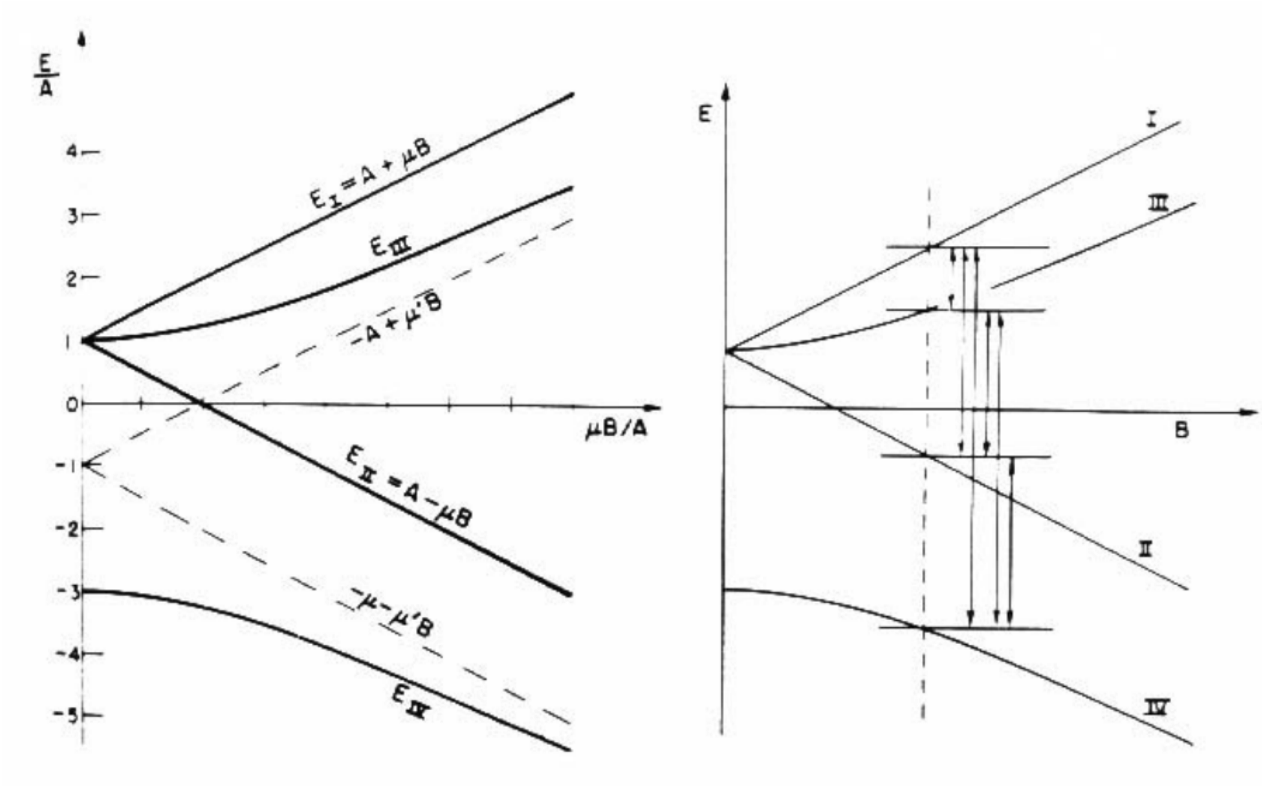

Figure 12.5.3.2:On left, Zeeman splitting of the hyperfine levels in the ground state $\left(1 s_{1/2}\right)$ of hydrogen. On right, some possible transitions between these states.

Footnote

1. See Feynman volume III chapter for a discussion of the calculation of

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12.6: Conclusion and References

To summarize the relative strengths of the effects discussed in this paper, table 4 gives some numbers for comparison of some energy splittings in the hydrogen atom. Note how much larger the principle energy splittings are than any of the other effects.

Table 12.6.1:Differences in energy of some particular pairs of states in the hy drogen atom The state of lower energy is listed rst

Effect	States	Energy difference (eV)
Principal splitting	$1s_(1//2), 2s_(1//2)$	10.2
Fine structure	$2p_(1//2), 2p_(3//2)$	$4.5xx10^(-5)$
Lamb shift	$2p_(1//2), 2s_(1//2)$	$4.4xx10^(-6)$
	$3d_(3//2), 3p_(3//2)$	$1.7xx10^(-8)$
Hyperfine structure	$1s_(1//2)(f=0), 1s_(1//2)(f=1)$	$5.9xx10^(-6)$
Zeeman effect (B=10 gauss)	$2s_(1//2)(m_(j)=-1//2), 2s_(1//2)(m_(j)=+1//2)$	$1.2xx10^(-7)$

The hydrogen atom is one of the most important dynamical systems in all of physics, for several reasons:

1. Hydrogen is the most abundant stuff in the known universe. About 92% by number of the nuclei in the universe are hydrogen, 75% by mass.
2. Even though it is a relatively simple system, the physics of the hydrogen atom contains many important quantum mechanical concepts that extend to more complex atoms and other systems.
3. Because of its relative simplicity, the hydrogen atom can be solved theoretically to very high precision. Experimental measurements involving hydrogen thus offer very sensitive tests of modern physical theories, like quantum electrodynamics.

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CHAPTER OVERVIEW

13: Miscellaneous Quantum Mechanics Topics

13.1: Bell's Theorem
13.2: Black Hole Thermodynamics
13.3: Complementarity and Copenhagen Interpretation
13.4: Double Slit
13.5: Flash Animations for Physics
13.6: Locality and Quantum Mechanics
13.7: Particle in a 2-dimensional box
13.8: Quantum Entanglement
13.9: Quantum Interference
13.10: Quantum Mechanics- a Poor Person's Guide
13.11: Quantum Mechanics- Interpretation
13.12: Quantum Teleportation
13.13: Schrödinger's Cat
13.14: Stern-Gerlach Experiment
13.15: The Bohr Model of the Atom
13.16: The Development of Quantum Mechanics
13.17: Two analogies to Bell's Theorem
13.18: Wave-Particle Duality

13.1: Bell's Theorem

INTRODUCTION

In 1975 Stapp called Bell's Theorem "the most profound discovery of science." Note that he says *science*, not *physics*. I agree with him.

In this document, we shall explore the theorem. We assume some familiarity with the concept of wave-particle duality. We also assume considerable familiarity with the Stern-Gerlach experiment and the concept of a correlation experiment.

A much simpler introduction to the theorem, with some loss of completeness, has been prepared. You may access an html or pdf version with the links to the right.

The origins of this topic is a famous paper by Einstein, Rosen and Podolsky (EPR) in 1935; its title was *Can Quantum-Mechanical Description of Physical Reality be Considered Complete?* They considered what Einstein called the "spooky action-at-a-distance" that seems to be part of Quantum Mechanics, and concluded that the theory must be incomplete if not outright wrong. As you probably already know, Einstein never did accept Quantum Mechanics. One of his objections was that "God does not play at dice with the universe." Bohr responded: "Quit telling God what to do!"

In the early 1950's David Bohm (not "Bohr") was a young Physics professor at Princeton University. He was assigned to teach Quantum Mechanics and, as is common, decided to write a textbook on the topic; the book is still a classic. Einstein was at Princeton at this time, and as Bohm finished each chapter of the book Einstein would critique it. By the time Bohm had finished the book Einstein had convinced him that Quantum Mechanics was at least incomplete. Bohm then spent many years in search of *hidden variables*, unobserved factors inside, say, a radioactive atom that determines when it is going to decay. In a hidden variable theory, the time for the decay to occur is not random, although the variable controlling the process is hidden from us. We will discuss Bohm's work extensively later in this document.

In 1964 J.S. Bell published his theorem. It was cast in terms of a hidden variable theory. Since then, other proofs have appeared by d'Espagnat, Stapp, and others that are not in terms of hidden variables. Below we shall do a variation on d'Espagnat's proof that I devised; it was originally published in the American Journal of Physics **50**, 811 - 816 (1982).

PROVING BELL'S INEQUALITY

We shall be *slightly* mathematical. The details of the math are not important, but there are a couple of pieces of the proof that will be important. The result of the proof will be that for any collection of objects with three different parameters, *A*, *B* and *C*:

The number of objects which have parameter A but not parameter B plus the number of objects which have parameter B but not parameter C is greater than or equal to the number of objects which have parameter A but not parameter C.

We can write this more compactly as:

Number(A, not B) + Number(B, not C) greater than or equal to Number(A, not C)

The relationship is called *Bell's inequality*.

In class I often make the students the collection of objects and choose the parameters to be:

A: male **B**: height over 5' 8" (173 cm) **C**: blue eyes

Then the inequality becomes that the number of men students who do not have a height over 5' 8" plus the number of students, male and female, with a height over 5' 8" but who do not have blue eyes is greater than or equal to the number of men students who do not have blue eyes. I absolutely guarantee that for any collection of people this will turn out to be true.

It is important to stress that we are not making any statistical assumption: the class can be big, small or even zero size. Also, we are not assuming that the parameters are independent: note that there tends to be a correlation between gender and height.

Sometimes people have trouble with the theorem because we will be doing a variation of a technique called *proof by negation*. For example, here is a syllogism:

All spiders have six legs. All six legged creatures have wings. Therefore all spiders have wings

If we ever observe a spider that does not have wings, then we know that at least one and possibly both of the assumptions of the syllogism are incorrect. Similarly, we will derive the inequality and then show an experimental circumstance where it is not true.

Thus we will know that at least one of the assumptions we used in the derivation is wrong.

Also, we will see that the proof and its experimental tests have absolutely nothing to do with Quantum Mechanics.

Now we are ready for the proof itself. First, I assert that:

Number(A, not B, C) + Number(not A, B, not C) must be either 0 or a positive integer

or equivalently:

Number(A, not B, C) + Number(not A, B, not C) greater than or equal to 0

This should be pretty obvious, since either no members of the group have these combinations of properties or some members do.

Now we add **Number(A, not B, not C) + Number(A, B, not C)** to the above expression. The left hand side is:

Number(A, not B, C) + Number(A, not B, not C) + Number(not A, B, not C) + Number(A, B, not C)

and the right hand side is:

0 + Number(A, not B, not C) + Number(A, B, not C)

But this right hand side is just:

Number(A, not C)

since for all members either **B** or **not B** must be true. In the classroom example above, when we counted the number of men without blue eyes we include both those whose height was over 5' 8" and those whose height was not over 5' 8".

Above we wrote "since for all members either **B** or **not B** must be true." This will turn out to be important.

We can similarly collect terms and write the left hand side as:

Number(A, not B) + Number(B, not C)

Since we started the proof by asserting that the left hand side is greater than or equal to the right hand side, we have proved the inequality, which I re-state:

Number(A, not B) + Number(B, not C) greater than or equal to Number(A, not C)

We have made two assumptions in the proof. These are:

- Logic is a valid way to reason. The whole proof is an exercise in logic, at about the level of the "Fun With Numbers" puzzles one sometimes sees in newspapers and magazines.
- *Parameters exist whether they are measured or not.* For example, when we collected the terms **Number(A, not B, not C) + Number(A, B, not C)** to get **Number(A, not C)**, we assumed that either **not B** or **B** is true for every member.

APPLYING BELL'S INEQUALITY TO ELECTRON SPIN

Consider a beam of electrons from an electron gun. Let us set the following assignments for the three parameters of Bell's inequality:

A: electrons are "spin-up" for an "up" being defined as straight up, which we will call an angle of zero degrees. **B**: electrons are "spin-up" for an orientation of 45 degrees. **C**: electrons are "spin-up" for an orientation of 90 degrees.

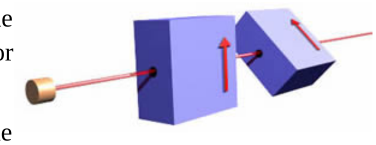
Then Bell's inequality will read:

Number(spin-up zero degrees, not spin-up 45 degrees) + Number(spin-up 45 degrees, not spin-up 90 degrees) greater than or equal to Number(spin-up zero degrees, not spin-up 90 degrees)

But consider trying to measure, say, **Number(A, not B)**. This is the number of electrons that are spin-up for zero degrees, but are not spin-up for 45 degrees. Being "not spin-up for 45 degrees" is, of course, being spin-*down* for 45 degrees.

We know that if we measure the electrons from the gun, one-half of them will be spin-up and one-half will be spin-down for an orientation of 0 degrees, and which will be the case for an individual electron is random. Similarly, if measure the electrons with the filter oriented at 45 degrees, one-half will be spin-down and one-half will be spin-up.

But if we try to measure the spin at both 0 degrees and 45 degrees we have a problem.

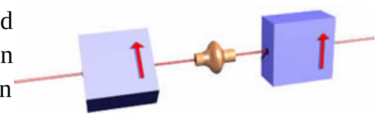


The figure to the right shows a measurement first at 0 degrees and then at 45 degrees. Of the electrons that emerge from the first filter, 85% will pass the second filter, not 50%. Thus for electrons that are measured to be spin-up for 0 degrees, 15% are spin-down for 45 degrees.

Thus measuring the spin of an electron at an angle of zero degrees irrevocably changes the number of electrons which are spin-down for an orientation of 45 degrees. If we measure at 45 degrees first, we change whether or not it is spin-up for zero degrees. Similarly for the other two terms in this application of the inequality. This is a consequence of the Heisenberg Uncertainty Principle. So this inequality is not experimentally testable.

In our classroom example, the analogy would be that determining the gender of the students would change their height. Pretty weird, but true for measuring electron spin.

However, recall the correlation experiments that we discussed earlier. Imagine that the electron pairs that are emitted by the radioactive substance have a total spin of zero. By this we mean that if the right hand electron is spin-up its companion electron is guaranteed to be spin-down provided *the two filters have the same orientation*.



Say in the illustrated experiment the left hand filter is oriented at 45 degrees and the right hand one is at zero degrees. If the left hand electron passes through its filter then it is spin-up for an orientation of 45 degrees. Therefore we are guaranteed that if we had measured its companion electron it would have been spin-down for an orientation of 45 degrees. We are simultaneously measuring the right-hand electron to determine if it is spin-up for zero degrees. And since no information can travel faster than the speed of light, the left hand measurement cannot disturb the right hand measurement.

So we have "beaten" the Uncertainty Principle: we have determined whether or not the electron to the right is **spin-up zero degrees, not spin-up 45 degrees** by measuring its spin at zero degrees and its companion's spin at 45 degrees.

Now we can write the Bell inequality as:

Number(right spin-up zero degrees, left spin-up 45 degrees) + Number(right spin-up 45 degrees, left spin-up 90 degrees) greater than or equal to Number(right spin-up zero degrees, left spin-up 90 degrees)

This completes our proof of Bell's Theorem.

The same theorem can be applied to measurements of the polarization of light, which is equivalent to measuring the spin of photon pairs.

The experiments have been done. For electrons the left polarizer is set at 45 degrees and the right one at zero degrees. A beam of, say, a billion electrons is measured to determine **Number(right spin-up zero degrees, left spin-up 45 degrees)**. The polarizers are then set at 90 degrees/45 degrees, another billion electrons are measured, then the polarizers are set at 90 degrees/zero degrees for another billion electrons.

The result of the experiment is that the inequality is violated. The first published experiment was by Clauser, Horne, Shimony and Holt in 1969 using photon pairs. The experiments have been repeated many times since.

The experiments done so far have been for pairs of electrons, protons, photons and ionised atoms. It turns out that doing the experiments for photon pairs is easier, so most tests use them. Thus, in most of the remainder of this document the word "electron" is generic.

Technical note: You may recall from our discussion of the Stern-Gerlach experiment that doing a correlation experiment for electrons with the polarisers at some relative angle is equivalent to doing the experiment for photons with the polarisers at half the relative angle of the electron polarisers. Thus, when we discuss an electron measurement with the polarisers at, say, zero degrees and 45 degrees, for a photon experiment it would be zero degrees and 22.5 degrees.

In the last section we made two assumptions to derive Bell's inequality which here become:

- Logic is valid.
- Electrons have spin in a given direction even if we do not measure it.

Now we have added a third assumption in order to beat the Uncertainty Principle:

- No information can travel faster than the speed of light.

We will state these a little more succinctly as:

1. Logic is valid.
2. There is a reality separate from its observation
3. Locality.

You will recall the we discussed proofs by negation. The fact that our final form of Bell's inequality is experimentally violated indicates that at least one of the three assumptions we have made have been shown to be wrong.

You will also recall that earlier we pointed out that the theorem and its experimental tests have nothing to do with Quantum Mechanics. However, the fact that Quantum Mechanics correctly predicts the correlations that are experimentally observed indicates that the theory too violates at least one of the three assumptions.

Finally, as we stated, Bell's original proof was in terms of hidden variable theories. His assumptions were:

1. Logic is valid.
2. Hidden variables exist.
3. Hidden variables are local.

Most people, including me, view the assumption of local hidden variables as very similar to the assumption of a local reality.

WHAT NOW?

As can be easily imagined, many people have tried to wiggle out of this profound result. Some attempts have critiqued the experimental tests. One argument is that since we set the two polarizers at some set of angles and then collect data for, say, a billion electrons there is plenty of time for the polarizers to "know" each other's orientation, although not by any known mechanism. More recent tests set the orientation of the the polarizers randomly *after* the electrons have left the source. The results of these tests are the same as the previous experiments: Bell's inequality is violated and the predicted Quantum correlations are confirmed. Still other tests have set the distance between the two polarizers at 11 km, with results again confirming the Quantum correlations.

Another critique has been that since the correlated pairs emitted by the source go in all directions, only a very small fraction of them actually end up being measured by the polarizers. Another experiment using correlated Beryllium atoms measured almost all of the pairs, with results again confirmed the Quantum correlations.

There is another objection to the experimental tests that, at least so far, nobody has managed to get totally around. We measure a spin combination of, say, zero degrees and 45 degrees for a collection of electrons and then measure another spin combination, say 45 degrees and 90 degrees, for *another* collection of electrons. In our classroom example, this is sort of like measuring the number of men students whose height is not over 5' 8" in one class, and then using another class of different students to measure the number of students whose height is over 5' 8" but do not have blue eyes. The difference is that a collection of, say, a billion electrons from the source in the correlation experiments always behaves identically within small and expected statistical fluctuations with every other collection of a billion electrons from the source. Since that fact has been verified many many times for all experiments of all types, we assume it is true when we are doing these correlation experiments. This assumption is an example of inductive logic; of course we assumed the validity of logic in our derivation.

Sometimes one sees statements that Bell's Theorem says that *information* is being transmitted at speeds greater than the speed of light. So far I have not seen such an argument that I believe is correct. If we are sitting by either of the polarisers we see that one-half the electrons pass and one-half do not; which is going to be the case for an individual electron appears to be random. Thus, the behavior at our polariser does not allow us to gain any information about the orientation of the other polariser. It is only in the *correlation* of the electron spins that we see something strange. d'Espagnat uses the word *influence* to describe what may be traveling at superluminal speeds.

Imagine we take a coin and carefully saw it in half so that one piece is a "heads" and the other is a "tails." We put each half in a separate envelope and carry them to different rooms. If we open one of the envelopes and see a heads, we know that the other envelope contains a tails. This correlation "experiment" corresponds to spin measurements when both polarisers have the same orientation. It is when we have the polarisers at different orientations that we see something weird.

So far we don't know which of the assumptions we made in the proof are incorrect, so we are free to take our pick of one, two or all three. We shall close this section by briefly considering the consequences of discarding the assumption of the validity of logic and then the consequences of discarding the assumption of a reality separate from its observation. In the next section we shall explore the idea of a non-local universe.

What If Logic Is Invalid?

It has been suspected since long before Bell that Quantum Mechanics is in conflict with classical logic. For example, deductive logic is based on a number of assumptions, one of which is the Principle of the Excluded Middle: *all statements are either true or false*.

But consider the following multiple choice test question:

1. The electron is a wave.
2. The electron is a particle.
3. All of the previous.
4. None of the above.

From wave-particle duality we know that both statements 1 and 2 are both sort of true and sort of false. This seems to call into question the Principle of the Excluded Middle. Thus, some people have worked on a multi-valued logic that they hope will be more consistent with the tests of Bells' Theorem and therefore with Quantum Mechanics. Gary Zukav's **The Dancing Wu Li Masters**has a good discussion of such a quantum logic; since numerous editions of this book exist and every chapter is numbered **0**, I can't supply a more detailed reference.

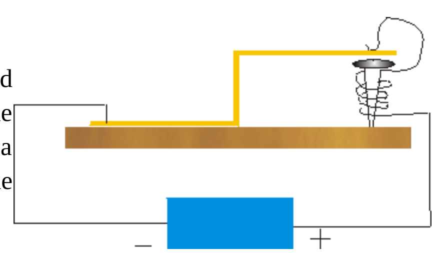
Mathematics itself can be viewed as just a branch of deductive logic, so if we revise the rules of logic we will need to devise a new mathematics

You may be interested to know that deductive logic has proved that logic is incomplete. The proof was published in 1931 by Gödel; a good reference is Hofstader's **Gödel, Escher, Bach**. The key to Gödel's work is *self-reference*; we shall see an example of self-reference in the next sub-section. What he proved was that any mathematics at all, unless it is trivially limited, will contain statements that are neither true nor false but simply unprovable.

By self-reference we mean a statement or set of statements that refer to themselves. For example, consider:
This statement is false.
Note that if this statement is true, then it must be false. If the statement if false, then it must be true. So we have a chain of *True » False » True » False ....*

New Yorker, Mar 5, 2001, pg. 78.

This may remind you a bit of a simple buzzer, such as a door buzzer.



A buzzer is shown to the right. A flexible piece of metal is bent into a double *L* shape and nailed to a board. A big nail is placed just under the right hand part of the metal, and the metal is adjusted so that it does not quite touch the big nail. A battery is wired in such a fashion that when the the metal *L*is at rest, the circuit is just completed, which causes the big nail to become an electromagnet.

This of course pulls the metal down, which breaks the circuit. Thus the metal springs back up, which completes the circuit again, which pulls the metal down, and so on. Thus, if the circuit is closed, it opens, and if the circuit is open, then it is closed. Or, we say we have a chain of *Closed* » *Open* » *Closed* » *Open* .... The difference between this example and the previous self-referential statement is that here the oscillations in value are occurring in time. You may access a Flash animation of a buzzer by clicking here.

In the late nineteenth century the logician Hilbert used to say "Physics is too important to be left to the physicists." In retaliation, J.A. Wheeler has stated: "Gödel is too important to be left to the mathematicians."

Finally, although *deductive* logic is fairly well understood, nobody has succeeded in codifying iron-clad rules for *inductive* logic that work consistently. Mills tried very hard to do this, but the following story by Copi shows one problem:

"A favorite example used by critics of the Method of Agreement is the case of the Scientific Drinker, who was extremely fond of liquor and got drunk every night of the week. He was ruining his health, and his few remaining friends pleaded with him to stop. Realizing himself that he could not go on, he resolved to conduct a careful experiment to discover the exact cause of his frequent inebriations. For five nights in a row he collected instances of a given phenomenon, the antecedent circumstances being respectively scotch and soda, bourbon and soda, brandy and soda, rum and soda, and gin and soda [ugh!]. Then using the Method of Agreement he swore a solemn oath never to touch soda again!"

Reference: I. Copi, **Introduction to Logic**, 2nd ed., (Macmillan, New York, 1961), pp 394-395.

Note the "hidden variable" in the above story.

What If There Is No Reality Separate From Its Observation?

As we have seen, the title of this sub-section is very similar to asking what are the consequences of having no hidden variables. We shall concentrate on the first form of the question.

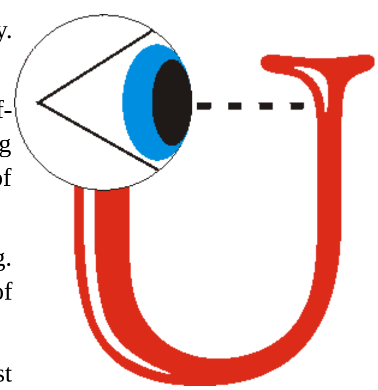
You may have already noticed that the question is a variation on the old philosophical saw regarding a tree that falls in the forest with nobody there to hear the sound.

A conflict between the assumption of reality and Quantum Mechanics has been suspected long before Bell. For example, in referring to the trajectory of the electron in, say, the double slit experiment Heisenberg stated "The path of the electron comes into existence only when we observe it."

People have long known that any measurement disturbs the thing being measured. A crucial assumption of classical sciences has been that at least in principle the disturbance can be made so small that we can ignore it. Thus, when an anthropologist is studying a primitive culture in the field, she assumes that her presence in the tribe is having a negligible effect on the behavior of the members. Sometimes we later discover that all she was measuring was the behavior of the tribe when it was being observed by the anthropologist.

Nonetheless, classically we assume a model where we, as *observers*, are behind a pane of glass where see what is going on "out there." Now we suggest that the pane of glass has been shattered. Wheeler suggests that we should drop the word *observer*entirely, and replace it with *participator*.

Wheeler has thought more deeply on the consequences of a participatory universe than anybody. He devised the figure to the right, whose caption is:



“Symbolic representation of the Universe as a self-excited system brought into being by ‘self-reference’. The universe gives birth to communicating participators. Communicating participators give meaning to the universe … With such a concept goes the endless series of receding reflections one sees in a pair of facing mirrors.”

Reference: J.A. Wheeler in Isham et al., eds, **Quantum Gravity** (Clarendon, Oxford, 1975), pg. 564-565. The colors were used by Wheeler in a colloquium in the Dept. of Physics, Univ. of Toronto some years ago.

You may have noticed a similarity between this view of Quantum Mechanics and the Idealist philosophy of Bishop Berkeley. Berkeley would likely have been very happy about Bell's Theorem. Dr. Johnson was, of course, opposed to Berkeley and used to argue against his philosophy by bellowing "I refute it thus!" while kicking a large rock. Apparently Johnson found sufficient comfort from his argument that he didn't mind hurting his foot.

d'Espagnat also tends to believe that the reality assumption is incorrect. Thus he wrote: "The doctrine that the world is made up of objects whose existence is independent of human consciousness turns out to be in conflict with quantum mechanics and with facts established by experiment."

In a participatory universe, I can argue that you owe your objective existence to my kind intervention in allowing you into my own consciousness. Thus, there is an inherent *solipsism* in this position. Wigner was one of many who was greatly troubled by this.

NON-LOCALITY AND DAVID BOHM

Recall that David Bohm set off in the early 1950's on a quest for the hidden variables. Nobody has explored the consequences of such variables being non-local more deeply than Bohm, and in the first sub-section below we shall discuss some of his work on this topic. In the next sub-section we shall discuss his later thinking about the nature of the world.

The Implicate Order

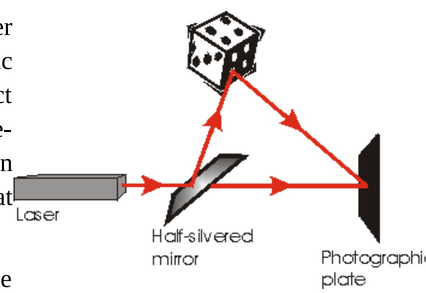
A good reference for the material of this sub-section is David Bohm, **Wholeness and the Implicate Order**. Although very deep the book is not technical except for Chapter 4, which I think should not have been included.

Bohm called our everyday world of space, time and causality the *explicate order*. He proposed that underlying this everyday world is an interconnected one which he calls the *implicate order*. He used a number of analogies and images to discuss these two orders.

In one analogy he imagined a large cylindrical glass container of glycerine mounted on a turntable. We place a spot of black ink in the glycerine. We slowly rotate the container, and the ink gradually disperses throughout the glycerine. If we slowly rotate the cylinder in the opposite direction the spot of ink gradually re-forms. When the ink is dispersed it is in an implicate state: it exists throughout the glycerine. When the ink is a spot it is explicate: it exists in one part of the glycerine but not in the other parts. If we continue rotating the cylinder in this opposite direction the spot disperses again.

We extend the image as follows. We place the spot of ink as before. We slowly rotate the cylinder one revolution, and the ink has begun to disperse. We place a second spot of ink just beside where the first spot was, and rotate for one more revolution. A third spot is placed beside where the second was, one more revolution, and we continue this for a few spots. Then we continue slowly rotating the cylinder until all the ink is fully dispersed. When we reverse the direction of rotation we see the last spot coalesce, then the next to last one right beside the last one, and so on. We could interpret what we are seeing as a single spot of ink that is moving. So in the implicate fully dispersed state we have enfolded the motion in space and time of an object throughout the glycerine. Reversing the rotation unfolds the reality back into space and time.

