

BPhO

Computational Challenge

Quantum, atoms, nuclear

Dr Andrew French.
December 2023.

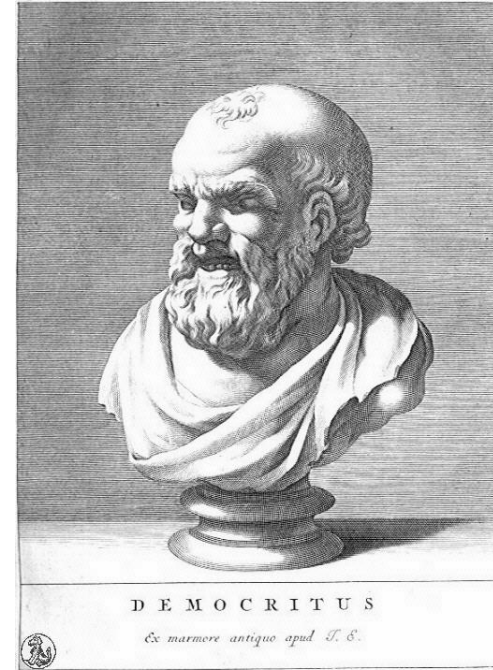
In ancient Greece, Democritus* proposed that matter is composed of 'uncuttable' *atomon* components. Today we call them **atoms**.

Unfortunately this idea only became scientific orthodoxy in the twentieth century!

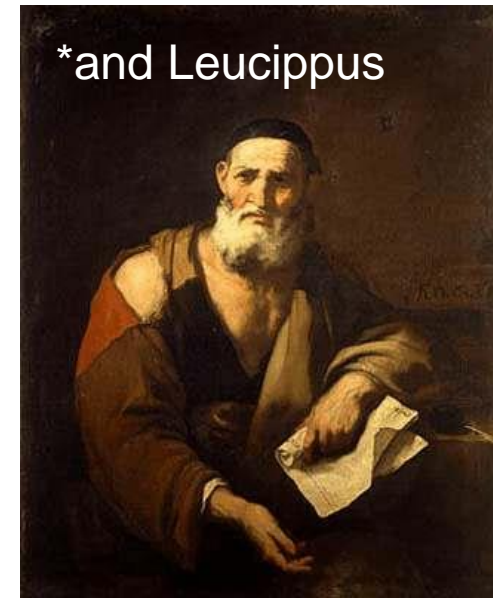
In the Standard Model of modern Physics, atoms are themselves composed of **fundamental particles**. **Quarks** are 'glued' together to form the **protons** and **neutrons** which comprise a tiny positively charged **atomic nucleus**, with radius 10^{-15}m (1femto-metre, fm). Around them is a cloud of negatively charged **electrons**. So what are these particles, and how do they interact?

Four key experiments at the turn of the twentieth century showed that the laws of Physics at these small scales are quite different, and much stranger, than the Classical theories of Newton, Maxwell etc.

This theory is called **Quantum Mechanics**

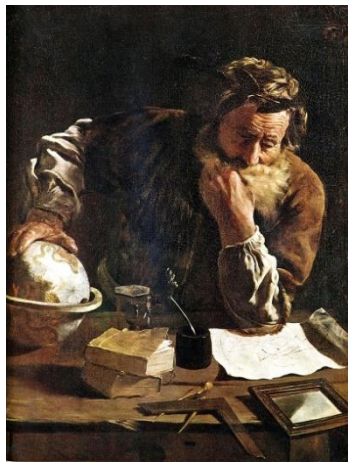


Democritus
460 BC – 370BC



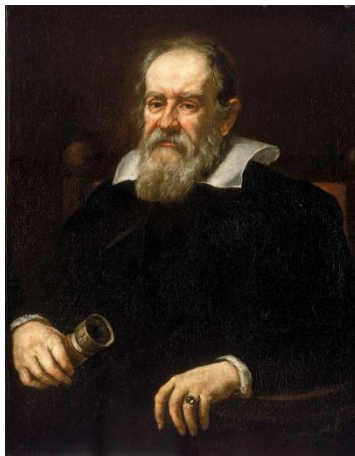
*and Leucippus

Mechanics



Archimedes
287BC - 212BC

Mechanics



Galileo Galilei
1564-1642

Orbits



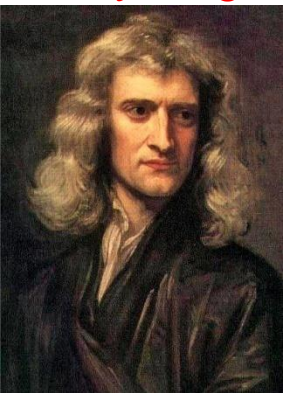
Johannes Kepler
1571-1630

Waves



Christiaan Huygens
1629 - 1695

Everything!



Isaac Newton
1642-1726

Waves, heat



Joseph Fourier
1768-1830

Electromagnetism



Michael Faraday
1791-1867

Entropy



Rudolf Clausius
1822-1888

Electromagnetism



James Clerk
Maxwell
1831-1879

A small selection of the

Pioneers of Classical Physics

Thermodynamics



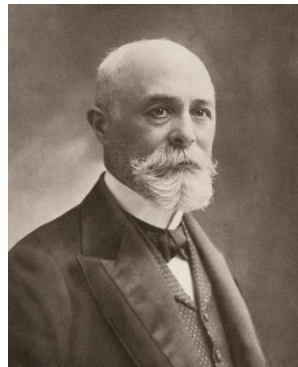
Ludwig Boltzmann
1844-1906

X-Rays



Wilhelm Röntgen
1845-1923

Radioactivity



Antoine Henri
Becquerel
1852-1908

Electron



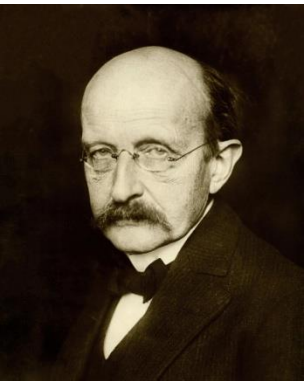
J.J. Thompson
1856-1940

Radio waves



Heinrich Hertz
1857-1894

Quanta



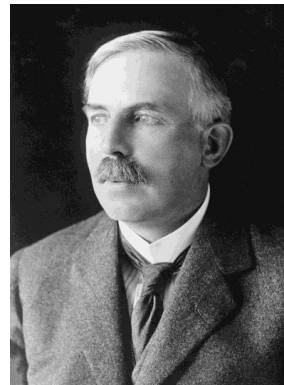
Max Planck
1858 – 1947

Radioactivity



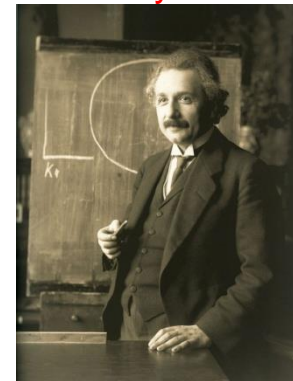
Marie Curie
1867-1934

Atomic nucleus



Ernest Rutherford
1871-1937

Quantum Theory Relativity



Albert Einstein
1879-1955

Quantum atom



Niels Bohr
1885-1962

A small selection of the

Pioneers of Atomic & Quantum Physics



Max Born
1882 –1970



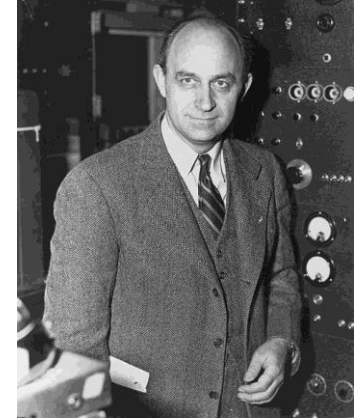
Erwin Schrödinger
1887 –1961



Louis de Broglie
1892 –1987



Wolfgang Pauli
1900 –1958



Enrico Fermi
1901-1954



Werner
Heisenberg
1901 – 1976



Paul
Dirac
1902-1984



George
Gamow
1904-1968



Richard
Feynman
1918-1988



Murray
Gell-Mann
1929-

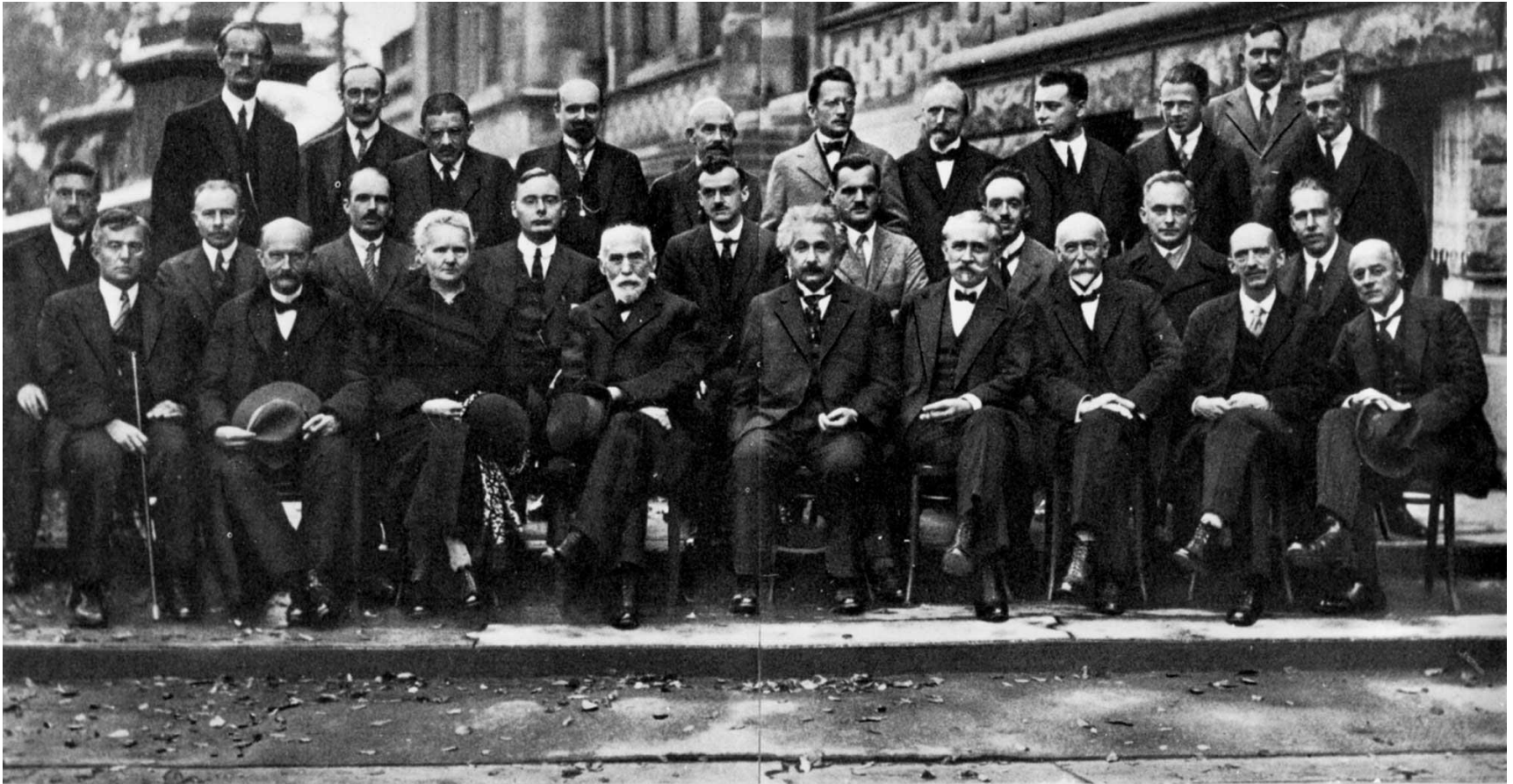


Peter Higgs
1929-

A small selection of the

Pioneers of modern Quantum Physics

The development of Quantum Mechanics was a truly collaborative effort, and unprecedented in terms of the speed at which the theory was assembled. The 1927 Solvay Conference in Brussels was devoted to Quantum Theory. Many of the pioneers of the subject attended. Nine were eventually Nobel laureates.