Another analogy is a hologram. As shown to the right, to make a hologram we split a laser beam into two pieces with a half-silvered mirror. One piece goes straight to a photographic plate, the other bounces off the object and then goes to the plate. In order to reconstruct the image of the object we shine a laser beam through the developed plate: the three-dimensional image appears. Note that in some sense the hologram on the plate is an interference pattern between the beam that has experienced the thing and the beam that experienced no-thing.

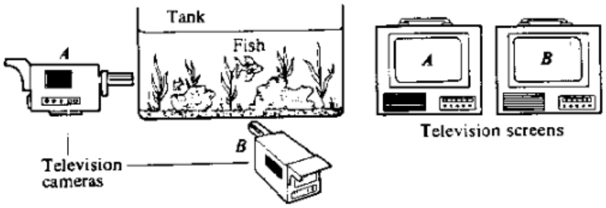


One characteristic of a hologram is that down to at least a few grains of the silver in the plate, each piece of the plate contains the entire image. If we cut the plate in half we do not lose half the image; instead we lose resolution and the image becomes more fuzzy. Thus each piece of the plate contains the entire space of the object in an enfolded way; this is an analogy to the implicate order. When we reconstruct the image, we have unfolded the implicate order into an explicate one.

There are "multiplexed" holograms that contain time information too. If the object is moving, we rotate the photographic plate. When we reconstruct the image if we look from different angles we see the object's motion. Here the object's time behavior is also enfolded into the totality.

We see that in the implicate order there is no spatial or time separation. Thus it is a non-local order.

Here is another image used by Bohm:



He comments: "The images on the screens are two dimensional *projections* (or facets) of a three dimensional reality. ... Yet, since these projections exist only as abstractions, the three-dimensional reality *is* neither of these. ... What is actually found [in the experimental tests of Bell's theorem] is that the behavior of the two [electrons] is correlated in a way that is rather similar to that of the two television images of the fish, as described earlier. Thus ... each electron acts as if it were a projection of a higher-dimensional reality. ... What we are proposing here is that the quantum property of a non-local, non-causal relation of distant elements may be understood through an extension of the notion described above." -- pg. 187-188.

The following table compares the explicate and implicate order:

Explicate	Implicate
parts make up the whole	whole makes up the parts
spatial separation	holographic
describable	"finger pointing to the moon"
things exist	'thing' and 'no-thing' interfere
"ten thousand things"	illusion
spacetime	spectra

Given the unbroken wholeness of the implicate order, Bohm asked why our thought is so dominated by fragmentation.

"... fragmentation is continually being brought about by the almost universal habit of taking the content of our thought for `a description of the world as it is'." -- pg. 3.

He also wrote about what to do about this:

"[Meditation] is particularly important because ... the illusion that the self and the world are broken into fragments originates in the kind of thought that goes beyond its proper measure and confuses its own product with the same independent reality. To end this illusion requires insight, not only into the world as a whole, but also into how the instrument of thought is working." -- pg. 25.

Bohm's Ontology of Quantum Mechanics

In philosophy, *epistemology* is the study of what we know and how we know it; this is as opposed to *ontology* which studies what actually exists. Most interpretations of Quantum Mechanics have been developed by people sympathetic to the idea of a participatory universe; we discussed this idea above. Therefore, these interpretations are essentially epistemology.

For Bohm, this wasn't good enough. He developed an ontology in his later years. His master work, **The Undivided Universe**, was written with his collaborator B.J. Hiley and published in 1993. It is written for physicists, and I can't really recommend it to a non-technical audience. Here we shall briefly explore some of the conclusions from this book.

Essentially, Bohm and his school re-interpreted the mathematics of Quantum Mechanics and extracted a part of the equation which they called the *quantum potential*. The quantum potential is non-local, and is responsible for all the non-local effects predicted by the theory.

The quantum potential guides, say, the path of an electron in a way similar to the way a radio beacon can guide an airplane coming in for a landing at the airport. It is the jets, ailerons, rudder, etc. on the plane that mechanically determines where the plane is going, but the beacon guides the way.

In Bohm's ontology electrons really are particles. For the case of, for example, the double slit experiment for electrons, each electron goes through either the upper slit or the lower slit; it has a definite path independent of its observation. However, the quantum potential is different depending on whether the other slit is open or closed; since this potential is non-local it can instantaneously change if the other slit is opened or closed. Thus the electron paths are different depending on whether or not the other slit is open.

You may recall that for a *chaotic* system, very small changes in initial conditions leads to radically different trajectories; you may read more about this here. It turns out that for the double slit experiment for electrons, the motion of the electron after it has passed the slits is chaotic in just this sense. Thus, even small thermal fluctuations in the electron's interaction with the slits cause the electron's future motion to be unknowable to us, even though it is strictly deterministic. Thus it seems to us that the path of the electron is random, although in reality it is not.

We call Physics before Quantum Mechanics *classical*; thus the theories of relativity are classical. Usually we characterise a classical theory as one that includes observers and strict determinism, while a non-classical theory has participators and randomness. If Bohm's interpretation is correct we need to change the way we characterise the distinction. A classical theory is local, while a non-classical one is non-local; both are strictly deterministic and have observers. Bohm had some hope that his ontology would have experimentally testable consequences, although no such experiments have yet been done.

You may wish to know that in Bohm's analysis the so-called photon is not a particle; it is an electromagnetic field whose particle-like behavior arises because of its interaction with the quantum potential.

Note that in this work, then, Bohm has finally identified the hidden variable he searched for for so many years: it is the quantum potential.

The non-locality of this potential led Bohm to invoke an image very similar to the one Wheeler used above in his discussion of the universe as a self-excited system:

"Classical physics provided a mirror that reflected only the objective structure of the human being who was the observer. There is no room in this scheme for his mental process which is thus regarded as separate or as a mere 'epiphenomenon' of the objective processes. ... [Through the] mirror [of quantum physics] the observer sees 'himself' both physically and mentally in the larger setting of the universe as a whole. ... More broadly one could say that through the human being, the universe is making a mirror to observe itself." -- Bohm and Hiley, **The Undivided Universe**, pg. 389

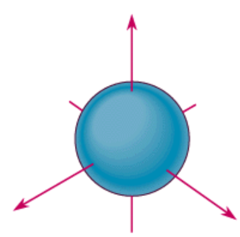
A colleague remarked to me that Bohm's heroic attempts to keep a reality separate from its observation, in this "final" form, is worse than the alternative of not having a reality. I don't know about the word *worse*, but after Bell's theorem something has to give, whether it is reality, locality and/or logic itself.

There are still some unresolved issues regarding Bohm's ontology. For example, as discussed elsewhere, the standard planetary model of the atom where the electrons orbit the nucleus just as the planets orbit the Sun is impossible, because according to classical electromagnetism such an electron is in a state of non-uniform accelerated motion and must radiate away its energy, causing it to spiral into the nucleus. However, when we think about the electron in its wave aspect, then when the waves are in a standing wave pattern, this corresponds to the allowed orbits of the Bohr model and the electrons do not radiate.

When the idea of treating the electron as a wave is fully developed by Quantum Mechanics, the orbits are more complicated then indicated in the document referenced in the previous paragraph.

To the right we show the "wave function" for the electron in its ground state orbital. It can be seen that it is spherically symmetric. In an earlier discussion we called this the orbit for which the quantum number n is equal to 1.

In Bohm's ontology, the electron is a particle. But for this orbit the electron is stationary, with the electric force trying to pull it into the proton being just balanced by the quantum potential. Thus, this electron will certainly not radiate away energy.



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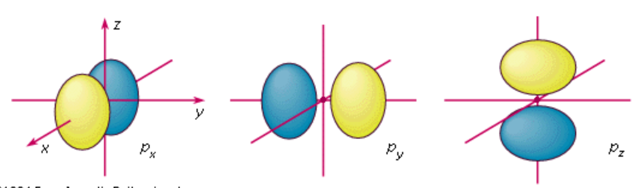

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For the state with principle quantum number 2, there is a spherically symmetric wave function that looks just like the one shown before for $n = 1$. But there are also three other orbitals, which look as shown above.

For the first two of these "p" orbitals, the electrons are moving and accelerating and would be expected to radiate away energy. The last p_z orbital turns out to represent an electron that is stationary.

This is clearly in conflict with the fact that the electrons in the atom do not radiate energy except when they change from one allowed orbit to another allowed orbit.

In fact, this difficulty manifests in another form in the double slit experiment for electrons. If the electron is a particle that changes its trajectory when it goes through the slits, it too should radiate away energy. One of Bohm's colleagues, Vigier, recently said that the wavelength of this radiation is very large and so the energy loss is negligible; some people believe that Vigier is wrong. Work on this problem is currently being pursued; one of the people working on it is Professor John Sipe of this Department. I became aware of this controversy in attempting to find the answer to a question asked by former JPU200Y student Sharmilla Reid.

CELLULAR AUTOMATA

A *cellular automaton* provides another approach to the study of the emergence of structures based on rules.

One of the best known automata is the *Game of Life*, devised by John Conway in 1970. This example is played on a large checkerboard-like grid. One starts with a configuration of cells on the board that are populated, and then calculates the population in succeeding generations using three simple rules:

1. Birth: an unoccupied cell with exactly 3 occupied neighbors will be populated in the next generation.
2. Survival: an occupied cell with 2 or 3 occupied neighbors will be populated in the next generation.
3. **Death**: in all other cases a cell is unoccupied in the next generation.

Despite the simplicity of the rules, truly amazing patterns of movement, self-organising complexity, and more arise in this game.

You can play an animation of the game of life on the web

- Click on the **Step** button to step from generation to generation. In this mode the number of occupied neighbors of each cell is shown.
- Click on **Play** to resume playing the animation.

There are many resources available on the web to explore this fascinating "game" in more detail.

It has been proposed that these sorts of automata may form a useful model for how the universe really works. Contributors to this idea include Konrad Zuse in 1967, Edward Fredkin in the early 1980's, and more recently Stephen Wolfram in 2002. Wolfram's work in particular is the outcome of nearly a decade of work, which is described in a mammoth 1200 page self-published book modestly titled **A New Kind of Science**.

There are two key features of cellular automata that are relevant for this discussion:

1. The rules are always strictly deterministic.
2. The evolution of a cell depends only on its nearest neighbors.

This seems to put a cellular automaton model of Physics in conflict with Bell's Theorem, which asserts that a logical local deterministic model of the universe can not be correct.

Advocates of the cellular automaton model attempt to argue that there is no essential conflict, just an apparent one. Arguments include:

- That the apparent randomness of quantum phenomena is only *pseudo-random*. To me, they seem to be re-introducing the idea of *hidden variables* via the back door. Plamen Petrov in one of the proponents of this argument.
- That there is some sort of higher-dimensional thread outside of the normal four dimensions of space and time. This "thread" will somehow allow for super-luminal connections. Wolfram and others have proposed this idea.
- Other Wolfram supporters have argued that the speed of light is or can be much greater than the "usual" value that we are used to. Whether or not it needs to be infinite is not clear.

In the previous **Bohm's Ontology of Quantum Mechanics** sub-section, we saw that Bohm's attempt to keep causality ended up with a totally non-local mechanism encapsulated in a *Quantum Potential*. Even there, we saw at the end that there are serious problems with the model.

It may be that there are even more serious problems with the Cellular Automaton model for the way the universe works. The controversy continues to be very active as of this writing (Spring, 2003). A semi-random list of further readings is:

- arxiv.org/PS_cache/quant-ph/pdf/0206/0206089.pdf
- http://www.math.usf.edu/~eclark/ANKOS_reviews.html
- http://digitalphysics.org/Publications/Petrov/Pet02m/Pet02m.htm

FINALLY ...

Einstein died many years ago, and so is not here to defend himself against claims of what he would or would not do today. Nonetheless, I tend to think that if he were alive today, Bell's theorem would force him to accept Quantum Mechanics.

Contributor

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13.2: Black Hole Thermodynamics

Introduction:

"Time and space are modes in which we think and not conditions in which we live." -- Einstein

"Space is the order of coexistence, and time is the order of succession of phenomena." -- Leibniz

"For the sage, time is only of significance in that within it the steps of becoming can unfold in clearest sequence." -- **I Ching**

Background Information

One of the features of Hawking and Bekenstein's development of black hole thermodynamics is that it ties many many pieces of physics together. Among those pieces are:

- The realisation from Quantum Mechanics that we can think of all matter-energy as waves. A document on this appears here.
- The realisation from classical physics that in a confined region, waves exist as *standing waves*. A document on this appears here.
- The realisation from thermodynamics that the *entropy* can be viewed as a measure of the number of combinations or permutations of an ensemble that are equivalent. This is equivalent to viewing the entropy more conventionally as a measure of the heat divided by the temperature of a body. According to the Second Law of Thermodynamics, in a closed system the entropy never decreases. A document on Entropy appears here.
- The realisation from Heisenberg's Uncertainty Principle that we can violate the principle of Conservation of Energy so long as we do it for only a short period of time. This is discussed in the next section of this document.
- The realisation from classical physics that all objects with a temperature above absolute zero radiate away energy as electromagnetic radiation. This is briefly discussed below.
- Feynman's theory of antimatter as regular matter going backwards in time. A document on antimatter appears here.

Finally, background information on black holes can be found here.

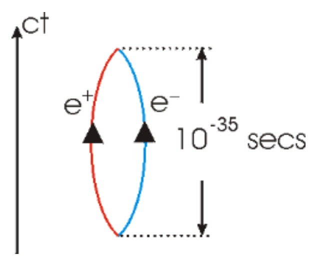
Virtual Pair Production

Recall Heisenberg's Uncertainty Principle. It basically puts a limit on how much we can reduce the disturbance we introduce in a system by doing a measurement on it. There are a number of forms of the principle, and here we shall use only one of them:

The uncertainty in any measurement of the energy of an object times the uncertainty in when the object had that energy will always be at least equal to a universal constant.

Technical note: The universal constant is *Planck's constant h* divided by 2 pi.

A moment's reflection on the implications of this form of the Uncertainty Principle may convince you that this means that the energy does not even *have* a definite value but only a lower and upper bound.
Thus the principle of conservation of energy can be violated so long as the violation occurs for only a brief period of time.
Now consider Dirac's infinite sea of negative energy electrons. One of those electrons can violate conservation of energy by spontaneously jumping into a positive energy state provided it falls back into the hole quickly enough. You will recall that we interpret the hole in the sea as a positron. Thus, we believe that this *virtual pair production* is occurring everywhere in the universe. The pair can only exist for a time of about 10^{-35} seconds, i.e. 34 zeroes followed by a 1 to the right of the decimal point; this is called the *Planck time*.



Similarly we believe virtual pairs of proton-antiprotons, neutron-antineutrons etc. are continually being formed and disappearing everywhere in the universe. Wheeler, then, characterizes the vacuum at a scale of very small distances as being *quantum foam*.

Thermal Radiation

Here is yet another "little" fact that we will need soon: Thermodynamics says that any body with a temperature above absolute zero will radiate its energy away.

Recall that heat is just the internal energy of motion and vibration of the molecules of the substance. And also recall that whenever a body with electric charge vibrates it radiates energy as electromagnetic radiation. These two facts explain the radiation process.

Your body is radiating at a rate of about 60 Watts, the same as a 60W light bulb. Most of that radiation is in the infrared region.

The higher the temperature of a body the faster it radiates energy away.

Technical note: for a perfect radiating body the rate of energy radiation is a universal constant times the fourth power of the absolute temperature.

Whether the radiation is mostly as infrared or visible light or X-rays etc. depends on the temperature of the body. For example, if we heat up a steel bar it starts to glow "red hot." Increasing the temperature shifts the radiation spectrum and it glows "white hot." Raise the temperature further and the radiation becomes blue.

Black Hole Thermodynamics

We consider here one of Stephen Hawking's contributions to Physics. A reference is his famous book **A Brief History of Time**. Sadly, a former tutor in JPU200Y was completely correct when he proposed the following multiple choice question for a test:

Stephen Hawking is:
A. a lousy writer.

Lost in the media blitz surrounding Hawking is that, working independently, Bekenstein also came to many of the realisations we describe here.

We imagine a black hole as the singularity in the center surrounded by a spherical *event horizon*.We know that when a black hole is created by a collapsing neutron star that the neutrons are crushed out of existence; by this I mean that all their *neutron*ness is wiped out. However their total mass-energy remains.

Another way of stating this is that outside of the event horizon all properties of the matter that formed it are gone except for the total mass-energy, rotation, and electric charge: this is sometimes called the *Black Hole Has No Hair* theorem.

The total mass-energy is manifested as the curvature of spacetime around the singularity.

We have seen that all matter has a wave aspect, and Quantum Mechanics describes the behavior of these waves. So, we shall think about representing the mass-energy inside the event horizon as waves.

Now, what kind of waves are possible inside the black hole? The answer is *standing waves*, waves that "fit" inside the black hole with a *node* at the event horizon. The possible wave states are very similar to the standing waves on a circular drum head that we saw earlier; they aren't exactly the same because the waves exist in three dimensions instead of just the two of the drumhead, but they are very close to the same.

Note that I just said "three dimensions." This is correct; we are using non-relativistic quantum mechanics.

The energy represented by a particular wave state is related to the frequency and amplitude of its oscillation. As we saw for the standing waves on a drumhead, the higher "overtones" have a higher frequency and thus these Quantum Mechanical waves contain more energy.

Assume that the total mass-energy inside the event horizon is fixed. So, we have various standing waves, each with a certain amount of energy, and the sum of the energy of all these waves equals the total mass-energy of the black hole. There are a large number of ways that the total mass-energy can distribute itself among the standing waves. We could have it in only a few high energy waves or a larger number of low energy waves.

It turns out that all the possible standing wave states are equally probable. Thus, we can calculate the *probability* of a particular combination of waves containing the total mass-energy of the black hole the same way we calculated the probability of getting various combinations for dice. Just as for the dice, the state with the most total combinations will be the most probable state.

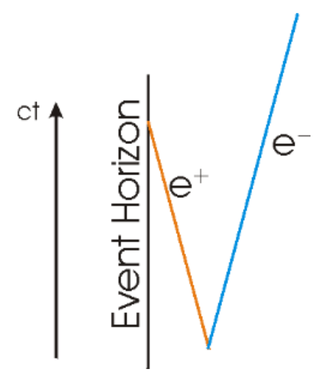
But we have seen that the *entropy* is just a measure of the probability. Thus we can calculate the entropy of a black hole.

We have also seen that the entropy measures the heat divided by the absolute temperature. The "heat" here is just the total mass-energy of the black hole, and if we know that and we know the entropy, we can calculate a *temperature* for the black hole.

So, as Hawking realised, we can apply all of *Thermodynamics* to a black hole.

In a previous section we saw that any body with a temperature above absolute zero will radiate energy. And we have just seen that a black hole has a non-zero temperature. Thus thermodynamics says it will radiate energy and evaporate. We can calculate the rate of radiation for a given temperature from classical thermodynamics.

How is this possible? Nothing can get across the event horizon, so how can the black hole radiate? The answer is via virtual pair production.
Consider a virtual electron-positron pair produced just outside the event horizon. Once the pair is created, the intense curvature of spacetime of the black hole can put energy into the pair. Thus the pair can become non-virtual; the electron does not fall back into the hole.
There are many possible fates for the pair. Consider one of them: the positron falls into the black hole and the electron escapes. According to Feynman's view we can describe this as follows:
The electron crosses the event horizon travelling backwards in time, scatters, and then radiates away from the black hole travelling forwards in time.
Using the field of physics that calculates virtual pair production etc., called *Quantum Electrodynamics*, we can calculate the rate at which these electrons etc. will be radiating away from the black hole. The result is the same as the rate of radiation that we calculate using classical thermodynamics.



The fact that we can get the radiation rate in two independent ways, from classical Thermodynamics or from Quantum Electrodynamics, strengthens our belief that black holes radiate their energy away and evaporate.

Technical note: if we measure the mass-energy **M** of a black hole in units where the mass of our Sun is one, then the absolute temperature of the black hole is $\mathbf{6 \times 10^{-8} / M}$ Kelvin and its lifetime, in seconds, is: $\mathbf{10^{71}\ M^3}$**.**

Black Holes and Information

Above we mentioned the *Black Hole Has No Hair* theorem, which states that no matter what falls into a black hole, the only properties that remain are the total mass, charge, and angular momentum of the object. Thus if, say, an encyclopedia falls into a black hole all the *information*in the encyclopedia is lost.

We can state this circumstance in another way using Quantum Mechanical terminology. Before it falls into a black hole the encyclopedia has in principle a single well defined *wave function*. This is called a *pure state*. After it falls into the hole, however, we have seen that the description of its mass-energy becomes a combination of the possible standing wave states that can exist with nodes on the event horizon. This is called a*mixed* state.

However, Quantum Mechanics provides no mechanism by which a pure state can become a mixed one. This is usually called the "Information Problem" with black holes.

Hawking, Kip Thorne and others believe that when this problem is resolved, it will turn out that the information really has been irretrievably lost. However, John Preskill and others firmly believe that a mechanism for the information to be released by the evaporating black hole must and will be found in a correct theory of quantum gravity.

Thus, in February 1997 Preskill offered a bet to Hawking and Thorne that:

"When an initial pure quantum state undergoes gravitational collapse to form a black hole, the final state at the end of black hole evaporation will always be a pure quantum state."

Hawking and Thorne accepted the bet. The wager is:

"The loser(s) will reward the winner(s) with an encyclopedia of the winner's choice, from which information can be recovered at will."

Thermodynamics of the Universe

Consider the universe. It has a size of about 15 billion light years or so. It also has a total amount of mass-energy. If we represent this mass-energy as quantum mechanical standing waves, just as we did for black holes, we can calculate the total entropy of the universe.

It turns out that the entropy of either a black hole or the universe is proportional to its size squared.

Thus for a given amount of total mass-energy, the larger the object the higher the entropy.

But the universe is expanding, so its size is increasing. Thus the total entropy of the universe is also increasing.

This leads us to the idea that the Second Law of Thermodynamics may be a consequence of the expanding universe. Thus cosmology explains this nineteenth century principle.

Put another way, recall that we have realised that the direction of time, "time's arrow," can come either from the fact that the universe is expanding or from the Second Law of Thermodynamics. We have now found a relationship between these two indicators of the direction of time.

It is amusing to speculate about what will happen to the Second Law of Thermodynamics if the universe is closed, so that at some point the expansion stops and reverses.

Even more wild is the idea that if the expansion of the universe determines the direction of time's arrow, then if the universe starts to contract the direction of time will also reverse.

Sentient Beings

Hawking and Bekenstein did much of the above work on the thermodynamics of black holes and the universe. In this section we consider a speculation for which I must take the blame.

Reference: D. Harrison, "Entropy and the Number of Sentient Beings in the Universe," Speculations in Science and Technology **5** (1982) 43.

First, we must think a bit about *information*.

The search for extra-terrestrial life has concentrated on scanning the universe for radio waves and trying to see if the patterns of the radiation could contain evidence of intelligence. When the *pulsars*, the radio sources that send blips at highly regular intervals, were first discovered some people got very excited and thought perhaps the search had yielded a positive result; now we believe that the pulsars are the radiation from rapidly rotating neutron stars.

If we receive a radio transmission that is just static, there is very little information in it. The information content of a signal depends on that signal being ordered, not random. Thus if the extra-terrestrial beings are sending information to us in radio waves the signal will be ordered in some way.

Thus, information must have low *entropy*. You may recall that earlier we mentioned the *negentropy*, which is the negative of the entropy: it measures the amount of order in a system. People who work in information theory customarily think about the negentropy.

We are, hopefully, acquiring information about the world, ourselves, our friends all the time. Thus we are creating negentropy in our mental system.

Now, the Second Law of Thermodynamics says that the entropy is increasing. This is a sort of strange law for a physicist: it says that the entropy is never conserved. This is as opposed to the types of laws that we are used to, which talk about conditions under which things are conserved.

You will also recall that Quantum Mechanics seems to say that there are no *observers* in the universe, only *participators*. Thus the universe is in some sense brought into being by communicating participators acquiring information about it (and vice versa).

What if the Second Law of Thermodynamics is not quite complete as stated? My speculation is that it could be extended to read:

The rate of production of physical entropy by the universe equals the rate of production of negentropy by sentient beings in the universe.

Now we have a conservation law.

However, the total physical entropy of the universe is increasing, and we can calculate the rate of that increase. If we could calculate the rate at which a typical human-like creature acquires information throughout its lifetime, then a simple division will allow us to calculate the number of such sentient beings there are in the universe.

To guess at the rate at which we produce negentropy we take our memory system to be essentially digital, with each of the 10^{14} synapses in our brain in either an *on* or *off* state. The combinations of synapse states are just the same as the combinations of black marble-white marble states that I insisted we think about when we discussed entropy in an earlier class. So, just as always, we count the number of combinations to calculate the entropy, whose negative is the negentropy.

We assume evolution is efficient, so the memory store is full after 100 years.

The result of dividing this rate of negentropy production into the rate at which physical entropy is being produced by our expanding universe is a number on the order of 10^{102} sentient human-like beings in the universe. To put this number into context, there are on the order of 10^{80}protons plus neutrons in the universe.

So, perhaps this is a failed speculation. Other alternatives include:

- Neutrons, protons, etc. are sentient.
- The human memory system contains a great deal more potential that we have allowed for.
- We have not included the negentropy production due to the communication that occurs between sentient beings.
- We, along with Hawking and Bekenstein, have calculated the rate of physical entropy production in the universe using equilibrium thermodynamics. A self-organising universe with negentropy production through dissipative structures makes our calculation of the rate of physical entropy production incorrect.

Author

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13.3: Complementarity and Copenhagen Interpretation

Introduction

Neils Bohr (1885 - 1962) was one of the giants in the development of Quantum Mechanics. He is best known for:

1. The development of the *Bohr Model of the Atom* in 1913. A small document on this topic is available here.
2. The principle of *Complementarity*, the "heart" of Bohr's search for the significance of the quantum idea. This principle led him to:
3. The *Copenhagen Interpretation of Quantum Mechanics*.

In this document we discuss Complementarity and then the Copenhagen Interpretation.

But first we shall briefly discuss the general issue of interpretations of Quantum Mechanics, and briefly describe two interpretations. The discussion assumes some knowledge of the *Feynman Double Slit*, such as is discussed here; it also assumes some knowledge of *Schrödinger's Cat*, such as is discussed here. Finally, further discussion of interpretations of Quantum Mechanics can be meaningfully given with some knowledge of *Bell's Theorem*; a document on that topic is here.

The level of discussion in what follows is based on an upper-year liberal arts course in modern physics without mathematics given at the University of Toronto. In that context, the discussion of Bell's Theorem mentioned in the previous paragraph is deferred until later.

A recommended reference on the material discussed below is:

F. David Peat, **Einstein's Moon** (Contemporary Books, 1990), ISBN 0-8092-4512-4 (cloth), 0-8092-3965-5 (paper).

Interpretations of Quantum Mechanics

Although the basic mathematical formalism of Quantum Mechanics was developed independently by Heisenberg and Schrödinger in 1926, a full and accepted interpretation of what that mathematics means still eludes us. If we found such an interpretation, then in some sense we could claim to understand Quantum Mechanics.

Richard Feynman stated that he never understood Quantum Mechanics. Certainly the author of this document does not understand Quantum Mechanics. This may be because Quantum Mechanics is not understandable, at least in the usual sense of the meaning of the word *understandable*.

Regrettably, some physicists claim that it is not important whether or not we understand Quantum Mechanics: what is important is that we know how to manipulate the mathematical formalism to get answers to our quantitative questions.

Here are some statements by physicists that take the opposite position on understanding:

- "Never make a calculation until you know the answer." -- Wheeler, **Spacetime Physics**, pg 60.
- "Our mathematical procedures seem to obscure our intuitive and imaginative understanding." -- Bohm, Foundations of Physics **5**, 93 (1975).
- I feel that we do not have definite physical concepts at all if we just apply working mathematical rules; that's not what the physicist should be satisfied with." -- Dirac, **Physicist's Conception of Nature**, pg 11.

In any case, the typical education of a physicist tends to ignore the issue of interpretations.

To the extent that the usual course in Quantum Mechanics for physics students discusses interpretations at all, it usually presents only a simple probability view. Quantum Mechanics describes the world in terms of a "wave function" or "state function." When we see, say, electrons in a two slit experiment forming an interference pattern, we say that a wave has split up, gone through the two slits, and then re-combined. This is the normal way of explaining two slit interference of any type of wave. The Quantum Mechanical wave, the wave function, is interpreted as being the amplitude of the probability of finding the electron at some position in space. Thus, when we don't look at what is happening at the slits, there is a 50% chance a given electron went through the upper slit and a 50% chance it went through the lower slit. Thus the wave function has an amplitude at both slits, and then when later the wave functions re-combine we get interference. If we set up an experiment at the slits to see what the electrons are doing, we see each electron going through either the upper slit or through the lower slit, never through both slits at once. But the process of doing this measurement "collapses the wave function" so that it has a non-zero amplitude only at the slit where we see the electron. And it is this collapse that destroys the interference pattern.

Similarly, before we look the Quantum Mechanical description of Schrödinger's Cat states that after one half-life the cat is 50% alive and 50% dead. When we open the box and look we similarly "collapse the state."

Deeper consideration of this "interpretation" will quickly lead to the conclusion that it is at least incomplete.

Another interpretation of Quantum Mechanics was devised by Hugh Everett, III as a PhD thesis when he was a graduate student of John Wheeler at Princeton in 1957. The thesis itself was nine pages in length, which is about typical for the length of the *bibliography* of a typical PhD thesis in physics.

In Everett's interpretation when we, say, look in the box and find that Schrödinger's Cat is alive, that measurement has created a parallel universe where we found that the cat is dead. And similarly, every conscious act of perception bifurcates the universe.

In this view, then, when we find, say, a live cat the apparent fixed outcome is *illusion*, because we have created another parallel universe where we found a dead cat. And the totality is both universes, one with a live cat and the other with a dead one.

Borges' **A Garden of Forking Paths** evokes images reminiscent of the many-worlds interpretation:

" ... a picture, incomplete yet not false, of the universe as Ts'ui Pen conceived it to be. Differing from Newton and Schopenhauer, ... [he] did not think of time as absolute and uniform. He believed in an infinite series of times, in a dizzily growing, every spreading network of diverging, converging and parallel times. This web of time - the strands of which approach one another, bifurcate, intersect or ignore each other through the centuries - embraces *every* possibility. We do not exist in most of them. In some you exist and not I, while in others I do, and you do not, and in yet others both of us exist. In this one, in which chance has favored me, you have come to my gate. In another, you, crossing the garden, have found me dead. In yet another, I say these very same words, but am an error, a phantom."

Complementarity

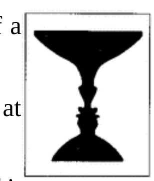
Here is a favorite statement of Bohr's Principle of Complementarity, based on so-called *wave-particle duality* for light:

> "But what is light really? Is it a wave or a shower of photons? There seems no likelihood for forming a consistent description of the phenomena of light by a choice of only one of the two languages. It seems as though we must use sometimes the one theory and sometimes the other, while at times we may use either. We are faced with a new kind of difficulty. We have two contradictory pictures of reality; separately neither of them fully explains the phenomena of light, but together they do." -- Albert Einstein and Leopold Infeld, The Evolution of Physics, pg. 262-263.

Incidentally, I have been told that Infeld wrote the entire book **The Evolution of Physics** in 1938, but was experiencing difficulty in getting anyone to publish it. Once Einstein put his name on it, all such difficulties disappeared.

John Wheeler, with his usual insight and striking prose, neatly summarizes the status of the principle:

"Bohr's principle of complementarity is the most revolutionary scientific concept of this century and the heart of his fifty-year search for the full significance of the quantum idea." -- Physics Today **16**, (Jan 1963), pg. 30.



A nice analogy is *Figure-Ground* studies such as the one shown to the right. Looked at one way, it is a drawing of a vase; looked at another way it is two faces.

We can switch back and forth between the two viewpoints. But we can not see both at once. But the figure *is* both at once.

Similarly, we can think of an electron as a wave or we can think of an electron as a particle, but we can not think of it as both at once. But in some sense the electron *is* both at once. Being able to think of these two viewpoints at once is in some sense being able to understand Quantum Mechanics.

I do not believe that Quantum Mechanics is understandable, at least for the usual meaning of the word *understand*.

Thus when we think of an electron in a Hydrogen atom, we can imagine it as a particle in orbit around the central proton. We can also imagine it as the *wave function*, its wave aspect; it turns out that the wave function for the electron in the Hydrogen atom is spherically symmetric with maximum density at the center of the atom.

A Flash animation of these two viewpoints of an electron in a Hydrogen atom may be accessed by clicking on the red button to the right. It will appear in a separate window, and has a file size of 9.6k In order to view it, you need to have the Flash player of Click Me

Version 5 or later installed on your computer; the Flash player is available free fromhttp://www.macromedia.com/

We can illustrate the Principle of Complementarity with some examples by Bohr himself:

1. "The opposite of a true statement is a false statement, but the opposite of a profound truth is usually another profound truth."
2. Life: a form through which matter streams.
   Life: a collection of matter.
3. Justice and love.

References to the above examples are:

1. Ken Wilbur, **Spectrum of Consciousness**, pg. 34.
2. Heisenberg, **Physics and Beyond**, pg. 105.
3. From the Chinese Taoist text **I Ching**, as reported in Reference 2, pg. 15.

In 1947 Bohr was awarded the Order of the Elephant from the Danish government. For a proud Dane like Bohr, this was a very big deal, and Bohr is the only person to be awarded it who was not royalty and/or a famous general. As part of the award, the winner's family coat of arms is carved into a sort of wall of fame. Bohr's family, though, did not have a coat of arms, so Bohr got to design one himself. The figure to the right is what he designed.

You will notice that he choose the ancient Chinese symbol for the Tao, the "Yin-Yang Symbol," for the centerpiece. He did not do this lightly. The inscription reads *CONTRARI SUNT COMPLEMENTA* or *Opposites Are Complements*. Thus he chose to represent his Principle of Complementarity as the centrepiece of his coat of arms.

As you probably know, in Taoist philosophy all is related to pairs of opposites which are called *Yang* and *Yin*. The table below illustrates. All the entries but the last are as given by the traditional Taoist classification.

Yang	Yin
Sunny	Shady
Masculine	Feminine
Active	Passive
Rational	Intuitive
Heavy	Light
Particle	Wave

The last entry in the above table is by the author of this document. You may wish to muse about whether I have got the right label in the correct column.

Similarly, the first two of the following quotations are famous to Taoists, while the last is not nearly as well-known:

1. "The ten thousand things carry yin and embrace yang.
   They achieve harmony by combining these forces."
   -- Lao Tsu, **Tao Te Ching 42**
2. "The Tao that can be told is not the true Tao."
   -- **Tao Te Ching 1**
3. "The electron that can be told is not the true electron."
   -- David Harrison

At the risk of pushing the illustration of Western physics by means of Eastern ideas too far, you may wish to consider the following:

"[In 1961] I had occasion to discuss Bohr's ideas with the great Japanese physicist [Yukawa], whose conception of the meson with its complementary aspects of elementary particle and field of nuclear force is one of the most striking illustrations of the fruitfulness of the new way of looking at things that we owe to Neils Bohr. I asked Yukawa whether the Japanese physicists had the same difficulty as their Western colleagues in assimilating the idea of complementarity ... He answered `No, Bohr's argumentation has always appeared quite evident to us; ... you see, we in Japan have not been corrupted by Aristotle." -- Rosenfeld, Physics Today **16**, (Oct 1963), pg. 47.

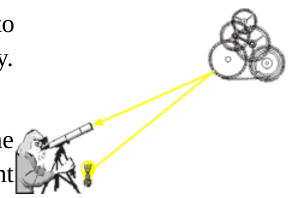
Finally, we close this section by considering the methodology used by Bohr, as well as many other creative geniuses both in and out of the sciences: *paradox*.

"Among all paradigms for probing a puzzle, physics proffers none with more promise than a paradox ... No one took the paradox [of quantum theory] more seriously than Bohr. No one worked around the central mystery with more energy wherever work was possible. No one brought to bear a more judicious combination of daring and conservativeness, nor a deeper feel for the harmony of physics." -- Misner, Thorne, and Wheeler, **Gravitation** pg. 1197

"The Copenhagen interpretation of quantum theory starts from a paradox." Heisenberg, **Physics and Philosophy**, pg. 44.

Similarly, in the Eastern traditions understanding is often achieved through deep consideration of paradox. A well-known example is the *koans* used in the Zen tradition. A famous koan is "What is the sound of one hand clapping?" There are more-or-less unique correct answers to the koans, which can be found by deep internal questioning.

Copenhagen Interpretation of Quantum Mechanics



If the Complementarity Principle is subtle, complex, and difficult to understand, then its extension into Bohr's interpretation of Quantum Mechanics will share these characteristics with some added subtlety. We begin by considering an apparatus making a measurement on some system:

The *apparatus* consists of a light source and a detector, which is the telescope and observer. The apparatus is making measurements on a *system* which in this example consists of some gears. The light source emits *photons*, the particulate aspect of light. The photons are "reflected" by the system, and enter the detector. The reflection of the photons off the gears necessarily disturbs the system we are attempting to measure.

If we attempt to reduce the disturbance on the system due to our measurements on it, we eventually reach a point where we have reached an irreducible minimum: this is when the interaction involves the exchange of a single quantum of energy, emitted by the light source, reflected off the system, and detected by the telescope and observer

The situation is actually even more complex than this. In fact, the photon from the light bulb is absorbed by the gears, which then emits another photon which ends up in the detector. If the "observer" were some sort of detector capable of detecting a single photon that would be the end of the story. But for the human observer shown, that single photon would have to enter his eye, be absorbed by the retina, which in turn causes an electrical impulse to go up the optic nerve to the brain where in principle the brain would process it; for real humans the minimum light level that is perceptible corresponds to a few photons, not a single one. So for a human to participate in this minimal observation, we would require a detector capable of registering a single photon and sending a larger signal, such as a flashing light, which a human can perceive.

The fact that the interaction cannot be reduced beyond a minimum amount, the interchange of a single photon, is the heart of the *Heisenberg Uncertainty Principle*. However, Bohr realised that it means even more than this. At this level we can not divide the quantum of energy into a contribution from the apparatus and a contribution from the system: the process is inseparable. Thus it is *holistic*.

This in turn means that at this level it is not meaningful to talk about the system at all separate from the apparatus observing it. As Bohr repeatedly said, "The quantum world does not exist."

Wheeler made a similar conclusion when he suggested that we should drop the word *observer* from our vocabulary, replacing it with the word *participator*.

In fact, the separation between the observer and the observed is always more-or-less arbitrary, although we customarily ignore that fact. An example by Bohr may clarify:

We customarily think of the outside world as separate from ourselves, and the boundary between the two is the surface of our skin. However, think of a blind person who gets around with the assistance of a cane. In time that person will probably treat the cane as part of his or her body, and will think of the outside world as beginning just at the tip of the cane. Now imagine the blind man's sense of touch extending out of the tip of the cane and into the roadway itself. Imagine it extending further, down the block, into the countryside, to the whole world. There is no point where the blind man ends and the world begins. Similarly, we can not say which is the system and which is us observing it.

This is the heart of the Copenhagen Interpretation of Quantum Mechanics.

We conclude this section with a further subtlety. The energy of a photon, the particulate aspect of light, is related to the wavelength of the wave aspect of the same light. We can reduce the energy of an individual photon by increasing the wavelength. Thus, we can reduce the disturbance on the system we are attempting to observe by using light of a larger wavelength. However, our ability to see the details of an object also depends on the wavelength of the light: we can not see details that are smaller than the wavelength. In the usual case we don't notice this because the wavelength of visible light is so small compared to everyday distances.

However, in the case of a quantum measurement we are typically investigating systems that are very small. Thus there is a meaningful maximum wavelength for the light we are using if we wish to see the system. So the minimum interaction between the apparatus and the system involves a single photon with a maximum wavelength, i.e. a single photon with a minimum energy. This minimum energy of the photon further constrains the minimum amount of disturbance we introduce by doing a measurement.

Technical note: the energy of the photon equals *h c / wavelength*, where *h* is Planck's constant and *c* is the speed of light.

Author

This document was written by David M. Harrison, Dept. of Physics, University of Toronto, harrison@physics.utoronto.ca in March 2000. This is version 1.6, date (m/d/y) 03/27/06.

13.4: Double Slit

The Feynman Double Slit

Here we discuss one of the two major paradoxes that we use to introduce Quantum Mechanics. It is the double slit experiment for bullets, water waves and electrons. Although many people have experimented with the systems to be discussed and written about them, Richard Feynman's treatment is so clear that physicists often call it the "Feynman" double slit. At the end, 2 references are given so you may read the "master" on this topic.

Operational Definitions for "Particles" and "Waves"

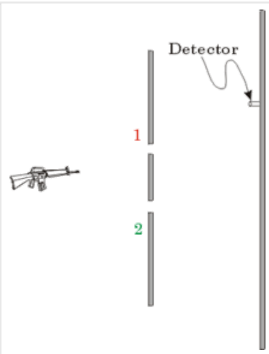
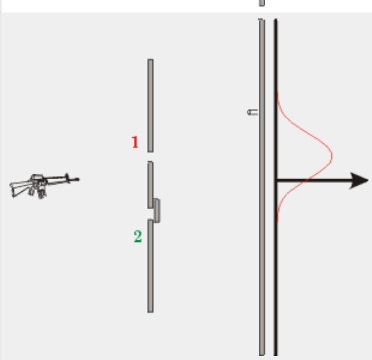
An "operational definition" is just a well-defined repeatable experimental procedure whose result defines a word or words. For example, one may have wide-ranging discussions of the meaning of the word *intelligence*. An operational definition of intelligence which side-steps these discussions could be:

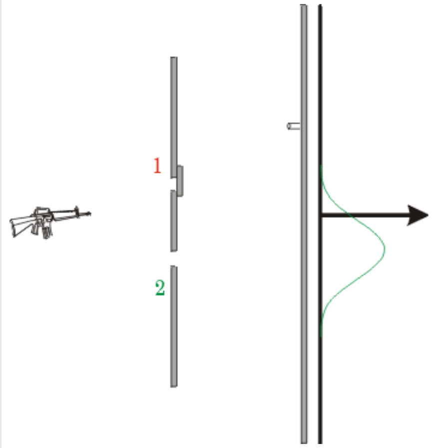
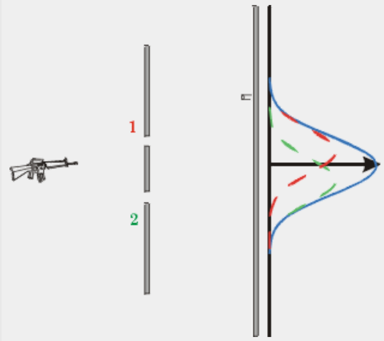
I administer the Stanford-Binet IQ test to a person and score the result. The person's intelligence is the score on the test.

Here we build operational definitions for the words "particles" and "waves."

First we discuss "particles" and will take as our prototype bullets from a machine gun. We have the machine gun, a piece of armor-plate in which two small slits have been cut, labeled"1" and "2", a detector and a solid armor-plate backstop. The detector is quite simple: it is a can in which we have placed some sand. We will turn the gunner loose for, say, a 1 minute burst, and then see how many bullets arrive in the can. We empty the can, and then move it to a different position on the backstop, turn the gunner loose for another 1 minute burst, and see how many bullets have arrived at the new position. By repeating the procedure, we can determine the distribution of bullets arriving at different positions on the backstop.

It turns out the the machine gunner is drunk, so that he is spraying the bullets randomly in all directions.

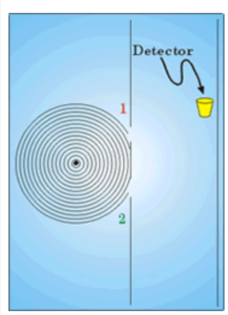
The apparatus is shown to the right. We will do three different "experiments" with this apparatus.	
First we close up the lower slit and measure the distribution of bullets arriving at the backstop from the upper slit. For some bullet sizes and slit widths, although many bullets will go straight through the slit a significant fraction will ricochet off the armor plate. So the distribution of bullets looks as shown by the curve to the right.	

Next we close up the upper slit, and measure the distribution of bullets arriving at the backstop from the lower slit. The shape, shown as the curve to the right, is the same as the previous one, but has been shifted down.	
Finally, we leave both slits open and measure the distribution of bullets arriving at the backstop from both slits. The result is the solid curve shown to the right. Also shown as dashed lines are the results we just got for bullets from the upper slit and bullets from the lower slit.	

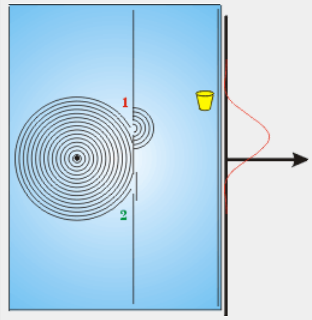
The result is just what you probably have predicted: the number of bullets arriving from both slits is just the sum of the bullets from the upper slit and the bullets from the lower slit.

It will be useful later for you to realize that since the path of a single bullet is random, the distributions we were measuring above are essentially measuring the *probability* that a given bullet will arrive at a particular position at the backstop.

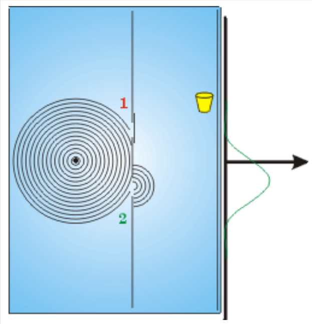
Now we turn our attention to waves. My high school physics teacher had a device called "ripple tank" which is just a tank made of plexiglass which could be filled with water. Various devices would tap the surface of the water, causing water waves to spread out from the device. One may insert slits and other objects in the path of the waves. The whole apparatus was mounted on an overhead projector, so could be used as a class demonstration. My teacher absolutely *loved* his ripple tank, so physics class was basically water-play. I don't know quite why he was so enamored with the device or what he expected us to learn from it, but to this day when I think of a prototype wave I think of water waves in a ripple tank. So we will repeat the double slit experiments we just did in a ripple tank.

First we show the apparatus. The thing that is tapping the surface of the water is the little black circle in the middle of all the concentric circles. The concentric circles are the water waves spreading out away from the source. Just as before we have two slits and a backstop. Just in front of the backstop is our "detector", which is just a cork floating on the surface of the water. Se we measure how much the cork bobs up and down and determine the amount of wave energy arriving at that position at the backstop. Moving the cork to other positions will allow us the determine the distribution of wave energy at the backstop.	

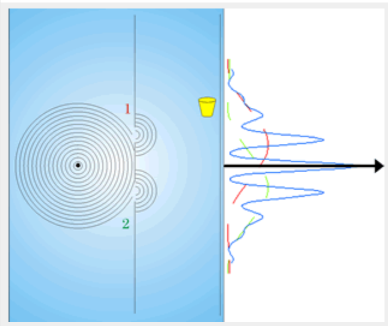
Now we close up the lower slit, and measure the distribution of wave energy arriving at the backstop just from the upper slit. For some combinations of slit width and wavelength, there will be significant spreading of the wave after it passes through the slit. If you have ever observed surf coming in through a relatively small slit in a seawall, you may have observed this.
The distribution is shown by the curve to the right. Note that it is very similar to the distribution of bullets from a single slit.



Now we close the upper slit and measure the distribution of wave energy arriving from the lower slit, as shown to the right.



Finally, we leave both slits open and measure the distribution. The result is shown to the right. As we did for the bullets, the dashed lines show the results we just obtained for the distribution from the upper and lower slits alone, while the solid line is the result for both slits open.
This looks nothing like the result for bullets. There are places where the total wave energy is much greater than the sum from the two slits, and other places where the energy is almost zero.
Such a distribution is called an *interference pattern*.

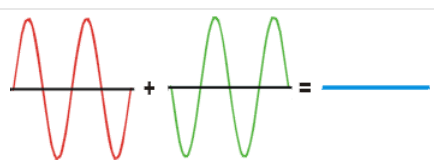


This completes the "operational definition" that we need to define waves and particles. In the two slit experiment, a **particle** does not show an interference pattern and the probability of a particle arriving at a location at the backstop with both slits open is just the sum of the probability of it arriving through the upper slit plus the probability of it arriving through the lower slit. A **wave** shows an interference pattern.

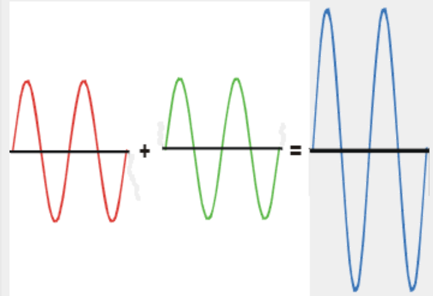
If you think about conservation of energy, you may worry a bit about the interference pattern for waves. There is no problem. The total energy in the interference pattern is equal to the energy arriving from the upper slit plus the energy arriving from the lower slit: the interference pattern re-arranges the energy but conserves the total amount of energy.

We can explain the interference pattern for waves. When the two waves from the two slits arrive at some position at the backstop, except for right in the middle they will have traveled different distances from the slits. This means that their "waving" may not be in sync.

The figure to the right shows two waves totally "out of phase" with each other. Their sum is always zero.
This is basically what is happening at the *minima* in the interference pattern.



The figure to the right shows the two waves in phase. The total wave is the sum of the two. This is what is occurring at the *maxima* in the interference pattern.



The Two Slit Experiment for Light

In ancient Greece there was a controversy about the nature of light. Euclid, Ptolemy and others thought that "light" was some sort of ray that travels from the eye to the observed object. The atomists and Aristotle assumed the reverse. Nearly 800 years after Ptolemy, circa 965 CE, in Basra in what is now Iraq, Abu Ali al-Hasan Ibn al-Haytham (Alhazen) settled the controversy with a clever argument. He said that if you look at the Sun for a long time you will burn your eyes: this is only possible if the light is coming from the Sun to our eyes, not vice versa.

In 1672 another controversy erupted over the nature of light: Newton argued that light was some sort of a particle, so that light from the sun reaches the earth because these particles could travel through the vacuum. Hooke and Huygens argued that light was some sort of wave. In 1801 Thomas Young put the matter to experimental test by doing a double slit experiment for light. The result was an interference pattern. Thus, Newton was wrong: light is a wave. The figure shows an actual result from the double slit experiment for light.

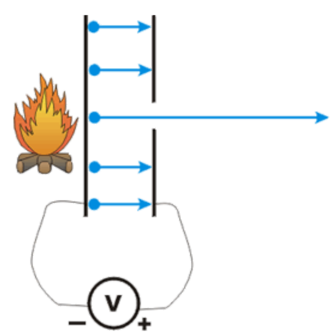
Of course, we haven't said anything about what is "waving" or in what medium it is waving. But, in terms of our operational definition it is clear that light is a wave of something.

Electron Guns

An electron gun, such as in a television picture tube, generates a beam of electrons. In this section we discuss how it works. These details are not important for our primary purpose here, so you may jump to the next section by clicking here.

A diagram of an electron gun appears to the right. There are two vertical metal plates; the right hand plate has a small hole cut in it. A voltage source, indicated by **V**, maintains a voltage across the plates, with the left hand plate negative and the right hand plate positive.

When a metal plate is heated, a process called *thermionic emission* literally boils electrons off the surface of the metal. Normally the electrons only make it a fraction of a millimeter away; this is because when the electron boiled off the surface of the metal, it left that part of the plate with a net positive electric charge which pulls the electron right back into the plate.



In the figure, we are heating up the left hand plate so thermionic electrons will be boiled off the surface. But because of the voltage difference being maintained across the plate, electrons that boil off between the two plates do not fall back into the plate, but instead are attracted to the right hand positive plate. Most of the electrons crash into the positive plate, as shown. However, the electron in the middle would have crashed into the plate except that we have cut a hole in that part of it. So we get a beam of electrons out of this "electron gun."

In real electron guns, such as at the back of a TV picture tube, the negative plate is not heated with a campfire as in our figure. Instead, a small filament of wire has a current passed through it. The filament heats up, glows red, and heats up the negative plate. You may have seen that red glow in the back of a TV picture tube.

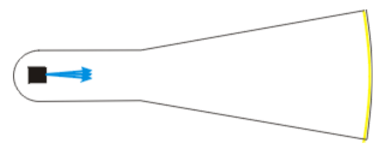
We control the speed of the electrons in the beam with the voltage, and the number of electrons by how hot we make the negatively charged plate.

One more small point. Because the hole in the right hand plate is not of zero size, electrons can emerge in directions slightly away from perfectly horizontal. Thus, the beam of electrons will tend to "spray" somewhat.

From now on we will put the electron gun in a black box, and represent the electron beam coming from it as shown to the right.

The Two Slit Experiment for Electrons

In the previous section we discussed how to produce a beam of electrons from an electron gun. Here we place the electron gun inside a glass tube that has had all the air evacuated. The right hand glass screen has its inside coated with a phosphor that will produce a small burst of light when an electron strikes it. In a TV picture tube, for example, fields direct the beam of electrons to the desired location, the intensities of the electrons are varied depending on where we are steering the beam, and our minds and/or eyes interpret the flashes as the image we are seeing on the television.

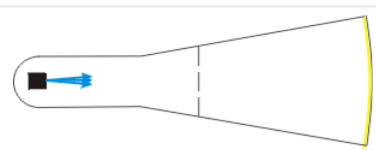


Property	Value
Mass	9.11×10^{-31}kg
Electric Charge	1.60×10^{-19}Coulombs
Spin angular momentum	5.28×10^{-35}Joule-seconds

Now, "everybody knows" that electrons are particles. They have a well defined mass, electric charge, etc. Some of those properties are listed to the right. Waves do not have well defined masses etc.

When an electron leaves the electron gun, a fraction of a second later a flash of light appears on the screen indicating where it landed. A wave behaves differently: when a wave leaves the source, it spreads out distributing its energy in a pattern as discussed at the beginning of this document.

Except, when we place two slits in the path of the electrons, as shown, on the screen we see an interference pattern! In fact, what we see on the screen looks identical to the double slit interference pattern for light that we saw earlier.



If this seems very mysterious, you are not alone. Understanding what is going on here is in some sense equivalent to understanding Quantum Mechanics. I do not understand Quantum Mechanics. Feynman admitted that he never understood Quantum Mechanics. It may be true that *nobody* can understand Quantum Mechanics in the usual meaning of the word "understand."

We will now extend our understanding of our lack of understanding. One possibility about the origins of the interference pattern is that the electrons going through the upper slit are somehow interacting with the electrons going through the lower slit. Note that we have no idea what such a mechanism could be, but are a little desperate to understand what is going on here. We can explore this idea by slowing down the rate of electrons from the gun so that only one electron at a time is in the system. What we do is fire an electron, see where the flash of light occurs on the phosphor screen, wait a while for everything to settle down, then fire another electron, noting where it lands on the screen.

After we have fired a large number of electrons, we will discover that the distribution of electrons is still the interference pattern.

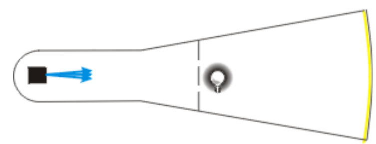
I have prepared a small Flash animation that simulates this result. You may access the animation by clicking on the red button to the right. The file size is 6.4k. You may get the Flash player free from http://www.macromedia.com/; our animation is for Version 5 or later of the player.

You may wish to know that in the animation, the position of the electron is generated randomly using a *Monte Carlo* technique. Thus, if you "Rewind" the animation to start it over, the build-up of the histogram is almost certain to not be identical to the previous "trial."

We conclude that whatever is going on to cause the interference pattern does not involve two or more electrons interacting with each other. And yet, with one electron at a time in the system, with both slits open there are places on the screen where the electrons do not go, although with only one slit open some electrons do end up at that position.

Now, to get an interference pattern we take a wave, split it up into two parts, send each part through one of the slits, and then recombine the waves. Does this mean that a single electron is somehow going through both slits at once? This too is amenable to experimental test.

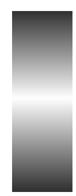
The result of doing the test turns out to be independent of the details of how the experiment is done, so we shall imagine a very simple arrangement: we place a light bulb behind the slits and look to see what is going on. Note that in a real experiment, the light bulb would have to be smaller than in the figure and tucked in more tightly behind the slits so that the electrons don't collide with it.



We will see a small flash of light when an electron passes through the slits.

What we see is that every electron is acting completely "normal": one-half the electrons are going through the upper slit, one-half are going through the lower slit, and which is going to be the case for a given electron appears to be random. A small (24k) gif animation of what we might see in this experiment may be seen here.