Photographie Benjamin Couprie

28, Avenue Louise, Bruxelles

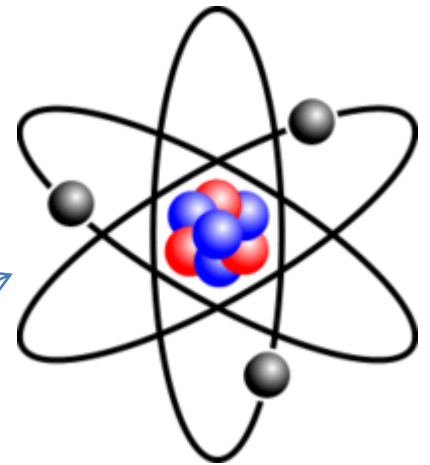
A. PICCARD	E. HENRIOT	ED. HERZEN	TH. DE DONDER	E. SCHROEDINGER	W. PAULI	W. HEISENBERG	R. H. FOWLER	L. BRILLOUIN
	P. EHRENFEST			E. VERSCHAFFELT				
P. DEBYE	M. KNUDSEN	W. L. BRAGG	H. A. KRAMERS	P. A. M. DIRAC	A. H. COMPTON	L. V. DE BROGLIE	M. BORN	N. BOHR
I. LANGMEIR	M. PLANCK	MADAME CURIE	H. A. LORENTZ	A. EINSTEIN	P. LANGEVIN	CH. E. GUYE	C. T. R. WILSON	O. W. RICHARDSON

But first we must start with

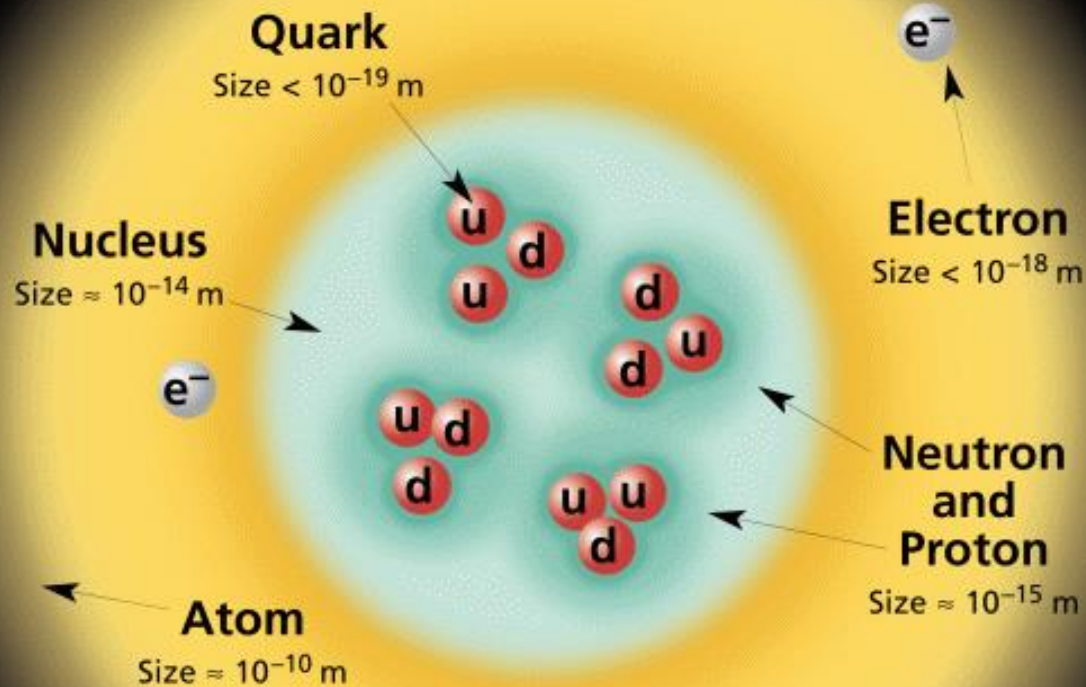
ATOMS

and why they exist at all

This model has
a serious flaw!



Structure within the Atom



If the protons and neutrons in this picture were 10 cm across, then the quarks and electrons would be less than 0.1 mm in size and the entire atom would be about 10 km across.

The size of an atom



Earth diameter
= 12,756km

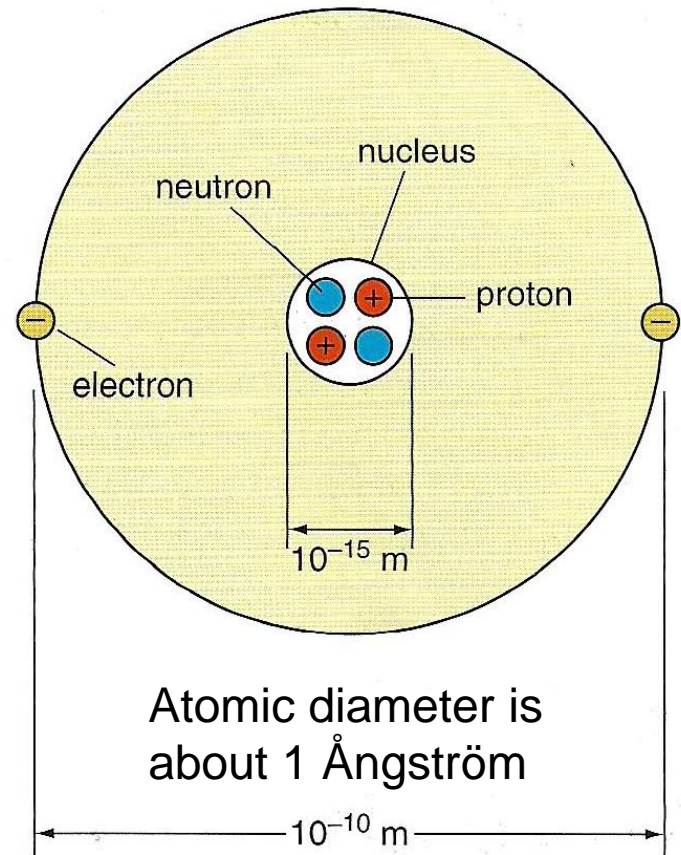


Marble diameter =
3.6cm

$$\left(\frac{1.2756 \times 10^7}{3.6 \times 10^{-2}} \right)^3 \approx 4.4 \times 10^{25}$$

Volume of Earth in marbles

**There are as many
atoms in a marble as an
Earth made of marbles!**

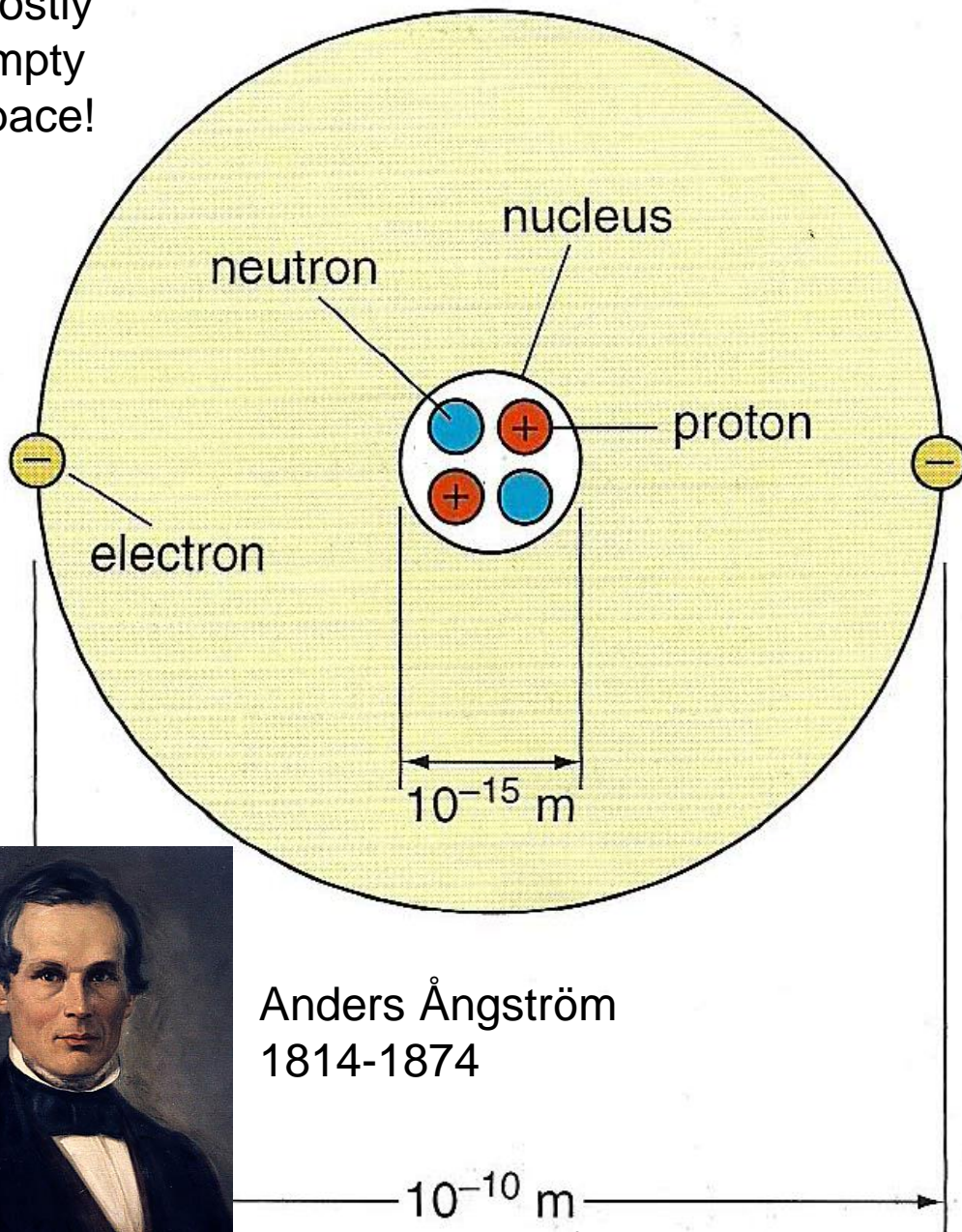


$$\left(\frac{3.6 \times 10^{-2}}{1 \times 10^{-10}} \right)^3 \approx 4.7 \times 10^{25}$$

Number of atoms in a marble

Atomic mass and density

Mostly
empty
space!



Anders Ångström
1814-1874

10^{-10} m
This is one Ångström

$$m_e = 9.109 \times 10^{-31} \text{ kg}$$

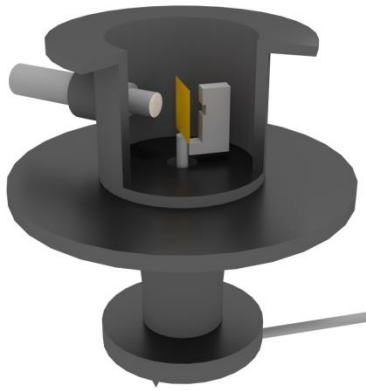
$$m_p = 1.673 \times 10^{-27} \text{ kg}$$

$$m_n = 1.675 \times 10^{-27} \text{ kg}$$

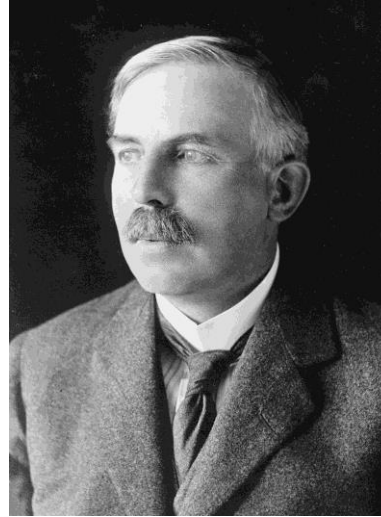
$$\rho \approx \frac{1.673 \times 10^{-27} \text{ kg}}{\frac{4}{3} \pi \times \left(\frac{1}{2} \times 10^{-10} \right)^3}$$

$$\rho \approx 3,200 \text{ kgm}^{-3}$$

$$\rho_{\text{water}} \approx 1,000 \text{ kgm}^{-3}$$



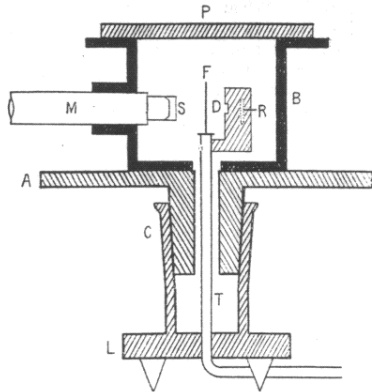
Ernest
Rutherford
1871-1937



Hans
Geiger

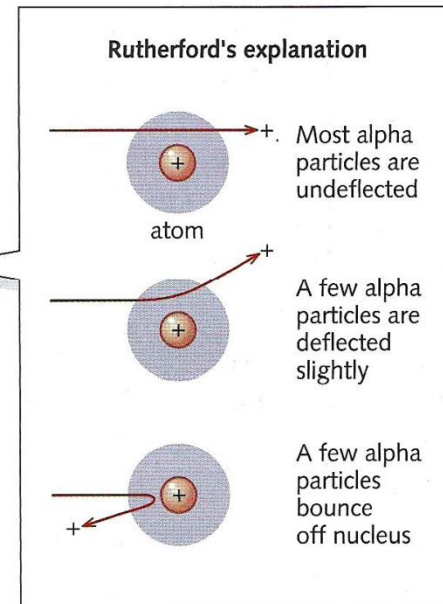
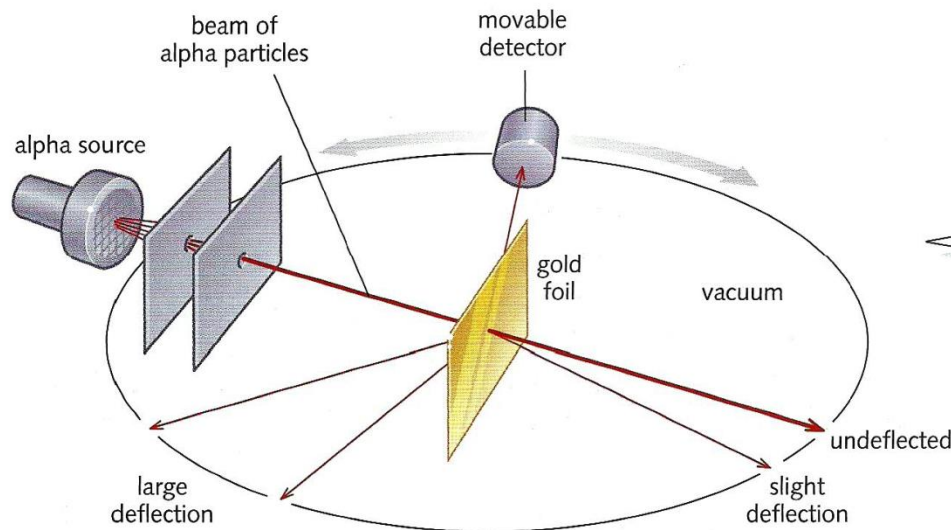


Ernest
Marsden



The **Rutherford scattering experiment** , performed 1908-1913 at the University of Manchester, provided convincing evidence for the modern nuclear model of **atoms**

alpha particle
is a helium nucleus



$$B = a_v A - a_s A^{2/3} - a_c \frac{Z^2}{A^{1/3}} - a_a \frac{(A - 2Z)^2}{A} + \delta(A, Z)$$

$$\delta(A, Z) = v \begin{cases} a_p A^{-3/4} & Z, A - Z \text{ even} \\ -a_p A^{-3/4} & Z, A - Z \text{ odd} \\ 0 & \text{otherwise} \end{cases}$$

$$a_v = 15.76 \text{ MeV}$$

$$a_s = 17.81 \text{ MeV}$$

$$a_c = 0.711 \text{ MeV}$$

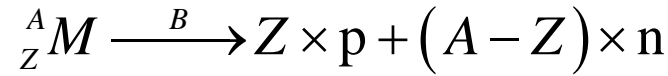
$$a_a = 23.702 \text{ MeV}$$

$$a_p = 34.0 \text{ MeV}$$

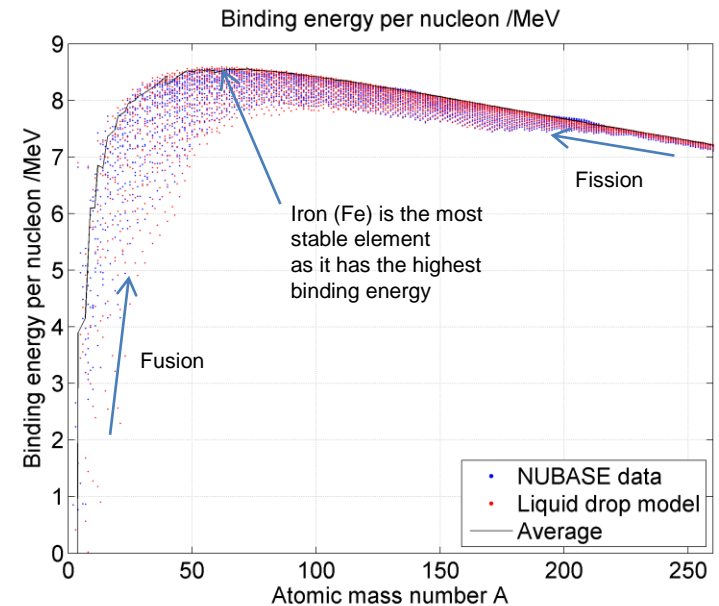
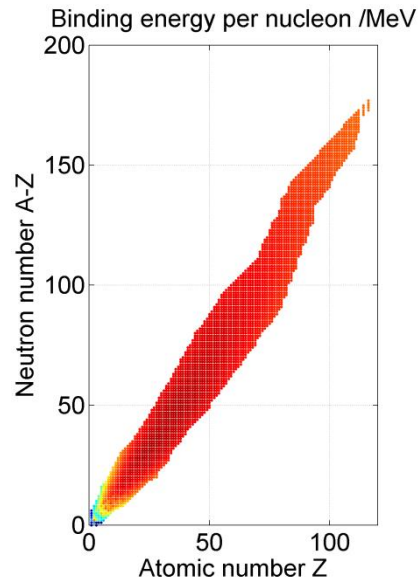
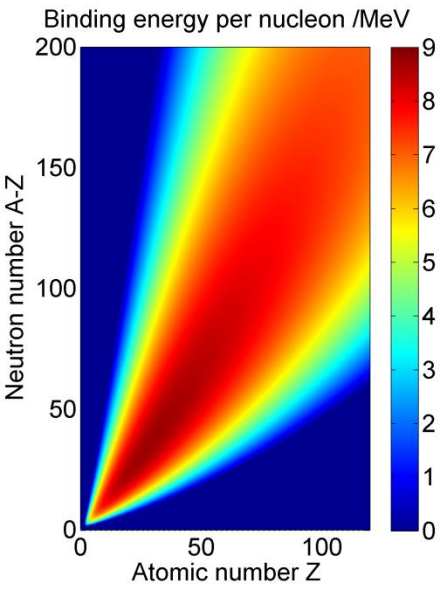
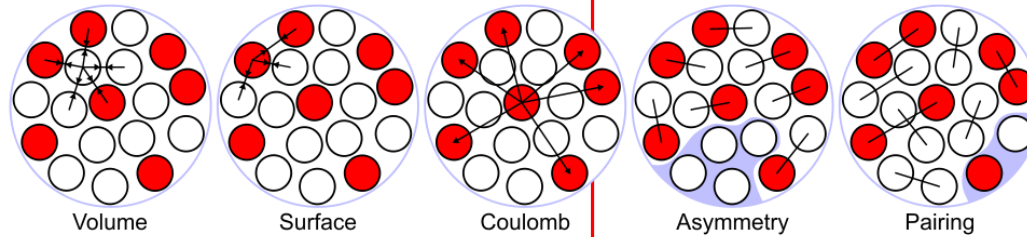
NUCLEAR BINDING ENERGY



Carl Friedrich von Weizsäcker
1912-2007
Liquid Drop Model
of Binding Energy

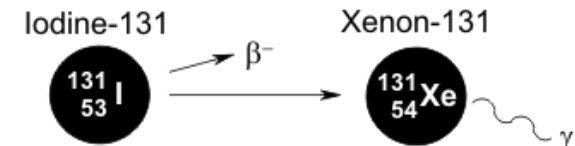
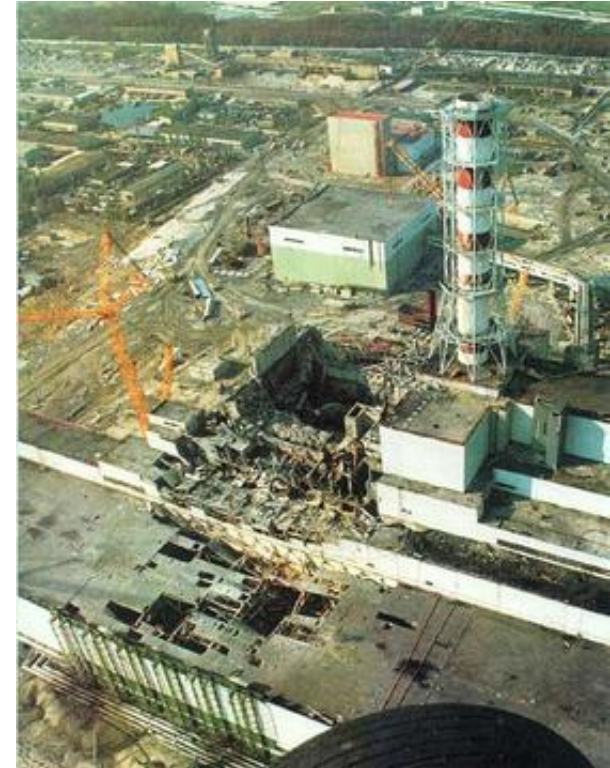
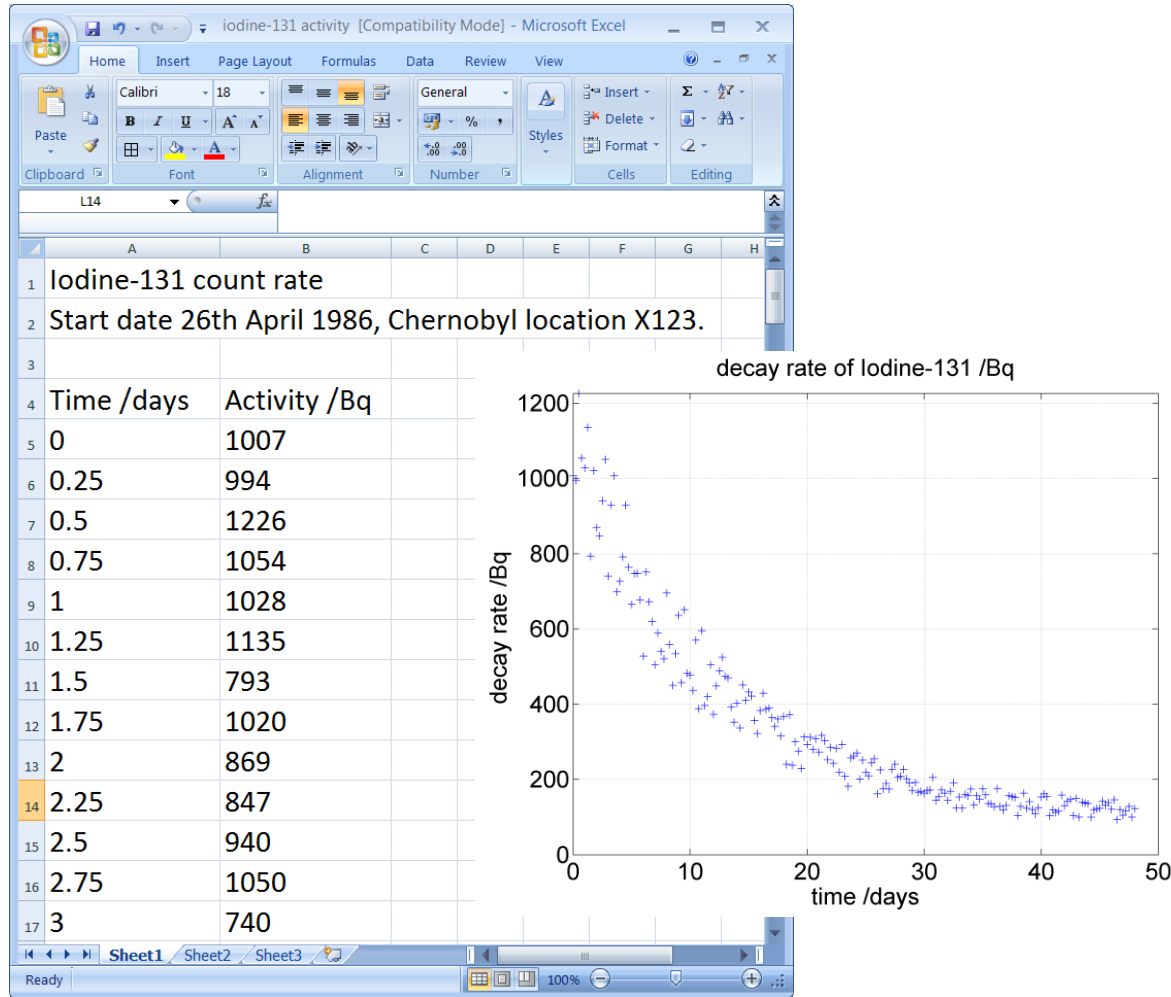


$$Mc^2 + B = Zm_p c^2 + (A - Z)m_n c^2$$



RADIOACTIVITY

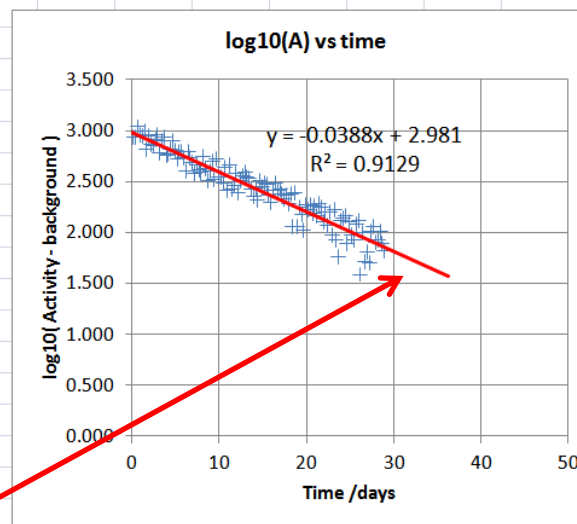
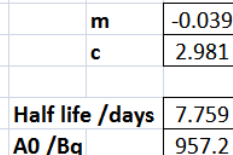
You are a soviet nuclear physicist sent to help with the Chernobyl disaster in 1986. You need to determine the presence of an isotope from its half life, but background levels are huge.... All you have is a text file of count rates. Your military commander demands results as soon as possible.



A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---

Start date 26th April 1986, Chernobyl location X123.

7.75	521	398	NOTE IGNORE DATA AFTER 28.75 DAYS FOR BEST FIT
8	695	572	
8.25	558	435	
8.5	450	327	
8.75	534	411	



Time /days	Activity /Bq
0	123
50	123

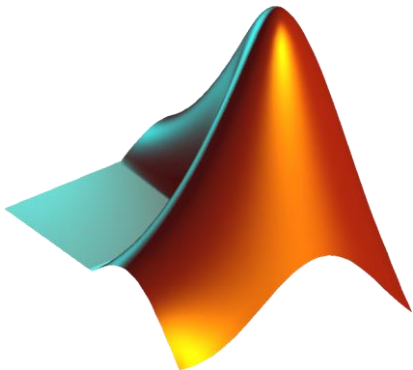
$$t_{1/2} = -\frac{\log_{10} 2}{m} \quad A_0 = 10^c$$

**NOTE IGNORE
DATA AFTER 28.75
DAYS FOR BEST
FIT**

Data flow Data processing and Information Presentation

is often best achieved
by *writing code*.