But meanwhile, we have a colleague watching the flashes of light on the phosphor coated screen who says "Hey, the interference pattern has just gone away!" And in fact the distribution of electrons on the screen is now exactly the same as the distribution of machine gun bullets that we saw above.
The figure to the right is what our colleague sees on the screen.



Evidently, when we look at what is going on at the slits we cause a qualitative and irreversible change in the behavior of the electrons. This is usually called the "Heisenberg Uncertainty Principle."

Everyone has always known that doing any measurement on any system causes a disturbance in the system. The classical paradigm has been that at least in principle the disturbance can be minimised to the point that it is negligible.

Is it possible to minimise the disturbance being caused by the light bulb? We can turn down the intensity of the light it is emitting. However, if we try it, just at the point that the light is getting so faint that we are missing some of the electrons, the interference pattern starts to come back! In fact, if the light intensity is, say, such that we are missing one-half of the electrons, we have one-half an interference pattern and one-half a particle distribution. So this attempt to minimise the disturbance didn't work out: we still don't know what is going on at the slits when we see the interference pattern.

There is yet another way to minimise the disturbance. The light contains energy, and it turns out that if we increase the wavelength of the light, towards the infrared, the energy of each part of the light goes down. Perhaps if we decrease the energy in the light we won't be scattering it off the electrons so violently. So, we start increasing the wavelength of the light emitted by the light bulb. We continue to see all the electrons, and at first we always see that one-half of them are going through the upper slit and one-half are going through the lower slit.

However, our ability to resolve two positions in space by looking depends on the wavelength of the light that we are seeing with. And just at the point that the wavelength of the light from the lightbulb gets so large that although we can see the electrons we can't tell which slit they went through, the interference pattern comes back.

A student once remarked that we should do a "better" experiment. The Heisenberg Uncertainty Principle says that such a better experiment does not exist. Einstein in particular devoted a lot of time trying to devise such a better measurement; all his attempts failed.

The conclusion of all this is that there is **no** experiment that can tell us what the electrons are doing at the slits that does not also destroy the interference pattern. This seems to imply that there is **no** answer to the question of what is going on at the slits when we see the interference pattern. The path of the electron from the electron gun to the screen is not knowable when we see the interference pattern. As Heisenberg said, "The path [of the electron] comes into existence only when we observe it."

We will be discussing interpretations of what all this may mean in great detail later. For now I will briefly mention a "standard" if incomplete interpretation. If we think that the probability of where the electron is in space is a wave, then when we don't look the probability wave has two pieces at the slits, representing the fact that there is a 50% chance the electron went through the upper slit and a 50% chance it went through the lower slit. These two probability waves from the two slits, then, recombine at the screen and cause the interference pattern.

When we look, we "collapse the state" in a 100% chance it went through one slit and a 0% chance it went through the other. And in this circumstance the two probability waves for the two slits cannot then recombine at the screen to cause an interference pattern: for each electron there is only one non-zero probability wave.

Finally, then, we have two contradictory yet complementary models of the two-slit experiment for electrons. In one model the electron is a particle that somehow exhibits an interference pattern. In the other model, the electron is a wave that somehow manifests as a particle whenever we look at it.

A Flash animation of these two models, both incomplete, may be accessed by clicking the red button to the right. The file size is 23k and will appear in a separate window.

Click Me

References

- Richard Feynman, **The Character of Physical Law** (MIT, 1965), Chapter 6
- Richard P. Feynman, Robert B. Leighton and Matthew Sands, **The Feynman Lectures on Physics** (Addison-Wesley, 1963), Vol III, Chapter 1

Author

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13.5: Flash Animations for Physics

We have been increasingly using Flash animations for illustrating Physics content. This page provides access to those animations which may be of general interest. The animations will appear in a separate window.

The animations are sorted by category, and the file size of each animation is included in the listing. Also included is the minimum version of the Flash player that is required; the player is available free from http://get.adobe.com/flashplayer/. The categories are:

- Chaos
- Classical Mechanics
- Electricity and Magnetism
- Fluid Mechanics
- Micrometer Caliper
- Miscellaneous
- Nuclear
- Optics
- Oscilloscope
- Quantum Mechanics
- Relativity
- Sound Waves
- Vectors
- Waves

In addition, I have prepared a small tutorial in using Flash to do Physics animations. It contains screen shots and embedded Flash animations, so the file size is a 173k. You may view it in a separate window at http://faraday.physics.utoronto.ca/PVB/Harrison/Flash/Tutorial/FlashPhysics.html.

Links to versions of these animations in other languages, other links, and license information appear towards the bottom of this page.

The Animations

There are 99 animations listed below. Some are simple; others are more complex. The most recent animations added to the list are identified.

Category	Title	Description/Comment	
Chaos	Bunimovich Stadium	Illustrating the chaotic Bunimovich Stadium. Requires Flash 6; file size is 17k.	View
Chaos	Logistic Map	The logistic map, which demonstrates the bifurcation of the population levels preceding the transition to chaos. Requires Flash 6; file size is 15k.	View
Chaos	Lorenz Attractor	Looking at the Lorenz Attractor in a chaotic regime, allowing the attractor to be rotated. Requires Flash 6; file size is **550k**.	View
Chaos	Three-body Gravitational Interaction	2 fixed suns and 1 planet. Initial conditions are controllable, and up to 4 different independent planets may be displayed. Requires Flash 6 and a computer with reasonable power; file size is 50k.	View
Classical Mechanics	Displacement and Distance	A simple animation showing the difference between the *distance* and the *displacement*. Requires Flash 5; file size is 5k.	View
Classical Mechanics	Constant Acceleration	1-dimensional kinematics of a body undergoing constant acceleration. Includes visually integrating the acceleration and velocity graphs, and visually differentiating the position and velocity graphs. Requires Flash 6; file size is 30k.	View
Classical Mechanics	Motion Animation	A car with a non-zero initial speed has a constant acceleration whose value can be controlled by the user. Requires Flash 6; file size is 27k.	View

Classical Mechanics	Dropping Two Balls Near the Earth's Surface	Two balls falling near the Earth's surface under the influence of gravity. The initial horizontal speed of one of the balls may be varied. Requires Flash 6; file size is 11k.	View
Classical Mechanics	Galilean Relativity	Illustrating Galilean relativity using his example of dropping a ball from the top of the mast of a sailboat. Requires Flash 6; file size is 22k.	View
Classical Mechanics	Foucault Pendulum	A simple animation viewing a Foulcault Pendulum at the North Pole from an inertial frame above the Earth. See also the Foucault Pendulum animation in the Relativity section. Requires Flash 7 and Action Script 2; file size is **1.3 M** .	View
Classical Mechanics	Projectile Motion	Firing a projectile when air resistance is negligible. The initial height and angle may be adjusted. Requires Flash 6; file size is 36k.	View
Classical Mechanics	Kinematics of Projectile Motion	A visualization exploration of the kinematics of projectile motion. Requires Flash 6; file size is 9k.	View
Classical Mechanics	The Monkey and the Hunter	An animation of the classic lecture demonstration. The actual demonstration is preferable if possible; then this animation can be given to the students for later review. Requires Flash 6; file size is 21k.	View
Classical Mechanics	Racing Balls	Two balls roll down two different low-friction tracks near the Earth's surface. The user is invited to predict which ball will reach the end of the track first. This problem is difficult for many beginning Physics students. Requires Flash 6 Release 79; file size is 140k.	View
Classical Mechanics	Racing Skiers	The "Racing Balls" animation which is accessed via the above line sometimes triggers cognitive dissonance and rejection in beginning students. For some of these, changing the balls to skiers helps to clarify the situation, and that is what this animation does. The "Racing Balls" one should be used with students first. Requires Flash 6 Release 79; file size is 145k.	View
Classical Mechanics	Air Track Collisions	Elastic and inelastic collisions on an air track, with different masses for the target cart. Requires Flash 6; file size is 70k.	View
Classical Mechanics	Newton's Cradle	A small animation of Newton's Cradle, sometimes known as Newton's Balls. Requires Flash 6; file size is 1k.	View
Classical Mechanics	Hooke's Law	A simple animation illustrating Hooke's Law. Requires Flash 6; file size is 13k.	View
Classical Mechanics	Coordinate System for Circular Motion	An unusual coordinate system for describing circular motion. Requires Flash 6; file size is 94k.	View
Classical Mechanics	Vertical Circular Motion	A mass is in circular motion in the vertical plane. We show the weight and force exerted by the tension in the string. Requires Flash 6; file size is 7k.	View
Classical Mechanics	Forces on a Pendulum	The weight, force due to tension, and total force exerted on the bob of a pendulum are shown. Requires Flash 6; file size is 8k.	View

Classical Mechanics	Motion in a Non-inertial Frame	The motion of a ball in uniform circular motion is viewed by an observer in a rotating reference frame. Requires Flash 6; file size is 12j,	View
Classical Mechanics	Rolling Disc	A simple animation that traces the motion of a point on a rolling disc. Requires Flash 6; file size is 31k.	View
Classical Mechanics	Right-Hand Screw Rule	The direction of the angular velocity vector given by a right-hand screw rule. Requires Flash 6; file size is 196k. Also linked to from the *Vectors* section.	View
Classical Mechanics	Direction of the Angular Velocity Vector	A simple animation of the direction of the angular velocity vector. Requires Flash 6; file size is 125k.	View
Classical Mechanics	Curling	Curling rocks and tori sliding across surfaces. Requires Flash 6; file size is **601k**.	View
Classical Mechanics	How Does a Cat Land on its Feet?	The saying is that cats always land on their feet. This animation explains how they do this. Requires Flash 6; file size is 81k.	View
Classical Mechanics	Precession of a Spinning Top	A simple animation of a spinning top which precesses. Requires Flash 5; file size is **739k.**	View
Classical Mechanics	Simple Harmonic Motion I	Demonstrating that one component of uniform circular motion is simple harmonic motion. Requires Flash 6; file size is 10k.	View
Classical Mechanics	Simple Harmonic Motion II	Illustrating and comparing Simple Harmonic Motion for a spring-mass system and for a oscillating hollow cylinder. Requires Flash 5; file size is 20k.	View
Classical Mechanics	Damped Simple Harmonic Motion	The damping factor may be controlled with a slider. The maximum available damping factor of *100* corresponds to critical damping. Requires Flash 6; file size is 12k.	View
Classical Mechanics	Driven Simple Harmonic Motion	A harmonic oscillator driven by a harmonic force. The frequency and damping factor of the oscillator may be varied. Requires Flash 6; file size is 199k.	View
Classical Mechanics	Coupled Harmonic Oscillators	Two simple pendulums connected by a spring. The mass of one of the pendulums may be varied. Within mathematical rounding errors, the resolution on the screen of one pixel, and a frame rate of 12 frames per second the animation is correct, not an approximation. Requires Flash 6; file size is 47k.	View
Electricity and Magnetism	Coulomb's Law	A simulation of an experiment to determine the dependence of the electrostatic force on distance. Requires Flash 6; file size is 15k.	View

Electricity and Magnetism	Comparing a DC circuit to the flow of water.	A simple DC circuit has a DC voltage source lighting a light bulb.Also shown is a hydraulic system in which water drives a turbine. The two systems are shown to be similar. Requires Flash 6; file size is 51k.	View
Electricity and Magnetism	A Light Switch	A simple animation of how a common light Switch works. Requires Flash 6; file size is 4kb.	View
Electricity and Magnetism	Field Lines	Illustrating representing an electric field with field lines. Requires Flash 5; file size is 22k.	View
Electricity and Magnetism	A Simple Buzzer	A simple buzzer consisting of a battery, a flexibile metal strip, a piece of iron, and some wire. Requires Flash 6; file size is 20k.	View
Electricity and Magnetism	Electric Field of an Oscillating Charge	An electric charge is executing simple harmonic motion, and the animation shows the electric field lines around it. Requires Flash 6 and a computer with reasonable power; file size is 40k.	View
Electricity and Magnetism	Electric and Magnetic Fields of an Oscillating Charge	A 3 dimensional animation of the "far" fields of an oscillating charge. Requires Flash 6; file size is 120k.	View
Electricity and Magnetism	Circular Polarization	Circular polarization generated from a linearly polarized electromagnetic wave by a quarter-wave plate. Requires Flash 6; file size is **785k.**	View
Electricity and Magnetism	Spinning Charges and an Inhomogeneous Magnetic Field 1	A spinning charged object passes through an inhomogeneous magnetic field. This animation is also used in a discussion of the Stern-Gerlach experiment. Requires Flash 6; file size is 74k.	View
Electricity and Magnetism	Spinning Charges and an Inhomogeneous Magnetic Field 2	A spinning charged object passes through an array of 3 magnets each producing an inhomogeneous magnetic field. This animation is also used in a discussion of the Stern-Gerlach experiment. Requires Flash 6; file size is 79k.	View
Fluid Mechanics	Viscous Motion	Dropping a ball in a viscous liquid. The densities, liquid viscosity, and size of the ball are controllable. Requies Flash 6; file size is 55k.	View
Fluid Mechanics	Dropping a Ball From the CN Tower	A ball is dropped through the air from 350 m above the ground. The ball may be a billiard ball, a 5-pin bowling ball or a 10-pin bowling ball. The 5-pin bowling ball clearly shows the *drag crisis*. Requires Flash 7; file size is 133k.	View
Micrometer Caliper	Measuring with a Micrometer	A simple animation of using a micrometer to measure the width of a pencil. Requires Flash 5; file size is 13k.	View
Micrometer Caliper	An Exercise in Reading a Micrometer	Provides controls to position the micrometer, and when a button is clicked displays the reading. Requires Flash 5; file size is 30k	View
Miscellaneous	A Simple Piston and Boyle's Law	A small animation showing a piston compressing a sample of gas. As the volume of the gas goes down, the density and therefore the pressure goes up. Requires Flash 5; file size is 3.9k.	View

Miscellaneous	Derivative of the Sine Function	An animation illustrating that the derivative of a sine function is a cosine. Requires Flash 6, file size is 20k.	View
Miscellaneous	Area of a Circle As a Limit	Illustrating that the area of a circle is a limit of the sum of the areas of interior triangles as the number of triangles goes to infinity. Requires Flash 5; file size is 12k.	View
Miscellaneous	Integration	Illustrating the meaning of the integral sign, including an example. Requires Flash 5; file size is 124k.	View
Nuclear	Scattering	Simulating nuclear scattering experiments by scattering ball bearings off targets. This is based on an experiment in the First Year Physics Laboratory at the University of Toronto. Requires Flash 6 Release 79; file size is 182k.	View
Nuclear	Nuclear Decays	The decay of 500 atoms of the fictional element Balonium. Uses a proper Monte Carlo engine to simulate real decays. Requires Flash 6, file size is 27k.	View
Nuclear	Pair Production	A simple illustration of electron-positron production and annihilation. Requires Flash 5, file size is 21k.	View
Nuclear	The Interaction of X-rays With Matter	Illustrating the 3 principle modes by which X-rays interact with matter. Requires Flash 6; file size is 47k.	View
Optics	Rotating a Mirror and the Reflected Ray	Illustrating that when a mirror is rotated by an angle, the reflected ray is rotated by twice that angle. Requires Flash 6; file size is 20k.	View
Optics	Reflection and Refraction	Illustrating reflection and refraction, including total internal reflection. Requires Flash 6; file size is 33k.	View
Optics	Object-Image Relationships	Ray tracing for a thin lens showing the formation of a real image of an object. Requires Flash 5; file size is 17k.	View
Optics	Using an Optical Bench	A simulation of an optical bench with a light source, object, thin lens and an image. The screen that displays the image is moved. Requires Flash 5, file size is 14k.	View
Oscilloscope	The Time Base Control 1	Shows the effect of changing the time base control on the display of an oscilloscope. There is no input voltage. Requires Flash 5; file size is 10k.	View
Oscilloscope	The Time Base Control 2	Shows the effect of changing the time base control on the display when there is an input voltage varying in time. Requires Flash 5; file size is 12k.	View

Oscilloscope	The Time Base Control 3	Shows the effect of changing the time base control on the display when there is an input voltage varying in time when the frequency of the voltage is high. Requires Flash 5; file size is 17k.	View
Oscilloscope	The Voltage Control	Shows the effect of changing the voltage control on the display. Requires Flash 5; file size is 10k.	View
Oscilloscope	The Trigger	Shows the effect of changing the trigger level on the display. Requires Flash 5; file size is 5.9k	View
Quantum Mechanics	The Bohr Model	The photon excitation and photon emission of the electron in a Hydrogen atom as described by the Bohr model. Requires Flash 6: file size is 77k.	View
Quantum Mechanics	Circular Standing Waves	Illustrating how thinking about the electron as a de Broglie wave "explains" the Bohr model.	View
Quantum Mechanics	Complementarity	Here we visualize a hydrogen atom, which consists of an electron in orbit around a proton. In one view the electron is a *particle* and in the other view it is a *probability distribution*. The reality is neither view by itself, but a composite of the two. Requires Flash 5; file size is 15k.	View
Quantum Mechanics	The Double Slit Experiment 1	The famous "Feynman Double Slit Experiment" for electrons. Here we fire one electron at a time from the electron gun, and observe the build-up of electron positions on the screen. Requires Flash 5; file size is 15k.	View
Quantum Mechanics	The Double Slit Experiment 2	Here we illustrate *Complementarity* using the double slit experiment. We view the path of the electron from the gun to the observing screen as a particle and as a wave. Requires Flash 5; file size is 33k.	View
Quantum Mechanics	Stern-Gelach Filters	Up to three Stern-Gerlach filters with user-controlled orientations are placed in an electron beam. Requires Flash 7; file size is 130k.	View
Quantum Mechanics	Bell's Theorem	Based on an analysis by Mermin, this animation explores correlation measurements of entangled pairs. Requires Flash 6; file size is 38k.	View
Relativity	Michelson-Morley Experiment	A simple analogy involving two swimmers that sets up the Michelson-Morley Experiment. Requires Flash 6; file size is 15k.	View
Relativity	Time Dilation	A demonstration that the phenomenon of time dilation from the special theory of relativity necessarily follows from the idea that the speed of light is the same value for all observers. Requires Flash 6; file size is 55k.	View
Relativity	Deriving Length Contraction	A tutorial that shows how relativistic length contraction must follow from the existence of time dilation. Requires Flash 5; file size is 37k.	View

Relativity	Length Contraction is Invisible	This series of animations demonstrates that the relativistic length contraction is invisible. Requires Flash 5; file size is 90k.	View
Relativity	Deriving the Relativity of Simultaneity	A tutorial that shows how the relative nature of the simultaneity of two events must follow from the existence of length contraction. Requires Flash 5; file size is 39k.	View
Relativity	Twin Paradox	There are many ways of approaching this classic "paradox". Here we discuss it as an example of the relativistic Doppler effect. Requires Flash 6; file size is 116k.	View
Relativity	Foucault Pendulum and Mach's Principle	This began as an animation of the Foucault Pendulum, but then I generalized it to illustrate Mach's Principle. See also the simple Foucault Pendulum in the Classical Mechanics section. Requires Flash 6, file size is **1.5M**.	View
Relativity	Advance of the Perihelion	A simple animation showing Newton's and Einstein's predictions for the orbit of Mercury. Requires Flash 6; file size is 7.0k.	View
Sound Waves	Beats	Illustrating beats between 2 oscillators of nearly identical frequencies. Requires Flash 6; file size is 215k.	View
Sound Waves	Doppler Effect: Wave Fronts	Illustrating the wave fronts of a wave for a moving source. There are a few similar animations on the web: this is my re-invention of that wheel. Requires Flash 6; file size is 11k	View
Sound Waves	Doppler Effect	Illustrating the classical Doppler Effect for sound waves. Requires Flash 6; file size is 43k.	View
Sound Waves	Tuning Fork	A small animation of a vibrating tuning fork producing a sound wave. Requires Flash 5; file size is 2.7k.	View
Sound Waves	Pressure and Displacement Waves	This animation shows air molecules vibrating, with each molecule "driving" its neighbor to the right. It is used to illustrate that when the displacement wave is at a maximum then the density of the molecules, and thus the pressure wave, is at a minimum and vice versa. Requires Flash 5; file size is 30k	View
Sound Waves	Temperament	A very brief introduction to the physics and psychophysics of music, with an emphasis on temperament, the relationship between notes. Requires Flash 6 and sound; file size is 151k.	View
Vectors	Adding 2 Vectors	A simple demonstration of adding 2 vectors graphically. Also demonstrates that vector addition is commutative. Requires Flash 5; file size is 7k.	View
Vectors	Adding 3 Vectors	A simple demonstration of adding 3 vectors graphically. Also demonstrates that vector addition is associative. Requires Flash 5; file size is 10k.	View

Vectors	Subtracting 2 Vectors	A simple demonstration that subtracting 2 vectors graphically is the same as adding the first one to the negative of the second one. Requires Flash 5; file size is 4.5k.	View
Vectors	Component Addition	A simple demonstration that to add 2 vectors numerically, just add the Cartesian components. Requires Flash 5; file size is 16k.	View
Vectors	Unit Vectors	A simple animation of unit vectors and vector addition. Requires Flash 6; file size is 12k.	View
Vectors	Dot Product	A simple demonstration of the relation between the dot product of 2 vectors and the angle between them. Requires Flash 6; file size is 8k.	View
Vectors	Right-Hand Screw Rule	The direction of the angular velocity vector given by a right-hand screw rule. Requires Flash 6; file size is 196k. Also linked to from the *Classical Mechanics* section.	View
Vectors	Cross Product	The direction of the cross product of 2 vectors is demonstrated. The magnitude shown is correct but not discussed. Requires Flash 6; file size is 44k.	View
Waves	Traveling Waves	Illustrating the sign of the time term for traveling waves moving from left to right or right to left. Requires Flash 6; file size is 42k.	View
Waves	A Plane Wave Traveling Through Two Mediums	Illustrating the relation between wavelengths and frequencies of a wave when it travels from one medium to another. Requires Flash 6; file size is 5.4k.	View
Waves	Refraction	The previous animation shows wave fronts entering the mediums with a zero angle of incidence. Here the angle of incidence is not zero. Requires Flash 6; file size is 11kb	View
Waves	Reflections From a Barrier	A wave is reflected from a barrier with a phase reversal. This is the behavior for transverse waves and the *displacement* aspect of a longitudinal wave. Requires Flash 5; file size is 42k.	View
Waves	Reflections From Two Barriers	A wave is reflected back and forth between two barriers, setting up a standing wave. Requires Flash 5; file size is 41k.	View
Waves	Standing Waves With a Node on Both Ends	The first three standing waves for nodes at both ends. The frequencies of the waves are proportional to one over the wavelength. Requires Flash 5; file size is 11k.	View
Waves	Standing Waves With a Node on One End	The first three standing waves for a node at one end and an anti node at the other. The frequencies are proportional to one over the wavelength. Requires Flash 5; file size is 18k.	View

Other Languages and Links

These animations have been translated into Catalan, Spanish and Basque:

En aquest enllaç http://www.meet-physics.net/David-Harrison podeu trobar la versió al català de les animacions Flash de Física.

Las animaciones Flash de Física se han traducido al español, y están disponibles en esta dirección: http://www.meet-physics.net/David-Harrison

Fisikako Flash animazioak euskeratu dira eta helbide honetan eskura daitezke http://www.meet-physics.net/David-Harrison

Many animations have been translated into Greek by Vangelis Koltsakis. The web site is: users.sch.gr/ekoltsakis/nt/harrison/harrison.htm

Many animations have been translated into Dutch by Jacques Bijvoet, Dalton Lyceum Barendrecht. http://www.xs4all.nl/~jafrma/Harrison/

Most animations have been translated into Hungarian by Sandor Nagy, Eötvös Loránd University. Üdv a magyar látogatónak! Nagy Sándor egyik gyűjteményében (http://nasa.web.elte.hu/Harrisonia/) 68 magyarított animációmat találja meg magyar szövegkörnyezetben.

Many animations have been translated into Polish by the edukator.pl team. Do wspaniałego dorobku Davida Harrisona polską wersję językową wykonał zespół edukator.pl - Fundacja Nauka i Wiedza. http://www.edukator.pl/APLETY,7365.html

Tags recommended by the template: article:topic

13.6: Locality and Quantum Mechanics

Introduction

You may be aware of the fact that Einstein never accepted Quantum Mechanics. He explained his objections by discussing two particular aspects of the theory. One was the fact that the theory is probabilistic, and seems to imply that the future is random. Einstein repeatedly said "God does not play dice with the universe," to which Bohr responded "Quit telling God what to do!" The probabilistic nature of cause and effect in Quantum Mechanics is pinpointed particularly well by the Schrödinger's Cat paradox.

The second aspect of Quantum Mechanics that greatly bothered Einstein is what he called a "spooky action at a distance" implied by the theory. Often this aspect of the theory is characterized as *non-locality*.

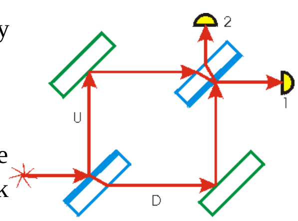
Locality means the reasonable assumption that no signal can travel faster than the speed of light. This imposes constraints on cause and effect. Thus, if we send a signal traveling at light speed to Alpha Centarui, which is 4.5 light years away from us, that signal will have no effect on Alpha Centauri for 4.5 years: locality says it is impossible to cause some effect on Alpha Centauri any faster than this. If we send a signal at light speed to the other side of a room which is about 10 meters away, the signal can have an effect in about 3 billionths of a second: the other side of the room is more local than Alpha Centauri.

As we shall see, locality is in some conflict with Quantum Mechanics.To illustrate the conflict we will only need the fact that we can view phenomena such as light as both a wave and as a particle.

The following discussion is at the level of an upper year liberal arts course in modern physics without mathematics that is given at the University of Toronto.

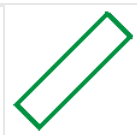
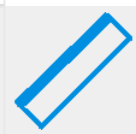
Mach-Zehnder Interferometer

We shall use the *Mach-Zehnder Interferometer* to illustrate non-locality. The device, co-invented by Ernst Mach, the "grandfather" of the Theories of Relativity, is shown to the right:



The legend for the figure is shown to the left.

Recall that a "half-silvered mirror" is a mirror that only reflects one-half of the light incident on it; the other half is transmitted through the mirror. In the figure, the reflecting surface is drawn as the thick one.

Light source:		Mirror:	
Detector:		Half-silvered mirror:	

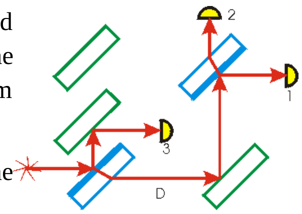
Light leaves the source and travels to the first half-silvered mirror. One half of the light is reflected as the upper *U* beam, which is reflected by the upper-left mirror, and travels to the upper-right half-silvered mirror. There, one half of the beam is transmitted to Detector *1*, and the other half is reflected into Detector *2*.

From the lower-left half-silvered mirror, the lower *D* beam is reflected by the lower-right mirror, and travels to the upper-right half-silvered mirror. There, one half of the beam is reflected to Detector *1*, and the other half is transmitted into Detector *2*

It turns out that, despite contrary appearances in the figure, all of the light that leaves the source ends up in Detector *1*; no light enters Detector *2*. What is happening is that the two beams, *U* and *D*, constructively interfere at Detector *1* and destructively interfere at Detector *2*. The details of why this is so are sort of complex and not important for our purpose here. Those details are related to the fact that when light goes from one medium to another various "phase changes" occur.

This type of interferometer is still in regular use in laboratories around the world. It turns out that the balance of constructive and destructive interference at the detectors is extremely sensitive to any phase changes in the two beams of light. Thus, by inserting, say, a gas sample into the path of one of the beams, the additional phase shift caused by the gas allows the deduction of information on the density, pressure and temperature of the gas by observing the changes in intensity of the signals arriving at the two detectors.

Another Interferometer Arrangement



Now consider the arrangement to the right. A third mirror deflects all of the upper *U* beam to a third detector. Now there can not be any interference effects at detectors 1 and 2 because there is only one beam reaching the upper-right half-silvered mirror. This beam is made up of one-half of the light from the source; the other half is reflected by the lower-left half-silvered mirror and ends up in detector 3.

In summary, for this arrangement, the percentages of the light leaving the source that arrive at the detectors are:

Detector	Percentage of Light from Source
1	25%
2	25%
3	50%

Now we begin to think of the light in the interferometer as *photons*, its particulate aspect. In the arrangement discussed in this section, 25% of the photons that leave the source end up in detector 2. Think for a moment about one of those photons. It travels along the lower path *D* and ends up in the detector. It can only end up in that detector if the third mirror is deflecting the *U* beam. But how did that photon "know" whether or not the *U* beam was being deflected? It was never anywhere near the third mirror.

It is here that we see a hint of non-locality. The existence of a third mirror that is deflecting the *U* beam has an immediate non-local effect on photons that were never near that mirror.

This non-locality is consistent with Quantum Mechanics, and can be demonstrated in other circumstances. For example, we consider the double slit experiment for electrons. There are positions at the observing screen where electrons will not go when both slits are open, the *minima* in the interference pattern. But with only one slit open, some electrons do go to that position on the screen. So if an electron goes through, say, the upper slit it seems to "know" whether or not the lower slit is open, so it knows whether or not it can go to one of the positions of the minima in the interference pattern.

Conclusion

The potential conflict between locality and Quantum Mechanics has been known since at least the early 1930's, and was the focus of a famous paper by Einstein, Pololsky and Rosen (EPR) in 1934. In that paper, they concluded that Quantum Mechanics must be at least incomplete.

The possible non-local and/or probabilistic nature of cause and effect is explored more deeply by Bell's Theorem of 1964 and its subsequent experimental tests. A document on Bell's Theorem is available here

Both for the material discussed here and especially in commentary about Bell's Theorem, one sometimes sees statements that according to Quantum Mechanics one may transmit *information* at speeds greater than the speed of light. I have never seen such an argument that I believe is correct. Whatever is being transmitted at superluminal speeds is somewhat less than information; d'Espagnat uses the word *influence*.

If we have some influence or even information being transmitted at superluminal speed from *A* to *B*, then according to the Special Theory of Relativity there are reference frames where the influence is traveling from B to A; the influence is still traveling faster than the speed of light with respect to all observers. The conclusion is that any superluminal influence has to be viewed as a *connection* between A and B, and identifying which is the cause and which is the effect is problematic.

A JPU200Y student recently made a startling suggestion that the *influence* can be traveling at superluminal speeds via a mini-blackhole wormhole connection, ie. through the *quantum foam* that we have seen pervades space time at very small distances.

Author

his document was written in March 2000 by David M. Harrison, Department of Physics, University of Toronto, mailto:harrison@physics.utoronto.ca. This is version 1.4, date (m/d/y) 03/12/02.

13.7: Particle in a 2-dimensional box

We learned from solving Schrödinger's equation for a particle in a *one*-dimensional box that there is a set of solutions, the stationary states, for which the time dependence is just an overall rotating phase factor, and these solutions correspond to definite values of the energy. An alternative way of finding that set of solutions is *separation of variables*. The basic strategy is to assume that the solution to the wave equation can be factored into a product of two functions, one depending only on time, the other on the spatial variable,

$$\Psi(x,t)=\psi(x)\varphi(t) \tag{13.7.1}$$

If this solution is substituted in the Schrödinger equation, and the result divided by $\Psi(x,t)$, we find

$$i\hbar\frac{\frac{\partial\phi(t)}{\partial t}}{\phi(t)}=\frac{-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+V(x)\psi(x)}{\psi(x)} \tag{13.7.2}$$

On writing the equation in this form, it is clear that the left hand side is only a function of t, not of x, and the right hand side is only a function of x! This can only make sense if in fact both sides are the same constant. If we denote this constant by E, we can write two equations:

$$i\hbar\frac{\partial\phi(t)}{\partial t}=E\phi(t) \tag{13.7.3}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+V(x)\psi(x)=E\psi(x) \tag{13.7.4}$$

The solution to the first equation just gives the phase time dependence,

$$\varphi(t)=Ae^{-iEt/k} \tag{13.7.5}$$

and the second is the time independent Schrödinger equation as before. The solutions to this equation are determined by the boundary conditions on ψ, in general there is a sequence of such eigenstates labeled by a quantum number n = 0,1,2,3,..., with corresponding values E_0, E_1, ..., which are put in the corresponding $\varphi(t)$.

A Two Dimensional Box

Let us now consider the Schrödinger equation for an electron confined to a two dimensional box, $0<x<a$ and $0<y<b$. That is to say, within this rectangle the electron wavefunction behaves as a free particle ($V(x,y)=0$), but the walls are impenetrable so the wavefunction $\Psi(x,y,t)=0$ at the walls. What do we expect the wavefunction to look like?

First notice that the separation of variables trick given above for one dimension works equally well here, writing

$$\Psi(x,y,t)=\psi(x,y)\varphi(t) \tag{13.7.6}$$

gives

$$i\hbar\frac{\partial\phi(t)}{\partial t}=E\phi(t) \tag{13.7.7}$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi(x)}{\partial x^2}+\frac{\partial^2\psi(x)}{\partial y^2}\right)=E\psi(x) \tag{13.7.8}$$

The surprising thing at this point is that we can do the separation of variables trick *again*—we can write

$$\psi(x,y)=f(x)g(t) \tag{13.7.9}$$

and substitute in the above equation to find

$$-\frac{\hbar^2}{2m}\left(\frac{\frac{\partial^2 f(x)}{\partial x^2}}{f(x)}+\frac{\frac{\partial^2 g(x)}{\partial y^2}}{g(y)}\right)=E \tag{13.7.10}$$

Again, we have an equation in which only one term is *x*-dependent, so it must be a constant (which we take to be negative for future convenience),

$$\frac{\frac{\partial^2 f(x)}{\partial x^2}}{f(x)} = -C \tag{13.7.11}$$

so

$$\frac{\partial^2 f(x)}{\partial x^2} = -C f(x) \tag{13.7.12}$$

This is exactly the same equation we dealt with in the one dimensional case, so we know

$$f(x) = A \sin \frac{n\pi x}{a} \tag{13.7.13}$$

with n an integer, and the constant C is equal to $n^2\pi^2/a^2$. Hence the energy levels in this rectangular well are given by

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n_x^2\pi^2}{a^2} + \frac{n_y^2\pi^2}{b^2}\right) \tag{13.7.14}$$

with n_x and n_y are the two quantum numbers needed to label each state.

The first nice probability distributions for a particle in a 2D box are viewable below.

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wiki.page("Visualizations_and_Simulations/CalcPlot3D/Probability_Wave_Function")
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Figure $\mathbf{13.7.1}$ *: Visualization of the probability for a particle in a 2D box. The quantum numbers (n_x and n_y) can be varied in the upper left.*

Degeneracy

Two distinct wavefunctions are said to be *degenerate* if they correspond to the same energy. If the sides *a*, *b* of the rectangle are such that *a*/*b* is irrational (the general case), there will be no degeneracies. The *most* degenerate case is the square, *a* = *b*, for which clearly $E_{m,n} = E_{n,m}$. Degeneracies in quantum physics are most often associated with symmetries in this way.

Figure $\mathbf{13.7.2}$ *: Contours of the $n_x = 2$ and $n_y = 3$ wavefunction (left) and $n_x = 3$ and $n_y = 2$ wavefunction (right).*

We give here examples of wavefunctions (3,2) and (2,3) for a rectangle. These are contour maps for the time-independent solution, with white being the highest point. These two wavefunctions do not correspond to the same energy, although they would, of course, for a square.

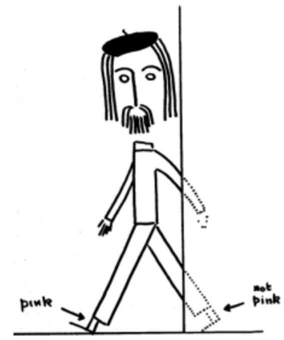
Contributors and Attributions

- Michael Fowler (Beams Professor, Department of Physics, University of Virginia)

13.8: Quantum Entanglement

The origins of this story are rooted in the very beginnings of Quantum Mechanics in 1926. A seminal paper was by Einstein, Podolsky and Rosen in 1935, so often the acronym EPR is associated with all this. In the early 1950's David Bohm re-cast the *EPR* argument in a clearer form, so sometimes the acronym becomes EPRB. In 1964 John Bell published a theorem that made the situation even clearer, so sometimes we refer to *Bell's Theorem*. Finally, the whole story is based on pairs of objects which somehow are interconnected even when they are spatially separated, and we say the objects are *entangled*.

Bertlmann's Socks



Bertlmann, a colleague of Bell at CERN, always wore mismatched socks. Which color he would have on a given foot on a given day was quite unpredictable. But when you see that the first sock is pink you can be sure that the second sock is not pink, even when you can't see it. The figure, drawn by Bell, illustrates. There is no mystery here.

An important question for a sock is: "Will it wash?" We imagine a consumer testing organization which wants to determine if a sock will withstand washing when the water is at 0° C, or at 45° C, or at 90° C. We assume, reasonably, that the washability goes down as the temperature increases.

We imagine a large collection of socks. There may be variability in the washability of them. We randomly divide the collection into thirds, and assume that we have a large enough collection that the washability of the socks is equally represented in each third. We wash one collection of socks at 0°, and those that survive we wash at 45°. We wash the second collection of socks at 45°, and those that survive we wash at 90°. We wash the third collection at 0° and those that survive we wash at 90°. Since the washability of each collection of socks is the same:

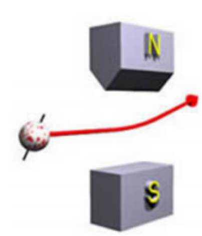
> The number that survive at 0° and not at 45° Plus
>
> The number that survive at 45° and not at 90° Is not less than
>
> The number that survive at 0° and not at 90°

There is no mystery here either. For each member of the third group, either it would not have survived at 45° and would have been in the first group, or it would have survived at 45° and would have been in the second group.

But Bertlmann's socks come in pairs. We assume that each individual pair of socks has different colours but identical washability. Then if we test a large sample of pairs of his socks the relation at the bottom of the previous page becomes:

> The number of pairs in which one survives at 0° and the other not at 45° Plus
>
> The number of pairs in which one survives at 45° and other not at 90° Is not less than
>
> The number of pairs in which one survives at 0° and other not at 90°

Electron Spin



When a charged classical object is spinning, if we throw it between the poles of a weird shaped magnet it will be deflected either up or down. The amount of deflection depends on:

- The total charge on the object and its distribution.
- The rate and orientation of the spin

If we take a beam of electrons from an electron gun and run it through the magnet, we see something strange: all electrons are deflected up by some fixed amount or deflected down by exactly the same amount, and which for each individual electron appears to be random. If the deflection is up, we say the electron is "spin up" and if it is deflected down we say it is "spin down."

There are substances which emit electrons in pairs. Each electron acts just like the electrons from the electron gun. But when we look at pairs of electrons we see that if one electron is "spin up" then its companion is "spin down" and vice versa. So we can call these Bertlmann's electrons: if you measure one and see that it is spin up, you know that its companion is not spin up, it is spin down. Physicists often say that these pairs have a total spin of zero and that the two electrons are *entangled*.

The fact that electrons can have only two spin states is a mystery. The fact that Bertlmann's electrons have a total spin of zero is not.

There is a further mystery about electrons, either from an electron gun or one of the Bertlmann pairs: if I rotate the magnet by, say, 45° or 90° about the axis of the initial path of the electrons I get the same result as before: all the electrons are deflected up by some fixed amount or deflected down by exactly the same amount, and which for each individual electron appears to be random. Note that the definition of "up" is determined by the orientation of the magnet.

We can extend the washability study for pairs of socks to entangled pairs of electrons with one trivial difference. For the socks if one survived washing at 45° we assumed that the other member of the pair would too. For Bertlmann's electrons if one is spin up for 45° its companion is spin down for 45°, i.e. its companion is not spin-up for 45°. So now the relation near the top of the previous page becomes:

> The number of pairs for which one is spin-up for 0° and the other is spin-up for 45° Plus
>
> The number of pairs for which one is spin-up for 45° and the other is spin-up for 90° Is not less than
>
> The number of pairs for which one is spin-up for 0° and the other is spin-up for 90°

This relation has been experimentally tested, and is not true! So evidently there is some difference between Bertlmann's socks and Bertlmann's electrons, and we have made at least one wrong assumption somewhere in deriving this relation for electrons.

It turns out that the actual experimental result is predicted by Quantum Mechanics, so whatever wrong assumptions we made are also violated by that theory.

The Assumptions

We have used some logic in deriving the relation for Bertlmann's socks and electrons. We also made two assumptions in deriving the relations. Both are so self-evident that it is easy to miss the fact that we made them at all.

First, when we talked about the number of socks or electrons at 0° and 90° we assumed that each would or would not pass the test at 45°. Put another way, we assumed the existence of washability at some temperature or spin at some angle, even if it was not actually measured. Put still another way, we have assumed that there is a reality independent of its observation. This is similar to the old philosophical saw about a tree falling in the forest: if no one is there was there any sound?

Second, when we talk about measuring the washability or spin of one member of a pair to determine something about its companion, we assumed that since we were doing simultaneous measurements of two different socks/electrons at different locations, the effect of one measurement can't possibly disturb the result of the measurement of the other member of the pair. Put another way, we assumed that no signal or influence can propagate infinitely fast. Sometimes this assumption is called *locality*.

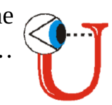
So experimentally we have proven that at least one of these two assumptions is wrong for entangled electrons.

So What?

The experimental tests have proved that there is no reality separate from its observation and/or different parts of the universe are instantaneously connected to every other part of the universe. So we have learned something profound about the physical world.

Nobody thought more deeply about a universe that does not exist independent of its observation than John Archibald Wheeler. He suggested that we should drop the word "observer" from our vocabulary, replacing it with "participator." The figure below was devised by him. He comments on the figure:

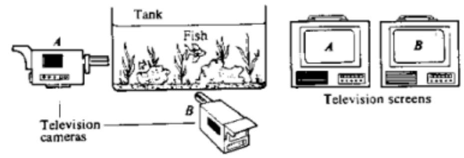
> Symbolic representation of the Universe as a self-excited system brought into being by 'self-reference'. The universe gives birth to communicating participators. Communicating participators give meaning to the universe … With such a concept goes the endless series of receding reflections one sees in a pair of facing mirrors.



David Bohm thought deeply about a universe which is instantaneously connected to every other part of the universe. He proposed that underlying our everyday universe, which he called the *explicate* order, there is an underlying order, the implicate, in which there is no separation in space or time. The figure is an analogy devised by Bohm.

We can only look at the television screens, and we see two fish at different locations. As we continue to look, we start noticing a correlation between the motions of the two fish. This is because underlying the reality of the two screens is a single unity, a single fish, that we can only observe from two different perspectives.

So this entanglement business is causing some deep thinking about the nature of the world. A pragmatist might say “So what?” Similarly, in the mid nineteenth century Faraday, Maxwell and others were thinking about the nature of electricity and magnetism. The British prime minister, Gladstone, is reported to have asked Faraday what possible use such idle speculations might have. Faraday replied: “Some day, sir, you will tax it.”



Entanglement almost certainly has practical applications, which presumably will eventually be taxed. These include quantum computers, which may have orders of magnitude more power than any conventional computer can possibly achieve, and quantum teleportation ala the transporter in Star Trek. Developing these applications is a “red hot” field of research and development.

To Learn More

Louisa Gilder, The Age of Entanglement: When Quantum Physics Was Reborn. (2008).

> Reading this book caused me to bring Louisa to Toronto for a Physics colloquium in January. The photograph was taken at the colloquium. The colloquium in turn led to an invitation for me to give this talk. The book is available in hardback, paperback, and on Kindle.

John S. Bell, “Bertlmann’s Socks and the Nature of Reality” (1980)

> The first few sections of my little document are almost plagiarised1 from Bell’s classic paper. It can easily be found via Google.

N. David Mermin, “Quantum Mysteries for Anyone” (J. Philosophy 78, p. 397, 1981) and “Bringing home the atomic world: Quantum mysteries for anybody” (Amer. J. Physics 49, p. 940, 1981).

> These nearly identical papers are brilliant. The first version had a large influence on Louisa Gilder. I have prepared a Flash animation based on Mermin’s papers:
>
> http://faraday.physics.utoronto.ca/P...in/Mermin.html

David Bohm, Wholeness and the Implicate Order (1980).

> This book discusses Bohm’s thinking about a non-local universe.

David Harrison, “Bell’s Theorem” (1999, last revision 2006).

> A long-winded discussion with some similarities to this document. It is available at:
>
> http://www.upscale.utoronto.ca/PVB/H...lsTheorem.html
>
> I am amazed and pleased that Googling bell’s theorem lists this document 2nd, just after the Wikipedia entry.

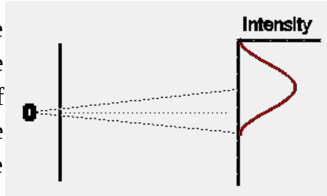
Author

13.9: Quantum Interference

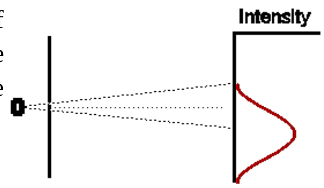
The Double Slit Experiment Revisited

Remember Young's double slit experiment ? If, instead of a light beam, we sent a beam of electrons into this double slit system, what would we see? Let us replace the source of light with an electron oven, which sends a stream of electrons towards the double slit system; at a good distance beyond the double slits lies a screen which can record the arrival of each electron. Let us suppose that the set-up has been carefully arranged so that of the electrons which reach the detection screen, exactly 50% of them have arrived from each slit.

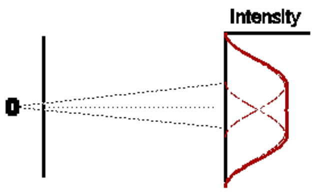
Firstly we notice that electrons are truly point particles; those that get through the double slit system and reach the detection screen arrive at one place and one place only on that screen.



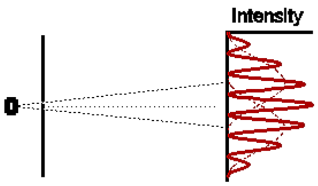
If we were to close one slit and wait for some time to allow a large number of electrons to reach the detection screen, the distribution of electrons would look somewhat as shown opposite. The intensity pattern is spread out somewhat, presumably because some of the electrons are scattered off the edges of the slit. Note that, as expected, the centre of the intensity pattern lies at a point in the direct line-of- sight back to the electron oven, and is displaced slightly from the exact centre of the detection screen.



In a similar way, if we were to close off the other hole, and open the first for the same amount of time, we would expect (given that our experiment has been set up with exact symmetry) that the intensity pattern would be identical in shape to the first case, but displaced an equal amount to the other side of the centre of the detection screen.



So if both slits were left open for the same amount of time, what would we expect ? Obviously, if electrons were classical particles, we would expect that the total intensity pattern is simply the sum of the two previous intensity patterns, shown opposite.



Astonishingly, this is not at all what we observe. In fact the observed intensity pattern shows interference bands, very similar to those produced by light passing through the double slit system; there are places on the detection screen where no electrons land, and other places where more electrons than the number we would expect from simply adding the contributions from each slit acting alone.

What is going on ??

The astonishing thing is that *the electrons, which each arrive individually as "particles", do so in such a way as to form an intensity pattern which we can only make sense of in terms of "waves"*. Indeed, using the very simple theory of waves which gives a description of the double slit experiment for waves, we get a complete description of the entire intensity pattern of this double slit experiment for electrons. To drive the point home, let's look at a couple of modifications to the experiment which may help dispel any lingering doubts that this is truly what is happening.

We might be concerned that some sort of interference effect may be going on between different electrons as they traverse the experimental system. To check this, we could reduce the intensity of the electron beam (by turning down the oven, for example) so that at any one time there was only **one** electron in the system. The extraordinary result is that, although it takes much longer for the interference pattern to develop, *exactly the same pattern does develop*.

But how can each individual electron "know" where it is supposed to land up, since the experiments tell us that this depends only on whether one or both slits are open. So maybe the electron somehow splits itself up and goes through both holes at once, recombining before it reaches the detection screen. To check this, we could design an apparatus to check whether the electron goes through one slit or the other, or both, when both slits are open **.**

Let us suppose that we have a small light placed just behind the double slit system. It sends out photons to bounce off the electrons that are coming through the slits; if an electron is hit, it deflects the photons into our eyes, and we observe the electron and can determine its position. (Of course this is a very crude piece of equipment to make such a measurement; in reality we would design things much better. However this "gedanken" experiment makes the discussion simpler, and represents the essentials of a real experiment). Now we can see which slit each electron comes through. What is the result? It turns out that indeed, every time the *electron* comes through one slit or the other. However we notice to our dismay that when we are making this observation, the *interference pattern disappears*!

Perhaps we have so many photons around that they are somehow interfering with the electrons' paths? Well, we can reduce the intensity of the light source (i.e. the number of photons flooding the system) to check this out. However, if we reduce the intensity too much, we will begin to miss some of the electrons, because there aren't enough around to ensure that every photon is struck, and thus observed. If we look at the distribution of the electrons that we miss, indeed the interference pattern is again observed. However, for those electrons for which we can determine which slit they have passed through (and, when detected, they are always seen to come through one slit or the other!), no interference pattern is observed.

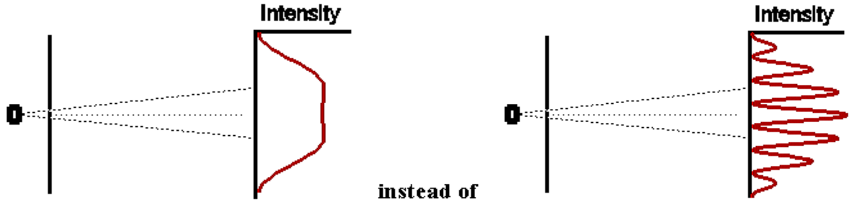
Perhaps, we might suggest, the photons we are using in this experiment are too energetic, so that their impact on the fragile electrons is too large. Well, we can reduce their impact by reducing their momentum; since their wavelength is inversely proportional to the momentum, that means we increase their wavelength. And indeed as we increase the wavelength of the observing photons, we do begin to

notice that the interference pattern re-establishes itself. However, to our dismay, just at that point we find that our resolution (which, remember, is proportional to the wavelength of the observing light) has become so poor that our ability to determine which slit these electrons have come through disappears!

In the words of Richard Feynman (in *The Character of Physical Law. (MIT Press)):*

"If you have an apparatus which is capable of telling which hole the electron goes through ... then you can say that it either goes through one hole or the other. It does; it is always going through one hole or the other - when you look. But when you have no apparatus to determine through which hole the thing goes, then you cannot say it goes through one hole or the other ... to conclude that it goes through one hole or the other when you are not looking is to produce an error in prediction. That is the logical tightrope on which we have to walk if we wish to interpret Nature."

Now it may be thought that our inability to pin the electron down to one slit or the other at the same time as we are observing the interference pattern is simply due to the fact that our observation of the system disturbs it too much. There is indeed some truth to this; most modern scientists would now accept that the old idea that the observer can stand outside of Nature in order to observe it is no longer tenable. John Wheeler has put this nicely, by saying that indeed there is no such thing as an "observer" - only "participants". However, there is something even deeper going on here: for if we had *any method whatsoever* to determine which slit each electron came through, simple logic would insist that the observed distribution would simply be the sum of the distributions of electrons from each slit, taken separately. That is, we should observe



Nature would then be placed in an irresolvable paradox. So the implication here is that indeed *the future is unpredictable;* we can never predict which slit the electron is going to go through.

Heisenberg's Uncertainty Principle.

There is a more formal mathematical statement of this fact, called the Heisenberg Uncertainty Principle, which sets clear limits on what we can observe. A simple "sort of proof" goes as follows:

Consider our attempt to view the electrons in the double slit system by shining light of wavelength λ on them. The photons of this light will have momenta $\mathbf{p_{photon}} = \mathbf{h}/\lambda$. If we manage to see an electron it will be because one of these photons has struck it. Clearly the electron momentum will have been affected by this interaction with the photon. Let us call the change we have so induced in the electron's momentum $\Delta p_{electron}$ (meaning a small change in $\mathbf{p_{electron}}$). Obviously, the greater the momentum of the photon, the greater this change in the momentum of the struck electron. Certainly $\Delta p_{electron}$ is proportional to $\mathbf{p_{photon}}$; the constant of proportionality will depend to some extent on the experimental set-up, but might typically be of the order of 0.1 or so. However, to the order of our present calculation, we can assume it is 1. Thus we can write that $\Delta \mathbf{p_{electron}} = \Delta \mathbf{p_{photon}} = \mathbf{h}/\lambda$ **.**

Now we know that the precision with which we can determine a distance is limited by the size of the wavelength of the light which we use to measure the distance. In fact this uncertainty in position is directly proportional to the wavelength of the light; again, at our present level of accuracy, we can set the proportionality constant to 1. In the double slit experiment, let us call this uncertainty in position $\Delta \mathbf{x}$. So, using the above arguments, we can write the uncertainty in our knowledge of the position of the electron, determined by shining a photon of wavelength **L** on it, to be $\Delta \mathbf{x_{electron}} = \lambda$. Combining the two equations for the uncertainty of the electron's momentum and its position, we obtain the following expression for their product: $\Delta \mathbf{p_{electron}} . \Delta \mathbf{x_{electron}} = (\mathbf{h}/\lambda)\lambda = \mathbf{h}$. It turns out that this expression is generally true for all particles, and we can write it finally as $\Delta \mathbf{p} . \Delta \mathbf{x} = \mathbf{h}$. This is one way of writing Heisenberg's Uncertainty Principle.

The difficulty with this derivation of the Uncertainty Principle is that it may encourage you to think that the uncertainty in the result, and indeed an explanation of the whole odd behavior that we observe in the Double Slit experiment is entirely due to the unavoidable disturbance that we make when we observe the experiment.

However **this is simply not true.** The Uncertainty Principle implies a built-in, unavoidable *limit to the accuracy with which we can make measurements*. NOR is it similar to experimental uncertainty as understood in Classical Physics. There, for example, when we want to measure the temperature of a beaker of water, it is certainly true that we disturb the temperature we want to measure by introducing a cold thermometer into it, so the temperature we measure is thus not exactly that of the beaker alone. However, in principle, we can remove this error, by measuring with smaller and smaller ther mometers and extrapolating to zero size; *in principle* (if not in practice) we can thus measure to arbitrarily high accuracy. This is not possible in the Quantum world, thanks to Heisenberg's Uncertainty Principle. A further implication is that the future is not predictable in the classical sense; for if we do not know the initial conditions exactly - and Heisenberg's principle tells us that we cannot - we cannot make accurate predictions about the future, no matter how precise and pre-determined are our equations.

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13.10: Quantum Mechanics- a Poor Person's Guide

The Wave Function

The observation of the world lets us know that something very odd is going on. The Double Slit Experiment is the prototypical experiment of Quantum Physics. Guided by this experiment and others like it, a mathematical theory, called Quantum Theory has been developed to give results which are in agreement with our observations; the "weirdness" we find in Nature is reflected in the way in which the Quantum Theory is constructed. It goes a bit like this.

The state of a physical system is described by a "wave function", usually denoted by the symbolΨ.. In particular cases, we will know more or less exactly what function this is - e.g a sine or a cosine, a quadratic expression, etc. This wave function can depend on time, spatial coordinates, etc. Quantum Theory tells us that to make calculations about real measurements that could be made on the system, we must **take the square of the wave function.** The value so obtained will give us the **probability** of obtaining, through measurement on the system, a particular value of the quantity we are interested in. We would expect a theory from Classical Physics to give us an **exact** value of the quantity we were interested in; here, however, the best we can do is calculate a probability of obtaining the value. The wave function is also called a Probability Amplitude, for this reason.

For example, if, on the basis of our knowledge of conditions in which a particle might find itself (in a box, with a magnetic field, for example) we knew how to write down the particle's wave function; and let's say this wave function depended on its position (call that x) and the time measured from some starting time (call that t). In that case, we would write its wave function as $\Psi(x,t)$. x could take any values of position that the particle could reach. If then, we wanted to know the chance, or probability, of finding the particle at a particular value of x, say x = 45 cm, at a particular time of, say 7 seconds, Quantum Theory tells us that the answer isΨ **$(45,7)^2$**. Note that this is very different from Classical Physics; there, we might know that the "equation of motion" of the particle was, e.g. $x = 6t$; then the answer to our question would be that the position of the particle at time 7 seconds, would be the exactly x = 42 cm.