In other words
a **text file** which
is interpreted
by a *programming
language* like
MATLAB or Python

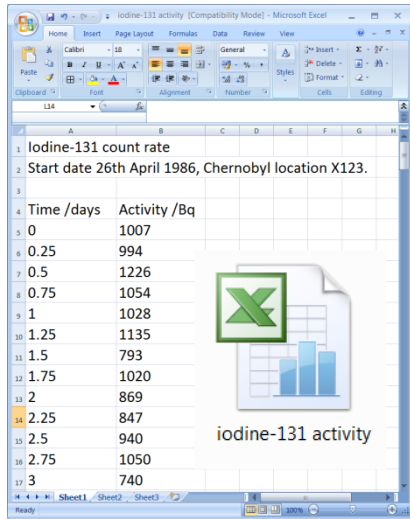


```
E:\Programming\A Course in Coding\2. MATLAB\Short Scientific Computing Course\1. The Signal and the Noise\radiactive_decay_analysis.m
File Edit Text Go Cell Tools Debug Desktop Window Help
[Icons] Stack: Base fx

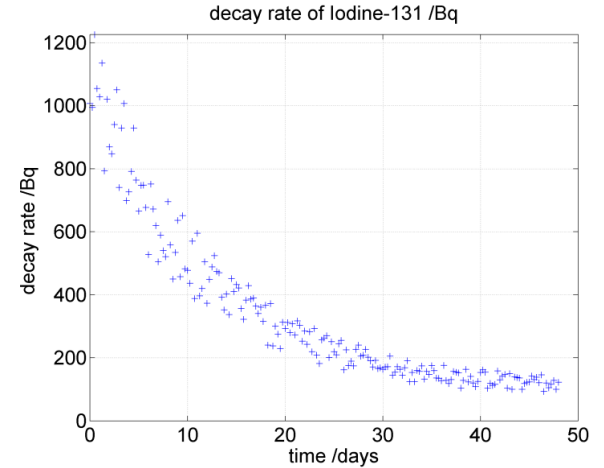
1      %radioactive_decay_analysis
2      % Analysis of Iodine-131 decay rate vs time data.
3      %
4      % LAST UPDATED by Andy French June 2019
5
6      function radioactive_decay_analysis
7
8      %Estimated background rate /Bq
9      B = 100;
10
11     %Fontsize for graphs
12     fsize = 18;
13
14     %
15
16     %Ingest Excel file of activity vs time
17     [num,txt,row] = xlsread( 'iodine-131 activity.xls' );
18
19     %Extract vectors for time /days and activity /Bq
20     t = num(:,1); A = num(:,2);
21
22     %Plot activity vs time
23     fig1 = figure('color',[1 1 1],'name','radioactive decay curve');
24     plot(t,A,'+');
25     xlabel('time /days','fontsize',fsize);
26     ylabel('decay rate /Bq ','fontsize',fsize);
27     set(gca,'fontsize',fsize);
28     grid on; ylim([0,max(A)]);
29
30     %Overlay background level
31     xlims = get( gca, 'xlim' ); hold on; plot( xlims,[B,B],'r-' );
32
```

radioactive_decay_analysis.m

make_decay_rate_data.m



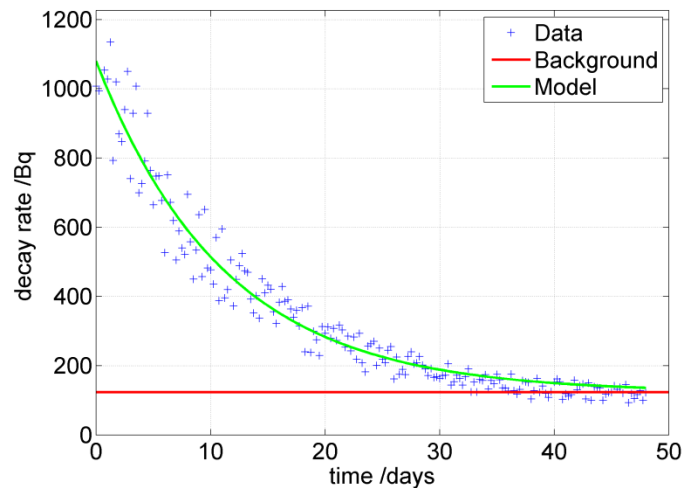
iodine-131 activity .xls



radioactive decay curve.png

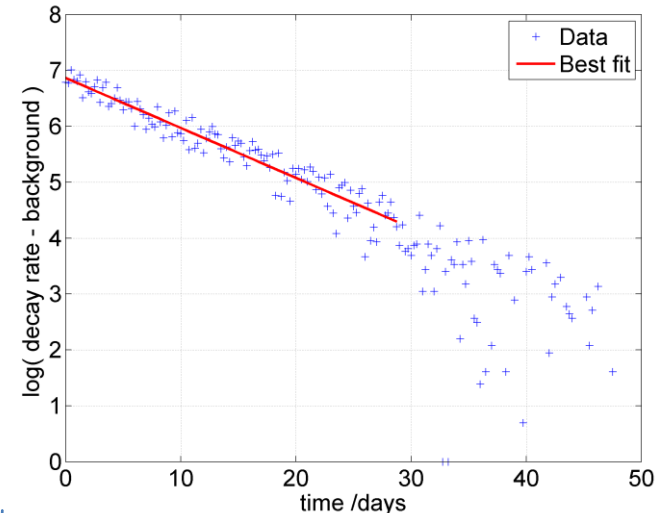
radioactive_decay_analysis.m

Activity of Iodine-131. Background = 123Bq
 $A_0 = 957\text{Bq}$, half life = 7.753 ± 0.225 days



radioactivity analysis graph.png

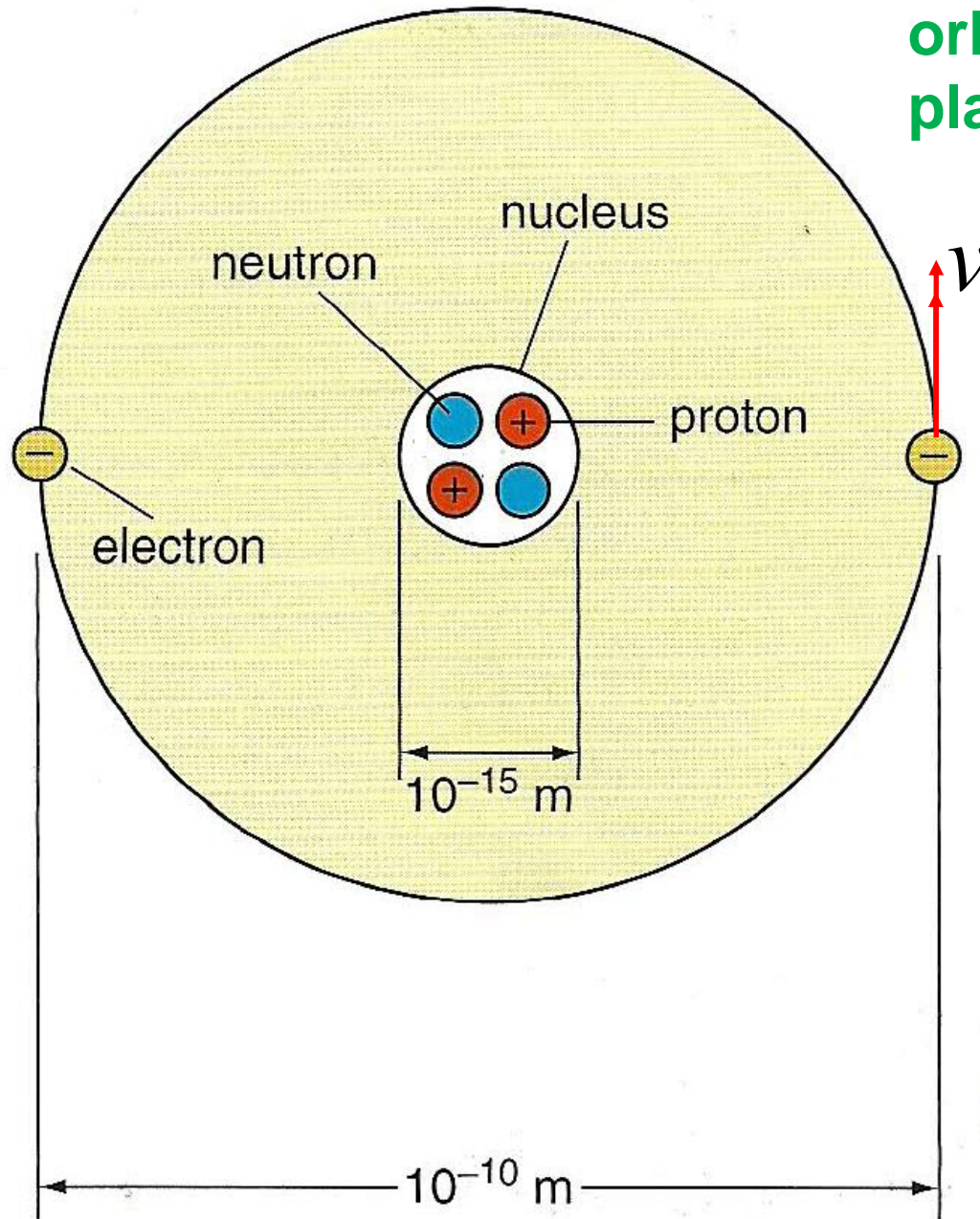
$A_0 = 957\text{Bq}$, half life = 7.753 ± 0.225 days



radioactivity analysis log graph.png

... Back to the atom!

So the electrons orbit the nucleus, just like planets orbit a star?

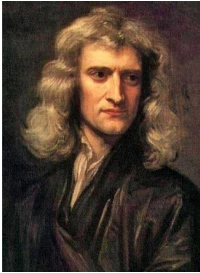


Gravity fields

$$F_G = \frac{GMm}{r^2}$$

$$F_E = \frac{Qq}{4\pi\epsilon_0 r^2}$$

Electric fields



But there is a **major problem here**. For electrons to 'orbit' a nucleus, they must be **accelerating**. Electromagnetism tells us that accelerating charges **radiate**.

A Classical calculation tells us that electrons should only exist for about 10^{-10} s!

$$\dot{E} = \frac{dE}{dt} = -\frac{e^2}{6\pi\epsilon_0 c^3} a^2 \quad \text{Radiated power}$$

$$\dot{E} = -\frac{e^2}{6\pi\epsilon_0 c^3} \times \left(\frac{Ze^2}{4\pi\epsilon_0 m_e r^2} \right)^2$$

$$\therefore \dot{E} = -\frac{Z^2 e^6}{96\pi^3 \epsilon_0^3 c^3 m_e^2 r^4}$$

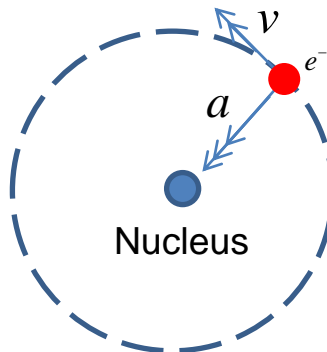
$$\tau = \frac{\frac{1}{2} m_e v^2}{|\dot{E}|} \quad \text{'electron lifetime'}$$

$$\tau = \frac{Ze^2}{8\pi\epsilon_0 r} \times \frac{96\pi^3 \epsilon_0^3 c^3 m_e^2 r^4}{Z^2 e^6}$$

$$\tau = \frac{12\pi^2 \epsilon_0^2 c^3 m_e^2 r^3}{Ze^4}$$

$$\tau \approx 4.7 \times 10^{-11} \text{ s}$$

$$\begin{aligned} \epsilon_0 &= 8.854187817 \times 10^{-12} \text{ Fm}^{-1} \\ e &= 1.6021766208(98) \times 10^{-19} \text{ C} \\ c &= 2.99792458 \times 10^8 \text{ ms}^{-1} \\ m_e &= 9.10938356(11) \times 10^{-31} \text{ kg} \end{aligned}$$



So how do atoms exist?

To answer the question “why do atoms exist?” we will need models which were developed to explain three perplexing problems of Classical Physics

1. The spectrum of radiation from a hot body
2. The photoelectric effect
3. The spectral lines of Hydrogen

The implications of these models are *profound*:

- All **particles** have an associated **wave-like character**
- These waves can interfere, diffract, tunnel through barriers
- The wave-pattern is related to the **probability** of finding a particle
- ***Uncertainty*** appears to be built into Physics

BLACK BODY RADIATION

Radiation power
per square metre

$$I = \epsilon \sigma T^4$$

Absolute
temperature /K

Emmissivity

Stefan-Boltzmann
constant

$$\sigma = 5.67 \times 10^{-8} \text{ Wm}^{-2} \text{ K}^{-1}$$

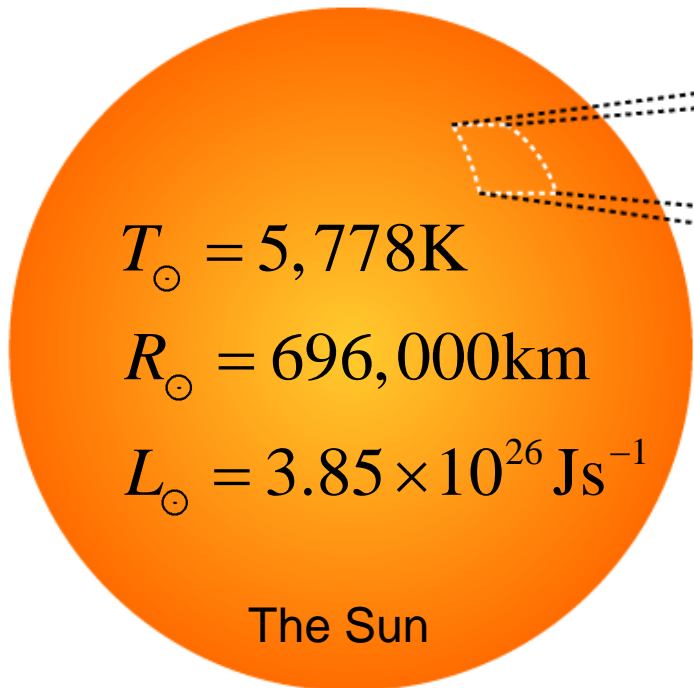
$$\epsilon = 1$$

A '**Black Body**'. i.e. all incident
radiation is absorbed and then
re-radiated

For a 'Black Body' at
 $20^\circ\text{C} = 293\text{K}$

$$I = 418 \text{ Wm}^{-2}$$

It is interesting to compare
this to the maximum solar
energy incident upon the
Earth, which is on average
about $1,361 \text{ Wm}^{-2}$



Energy Produced by
1 square meter $= \sigma T^4$

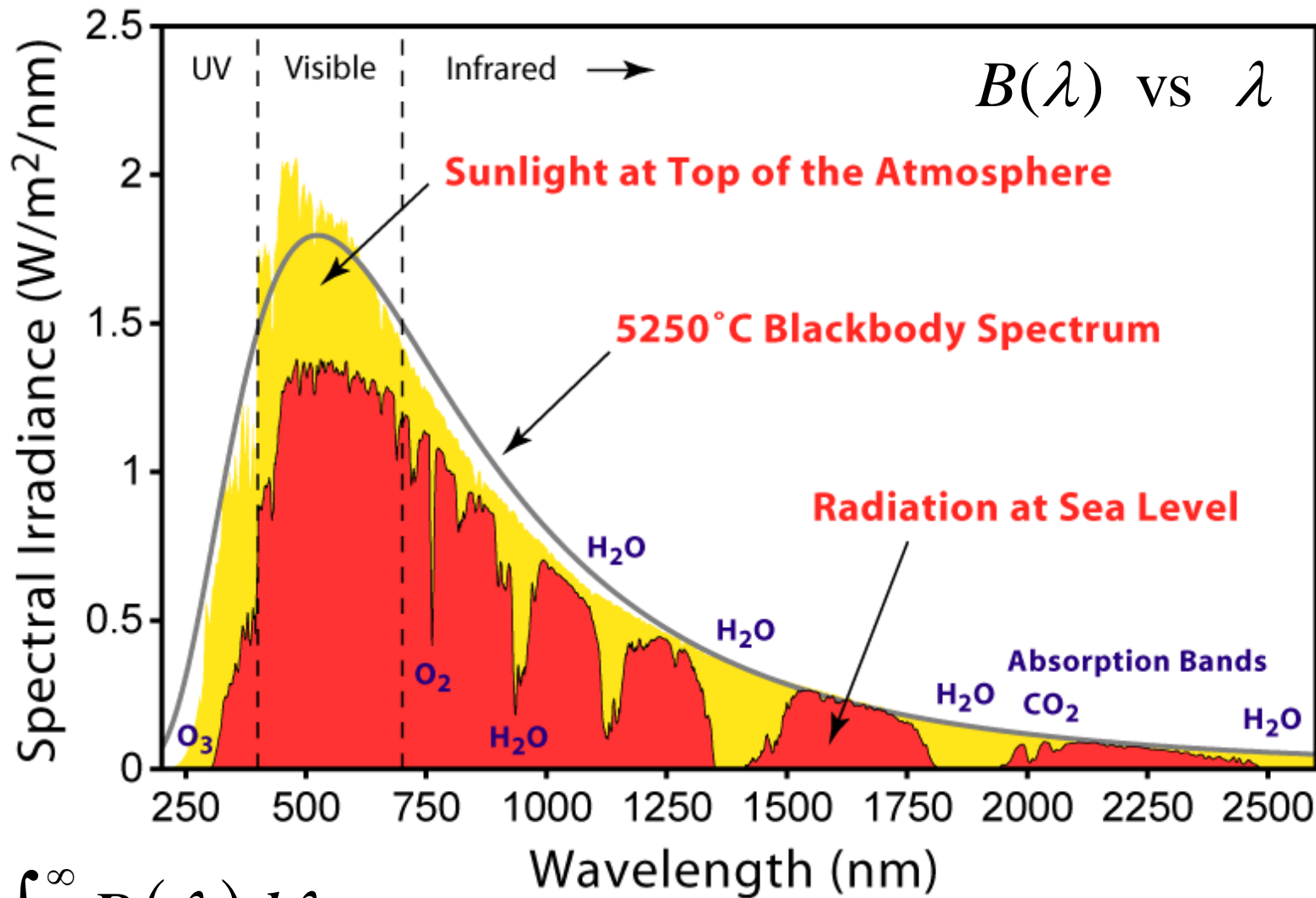
Total Square Meters
 $A = 4\pi R^2$

Total Energy Produced
 $L = (4\pi R^2)(\sigma T^4)$

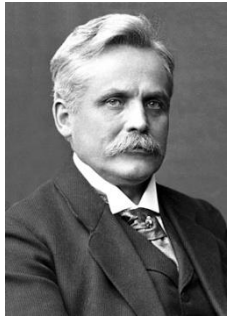
The measured solar irradiance (i.e. power received on Earth per square metre within a wavelength interval

i.e. $\lambda \rightarrow \lambda + d\lambda$

What is the model for $B(\lambda)$?



$$I = \int_0^{\infty} B(\lambda) d\lambda$$



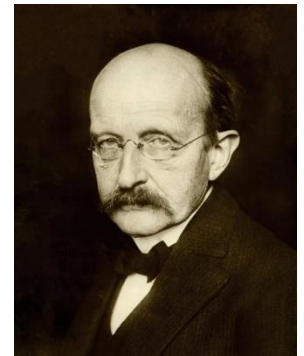
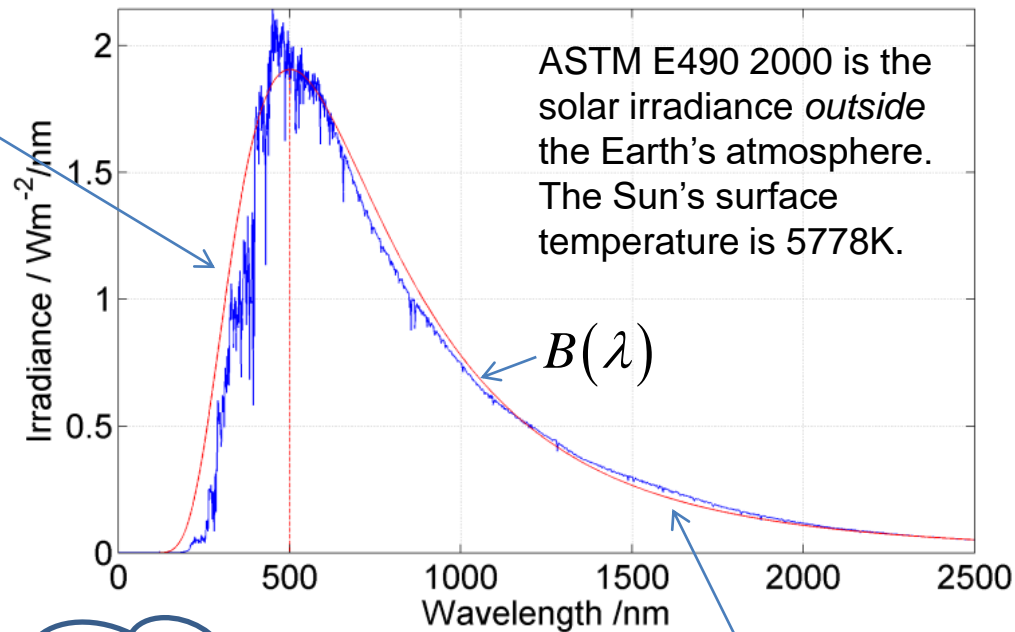
Wilhelm Wien
1864-1928

Predicted
the short wavelength
part well.....

But not the
spectrum at long
wavelengths

$$I = \int_0^{\infty} B(\lambda) d\lambda$$

— ASTM E490 2000 (1361.6441 Wm⁻²)
— Planck law (1453.6234 Wm⁻²)
Solar Irradiance vs Wavelength



Max Planck
'guessed'
what the law
should be. But this
led to a strange
conclusion

$$\bar{E} = \frac{3}{2} k_B T$$



**John Strutt
(Lord Rayleigh)**
1842-1919



James Jeans
1877-1946

Considered
waves in a 3D box
and predicted the long
wavelength spectrum.
But an 'ultraviolet
catastrophe' at short
wavelengths!

Max Planck
1858 – 1947





Max Planck
1858 – 1947

Let's start from the Rayleigh-Jeans analysis

$$I = \sigma T^4 = \frac{1}{4} u c$$

Radiant energy flux upon the walls of a black cavity containing energy per unit volume u (from Kinetic theory).

$$u = \int_0^\infty \phi(f) df$$

Energy density (energy per unit volume)

$$\phi(f) = \eta \times \bar{E}$$

Energy density within frequency range

Rayleigh
Jeans

$$\eta = \frac{8\pi f^2}{c^3}$$

This is the clever bit. Planck had to **quantize** radiation energy. h turned out to be very small, but *not* zero

is the 'density of states' i.e. number of photons per unit volume that can be activated within frequency range

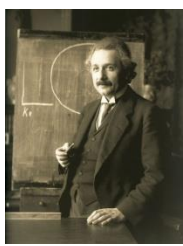
$$f \rightarrow f + df$$

But $\bar{E} = \frac{3}{2} k_B T$ means

$$I = \infty$$

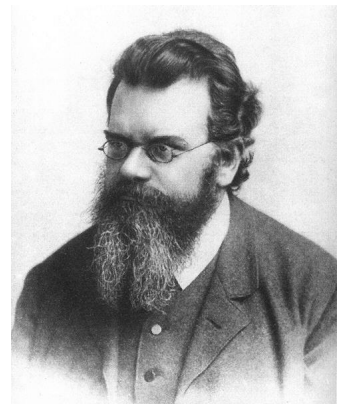
$$\bar{E} = \frac{hf}{e^{\frac{hf}{k_B T}} - 1}$$

Ludwig
Boltzmann
1844-1906



I worked this out!

is the average energy of a *photon* of frequency f

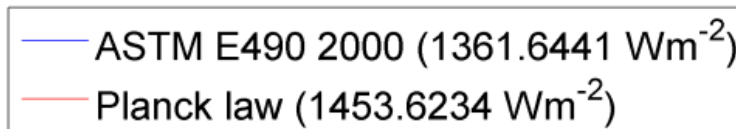


Red	620-750nm
Yellow	570-590nm
Green	495-570nm
Blue	450-495nm

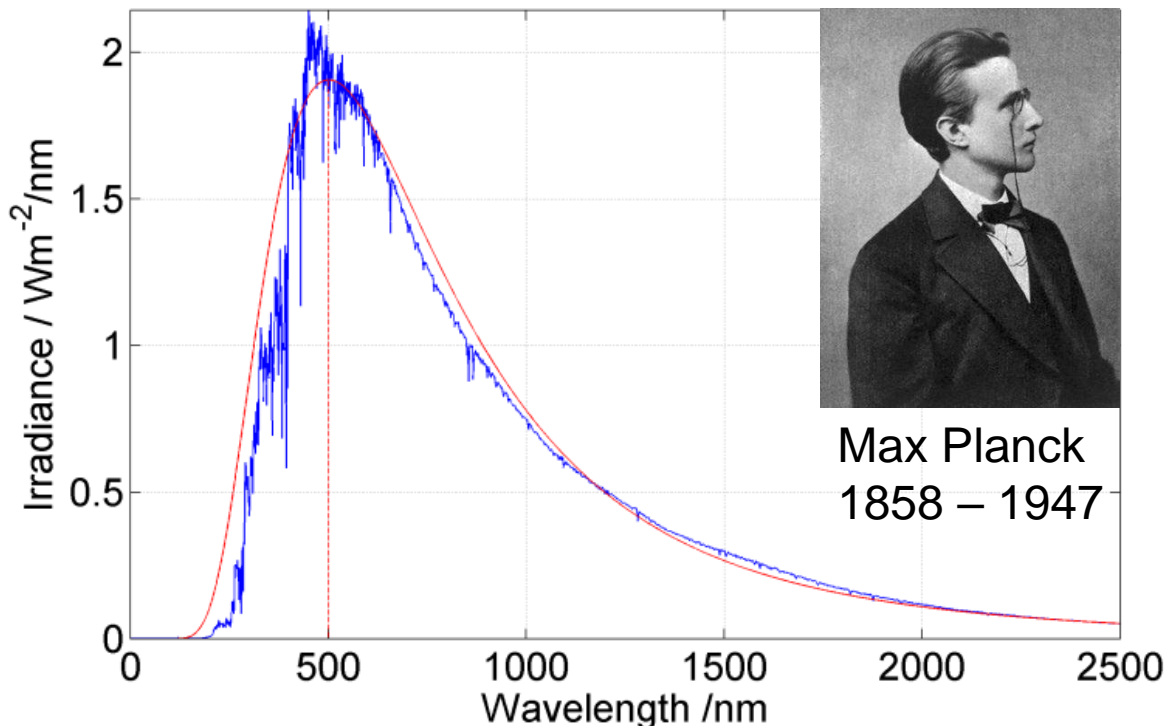
Boltzmann's constant $k_B = 1.381 \times 10^{-23} \text{ m}^2 \text{ kgs}^{-2} \text{ K}^{-1}$

Planck's constant $h = 6.626 \times 10^{-34} \text{ m}^2 \text{ kgs}^{-1}$

Speed of light $c = 2.998 \times 10^8 \text{ ms}^{-1}$



Solar Irradiance vs Wavelength



$$I = \int_0^{\infty} B(\lambda, T) d\lambda = \sigma T^4$$

$$\sigma = \frac{2\pi^5 k_B^4}{15c^2 h^3}$$

$$B(\lambda, T) = \frac{2hc^2}{\lambda^5} \frac{1}{e^{\frac{hc}{\lambda k_B T}} - 1}$$