Now let us look at the odd way in which Quantum Theory does its calculations about the world. Suppose we have an experiment about a physical process which can happen in more than one way, and we know the Probability Amplitude (or wave function) for each way. To calculate what results we would expect in an experiment which does not distinguish which way actually happens, we have to **first** add the Probability Amplitudes; **then** we square the result of this addition to get the answer to compare to measurement. If, on the other hand, the experiment does distinguish which way actually happens, we **square** the Probability Amplitudes **before** adding them. To see how this works, let's look at the Double Slit Experiment for electrons.

The Double Slit Experiment Again

Suppose thatΨ_1 is the Probability Amplitude for the electron's going through one slit, andΨ_2 is the Probability Amplitude for its going through the other slit; then the Probability Amplitude to calculate the results of an experiment which does not determine through which slit the electron goes (call it Experiment **I**) is written as $\Psi_I = \Psi_1 + \Psi_2$. [This is called a "(linear) superposition of probable states"]. Now, if we want to make a theoretical calculation of the results of a real experiment we might carry out (e.g. the distribution of the electrons on the detecting screen), we have to take the **square** of this total Probability Amplitude, i.e. $\Psi_I^2 = \{\Psi_1 + \Psi_2\}^2$. Multiplying out, this result can be written as $\Psi_I^2 = \Psi_1^2 + \Psi_2^2 + 2\Psi_1\Psi_2$. (In this not-quite-correct formulation, Ψ_1 can equal $-\Psi_2$).

Suppose we have a set-up which has equal size slits, located at the same distance from the source of electrons, then the probability that the electron goes through slit number 1 is equal to the probability that it goes through slit number 2. We express this fact by writing $\Psi_1^2 = \Psi_2^2 = 0.5$ (or 50%).

Then : EITHER$\Psi_1 = +\Psi_2$ and the result is **1** (or 100%);
OR$\Psi_1 = -\Psi_2$, and the result is **0** (or 0%).

For the Double Slit Experiment, this is obviously (??) a calculation of the interference pattern, with its maxima (**1**, in some arbitrary units) and minima (**0**) which we observe. However, if our experiment has some means for detecting, even in principle, which hole the electron goes through (Experiment **II**), the result of **this** experiment must be written as $\Psi_{II}^2 = \Psi_1^2 + \Psi_2^2$. This is clearly (??) the case in which **no** interference is observed.

Thus the Quantum Theory has managed to come up with a recipe to give calculations which agree with the observations we make on this weird world in which we live.

What can we say about the wave function (Probability Amplitude) of the electron after it has gone through the slit system, but **just before** we look at it to decide which slit it went through? In this case, Nature tells us we must write its wave function as $\Psi = \Psi_1 + \Psi_2$, as explained above. But if we make a measurement to determine which slit the electron did go through, we know we must get the result Ψ_1 (if it went through slit number 1) OR Ψ_2 (if it went through slit number 2). Then we say that the wave function has **collapsed** on to its final value.

What is an Electron?

According to Schrödinger, the electron can be represented by a wave-function, which contains all the information we can know about the particle. If an electron looks like anything we are familiar with (and it doesn't!!), it comes closest to a small "packet" of waves confined to a region of space Δx. This wave function obeys a wave equation first written down by Schrödinger. The **square** of the wave function gives the probability of finding it at a given place (and time).

(MATH NOTE: To represent such a function, we need a superposition of many wave forms, with a "spread" of wavelengths. Since $p = h/\lambda$ this implies a corresponding spread in momentum; this can be calculated to be $\Delta p = h/\Delta x$ - as we might have expected from Heisenberg's Uncertainty Principle).

Schrödinger's Cat (or Is the Moon There when Nobody Looks?)

By analogy, in the case of Schrödinger's cat, the state of the cat **before we open the box** is :
$\Psi_{cat} = \Psi_{alive} + \Psi_{dead}$. If we have designed the experiment so that there is equal probability for finding the cat alive or dead, we must have $\Psi_{alive}^2 = \Psi_{dead}^2$. When we open the box, since the cat must be alive OR dead, the total wave function, Ψ_{cat} must be EITHER $= \Psi_{alive}$ OR $= \Psi_{dead}$; we don't know which before we open the box. However, it appears that **just before** we open the box, the cat is NEITHER alive OR dead, but a superposition of the two states! Just try telling that to your grand mother!

The Implications of the Quantum

Quantum Physics forces us to the conclusion that:

a. there are no certainties, only probabilities - and the future is unpredictable.
b.Physical properties have no objective reality independent of the act of observation OR the act of measurement can, in principle, act *instantaneously* over enormous distances (i.e. non- local interactions exist). (*Bell's Theorem and the experiments of Aspect et al.*)

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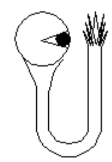
13.11: Quantum Mechanics- Interpretation

Albert Einstein - Einstein objected to the Quantum Theory on several grounds. Firstly it does not seem to give objective reality to individual events; he believed that an objective world exists, independent of any observer or observing process. Yet Quantum theory seems to imply that our method of observation determines what we will see. Secondly it does not seem to be a complete theory; it is essentially statistical in its predictions and cannot completely describe individual quantum events. His other objections were formalized in the Einstein-Podolsky-Rosen paper, and concerned what he called "spooky actions at a distance". (**NOTE:** in this area at least, Einstein seems to have been wrong. Bell's Theorem and the experiments of Aspect et al have proven conclusively that EITHER there is no objective reality OR that these "spooky" non-local interactions exist).

Neils Bohr - *the Copenhagen collapse*. Bohr believed that the wave function represents our knowledge of the physical phenomena we are studying, not the phenomena itself. In this sense, it is a potential which is realised only when we make an observation; this observation causes the wave function to "collapse" into the actual manifestation of the route taken.

David Bohm - *A Higher Multi-Dimensional Order*. In his book "Wholeness and the Implicate Order" Bohm suggests that the strange effects of the Quantum world may imply the existence of a a deeper, non-local level of reality. At this level - called the implicate order - all things are interconnected in an unbroken whole; "everything interpenetrates everything". Our observational world - which Bohm calls the explicate order - has access to this underlying reality in only a partial and incomplete fashion. Bohm's view has been likened to the suggestion that the Universe is a multi-dimensional hologram; any little piece of the hologram will recover the image, but not the full reality. We are reminded of Blake's wish - "to see the world in a grain of sand".

Eugene Wigner - *Human consciousness*. Wigner goes even further than Bohm by claiming that it is the entry of human consciousness into the picture that causes the wave function to collapse. The Cartesian mind-body dualism is re-established and the influence of the mind on the physical world is explicit. Wigner believes that the Newtonian concept of action-reaction and quantum physics both are evidence for this belief.



John Wheeler - *The Participatory Universe*. The renowned mathematician, John von Neumann was also an adherent to this view, which claims that the universe does not exist until a human mind is there to observe it. In this view, the universe is a self-observing system; the early stages of the universe can be promoted to concrete reality through its later observation by conscious ness, which itself depends on that reality (!!)

Hugh Everett and Bryce de Witt - *The Many Worlds Interpretation*. Far-fetched though this sounds it provides one of the cleanest explanations of the wave function collapse. The idea is that at each observation of the world ALL possibilities allowed by the wave function of the system are actually realised. The universe splits into branches, each corresponding to one of the possibilities available to it. Each branch is completely independent of the others, and no communication can take place between branches.

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13.12: Quantum Teleportation

INTRODUCTION

In March 1993 Charles H. Bennett from IBM proposed a scheme, based on Quantum Mechanics, that in principle could be used to teleport an object. The scheme was experimentally verified by Dik Bouwmeester et al. in the Fall of 1997. In 2004 researchers at the University of Vienna and the Austrian Academy of Science used an 800m-long optical fibre fed through a public sewer system tunnel to connect labs on opposite sides of the River Danube to achieve such teleportation..

Here we explore this phenomenon of *Quantum Teleportation*. We will then extend the discussion to *Quantum Information* and *Quantum Cryptography*. The document is based on a discussion with an upper year course in modern Physics without mathematics given at the University of Toronto.

Although the discussion is almost totally non-mathematical, it requires considerable understanding of the Quantum Correlation experiments used in describing *Bell's Theorem*.

TELEPORTATION

In *Star Trek*, when Captain Kirk is beamed from the starship Enterprise to the surface of a planet, Captain Kirk de-materialises on the Enterprise, and then re-materialises on the planet. On the TV show, an unanswered question is whether the transporter physically disassembles Captain Kirk, moves the atoms from his body to the planet, and then reassembles them. Another perhaps more reasonable alternative would be to scan all the information about Captain Kirk's physical state, and transmit that information to the planet surface where it is used to construct a new Captain Kirk out of raw materials found on the planet. Note that in either case the transporter needs to have complete information on Kirk's physical state in order to reconstruct him.

However, the Heisenberg Uncertainty Principle means that it is impossible to obtain this complete information about Kirk. Thus, it seems that the best the transporter can do is make an approximate copy of him on the planet surface. Quantum Teleportation provides a way to "beat" the Uncertainty Principle and make an exact copy.

As we shall see, the mechanism that beats the Uncertainty Principle is the same one used to beat it in the Quantum Correlation experiments we examined when we discussed Bell's Theorem. We shall also see that although the collapse of the state for the two measurements in the correlation experiments occurs instantaneously, the teleportation can not occur faster than the speed of light.

Finally, a little terminology. Before we were discussing Quantum Correlation experiments in which we were measuring the spins of two separate electrons whose total spin was zero. We call the states of those two electrons *entangled*.

BELL-STATE MEASUREMENTS

In previous discussions we almost always talked about the spin state of electrons, although we regularly pointed out that the same situations exist for the polarization of light, albeit with a difference of a factor of 2 in the angles being used. Here we will reverse the situation, and mostly talk about polarization states for photons, although the arguments also apply to spin states of electrons.

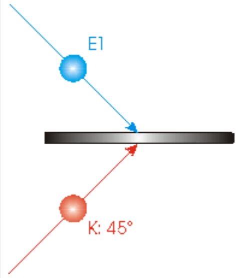
The fact that we may talk about light polarization in almost the same way that we discuss electron spin is not a coincidence. It turns out that photons have spins which can exist in only two different states. And those different spins states are related to the polarization of the light when we think of it as a wave.

Here we shall prepare pairs of entangled photons with opposite polarizations; we shall call them *E1* and *E2*. The entanglement means that if we measure a beam of, say, *E1* photons with a polarizer, one-half of the incident photons will pass the filter, regardless of the orientation of the polarizer. Whether a particular photon will pass the filter is random. However, if we measure its companion *E2* photon with a polarizer oriented at 90 degrees relative to the first, then if *E1* passes its filter *E2* will also pass its filter. Similarly if *E1* does not pass its filter its companion *E2* will not.

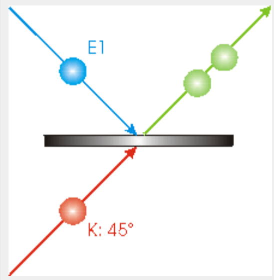
Earlier we discussed the Michelson-Morley experiment, and later the Mach-Zehnder interferometer. You will recall that for both of these we had half-silvered mirrors, which reflect one-half of the light incident on them and transmit the other half without reflection. These mirrors are sometimes called *beam splitters* because they split a light beam into two equal parts.

We shall use a half-silvered mirror to perform *Bell State Measurements*. The name is after the originator of Bell's Theorem.

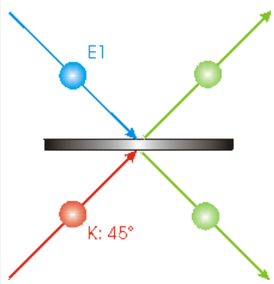
We direct one of the entangled photons, say *E1*, to the beam splitter.
Meanwhile, we prepare another photon with a polarization of 45^0, and direct it to the same beam splitter from the other side, as shown. This is the photon whose properties will be transported; we label it *K* (for Kirk). We time it so that both *E1* and *K* reach the beam splitter at the same time.



The *E1* photon incident from above will be reflected by the beam splitter some of the time and will be transmitted some of the time. Similarly for the *K* photon that is incident from below. So sometimes both photons will end up going up and to the right as shown.
Similarly, sometimes both photons will end up going *down* and to the right.



But sometimes one photon will end up going upwards and the other will be going downwards, as shown. This will occur when either both photons have been reflected or both photons have been transmitted.
Thus there are three possible arrangements for the photons from the beam splitter: both upwards, both downwards, or one upwards and one downwards.
Which of these three possibilities has occurred can be determined if we put detectors in the paths of the photons after they have left the beam splitter.
However, in the case of one photon going upwards and the other going downwards, we can not tell which is which. Perhaps both photons were reflected by the beam splitter, but perhaps both were transmitted.
This means that the two photons have become *entangled*.
If we have a large beam of identically prepared photon pairs incident on the beam splitter, the case of one photon ending up going upwards and the other downwards occurs, perhaps surprisingly, 25% of the time.



Also somewhat surprisingly, for a single pair of photons incident on the beam splitter, the photon *E1* has now collapsed into a state where its polarization is -45^0, the opposite polarization of the prepared 45^0 one. This is because the photons have become entangled. So although we don't know which photon is which, we know the polarizations of both of them.

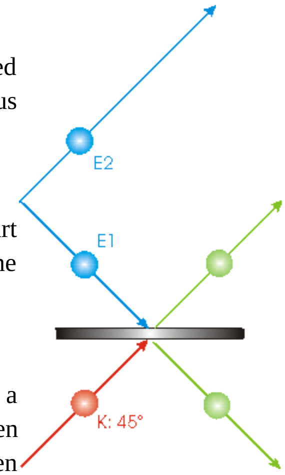
The explanation of these two somewhat surprising results is beyond the level of this discussion, but can be explained by the *phase shifts* the light experiences when reflected, the mixture of polarization states of *E1*, and the consequent *interference* between the two photons.

THE TELEPORTER

Now we shall think about the *E2* companion to *E1*.

25 percent of the time, the Bell-state measurement resulted in the circumstance shown, and in these cases we have collapsed the state of the *E1* photon into a state where its polarization is -45^0.

But since the two photon system E1 and E2 was prepared with opposite polarizations, this means that the companion to E1, *E2*, now has a polarization of $+45^0$. Thus the state of the *K* photon has now been transferred to the *E2* photon. We have teleported the information about the *K* photon to *E2*.



Although this collapse of *E2* into a 45^0 polarization state occurs instantaneously, we haven't achieved teleportation until we communicate that the Bell-state measurement has yielded the result shown. Thus the teleportation does not occur instantaneously.

Note that the teleportation has destroyed the state of the original *K* photon.

Quantum entanglements such as exist between E1 and E2 in principle are independent of how far apart the two photons become. This has been experimentally verified for distances as large as 10km. Thus, the Quantum Teleportation is similarly independent of the distance.

The Original State of the Teleported Photon *Must* Be Destroyed

Above we saw that the K photon's state was destroyed when the E2 photon acquired it. Consider for a moment that this was not the case, so we end up with two photons with identical polarization states. Then we could measure the polarization of one of the photons at, say, 45^0 and the other photon at 22.5^0. Then we would know the polarization state of both photons for both of those angles.

As we saw in our discussion of Bell's Theorem, the Heisenberg Uncertainty Principle says that this is impossible: we can never know the polarization of a photon for these two angles. Thus any teleporter must destroy the state of the object being teleported.

OTHER APPLICATIONS

Teleporting the polarization state of a single photon a quarter of the time is a long long way from reliably teleporting Captain Kirk. However, there are other applications of the above sort of apparatus that may be closer to being useful.

Quantum Information

As you probably know, computers store information as sequences of *0*'s and *1*'s. For example, in the *ASCII* encoding the letter *A* is represented by the number 65. As a binary number this is:

```
1,000,001
```

Inside the computer, there are transistors that are either on or off, and we assign the on-state be *1* and the off state *0*. However, the same information can be stored in exactly the same way in any system that has two mutually exclusive binary states.

For example, if we have a collection photons we could represent the *1*'s as photons whose polarization is $+45^0$ and the *0*'s as polarizations of -45^0. We could similarly use electrons with spin-up and spin-down states to encode the information. These quantum bits of information are called *qubits*.

Above we were thinking about an apparatus to do Quantum Teleportation. Now we see that we can think of the same apparatus as transferring Quantum Information. Note that, as opposed to, say, a fax, when transferring Quantum Information the original, the polarization of the *K* photon, is destroyed.

Quantum Cryptography

Cryptography depends on both the sender and receiver of the encrypted information both knowing a *key*. The sender uses the key to encrypt the information and the receiver uses the same key to decrypt it.

The key can be something very simple, such as both parties knowing that each letter has been shifted up by 13 places, with letters above the thirteenth in the alphabet rotated to the beginning. Or they can be very complex, such as a very very long string of binary digits.

Here is an example of using binary numbers to encrypt and decrypt a message, in this case the letter *A*, which we have seen is `1,000,001` in a binary ASCII encoding. We shall use as the key the number 23, which in binary is `0,010,111`. We will use the key to encode the letter using a rule that if the corresponding bits of the letter and key are the same, the result is a *1*, and otherwise a *0*.

A	1	0	0	0	0	0	1
Key	0	0	1	0	1	1	1
Encrypted	0	1	0	1	0	0	1

The encrypted value is 41, which in ASCII is the right parenthesis:)

To decrypt the message we use the key and the same procedure:

Encrypted	0	1	0	1	0	0	1
Key	0	0	1	0	1	1	1
A	1	0	0	0	0	0	1

Any classical encryption scheme is vulnerable on two counts:

- If the "bad guys" get hold of the key they too can decrypt the message. So-called *public key* encryptation schemes reveals on an open channel a long string of binary digits which must be converted to the key by means of a secret procedure; here security is based on the computational complexity of "cracking" the secret procedure.
- Because there are patterns in all messages, such as the fact that the letter *e* predominates, then if multiple messages are intercepted using the same key the bad guys can begin to decipher them.

To be really secure, then, there must be a unique secret key for each message. So the question becomes how can we generate a unique key and be sure that the bad guys don't know what it is.

To send a key in *Quantum Cryptography*, simply send photons in one of four polarizations: -45, 0, 45, or 90 degrees. As you know, the receiver can measure, say, whether or not a photon is polarized at 90 degrees and if it is not then be sure than it was polarized at 0 degrees. Similarly the receiver can measure whether a photon was polarized at 45 degrees, and if it is not then it is surely polarized at -45 degrees. However the receiver can not measure both the 0 degree state and 45 degree state, since the first measurement destroys the information of the second one, regardless of which one is performed first.

The receiver measures the incoming photons, randomly choosing whether to measure at 90 degrees or 45 degrees, and records the results but keeps them secret. The receiver contacts the sender and tells her on an open channel which type of measurement was done for each, without revealing the result. The sender tells the receiver which of the measurements were of the correct type. Both the sender and receiver keep only the qubits that were measured correctly, and they have now formed the key.

If the bad guys intercept the transmission of photons, measure their polarizations, and then send them on to the receiver, they will inevitably introduce errors because they don't know which polarization measurement to perform. The two legitimate users of the quantum channel test for eavesdropping by revealing a random subset of the key bits and checking the error rate on an open channel. Although they cannot prevent eavesdropping, they will never be fooled by an eavesdropper because any, however subtle and sophisticated, effort to tap the channel will be detected. Whenever they are not happy with the security of the channel they can try to set up the key distribution again.

By February 2000 a working Quantum Cryptography system using the above scheme achieved the admittedly modest rates of 10 bits per second over a 30 cm length.

There is another method of Quantum Cryptography which uses entangled photons. A sequence of correlated particle pairs is generated, with one member of each pair being detected by each party (for example, a pair of photons whose polarisations are measured by the parties). An eavesdropper on this communication would have to detect a particle to read the signal, and retransmit it in order for his presence to remain unknown. However, the act of detection of one particle of a pair destroys its quantum correlation with the other, and the two parties can easily verify whether this has been done, without revealing the results of their own measurements, by communication over an open channel.

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13.13: Schrödinger's Cat

Radioactive Decay

Some elements are unstable, decaying via the weak interaction into other elements. Such substances are called *radioactive*. For example, Nitrogen-13 decays into Carbon-13 plus an electron plus an anti-neutrino.

There are two factors that determine that rate at which a sample of radioactive atoms decays:

1. How many atoms are there? Twice as many atoms will have a total decay rate that is double.
2. What is the tendency of a particular atom to decay.

The tendency of an element to decay is expressed by its *half-life*.

The half-life of Nitrogen-13 is almost exactly 10 minutes. What this number means is that if we have a large "pot" of Nitrogen-13 and wait 10 minutes one half of the Nitrogen-13 atoms will have decayed and one half will not have decayed. If we wait a further 10 minutes one half of the remaining sample of atoms will have decayed and one half will not. After a further 10 minutes one half of that remaining sample will have decayed.

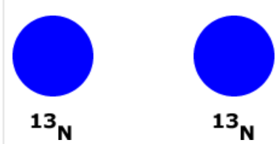
The concept of half-live is sort of reminiscent of a famous paradox by Xeno, who argued that we can never walk out of a room. If we head towards the door, eventually we get half way towards it. If we keep walking we will have gotten half way through the remaining distance to the door. And then if we keep walking we get half way through that remaining distance. So we keep getting half way towards the door and never actually get there.

Here are some half-lives:

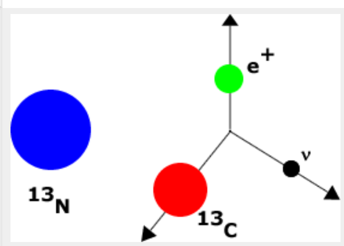
Atom	Half-Life
protons	> 10^{32} years (i.e. consistent with being stable
Carbon-14	5,730 years
Cobalt-60	1,925 days
Nitrogen-13	10 minutes

You may access a Flash animation of 500 radioactive atoms of the fictitious element *Balonuim* by clicking here.

For radioactive substances, one crucial factor in discussing the half-life is that we were discussing a *large* collection of atoms. What if we only have two such Nitrogen-13 atoms? Then if we wait 10 minutes, one-half life, there is a 50% chance that one of the atoms will have decayed. So this is sort of similar to flipping two coins. Whether a particular coin comes up heads is about a 50% chance. For flipping two coins we can get both heads, one head and one tail, or both tails. Similarly for two radioactive atoms we could end up with both decaying, one decaying and the other not, or both not decaying.



Imagine that after 10 minutes the atom on the right decayed and the one on the left did not decay.



We ask a basic question: **What is the difference between the two Nitrogen-13 atoms?**

The answer to this is trivially easy: one atom decayed and the other did not.

A more interesting question is: **What *was* the difference between the two Nitrogen-13 atoms before we waited 10 minutes?**

The answer to this better question is sort of hard. According to Quantum Mechanics there was no difference between the two atoms: we had two completely identical atoms but one decayed and the other did not.

Einstein never accepted Quantum Mechanics, and this part of the theory is one of the reasons. He summarised his objections by saying "God does not play at dice with the universe." Bohr responded "Quit telling God what to do!"

Einstein's God may not play at dice, but there are other views of divinity. For example, in the **Bhagavad Gita** Krishna says:

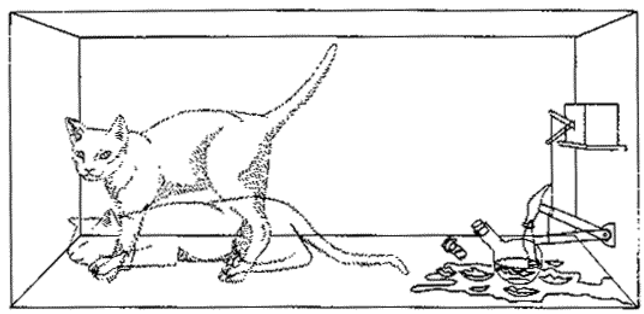
"I am the game of dice. I am the *self* centered in the heart of all beings."

If, with Einstein, we reject the idea that completely identical initial states can evolve to different outcomes, then we conclude that initially there must have been some difference, some variable, that distinguishes the two Nitrogen-13 atoms. To date all attempts to discover what that variable is have failed; thus we would say that there is some *hidden variable* inside the atoms. In Quantum Mechanics there are no such variables.

The Cat Paradox

In the early 1930's Erwin Schrödinger published a way of thinking about the circumstance of radioactive decay that is still useful. We imagine an apparatus containing just one Nitrogen-13 atom and a detector that will respond when the atom decays. Connected to the detector is a relay connected to a hammer, and when the atom decays the relay releases the hammer which then falls on a glass vial containing poison gas. We take the entire apparatus and put it in a box. We also place a cat in the box, close the lid, and wait 10 minutes.

We then ask: **Is the cat alive or dead?**
The answer according to quantum mechanics is that it is 50% dead and 50% alive.



Quantum Mechanics describes the world in terms of a *wave function*. DeWitt wrote about the cat that "at the end of [one half-life] the total wave function for the system will have a form in which the living cat and dead cat are mixed in equal portions." (Reference: B.S. DeWitt and N. Graham, eds., **The Many-Worlds Interpretation of Quantum Mechanics** (Princeton, 1973), pg. 156.)

When we open the box, we "collapse the wave function" or "collapse the state" and have either a live cat or a dead cat.

Of course, this is just a thought experiment. So far as I know nobody has actually every done this experiment.

In a sense the cat is a "red herring" [sorry!]. The paradox is just an illuminating way of thinking about the consequences of radioactive decay being totally random.

Imagine we have a friend waiting outside when we open the box. For us the wave function collapses and we have, say, a live cat. But our friend's wave function does not collapse until he comes into the room. This leads to a strong solipsism, since our friend can they say that we owe our objective existence to his kind intervention in coming into the room and collapsing our state.

As Heisenberg said, then, "The wave function represents partly a fact and partly our knowledge of a fact."

Our friend needn't have come into the room to collapse his wave function: if we have a cell phone we can call him and tell him the result of the experiment. Of course, this assumes that we don't lie to him and tell him the cat is dead when it is alive.

Unexplained but apparently true is the fact that when a state collapses, it collapses into the same state for everybody. If we see a live cat everybody sees a live cat (unless they or us are hallucinating).

As de Beauregard commented: "Finally, the need for consistency of the whole scheme leads me to think of the world we are living in as a Leibnitzian world, where cats are rather high in the hierarchy of monads." Reference: Foundations of Physics **6**, 539 (1976).

Paradoxes of Quantum Mechanics

There are two major paradoxes of Quantum Mechanics, each illustrating different aspects of the quantum mystery. Schrödinger's Cat is one of them, and the other is the *Double Slit*. Notes on the double slit may be accessed either in html or pdf by clicking on the links to the left.

Each paradox shows different aspects of the "collapse of the state."

Double Slit

Shows that the collapse of the state is real, irreversible, and causes a qualitative change in the later time evolution of the system.

Schrödingers Cat

Shows that our consciousness and knowledge are somehow mixed up in this process.

Tags recommended by the template: article:topic

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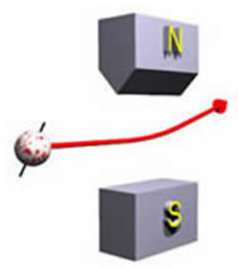
13.14: Stern-Gerlach Experiment

This page summarizes the classic Stern-Gerlach experiment on "spin" and extends the treatment to a discussion of correlation experiments. As is often the case, I build up maximum complexity as I examine the experimental details, and then hide them in a 'box'. This time the box will turn out to be literal.

Here we concentrate on electrons, which have only two spin-states. We also mention photons, which also have two spin-states. The approach is largely based on one by Feynman which he used for objects with three spin states: see R.P. Feynman, R.B. Leighton and M. Sands, **The Feynman Lectures on Physics**, Vol III, Chapter 5 for this discussion.

Classical Charged Spinning Objects

We begin by considering a macroscopic charged ball that is thrown between the poles of a magnet. If the ball is not spinning, a "knuckleball" to a baseball fan, it will not be deflected. However, if it is spinning it will be deflected as shown:



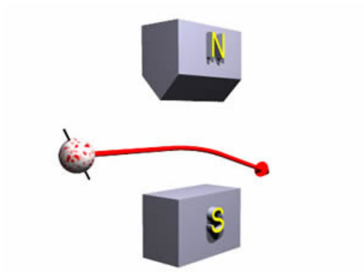
We ignore:

- The weird shape of the magnet pole pieces.
- The fact that there will be horizontal deflections. These can be cancelled by putting an electric field perpendicular to the plane of the ball's trajectory.

For the case shown above, the figure to the right shows the spin of the charge. We shall call this orientation "spin up" since it is deflected up by the magnets. The total amount of deflection is a function of

- The total amount and distribution of electric charge on the ball.
- The orientation and rate of spin. As the rate of spin increases, so does the deflection. As the axis of the spin becomes more vertical, that amount of deflection also increases.