So radiation is **quantized**
into **photons** of energy

$$E = hf$$

PHOTO ELECTRIC EFFECT

Maximum
Kinetic energy of
emitted electrons

$$E = hf - W$$

Photon
energy

'Work function' or
'binding energy' of
electron in the surface



Robert Millikan
1868-1953

To **stop** the electrons
reaching the cathode

$$eV = E = hf - W$$

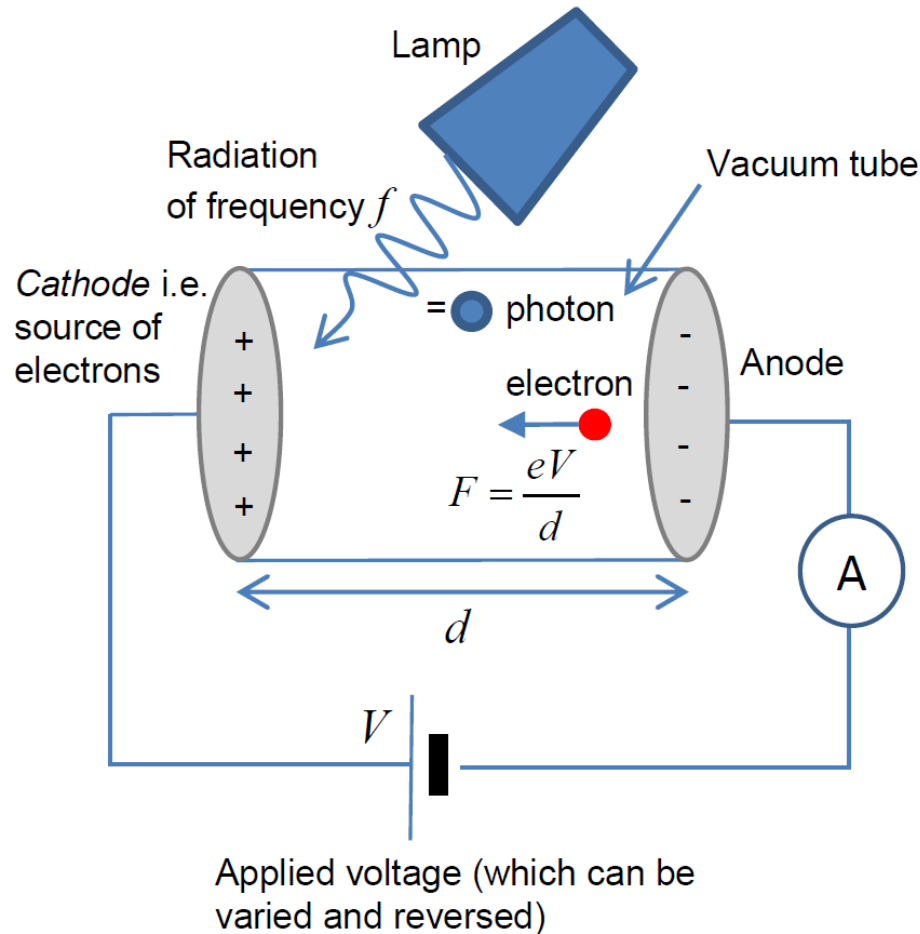
$$\therefore V = \frac{h}{e} f - \frac{W}{e}$$

$$f_{cutoff} = \frac{W}{h}$$

Light above a certain 'cutoff' frequency
causes surfaces to emit electrons.

More photons mean more electrons
but the electron energy only depends
of frequency

**This is *not* a classical
prediction!**



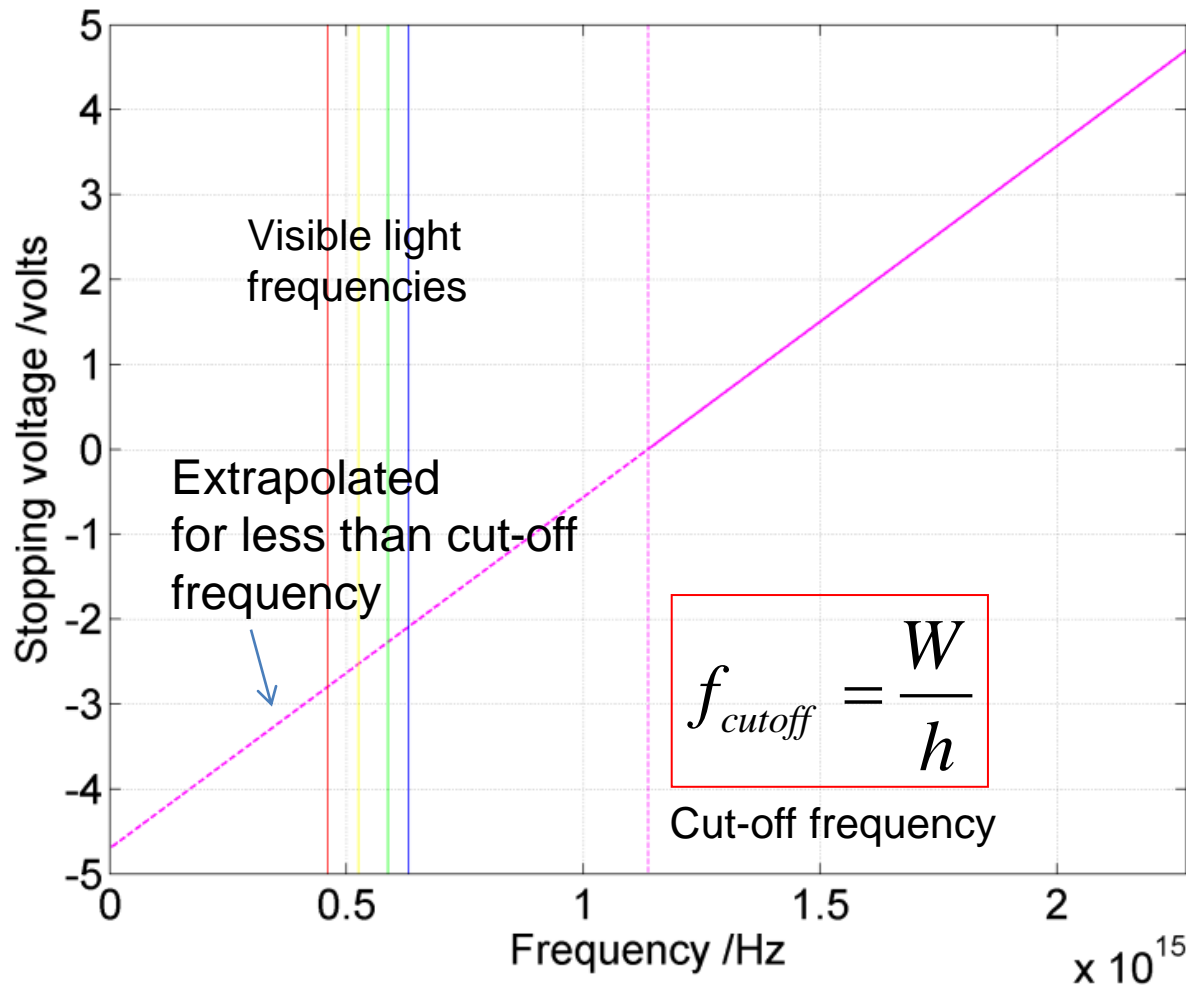
$$e = 1.6021766208(98) \times 10^{-19} \text{ C} \quad \text{electron charge}$$

$$eV = E = hf - W$$

$$\therefore V = \frac{h}{e} f - \frac{W}{e}$$

Therefore **UV light**
is needed to stimulate
the photoelectric effect
in most metals

Photoelectric effect: $W = 4.7\text{eV}$

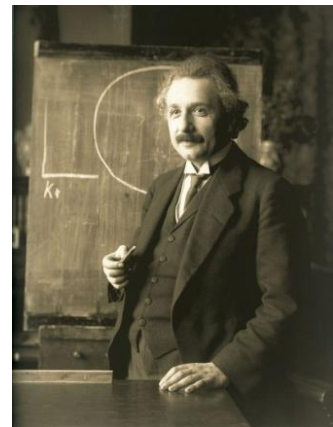


$$f_{cutoff} = \frac{W}{h}$$

Cut-off frequency

Material	Work function /eV
Silver (Ag)	4.3
Aluminium (Al)	4.3
Gold (Au)	5.1
Copper (Cu)	4.7
Tin (Sn)	4.4
Lead (Pb)	4.3
Tungsten (W)	4.5
Nickel (Ni)	4.6
Sodium (Na)	2.4

Albert Einstein
1879-1955



Yes, me
again!

HYDROGEN SPECTRA

Hydrogen Absorption Spectrum



Hydrogen Emission Spectrum

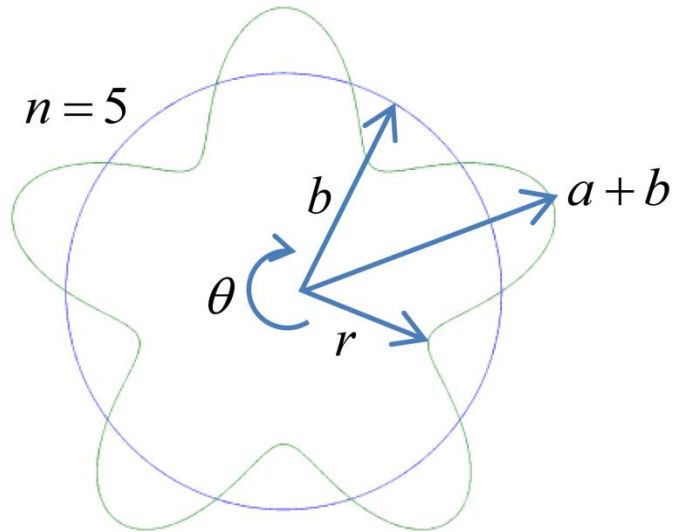


Johann Balmer
1825-1898

Hydrogen only re-radiates absorbed electromagnetic waves at particular frequencies. Classical Physics had no sensible explanation for this phenomenon. The Swiss Maths teacher J. Balmer proposed an empirical formula to predict the lines in the visible part of the electromagnetic spectrum

$$\lambda_n = 91.13\text{nm} \left(\frac{1}{m^2} - \frac{1}{n^2} \right)^{-1} \quad n \geq 3, m = 2$$

The strange formula can be explained by combining quantum ideas from de Broglie and Bohr, and a bit of classical physics



'Circular sine waves' of the form

$$r = a \sin n\theta + b$$

$$n\lambda = 2\pi b \quad \text{for waves to 'fit'}$$

$$\therefore r = a \sin \left(2\pi \times \frac{b\theta}{\lambda} \right) + b$$

Electrons are 'standing waves' around the nucleus

$$2\pi r = n\lambda$$

n is an **integer**



Louis de Broglie
1892 –1987



Niels Bohr
1885-1962

de Broglie relationship

$$m_e v = \frac{h}{\lambda}$$

momentum

$$\therefore m_e v = \frac{nh}{2\pi r}$$

Angular momentum is quantized!

$$\therefore m_e r v = n\hbar$$

$$m_e r_n v_n = n\hbar$$

From
Classical
Physics

Total energy of electron in orbit
about a nucleus of charge Ze

$$E_n = -\frac{Ze^2}{8\pi\epsilon_0 r_n}$$

Circular orbits, Coulomb force ...

$$\therefore E_n = -\frac{Ze^2}{8\pi\epsilon_0} \times \frac{m_e Ze^2}{4\pi\epsilon_0 n^2 \hbar^2}$$

for Hydrogen
 $Z = 1$

$$E_n = -\frac{m_e Z^2 e^4}{8\epsilon_0^2 h^2} \frac{1}{n^2} \approx \boxed{\frac{-13.6\text{eV}}{n^2}}$$

$$\therefore hf_{nm} = E_n - E_m \quad \text{Photon energy}$$

$$hf_{nm} = \frac{m_e Z^2 e^4}{8\epsilon_0^2 h^2} \left(\frac{1}{m^2} - \frac{1}{n^2} \right)$$

$$f_{nm} = \frac{m_e Z^2 e^4}{8\epsilon_0^2 h^3} \left(\frac{1}{m^2} - \frac{1}{n^2} \right)$$

$$c = f_{nm} \lambda_{nm}$$

$$\lambda_{nm} = \frac{c}{f_{nm}}$$

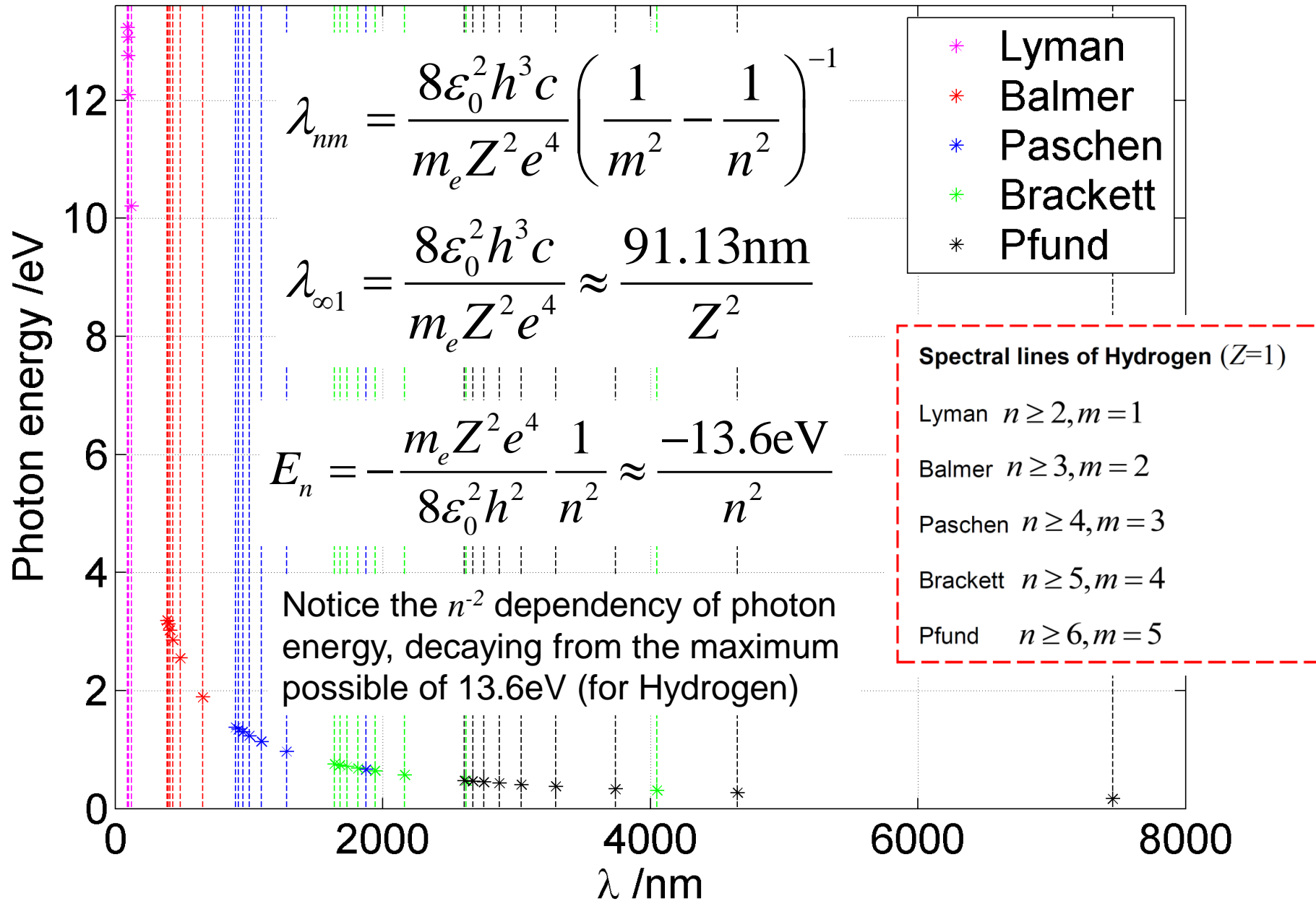
i.e. photons are
emitted when
electron energies
change from one
quantum state to
another

$$\lambda_{nm} = \frac{8\epsilon_0^2 h^3 c}{m_e Z^2 e^4} \left(\frac{1}{m^2} - \frac{1}{n^2} \right)^{-1}$$

$$\lambda_{\infty 1} = \frac{8\epsilon_0^2 h^3 c}{m_e Z^2 e^4} \approx \frac{91.13\text{nm}}{Z^2}$$

Bohr model of Hydrogenic atom

photon emissions: $Z = 1$



Orbital velocity

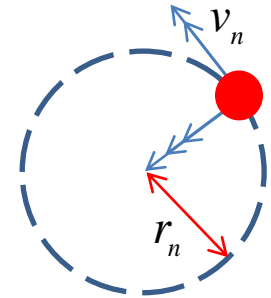
$$v_n = \frac{n\hbar}{m_e r_n}$$

$$v_n = \frac{1}{n} \frac{\hbar m_e Z e^2}{4\pi\epsilon_0 \hbar^2} = \frac{Z e^2}{4\pi\epsilon_0 \hbar} \frac{1}{n}$$

$$v_n = \frac{\alpha Z}{n} c$$

This is called the **Fine Structure Constant**
Note it is dimensionless!

$$\alpha = \frac{e^2}{4\pi\epsilon_0 \hbar c} \approx \frac{1}{137}$$



So electrons can 'orbit' about 1% of the speed of light. This is large enough for **relativistic effects** to be apparent.

Careful inspection of the Hydrogen emission spectrum shows indeed a small deviation from the Balmer formula

ELECTRON DIFFRACTION

$$eV = \frac{1}{2} m_e v^2$$

$$p = m_e v$$

$$\therefore eV = \frac{1}{2} m_e \left(\frac{p}{m_e} \right)^2 = \frac{p^2}{2m_e}$$

$$p = \sqrt{2m_e eV}$$

$$\lambda = \frac{h}{\sqrt{2m_e eV}}$$

Apply **relativity**
and you get a
small correction
to this formula

Louis de Broglie
1892 –1987



**All particles
have an
associated
wave**



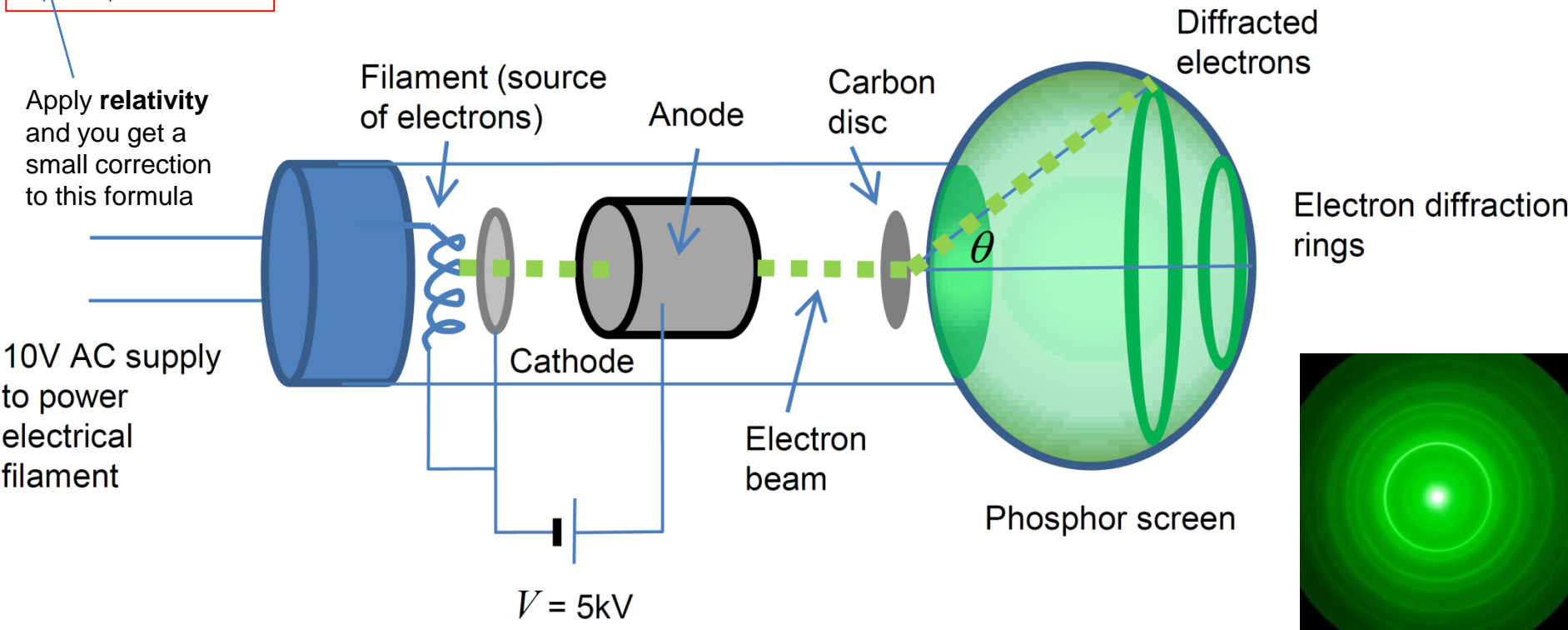
Lester Germer
(right) with Clinton
Davisson in 1927

wavelength

$$\lambda = \frac{h}{p}$$

Planck's
constant

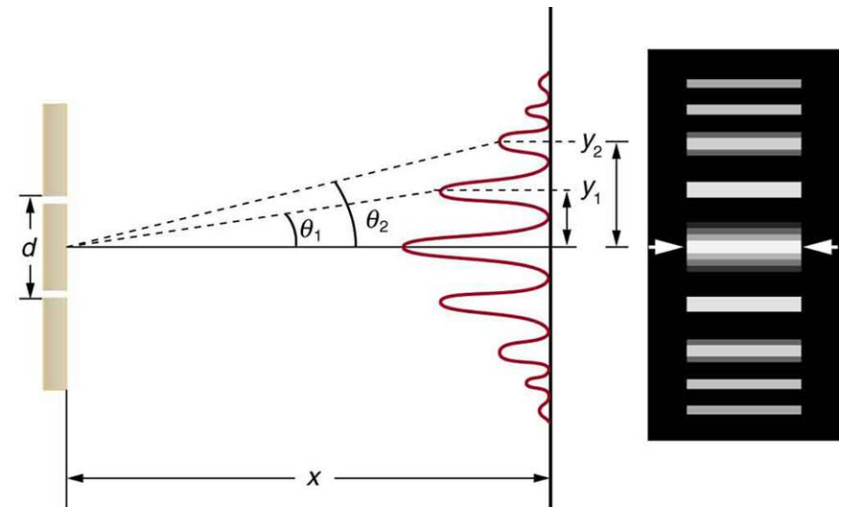
momentum





Young's slits and photons

Young's double slits cause incident waves to diffract, resulting in an **interference pattern**



Thomas Young
1773-1829

$$\psi(r,t) \approx \frac{Ae^{i(kr-\omega t)}}{r} \left(e^{-i\frac{1}{2}kd \sin \theta} + e^{i\frac{1}{2}kd \sin \theta} \right)$$

$$\psi(r,t) \approx \frac{2Ae^{i(kr-\omega t)}}{r} \cos\left(\frac{1}{2}kd \sin \theta\right)$$

$$|\psi|^2 \approx \frac{A^2}{r^2} \cos^2\left(\frac{1}{2}kd \sin \theta\right)$$

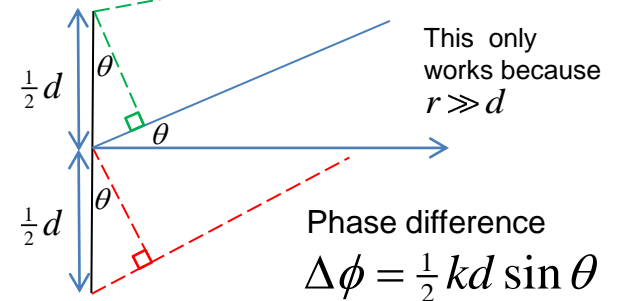
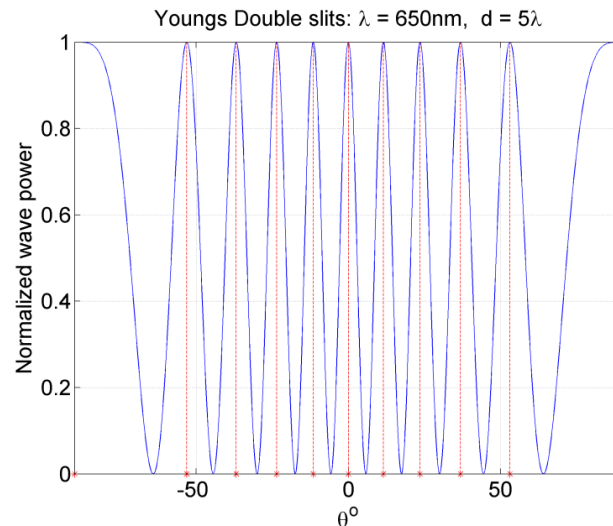
Hence *maxima* when

$$\frac{1}{2}kd \sin \theta = n\pi$$

$$\theta = \sin^{-1}\left(\frac{2n\pi}{kd}\right) = \sin^{-1}\left(\frac{n\lambda}{d}\right)$$

Equivalent geometry is wavelet sources are at the same angle (i.e. *plane waves*) but separated by $d \sin \theta$

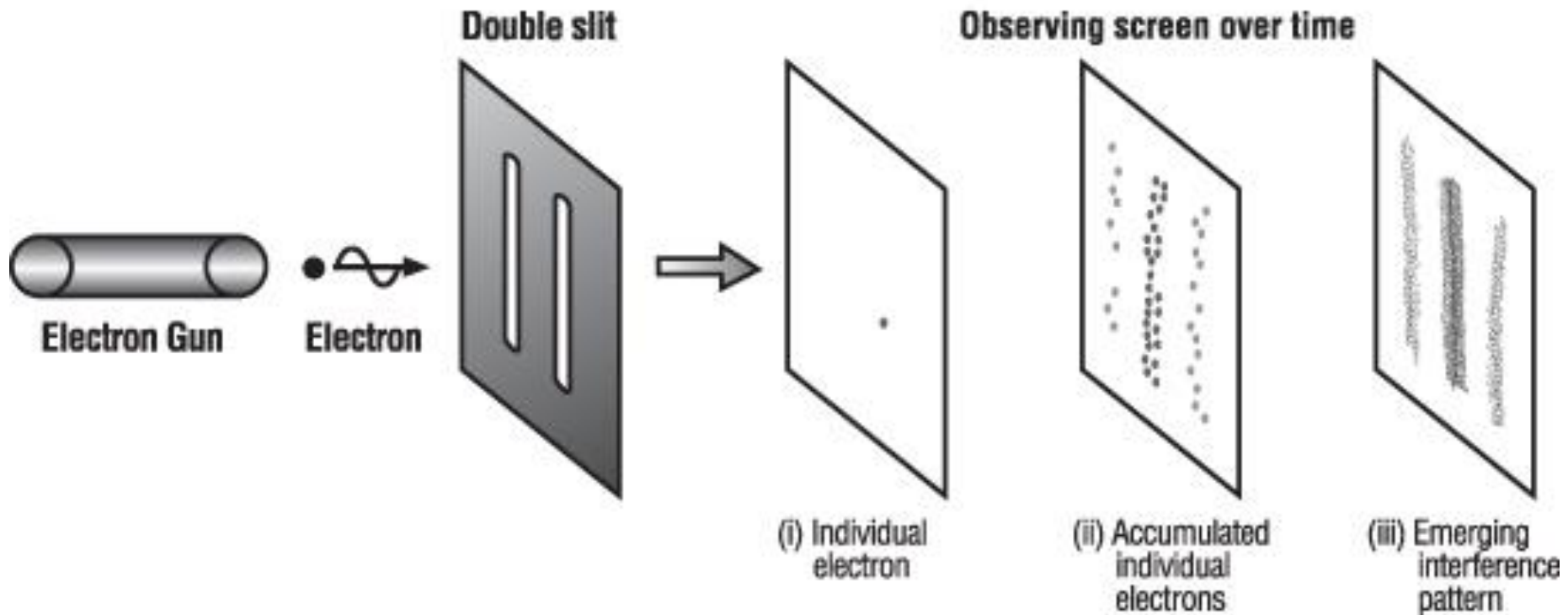
Phase difference
 $\Delta\phi = -\frac{1}{2}kd \sin \theta$



Amazingly, the same interference pattern is seen if single electrons are fired through a double slit arrangement. The wavefunction appears to interfere in exactly the same way as if the electron were an electromagnetic wave.