By contrast a "spin down" electron would have its spin oriented as shown below:

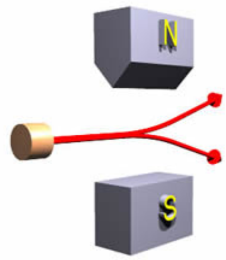


Such an object is deflected down by the magnets.

All of the above is just classical 19th century electricity and magnetism.

The Spin of the Electron

If the beam from the electron gun is directed to the magnets, as shown to the right, the beam is split into two parts. One half of the electrons in the beam are deflected up, the other half were deflected down. The amount of deflection up or down is exactly the same magnitude. Whether an individual electron is deflected up or down appears to be random. Stern and Gerlach did a version of this experiment in 1922.



This is very mysterious. It seems that the "spin" of electrons comes in only two states. If we assume, correctly, that the rate of spin, total charge, and charge distribution of all electrons is the same, then evidently the *magnitude* of the angle the spin axis makes with the horizontal is the same for all electrons. For some electrons, the spin axis is what we are calling "spin up", for others "spin down".

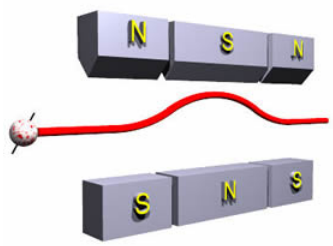
You should beware of the term "spin." If one uses the "classical radius of the electron" and the known total angular momentum of the electron, it is easy to calculate that a point on the equator of the electron is moving at about 137 times the speed of light! Thus, although we will continue to use the word "spin" it is really a shorthand for "intrinsic angular momentum."

Building a Spin Filter

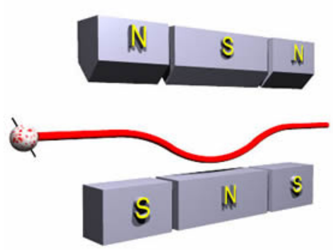
As promised at the beginning, we now make the situation a bit more complex. Consider the arrangement shown to the right:

Note that the polarity of the middle longer magnet is reversed from the other two. We have also drawn the path of a "spin up" object. When the object emerges from the magnets it is going the same direction as before it entered them with the same speed.

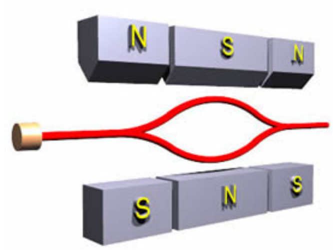
A Flash animation of this case may be viewed by clicking here.



The path of a "spin down" object is:

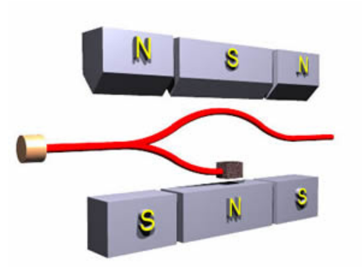


For a beam of electrons, one-half will go follow the upper path while and other half will follow the lower path:

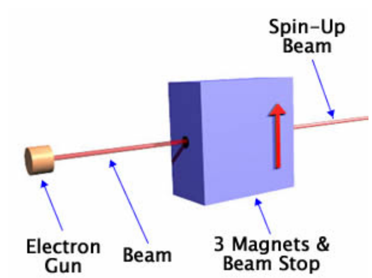


Finally, we imagine putting a small block of lead in the path of the "spin down" electrons.

Here, one-half of the incident beam, the spin-down electrons, will be stopped inside the apparatus, while all the spin-up electrons will emerge in the same direction as before they entered the magnets and at the same speed. Thus this is a "filter" that selects spin-up electrons.

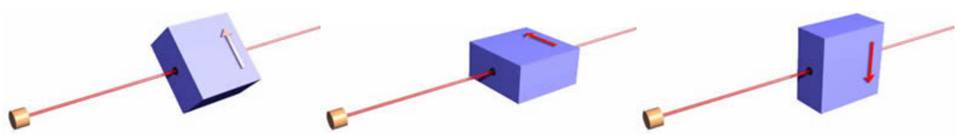


Now, again as promised, we simplify by taking all three magnets and the beam stopper and put it in a box. In the figure we also have included an electron gun firing a beam of electrons at the box. So one-half of the incident beam of electrons will emerge. It will be important to notice that we have painted an arrow on the front side of the box to indicate what direction is "up." You can't see it yet, but there is also an arrow pointing in the same direction on the back of the box.

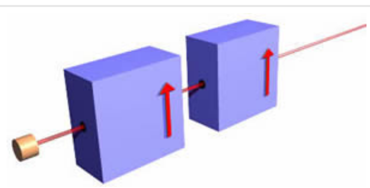
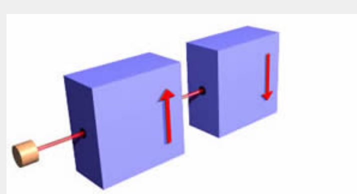


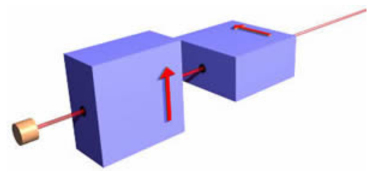
Using the Spin Filter

Note that one-half of the incident beam of electrons on the filter emerge from the box, while the other half do not. This is independent of the orientation of the filter; in all the orientations shown below one-half of the incident electrons emerge, while the other half do not.



Evidently the direction of "up" is defined by the orientation of the filter doing the measurement. This is sometimes called *spatial quantisation*, a term I do not like.

We now put a second filter behind the first with the same orientation. The second filter has no effect. Half of the electrons from the electron gun emerge from the first box, and **all** of those electrons pass through the second filter. So, once "up" is defined by the first filter, it is the same as the "up" defined by the second.	
Now we put the second filter behind the first and upside down relative to the first. As always, half of the beam of electrons from the electron gun emerge from the first filter, and **none** of those electrons emerge from the second filter. So, evidently once the first filter defines "up" that definition is the second filter's definition of "down."	

Here is another orientation for the second filter, this time oriented at 90° relative to the first one. To repeat once again, half of the beam of electrons from the electron gun emerge from the first filter. It turns out that one-half of those electrons pass through the second filter. So if we have two definitions of "up" from two filters at right angles to each other, one half of the electrons will satisfy both definitions.	

If we slowly rotate the orientation of the second filter with respect to the first one from zero degrees to 180 degrees, the fraction of the electrons that passed the first filter that get through the second filter goes continuously from 100% to 0%.

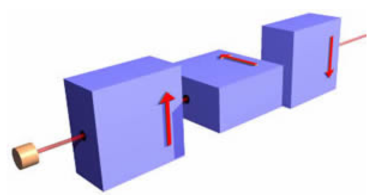
Technical note: if the relative angle is A, the percentage is $100 \cos^2(A/2)$.

All of the above may remind you of polaroid filters for light. One half of a beam of light from, say, an incandescent lamp will pass through such a filter. If a second filter is placed behind the first one with the same orientation, all the light from the first filter passes through the second (at least in the case of perfect polaroid filters). A brief summary of light polarisation appears here.

If the relative orientation of the two polaroid filters for light is 90°, then **no** light emerges from the second filter. This corresponds to the case above for electron filters when the relative orientation is 180°.

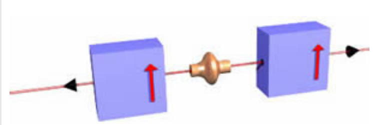
If the relative orientation of the two polaroid filters for light is 45°, one half of the light from the first filter will emerge from the second. This corresponds to the case above for electron filters when the relative orientation is 90°.

We conclude that the only difference between electron and light filters is a factor of 2 in the relative orientations. Thus, often we call the electron filters "polarisers."

Here is a final example of combining electron filters. One-half of the beam from the electron gun emerges from the first polariser; one-half of those electrons emerge from the second filter. And one-half of those electrons will make it through the third upside-down filter! Note that if the second filter were not present, **no** electrons will emerge from the upside-down filter. So we see that the middle filter actually changes the definition of "up" for the electrons. This is yet another manifestation of the Heisenberg Uncertainty Principle.	

A Flash animation of up to 3 of these Stern-Gerlach filters has been prepared. It requires Flash 7, and has a file size of 130k. It will appear in a separate window. To access the animation, click here.

Correlation Measurements

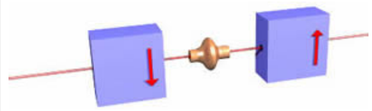
We imagine a radioactive substance that emits a pair of electrons in each decay. These two electrons go in opposite directions, and are emitted nearly simultaneously. When another nucleus in the sample decays, another pair of electrons are emitted nearly simultaneously and in opposite directions. So we can have a sample emitting these pairs of electrons. To the right we show such a sample, enclosed in a copper colored device, and electron filters measuring the spin of each member of the pair:	

For the radioactive substance we will be considering here, one-half of the electrons incident on the right hand filter emerge and one-half do not. Similarly, one-half of the electrons incident on the left hand filter emerge and one-half do not.

But if we look at the *correlation* between these electrons, we find that if, say, the right hand electron does pass through the filter, then its left hand companion does not pass its filters. Similarly, if the right hand electron does not pass through the filter, then its left hand companion always emerges from its filter.

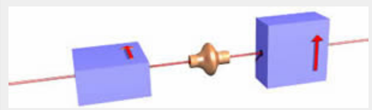
We say that each radioactive decay has a total spin of zero: if one electron is spin up its companion is spin down. Of course, this is provided that both filters have the same definition of up.

To the right is a case where the two filters have opposite definitions of up.
Again, one-half of the right hand electrons pass through their filter and one-half of the left hand electrons pass through their filter. But this time if a particular right hand electron passes its filter, then its companion left hand electron always passes its filter. Similarly, if the right hand electron does not pass its filter, its companion electron doesn't pass through its filter either.

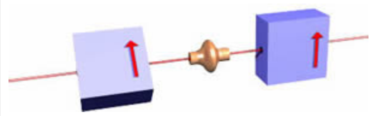


Now we consider yet another example. The two filters define "up" to be in perpendicular directions to each other. If you are still following this business with electron filters, you will not be surprised to learn that:

1. One-half of the right hand electrons emerge from their filter.
2. One-half of the left hand electrons emerge from their filter.
3. If a particular right hand electron passes its filter, one-half of the time its companion left hand electron will emerge from its filter, one-half of the time it will not.



These sorts of measurements are called *correlation experiments*. We show an arbitrary relative orientation of the two filters.



We summarise all of the above by saying that when the two filters have the same orientation, the correlation is zero: if the right hand electron passes its companion does not. When the two filters have opposite orientations, the correlation is 100%: if the right hand electron passes, so does its companion, while if the right hand electron does not pass, neither does its companion. When the two filters have perpendicular orientations, the correlation is 50%. It turns out that the correlation goes smoothly from zero to 100% as the relative orientation goes from 0° to 180°. For the mathphilic student, the actual formula is that the correlation is sin(a/2) squared, where a is the relative angle between the filters.

There are radioactive substances that emits pairs of photons similar the the pairs of electrons we have been consider so far. Some such substances have similar correlations to the electron source we have been considering, except that there is a difference of a factor of two in the relative orientations of the polarisers. If the light polarisers have the same orientation, the correlation is zero; this is the same as for electrons.

If the light polarisers have a relative orientation of 90°, the correlation is 100%: if the right hand photon passes through its polariser it companion photon will pass its polarisers, while if the right hand photon does not pass, neither does its companion. This corresponds to the case for electrons where the relative orientation of the filters was 180°.

Similarly, if you are still following all this, the correlation when the relative orientation of the light polarisers is 45° is 50%, just the correlation for electron with relative filter orientations of 90°.

As we shall see these correlation experiments, both for electrons and photons, have been performed and turn out to give us important information about the way the world is put together. This is the thrust of *Bell's Theorem*, also sometimes known as the *Einstein-Podolsky-Rosen (EPR)* paradox.

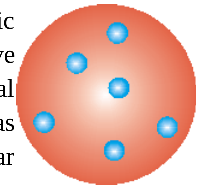
Author

This document was written by David M. Harrison, Department of Physics, University of Toronto, mailto:harrison@physics.utoronto.ca in March 1998. This is $Revision: 1.26 $, $Date: 2006/03/12 18:11:55 $ (y/m/d UTC).

13.15: The Bohr Model of the Atom

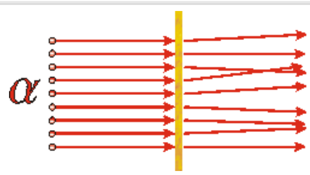
The Structure of the Atom

By the late nineteenth century, most people had accepted Dalton's proposal of 1808 that matter was made of *atoms*. Dalton "proved" his theory with a number of assumptions, each of which is either factually wrong or was used in a logically inconsistent manner. Nonetheless opposition from critics such as Mach, who never believed in atoms, was largely ignored. Throughout the nineteenth century atomism became an idea that came to dominate thought in a number of fields, including political science, sociology, psychology, biology and more.

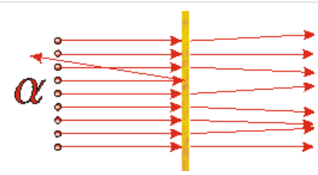


Then, in 1897 J.J. Thomson discovered the electron. He determined that these electrons had a negative electric charge and compared to the atom had very little mass. Thus he proposed that atoms consisted of a large massive positively charged body with a number of small negatively charged electrons scattered throughout it. The total charge of the electrons exactly balanced the positive charge of the large mass, so the total electric charge was zero. This was called the *plum pudding* model of the atom. The number of electrons determines the particular chemical element. Hydrogen, for example, has one electron; helium has two; carbon has six, etc.

In the early twentieth century Rutherford was experimenting with one of the newly discovered radioactive substances, one that emitted *alpha* particles. He knew that these particles had a mass much larger than the electron and had a net positive electric charge; now we know that these particles are identical to the nucleus of the helium atom. He was directing a beam of these alpha particles onto a very thin piece of gold foil. If Thomson's plum pudding model was correct, the experiments would be sort of similar to firing BB's from a BB gun into a thin slab of cream cheese with chives. And in fact the results of Rutherford's experiments usually followed this model: almost all of the alpha particles emerged on the other side slightly deflected by their interaction with the gold. However, once in a while he observed an alpha particle that was scattered right back towards the radioactive source.

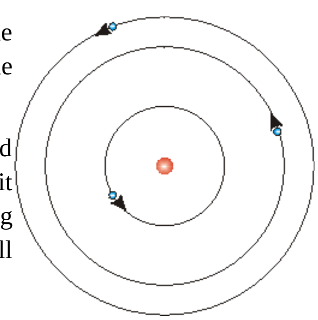


The above diagram shows what we would expect the result of Rutherford's experiment to be if the "plum pudding" model of the atom is correct.



The above indicates the actual result. Most of the alpha particles are only slightly deflected, as expected, but occasionally one is deflected back towards the source.

If you were doing the experiment involving the BB's and the cream cheese and occasionally had a BB scattered back towards you, you would probably conclude that there was something fairly small and very massive inside the slab. Similarly, Rutherford concluded that inside the gold foil there must be something fairly small, very massive, and positively charged. Thus the plum pudding model of the atom collapsed: most of the mass and the positive charge of the atom was concentrated into a very small volume. This small massive positively charged object is called the *nucleus*.



Soon, people proposed a *planetary* model of the atom. The electrons were in orbits around the nucleus, held in their orbits by the electric force that attracts negatively charged electrons to the positively charged nucleus.

However this model makes no sense. We know from classical electromagnetic theory that any charged body that is in a state of motion other than at rest or in uniform motion in a straight line will emit energy as electromagnetic radiation. Thus the electrons is this planetary model will be radiating energy. As they lose energy they will spiral into the nucleus and in a matter of nanoseconds will collide with it. Thus this atom can not be stable.

Bohr's Model

Neils Bohr knew about all of these facts, and in the early part of the century was collaborating with Rutherford. He also knew about the existence of line spectra from chemical elements; a document on this topic may be found here. He was struggling to make sense of all of this. As was common with Bohr when confronted with a puzzle, this struggle was nearly all-consuming.

Then in 1913 Bohr, by accident, stumbled across Balmer's numerology for the hydrogen spectrum, and in a flash came up with a workable model of the atom. The model asserts that:

- The planetary model is correct.
- When an electron is in an "allowed" orbit it does not radiate. Thus the model simply throws out classical electromagnetic theory. Technical note: an allowed orbit is one in which the electron mass times its speed times the radius of the orbit is equal to a positive integer **n** times Planck's constant divided by 2 pi. The integer **n** can be 1, 2, 3, 17, 108, etc. In fact, there are an infinite number of allowed orbits corresponding to the infinite number of positive integers.
- When an electron absorbs energy from incident electromagnetic radiation, it "quantum jumps" into a higher energy allowed state. This higher energy state corresponds to an allowed orbit with a higher value of the integer **n**.
- When an electron is in a higher energy state, it can quantum jump into a lower energy state, one with a smaller value of **n**, emitting all of its energy as a single photon of electromagnetic energy.

A Flash animation of Bohr's model showing the excitation and photon emission of the electron in a Hydrogen atom has been prepared. It requires the Flash player of Version 6 or better; the player is available free from http://www.macromedia.com/. The file size is 74k, and the animation will appear in a separate window. To access the animation click here.

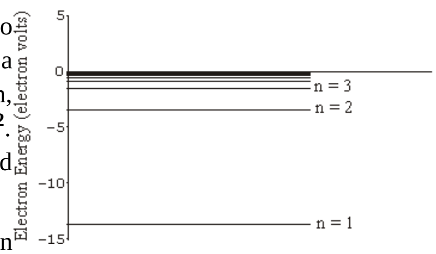
Technical note: the allowed orbits are given by the equation to the right, where **m** is the mass of the electron, **v** is its speed, **r** is the radius of the orbit, and **h** is Planck's constant.

$$m\, v\, r = n \frac{h}{2\pi}$$

As Bohr fully realised, this model is largely *ad hoc*, if not downright ugly. It does, however, "explain" the line spectra of the elements.

When Bohr published his model Otto Stern, who was Einstein’s student, and Max von Laue, who was Planck’s student, made an earnest vow: "If this nonsense of Bohr should in the end prove to be right, we will quit physics!"

Given these assertions plus the standard classical laws of attraction between two oppositely charged objects one can calculate the energy of the electrons in their orbits as a function of the value of **n**. It turns out to depend on the mass and charge of the electron, Planck's constant, some constants from electromagnetic theory, and also depends on $\mathbf{1/n^2}$. The energy of allowed orbits for hydrogen is shown to the right; we have also indicated the value of **n** for three of those energy levels.



Technical note: the fact that the energies are negative is only due to a common convention as to where we choose the zero point of energy in a non-relativistic analysis.

Recall Balmer's formula:

$$\frac{1}{\text{wavelength}} = R\left(\frac{1}{2^2} - \frac{1}{n^2}\right)$$

Here **R** is a constant equal to about 10,970,000 and **n** is any integer greater than 2, such as 3, 4, 5, 108, etc. Each different value of **n** gives the wavelength of a different line in the Hydrogen spectrum. The constant **R** is usually called the *Rydberg constant*.

The wavelengths described by this formula correspond exactly to the radiation emitted when an electron in the Bohr model quantum jumps from a high energy orbit, described by some **n** greater than 2, to an orbit whose value of **n** is equal to 2. In the model transitions to other "final" states such as **n** equal to 1 or 3, 4, 5, etc. are also predicted and the wavelengths in the spectrum for these are found experimentally to exist. Further, the constant **R** turns out to be expressed in terms of fundamental physical constants. So we have pushed the numerology of Balmer's work a bit back.

Technical note: the Rydberg constant is given by the equation to the right, where **m** is the mass of the electron, **e** its charge, **c** is the speed of light, **h** is Planck's constant, and ϵ_0 the constant relating the forces exerted by charged bodies on each other and the magnitudes of the charges.

$$R = \frac{\pi^2\, m\, e^4}{8\, c\, h^3\, \epsilon_0^2}$$

The lowest energy allowed orbit, the one with **n** equal to one, is the *ground state* of the atom. An unexcited hydrogen atom will have its electron in this state.

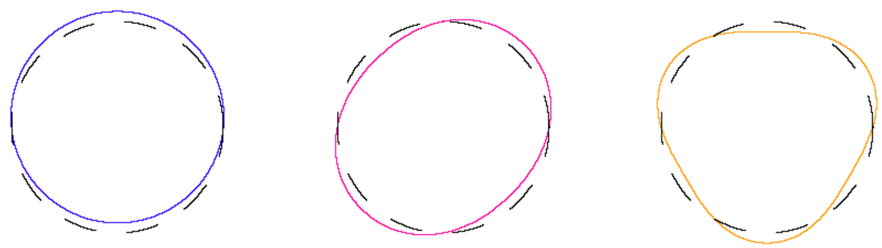
Explaining the Bohr Model

In 1924 Louis de Broglie proposed that electrons have a wave nature. As part of that proposal he also described the relationship between the wavelength of the wave aspect and the mass and speed of its particle aspect. The proposal has been experimentally confirmed and is one of the fundamental aspects of Quantum Mechanics.

Imagine a planetary model of the atom, but now think of the electrons as waves. Which waves states might be allowed?

You may recall that waves that "fit" into their available space, *standing waves*, are the ones that are allowed. A document discussing this is available here.

We show some of the standing waves that can exist for a circular orbit.



So in general the circumference equals **n** times the wavelength, where **n** is any positive integer. In the above figures the value of **n** is 1, 2 and 3 respectively.

You can view a simple animation of any of the three orbits above by pointing at it and clicking the left button. If you are using a fairly modern browser the animation will appear in a separate window; close that window whenever you wish. If you are using an older browser the animation will appear in this window; use the *Back* button of your browser to return here.

It turns out that these standing wave states for electrons correspond exactly to the "allowed" electron orbits in Bohr's model. So, Quantum Mechanics explains Bohr's ad-hoc model of the atom.

Now we call the integer **n** the *principle quantum number*. Note that for the hydrogen atom it completely describes the state of the electron.

"We are tracing the description of natural phenomena back to combinations of pure numbers which far transcends the boldest dreams of the Pythagoreans." -- Bohr

Tags recommended by the template: article:topic

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This document was written in March 1999 by David M. Harrison, Department of Physics, University of Toronto, mailto:harrison@physics.utoronto.ca. This is version 1.10, date (m/d/y) 11/19/07.

13.16: The Development of Quantum Mechanics

Introduction

Working essentially independently, in the mid-1920's Heisenberg and Schrödinger both created a full form of Quantum Mechanics. How these two extraordinary events occurred has been extensively studied; a favorite reference is Max Jammer, **The Conceptual Development of Quantum Mechanics** (McGraw-Hill 1966).

Here we briefly outline some of the key features of these developments. Some of the material is well-known, but other parts of what follows are not. The level is consistent with an upper-year liberal arts course in modern physics without mathematics that is given at the University of Toronto.

Heisenberg's Matrix Mechanics

Heisenberg's starting point was the Bohr model of the atom. This model had been extended by Sommerfeld, and by the Summer of 1925 many physicists had learned through trial and error how to navigate through some of the morass of atomic physics. This circumstance, however, is far short from having a good *theory* of atomic physics.

Heisenberg attempted to build such a theory, and immediately ran into difficulties. He was attempting to make an analogy between the orbit of an electron about a nucleus and the familiar problem of a simple pendulum. However, he ended up in a "morass of complicated mathematical equations, with no way out." (Physics and Beyond, pg. 60.)

Then Heisenberg remembered a principle of Einstein's: that the theory decides what can be observed. Heisenberg applied this idea to his attempts to build an atomic theory by throwing out any attempt to describe the orbits of the electrons directly. Instead he restricted the variables in the theory to the observables, which in this case are the wavelengths and the intensities of the lines in the atomic spectra. As he commented, "I thought it more fitting to restrict myself to these, treating them, as it were, as representatives of the electron orbits." (op. cit. pg. 63.) And from this principle he built his complete form of Quantum Mechanics.

In a later conversation, Einstein admitted that he had used a similar principle in developing the theories of relativity, but in this case thought that Heisenberg had gone much too far. (*ibid.*)

In any case, since the observables, the wavelengths of the line spectra, are discontinuous the theory that Heisenberg built is similarly discontinuous. This formulation of Quantum Mechanics is often called *Matrix Mechanics*; we shall see that this distinguishes it from Schrödinger's theory.

Heisenberg first published his Matrix Mechanics in 1926 in the journal *Zeitschrift der Physick*.

Schrödingers's Wave Mechanics

In 1905 Einstein proposed that light, in addition to its well known nature as a wave of electric and magnetic fields, can be thought of as a particle, which now we call the *photon*. In 1923 Louis de Broglie proposed that particle-like objects, such as electrons, could also be thought of as some sort of wave. At this time de Broglie was a graduate student, and his proposal was part of his PhD thesis. His supervising committee didn't know what to make of this outlandish proposal and asked Schrödinger, who pronounced that the idea was "rubbish!" The committee went to Einstein, who essentially said that they should give the kid his PhD, since "there might be something to it." So that is how de Broglie got his PhD, and in 1926 Davisson and Germer actually saw electrons demonstrating an interference pattern.

In 1926 Schrödinger published a series of papers giving a full form of Quantum Mechanics; in this formulation the central idea is de Broglie's hypothesis. This formulation, then, is called *Wave Mechanics*. When earlier we stated that we could "explain" the ad hoc Bohr model by realising that the 'allowed orbits' of that model correspond to standing waves of electrons, we were describing how Wave Mechanics describes the theory of an atom.

It is interesting to note that the first of these papers appeared simultaneously to Heisenberg's first publication. Schrödinger's paper was in the journal *Annelen der Physick*, a competitor to the *Zeitschrift* journal that had published Heisenberg's work.

It is obvious that Schrödinger changed his mind about a wave aspect to electrons between 1923 and 1926. There is some controversy about how Schrödinger actually arrived at Wave Mechanics, but in the Fall of 1925, presumably as he was building his theory, he wrote an essay, **Seek for the Road**, which may provide some clues. (Reference: **My View of the World**, (Cambridge, 1964).

You may recall the Schrödinger's Cat paradox, which was first published in its "scientific form" in 1935 in *Zeitschrift der Physick*. However in his 1925 essay he recounts an ancient Sankhya Hindu paradox that, jazzed up with some technology, became the cat paradox. In that original form the paradox was cast in the form of two people, one looking at a garden, the other in a dark room. The modern equivalent would be one person looking in the box to see if the cat is alive or dead, while a second person waits out in the hall. As we discussed, in this modern form the state "collapses" for the first person while it does not collapse for the second person.

In 1925 Schrõdinger resolved that paradox the way the Vedantists did: he asserted that all consciousness is one. As he wrote:

"But it is quite easy to express the solution in words, thus: the plurality [of viewpoints] that we perceive is only *"an appearance*; *it is not real*. Vedantic philosophy, in which this is a fundamental dogma, has sought to clarify it by a number of analogies, one of the most attractive being the many-faceted crystal which, while showing hundreds of little pictures of what is in reality a single existent object, does not really multiply the object."

Here is another fragment of that essay:

"... you may suddenly come to see, in a flash, the profound rightness of the basic conviction of Vedanta: ... knowledge, feeling and choice are essentially eternal and unchangeable and numerically *one* in all men, nay in all sensitive beings."

Do you think that Schrödinger had such a flash of insight? Is this the sort of insight which in the Eastern traditions is sometimes called *enlightenment*?

Finally, Schrödinger himself makes an interesting analogy between Vedantic philosophy and modern physics:

"If finally we look back at that idea of Mach [that `the universe is not twice given'], we shall realize that it comes as near to the orthodox dogma of the Upanishads as it could possibly do without stating it *expressis verbis*. The external world and consciousness are one and the same thing."

Comparing the Two Forms of Quantum Mechanics

Despite their radically different worldview, shortly after their publication it was shown that Matrix Mechanics and Wave Mechanics are mathematically identical. In fact, Schrödinger was one of the people who did the proof.

Despite their formal equivalence, there seems to be more than just logic involved in the interpretation of the mathematics. For example, Heisenberg wrote:

"The more I ponder the physical part of Schrðdinger's theory, the more disgusting it appears to me."

while Schrödinger wrote:

"If one has to stick to this damned quantum jumping, then I regret ever having been involved in this thing."

In the 5th century of the current era, there was a bitter argument in India between the Sankhya Hindus and the Buddhists about the nature of Universal Flux. Debates were held which lasted for days, and would attract huge crowds. According to the Buddhists:

The phenomena consist of an infinity of discrete moments following one another almost without intervals.... There is no matter at all, flashes of energy follow one another and produce the illusion of stabilized phenomena. The universe is a *staccato* movement.

while according to the Hindus:

The phenomena are nothing but waves or fluctuations standing out upon the background of an eternal, all-pervading undifferentiated Matter with which they are identical. The universe represents a *legato* movement.

Reference: F. Theodor Stcherbatsky, **Buddhist Logic**, Vol I, pg 83.

Even allowing for the possibility that Schrödinger's Wave Mechanics may have been influenced by Hindu philosophy, the parallels between the Buddhist-Hindu argument and the Heisenberg-Schrödinger aesthetic clash are striking.

Discussion

Earlier we saw that two formally identical theories of antimatter, due to Dirac and Feynman, are interpreted in radically different ways. Now we see two formally identical formulations of Quantum Mechanics, which not only have radically different interpretations, but those interpretations apparently have a huge emotional and aesthetic content. In this section I shall briefly discuss some ideas about how this can be so.

In the humanities, the field of *Literary Criticism* is involved in part with trying to interpret what some author actually means when they wrote some particular passage. For an outsider like me, it is absolutely amazing how just a few words in a poem can be interpreted so differently by different scholars.

This circumstance is one of the reasons why some have claimed that there really isn't any meaning in those few words, or much of anything else. This leads to the post-modern excesses of deconstruction, in my view.

I prefer to view these different interpretations as just a consequence of the fact that all *natural languages* are inherently ambiguous.

For example, consider the simple statement: *The plant is complete.* What is it that is complete? It could be a vegetable. It could be the act of fixing something in place. Or it could be a factory. In the usual case the meaning of a simple phrase like this is given by its context.

But in more sophisticated situations, there may be a range of meanings for a phrase and for a good writer all of those meanings are simultaneously being deployed.

Similarly, in mathematics one often puts a dot over a character: $\dot{A}$. The meaning of the dot is ambiguous. It could mean we are referring to a unit of length called the Angstrom. It could mean that we are referring to the derivative of the variable A with respect to time. It could mean other things as well.

Thus, it is fair to argue that mathematics, the language of Physics, is a natural language with all of the levels of multiple meaning and ambiguity of other such languages. In this view, then, the strong positions of Heisenberg and Schrödinger on the worldview of Quantum Mechanics is similar to an argument between two scholars of literary criticism on the meaning of a T.S. Eliot poem.

About a half century ago, C.P. Snow wrote about how our culture seems to have bifurcated into two cultures, a scientific one and a non-scientific one. One contributing factor to this possible bifurcation is that scientists when they communicate amongst themselves use mathematics as one of the primary languages of that communication. For the many people who are math-phobic, then, this communication is unintelligible.

Of course, one of the major points of this course is a demonstration that one may discuss and understand science at a deep level without mathematics.

In any case, the analogy between interpretations of poems and interpretations of scientific theories that I made above puts me into direct opposition to much of the following by D.H. Lawrence:

"[Literary] criticism can never be a science: it is, in the first place, much too personal, and in the second, it is concerned with values that science ignores. The touchstone is emotion, not reason." -- **Phoenix: The Posthumous Papers**

Author

This document was written in March 2000 by David M. Harrison, Department of Physics, University of Toronto, mailto:harrison@physics.utoronto.ca.. This is version 1.6, date (m/d/y) 04/30/04.

13.17: Two analogies to Bell's Theorem

Background

There are a couple of facts which we will need for our discussion. One is from human biology, and the other from physics.

Issues in the Development of People

The context of our analogy is the *nature* versus *nurture* debate about the development of people. Adherents of the nurture position believe that at birth humans are essentially a blank slate, and that their environment as they grow and develop is the only factor that determines characteristics of the individual. Thus matters of choice of profession, mate, musical preferences, morality, etc. are determined by society. Believers in the nature position, on the other hand, say the genetics is crucial in development, and that the characteristics of an individual are determined at birth.

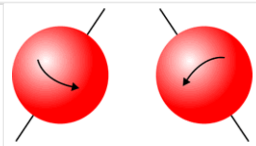
The data are fairly clear that both genetics and environment are approximately equally important in the development of an individual.

One of the types of studies that lead to this conclusion involve identical twins who were separated at birth. Such twins have almost completely identical DNA, and sometimes were raised in very different social environments. Nonetheless, there are often strong correlations between the later behavior of such twins: if one is, say, a firefighter than often the other is also a firefighter. Other characteristics that twins tend to share, even if raised in very different environments, include physical characteristics of their choice of mate, preferences in music, and more.

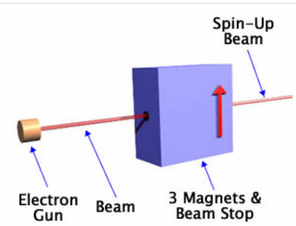
Later it will be important to note that the correlations are not 100%. Just because one twin is a firefighter does not guarantee that the other is too. Similarly, if one twin really hates the music of Twisted Sister does not guarantee that the other twin will also despise that type of "music." Nonetheless, the correlations are sufficiently strong that it is almost certain that they did not arise by pure chance.

Pairs of Spinning Particles in Physics

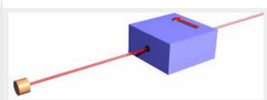
Most elementary particles, such as electrons, photons, etc., have an intrinsic angular momentum which is usually called *spin*. For our purposes, we can imagine the particle as a small ball that is spinning about some axis.
It turns out that the spin of an electron has only two states, which we call *up* and *down*. The origins of this terminology are not important for our purposes here. In the figure, the electron on the left is spin-up and the electron on the right is spin-down.



It is possible to construct a "filter" that selects only spin-up electrons. Again the details of what is in the box are not important for our purposes.
What is important here is that one-half of the electrons from the electron gun will emerge from the filter with the same speed in the same direction as before they entered the box, and one-half of the electrons will not emerge. Which is the case for an individual electron is random.
You will also want to notice that we have painted an arrow on the side of the box to indicate what direction is *up*.



The apparatus actually defines the direction of up. If we rotate it by some angle, again one-half of the incident electrons emerge from the filter, and which is the case for an individual electron is random.



There are some radioactive materials for which when an individual atom decays it simultaneously emits two electrons in opposite directions. These pairs of electrons have a total spin of zero: if one electron is spin-up, its companion electron is spin-down and vice versa. Such pairs of particles are called *entangled quantum pairs*.

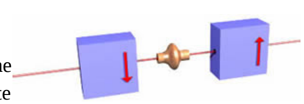
The Analogy

We shall begin by assuming that the *nurture* position on human development is correct. This assumption means that we would expect that for identical twins separated at birth, any later correlations in their choices of profession, mate, etc. are due to similarities in the environment in which the twins were raised. Each twin's environment is *local* to the separate individual, and we are assuming that this local environment causes the later behavior of the individual. In Physics-speak, we call this assumption **local causality**.

There are two kinds of correlation experiments that we can do.

1. Correlations in the choice of profession, or the taste in music, or some other characteristic.
2. Correlations of the choice of profession of one twin with the musical taste of the other twin. This is a more sophisticated experiment, and the analysis will require more statistical information.

The studies of the correlations of twin behavior, then, show that the assumption of local causality is incorrect.



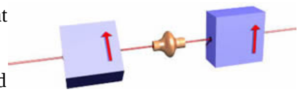
We can also do correlation experiments for the entangled quantum pairs of electrons that we discussed above. The source of the total spin-zero entangled electron pairs is in the center of the figure, and the two electrons from each decay go in opposite directions.

Note that the two filters have opposite orientations.

It turns out that one-half of the electrons traveling to the right pass through its filter and one-half do not, and which is the case for an individual electron is random. Similarly one-half of the electrons traveling to the left pass through its filter and one-half do not, and which is the case for an individual electron is random. However, when we examine the correlations, if the right-hand electron passes through its filter its companion left-hand electron also passes through its filter. If the right-hand electron does not pass through its filter its companion left-hand electron does not pass through its filter. This is a consequence of the fact that the two electrons have a total spin of zero, so if one is spin-up the other is spin-down *provided the direction of "up" is the same for both measurements*. Here the direction of "up" is opposite for the two filters.

For the identical twins, correlations in the same characteristic such as profession showed that local causality is not true in the nature vs. nurture debate. However, this correlation in electron spins does not violate local causality. This circumstance is more analogous to the following:

We carefully saw a coin in half along its plane, so one piece has the "head" and the other has the "tails." We put each piece in an envelope and walk the two envelopes away from each other. If we open one envelope and see a heads, we are guaranteed that the other piece contains a tails.



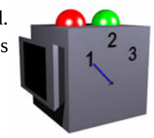
However, when we set the electron filters at orientations other than opposite each other we see strange correlations. To the right we have the right-hand filter oriented at zero degrees, and the left-hand filter tipped by 45 degrees.

In fact, the conflict with local causality for entangled electron spin correlations only shows up when we set the right and left hand filters at different angles. This is analogous the the twin correlation measurements where we try to correlate the profession of one with the musical taste of the other. The actual tests involve orienting the filters at zero degrees, 45 degrees, and 90 degrees.

We explore in more detail how this conflict arises in the next section.

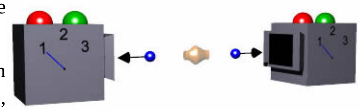
The Second Analogy: More Boxes

A Flash animation that duplicates much of the discussion of this section is available. It requires Flash 6, and has a file size of 78k. You may access it by clicking here. It will appear in a separate window.



We imagine a box, such as is shown to the right. Although nobody has every made such a box, there is no reason why it could not be constructed. It has a red and green light on top, and a switch that can be set to three positions: 1, 2, and 3. The apparatus is self contained, and has batteries inside to drive the lights and whatever mechanism is inside.

The box is a detector, and one of the lights will light up when a particle enters it from the left.



We have two of these detectors, and place them on either side of some device which emits pairs of particles in opposite directions.

We have bazillions of pairs of these particles go through the detectors, and set the switch positions randomly for each pair. If the boxes are measuring electron spin, then the switches could correspond to orienting the spin filters at zero, 45, and 90 degrees, and the pairs of particles could be entangled electron pairs. Soon we shall attempt to build another more classical model of what is being measured, and will run into trouble with it.

We record which lights flash for each pair and what are the switch positions. There are two cases:

1. If both switches on the boxes are set to the the same positions, either 1 or 2 or 3, the same light flashes on both boxes. Either both red lights flash or both green lights flash. Half of the time both red lights flash, the other half of the time both green lights flash.
2. If the switches are set to different positions both detectors flash the same color one-quarter of the time, either both red or both green. One half of the time when both colors flash they are both red, the other half of the time they are both green. Three-quarters of the time the detectors flash different colors, either red on the left and green on the right or green on the left and red on the right; in this case each of the two possibilities occur half of the time.

Explaining Case 1

Imagine that when the switch is in position 1 it measures the speed of the object, when it is position 2 it measures the size, and in position 3 it measure the shape of the object.

Switch Position	Measures	Green Light	Red Light
1	Speed	Flashes when particle is going fast	Flashes when particle is going slow
2	Size	Flashes when particle is big	Flashes when particle is small
3	Shape	Flashes when the particle is a sphere	Flashes when the particle is not a sphere

Then the experimental results are easy to explain:

- The pairs of particles always have the same speeds, the same size, and the same shape.
- Half of the time both the particles are moving fast, half of the time both are moving slow.
- Half of the time both the particles are big, half of the time they are both small.
- Half of the time both particles are spheres, half of the time they are not.
- There are eight different states the pairs of particles can be in, each occurring with equal frequency:
    1. Fast big spheres.
    2. Slow big spheres.
    3. Fast little spheres.
    4. Slow little spheres.
    5. Fast big non-spheres
    6. Slow big non-spheres
    7. Fast little non-spheres.
    8. Slow little non-spheres.

What About Case 2?

There are six settings of the switches which are different.

For the case of fast big spheres here are the possible switch settings and the results:

Left Switch	Left Light	Right Switch	Right Light
1	Green	2	Green
2	Green	1	Green
2	Green	3	Green
3	Green	2	Green
1	Green	3	Green
3	Green	1	Green

So for this case all the switch settings end up with the both green lights flashing. For slow small non-spheres, similarly, both red lights will flash for all six switch positions. We expect one-quarter of the bazillion pairs of particles to be either fast big spheres or slow small non-spheres. So far so good: the experimental result is that the lights flash the same color one-quarter of the time.

But imagine the case of pairs of fast big non-spheres. Here are the possible switch settings and the results:

Left Switch	Left Light	Right Switch	Right Light
1	Green	2	Green
2	Green	1	Green
2	Green	3	Red
3	Red	2	Green
1	Green	3	Red
3	Red	1	Green

Only two of the six possible settings have both lights flash the same color, green in this case. But the switch settings are made at random, so we expect each of the six possible results in the above table to occur with equal frequency. So both lights flash the same color one-third of the time.

The same argument can be made for the other five pairs that are not big fast spheres or small slow non-spheres: both lights will flash the same color one-third of the time.

Imagine we take data for 24 bazillion pairs of particles. We expect each of the eight possible states of speed, size, and shape to occur with equal frequency, so our sample will have 3 bazillion pairs of each type. We then expect the following results when the switches are set to different positions:

Switches are in different positions

Type	Number	Number of Pairs For Which the 2 Lights Flash the Same Color	Color	Fraction
fast big spheres	3 bazillion	3 bazillion	both green	1
slow big spheres	3 bazillion	1 bazillion	both green	1/3
fast little spheres	3 bazillion	1 bazillion	both green	1/3
slow little spheres	3 bazillion	1 bazillion	both red	1/3

fast big non-spheres	3 bazillion	1 bazillion	both green	1/3
slow big non-spheres	3 bazillion	1 bazillion	both red	1/3
fast little non-spheres	3 bazillion	1 bazillion	both red	1/3
slow little non-spheres	3 bazillion	3 bazillion	both red	1
Total	24 bazillion	12 bazillion	half both red, half both green	1/2

So when we summarise the data for all the pairs of particles that we measured, we would not expect to have different colors flashing on the two detectors one-quarter of the time, but instead one-half of the time. But the experimental result is one-quarter, not one-half.

This example has been thinking about classical objects, which is tantamount to assuming local causality. Thus we see that these correlation measurements violate local causality, in exactly the same way the the electron spin measurements of entangled electron pairs violate local causality.

This entire section is a slight simplification of Mermin's analysis, which is listed in the references. I close with the conclusion of that lovely paper:

I shall not describe how contemporary physical theory accounts for the behavior of the device except to note that although, in its own way, the explanation is very simple, it is far from obvious, and, some might argue, hardly an explanation at all. Instead, I only emphasize again that we live in a world where such a device can be built; nature is stranger and more wonderful than we had once thought or could possible [sic] have imagined. Ponder the device a little more if that seems too extreme a conclusion.

Further Study

Here are some documents on particle spin, Bell's Theorem, and the Nature vs. Nurture debate which are accessible to the layperson.

Spin

- A non-mathematical treatment, by the author of this document, is available on the web at:
  http://www.upscale.utoronto.ca/PVB/Harrison/SternGerlach/SternGerlach.html (html)
  http://www.upscale.utoronto.ca/PVB/Harrison/SternGerlach/SternGerlach.pdf (pdf)
- A wonderful discussion which does do a bit of the mathematics is Richard P. Feynman, Robert B. Leighton and Matthew Sands, **The Feynman Lectures on Physics**, Vol. III, Chapters 5 - 6, ISBN: 0201500647.

Bell's Theorem

- A brilliant example, which is non-mathematical but subtle, is N.D. Mermin, American Journal of Physics **49**, 940 (1981). Many institutions, including the University of Toronto, have subscriptions to this journal so they may be accessed from any computer whose IP number corresponds to the subscribing institution. The American Journal of Physics is available on-line at: scitation.aip.org/ajp/
- A clever proof, using simple Venn diagrams, is B. d'Espagnat, Scientific American **241**, 158 (November 1979).
- A "chaotic ball" analogy is C.H. Thompson and H. Holstein, Foundations of Physics Letters **9**, 357 (1996), http://www.arxiv.org/format/quant-ph/9611037 .
- A mostly non-mathematical treatment, by the author of this document, is available on the web at:
  http://www.upscale.utoronto.ca/PVB/Harrison/BellsTheorem/BellsTheorem.html (html)
  http://www.upscale.utoronto.ca/PVB/Harrison/BellsTheorem/BellsTheorem.pdf (pdf)

Nature versus Nurture

- Judith Rich Harris, **The Nurture Assumption** (Free Press,1999), ISBN**:** 0684857073
- Steven Pinker, **The Blank Slate** (Viking, 2002), ISBN: 0670031518

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13.18: Wave-Particle Duality

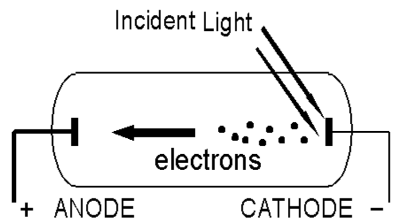
QUOTABLE QUOTES

1. Common sense is the deposit of prejudice laid down in the mind before the age of 18. A. Einstein

2. God is a mathematician of a very high order and He used very advanced mathematics in constructing the Universe. P.A.M. Dirac

3. If you are not confused by Quantum Physics then you haven't really understood it. N.Bohr

What is the Photo-Electric Effect?



In the Photo-Electric effect, a metal is illuminated with light. Under certain circumstances, electrons are emitted from the illuminated surface. We can vary the intensity of the light and its frequency (its colour).

Expectations of Classical Physics.

These expectations are based on the belief that light is an electromagnetic wave; if we increase the intensity of the light this is equivalent to increasing the amplitude of the oscillating electric field of which the light wave is composed. Since the energy of the light beam is spread uniformly over the beam, it is transferred continuously to the electrons, which require a certain minimum of energy to escape the attractive forces of the metal. In the following, "The maximum energy of the electrons" means "The energy of the most energetic electrons".

- c. There may be a time delay between the switching on of the light and the appearance of the first electrons; the lower the light intensity, the longer will be this time delay.

Experimental Observations.

- c. No matter how weak the light, as long as its frequency is above the threshold frequency, the emission of electrons starts IMMEDIATELY the light is switched on.

(In case you were wondering; an increase in the light intensity increases the number of electrons emitted per second, while leaving the energy of each electron unchanged).

Einstein's Explanation.

- c. The interaction between a photon and an electron in the metal is a unique, elemental act, in which the photon can give up some, or all of its energy to the electron, which then might have enough energy to escape from the metal.

Why does this explain the observations?

The electron is kept in the metal by the electric forces, and can only escape if a certain minimum amount of energy is given to it. If the photon energy (i.e. frequency) is too low to overcome this attractive force between the electrons and the metal, the electron can't escape. Thus the frequency of the photon must be above a certain value (which depends on the particular metal). Once we are above this threshold, the photon either hits an electron or it doesn't. If it does, and if enough energy is transferred to the the electron from the photon, the electron will have enough energy to escape IMMEDIATELY, with no time delay. Also, if we increase the energy of the photon by increasing its frequency, the electrons which interact with these electrons can come off with increased energy).

Einstein's conjecture that the energy of a photon is proportional to its frequency can be written $\mathbf{E_{photon} = h\ f}$; here **h** is Planck's constant.

Particles are also Waves.

The great success of Einstein's theory for the photoelectric effect stimulate de Broglie to postulate in his Ph.D. thesis at the University of Paris, that particles might exhibit wave-like properties. Starting from Einstein's relation, $\mathbf{E_{photon} = h\ f}$ and using the relation given by Maxwell's equations for the momentum of a light wave, $\mathbf{E_{light} = pc}$ (where **p** is the momentum of the light, and **c** is the speed of light), de Broglie derived the expression $\mathbf{p = h/\lambda}$, where λ is the wavelength of light; he proposed that this relation could be taken over to refer to particles, whose "wavelength" (whatever that means!) would be given by λ= h/p.

[Note the deliciously schizophrenic appearance of these formulae; on the right hand side there is a "particle" property - energy or momentum, while on the right hand side there is a "wave" property - frequency or wavelength.]

How could these particle wavelengths be observed? Remember that one identifying feature of waves is their ability to interfere, as in the double slit experiment. However, for electrons, for instance, this wavelength turns out to be very small. Now remember (see Waves) that wave effects (i.e. diffraction effects or interference) are difficult to see if we use measuring devices which are much larger than the wavelengths involved. So it was not surprising that the first confirmation of de Broglie's apparently fantastic proposal should find experimental support in the study of the interaction of electrons with metals. For the regular planes of atoms which are found crystals turn out to be just of the correct order of magnitude to allow observation of interference effects of electrons which are being reflected from metal crystal surfaces. In fact such crystal planes had already been used to show the effects of interference for X-rays - which are just very short wavelength electromagnetic waves; the wavelength of X-rays is around a few Angstroms - 1A = 10^{-10}m - so we need a "diffraction grating" which has line spacing between the slits of the same order of magnitude as this wavelength, and crystal planes do the job!

In 1927, three years after de Broglie's proposal, Davisson and Germer, working at Bell Labs in the US, and, independently G.P. Thomson working at Cambridge University, observed interference patterns in the scattering of electrons. The "wavelength" of the electrons, calculated from the observed interference patterns, agreed exactly with de Broglie's formula.

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Index

B

Bell's theorem
- 13.14: Stern-Gerlach Experiment
- 13.17: Two analogies to Bell's Theorem

Black Hole Thermodynamics
- 13.2: Black Hole Thermodynamics

C

conservative force
- 2.1: Conservative Fields

E

entanglement
- 13.8: Quantum Entanglement

L

Ladder operators
- 9: Ladder operators

Lamb shift
- 12.5.2: The Lamb Shift

O

Operators
- 3.2: Operators

P

probability density
- 3.1: The State of a Quantum System

R

reflection coefficient
- 6.2: Potential step

S

Scattering
- 6: Scattering from Potential Steps and Square Barriers

Spherical harmonics
- 11.6: Spherical Harmonics

Square Barrier
- 6.3: Square Barrier

T

transmission coefficient
- 6.2: Potential step

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    - 4.3: A_2= 0 - *CC BY-NC-SA 2.0*
    - 4.4: Some Consequences - *CC BY-NC-SA 2.0*
    - 4.5: Lessons from the square well - *CC BY-NC-SA 2.0*
    - 4.6: A physical system (approximately) described by a square well - *CC BY-NC-SA 2.0*
  - 5: Infinite Wells - *CC BY-NC-SA 2.0*
    - 5.1: Zero of Energy is Arbitrary - *CC BY-NC-SA 2.0*
    - 5.2: Solution - *CC BY-NC-SA 2.0*
  - 6: Scattering from Potential Steps and Square Barriers - *CC BY-NC-SA 2.0*
    - 6.1: Non-normalizable Wavefunctions - *CC BY-NC-SA 2.0*
    - 6.2: Potential step - *CC BY-NC-SA 2.0*
    - 6.3: Square Barrier - *CC BY-NC-SA 2.0*
  - 7: The Harmonic Oscillator - *CC BY-NC-SA 2.0*
    - 7.1: Prelude to Harmonic Oscillators - *CC BY-NC-SA 2.0*
    - 7.2: Dimensionless Coordinates - *CC BY-NC-SA 2.0*
    - 7.3: Behaviour for large |y| - *CC BY-NC-SA 2.0*
    - 7.4: Taylor Series Solution - *CC BY-NC-SA 2.0*
    - 7.5: A Few Solutions - *CC BY-NC-SA 2.0*
    - 7.6: Quantum-Classical Correspondence - *CC BY-NC-SA 2.0*
  - 8: The Formalism Underlying Quantum Mechanics - *CC BY-NC-SA 2.0*
    - 8.1: Key Postulates - *CC BY-NC-SA 2.0*
    - 8.2: Expectation Values of x^2 and p^2 for the Harmonic Oscillator - *CC BY-NC-SA 2.0*
    - 8.3: The Measurement Process - *CC BY-NC-SA 2.0*
  - 9: Ladder operators - *CC BY-NC-SA 2.0*
    - 9.1: Harmonic oscillators - *CC BY-NC-SA 2.0*
    - 9.2: The operators $\hat{A}$ and $\hat{A}^\dagger$. - *CC BY-NC-SA 2.0*
    - 9.3: Eigenfunctions of H through ladder operations - *CC BY-NC-SA 2.0*
    - 9.4: Normalisation and Hermitean conjugates - *CC BY-NC-SA 2.0*
  - 10: Time-Dependent Wavefunctions - *CC BY-NC-SA 2.0*
    - 10.1: Correspondence between time-dependent and time-independent solutions - *CC BY-NC-SA 2.0*

- 10.2: Superposition of time-dependent solutions - *CC BY-NC-SA 2.0*
- 10.3: Completeness and time-dependence - *CC BY-NC-SA 2.0*
- 10.4: Simple Example - *CC BY-NC-SA 2.0*
- 10.5: Wave packets (states of minimal uncertainty) - *CC BY-NC-SA 2.0*

- 11: 3D Schrödinger Equation - *CC BY-NC-SA 2.0*
  - 11.1: The momentum operator as a vector - *CC BY-NC-SA 2.0*
  - 11.2: Spherical Coordinates - *CC BY-NC-SA 2.0*
  - 11.3: Solutions independent of angular variables - *CC BY-NC-SA 2.0*
  - 11.4: The hydrogen atom - *CC BY-NC-SA 2.0*
  - 11.5: Now where does the probability peak? - *CC BY-NC-SA 2.0*
  - 11.6: Spherical Harmonics - *CC BY-NC-SA 2.0*
  - 11.7: General solutions - *CC BY-NC-SA 2.0*
- 12: Quantum Mechanics of the Hydrogen Atom - *CC BY-NC-SA 2.0*
  - 12.1: The Uncertainty Principle - *CC BY-NC-SA 2.0*
  - 12.2: Bohr Model of the Hydrogen Atom - *CC BY-NC-SA 2.0*
  - 12.3: Schrödinger Theory of the Hydrogen Atom - *CC BY-NC-SA 2.0*
    - 12.3.1: Schrödinger Theory of Hydrogen - *CC BY-NC-SA 2.0*
    - 12.3.2: The Spin-Orbit Effect - *CC BY-NC-SA 2.0*
    - 12.3.3: Kinetic Energy Corrections - *CC BY-NC-SA 2.0*
  - 12.4: Dirac Theory of the Hydrogen Atom - *CC BY-NC-SA 2.0*
  - 12.5: Smaller Effects - *CC BY-NC-SA 2.0*
    - 12.5.1: Hyperfine Structure - *CC BY-NC-SA 2.0*
    - 12.5.2: The Lamb Shift - *CC BY-NC-SA 2.0*
    - 12.5.3: The Zeeman Effect - *CC BY-NC-SA 2.0*
  - 12.6: Conclusion and References - *CC BY-NC-SA 2.0*
- 13: Miscellaneous Quantum Mechanics Topics - *CC BY-NC-SA 2.0*
  - 13.1: Bell's Theorem - *CC BY 2.0*
  - 13.2: Black Hole Thermodynamics - *CC BY-NC-SA 2.0*
  - 13.3: Complementarity and Copenhagen Interpretation - *CC BY-NC-SA 2.5*
  - 13.4: Double Slit - *CC BY-NC-SA 2.0*
  - 13.5: Flash Animations for Physics - *CC BY-NC-SA 2.0*
  - 13.6: Locality and Quantum Mechanics - *CC BY-NC-SA 2.0*
  - 13.7: Particle in a 2-dimensional box - *CC BY-NC-SA 2.0*
  - 13.8: Quantum Entanglement - *CC BY-NC-SA 2.0*
  - 13.9: Quantum Interference - *CC BY-NC-SA 2.0*
  - 13.10: Quantum Mechanics- a Poor Person's Guide - *CC BY-NC-SA 2.0*
  - 13.11: Quantum Mechanics- Interpretation - *CC BY-NC-SA 2.0*
  - 13.12: Quantum Teleportation - *CC BY-NC-SA 2.0*
  - 13.13: Schrödinger's Cat - *CC BY-NC-SA 2.0*
  - 13.14: Stern-Gerlach Experiment - *CC BY-NC-SA 2.0*
  - 13.15: The Bohr Model of the Atom - *CC BY-NC-SA 2.0*
  - 13.16: The Development of Quantum Mechanics - *CC BY-NC-SA 2.0*
  - 13.17: Two analogies to Bell's Theorem - *CC BY-NC-SA 2.0*
  - 13.18: Wave-Particle Duality - *CC BY-NC-SA 2.0*
- Back Matter - *Undeclared*
  - Index - *Undeclared*
  - Glossary - *Undeclared*
  - Detailed Licensing - *Undeclared*