Electron wavelength
from de-Broglie relation

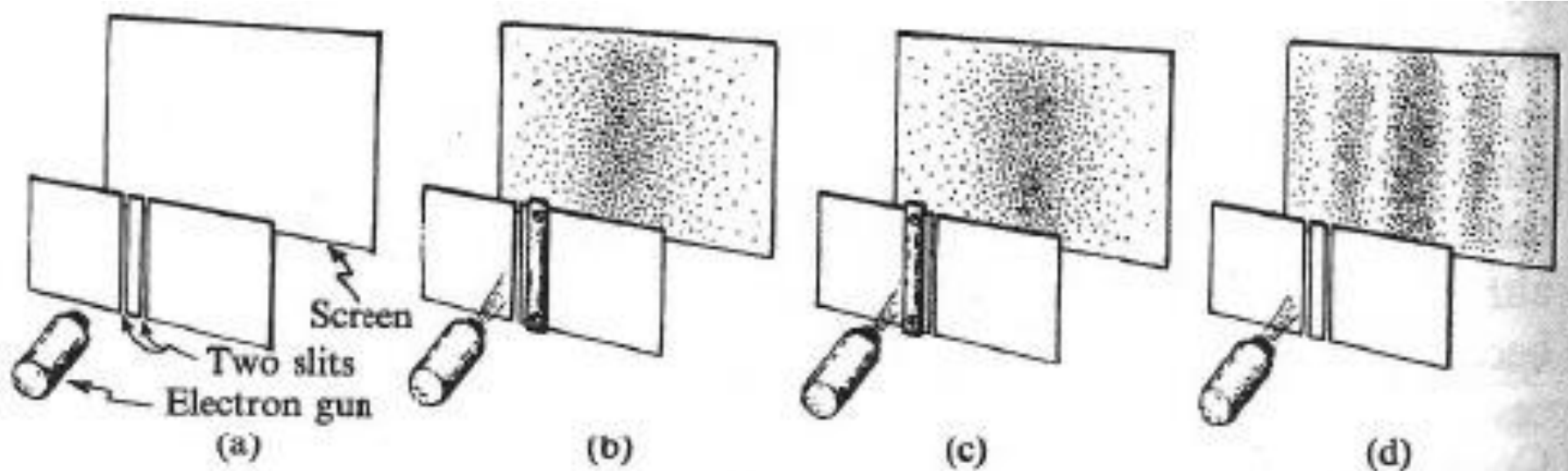
$$\lambda = \frac{h}{p}$$



Double-slit apparatus showing the pattern of electron hits on the observing screen building up over time.

If one of the slits is blocked off, the *interference pattern is broken*.

Does the electron go through 'both slits at the same time' ?



(a) Arrangement for the two-slit experiment. One electron is emitted at a time, aimed at the screen through the pair of slits. (b) Pattern on the screen when the right-hand slit is covered. (c) The same, when the left-hand slit is covered. (d) Interference occurs when both slits are open. Some regions on the screen cannot now be reached despite the fact that they can be with just one or the other slit open.

THE WAVE EQUATION & UNCERTAINTY PRINCIPLE

Combine:

The wave equation

Wave amplitude

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2}$$

Conservation of energy

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

de-Broglie relation

$$\lambda = \frac{h}{p}$$



Erwin Schrödinger
1887 – 1961

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi = E\psi$$

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

Schrödinger Equation



Erwin Schrödinger
1887 – 1961



Max Born
1882 – 1970

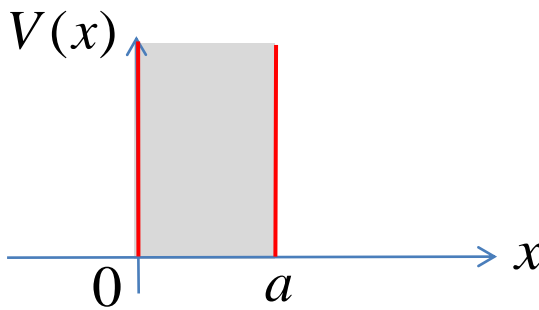
Born interpretation

$$|\psi(x, t)|^2 dx$$

is the *probability* of
a particle being at location
between x and $x + dx$

Particle in a box

$$V(x) = \begin{cases} \infty & x \leq 0, x \geq a \\ 0 & 0 < x < a \end{cases}$$



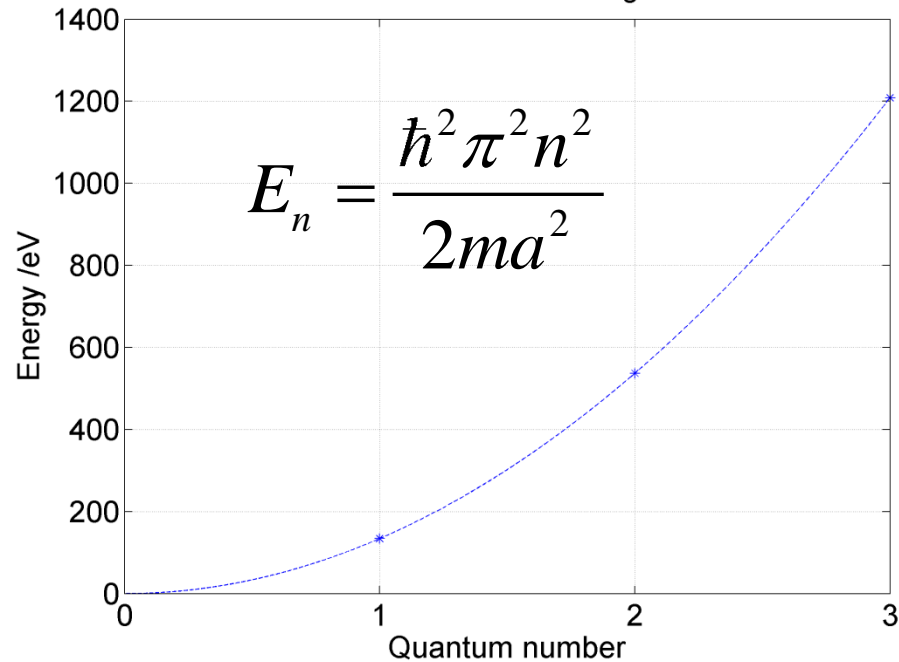
$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi = i\hbar \frac{\partial \psi}{\partial t}$$

Schrödinger Equation

$$\psi_n(x, t) = \begin{cases} \sqrt{\frac{2}{a}} e^{-\frac{iEt}{\hbar}} \sin\left(\frac{n\pi x}{a}\right) & 0 < x < a \\ 0 & x \leq 0, x \geq a \end{cases}$$

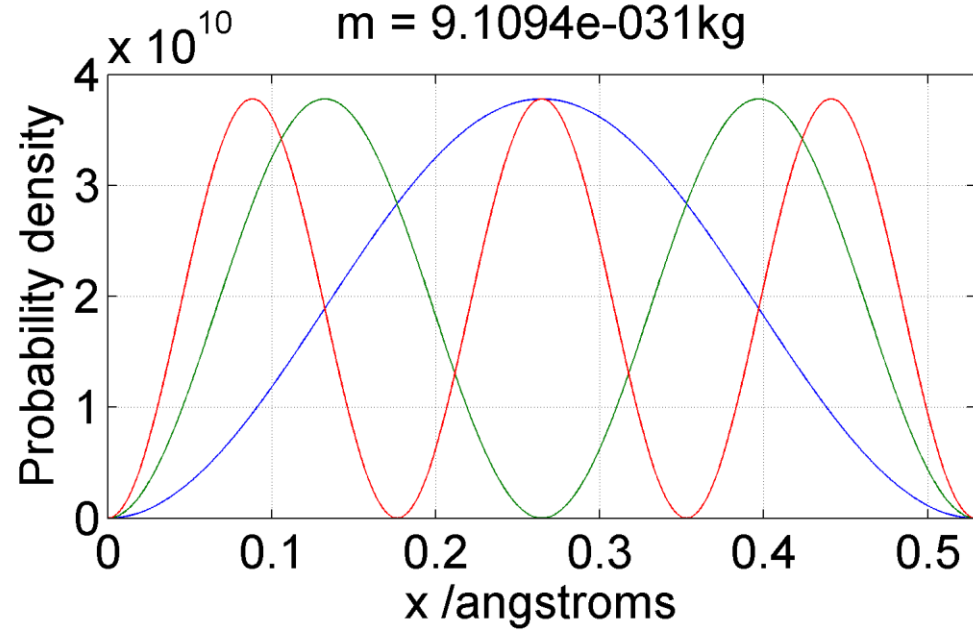
Particle in a box energy /eV
m = 9.1094e-031kg

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}$$



— n = 1 E = 134.2829eV
 — n = 2 E = 537.1314eV
 — n = 3 E = 1208.5457eV

Particle in a box
m = 9.1094e-031kg



Harmonic oscillator

$$V(x) = \frac{1}{2} m \omega^2 x^2$$

$$\psi_n(x, t) = \frac{e^{-\frac{x^2}{2a^2}}}{\sqrt{2^n a \sqrt{\pi n!}}} H_n\left(\frac{x}{a}\right) e^{-\frac{iEt}{\hbar}}$$

$$a = \sqrt{\frac{\hbar}{m\omega}}$$

Angular frequency
of oscillator $\omega = 2\pi f$

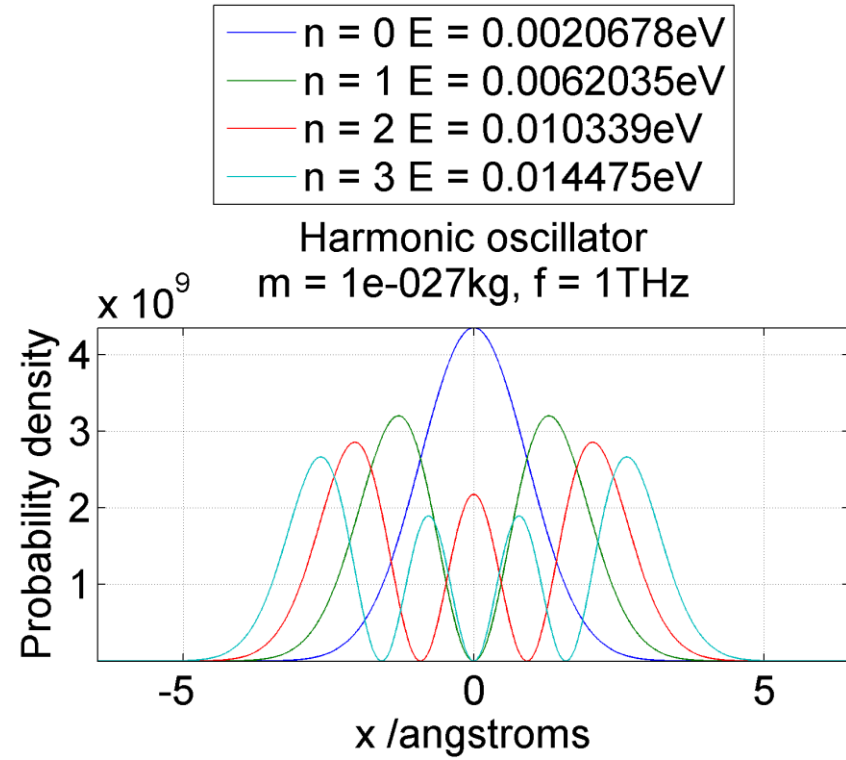
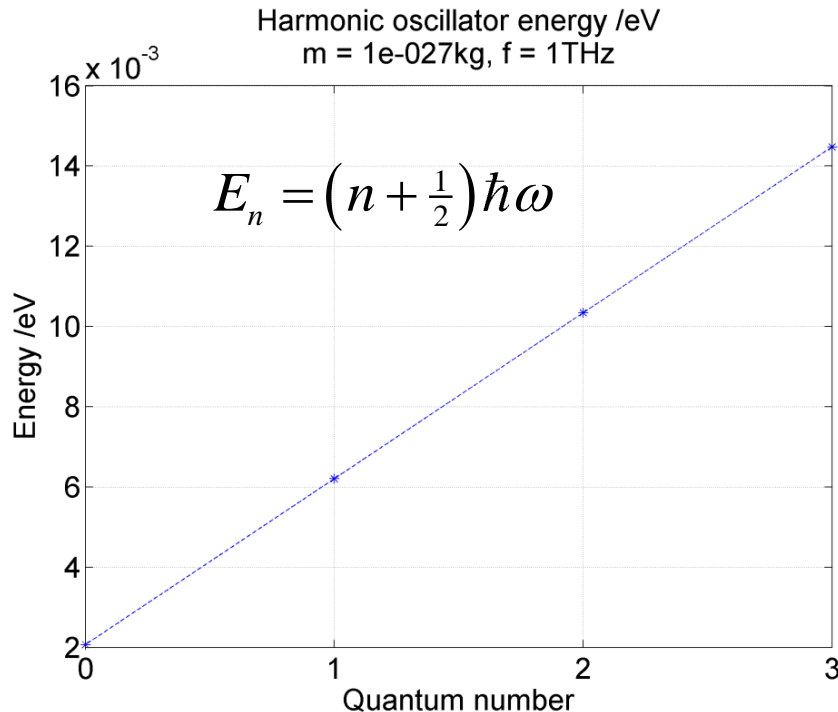
$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi = i\hbar \frac{\partial \psi}{\partial t}$$

Schrödinger Equation

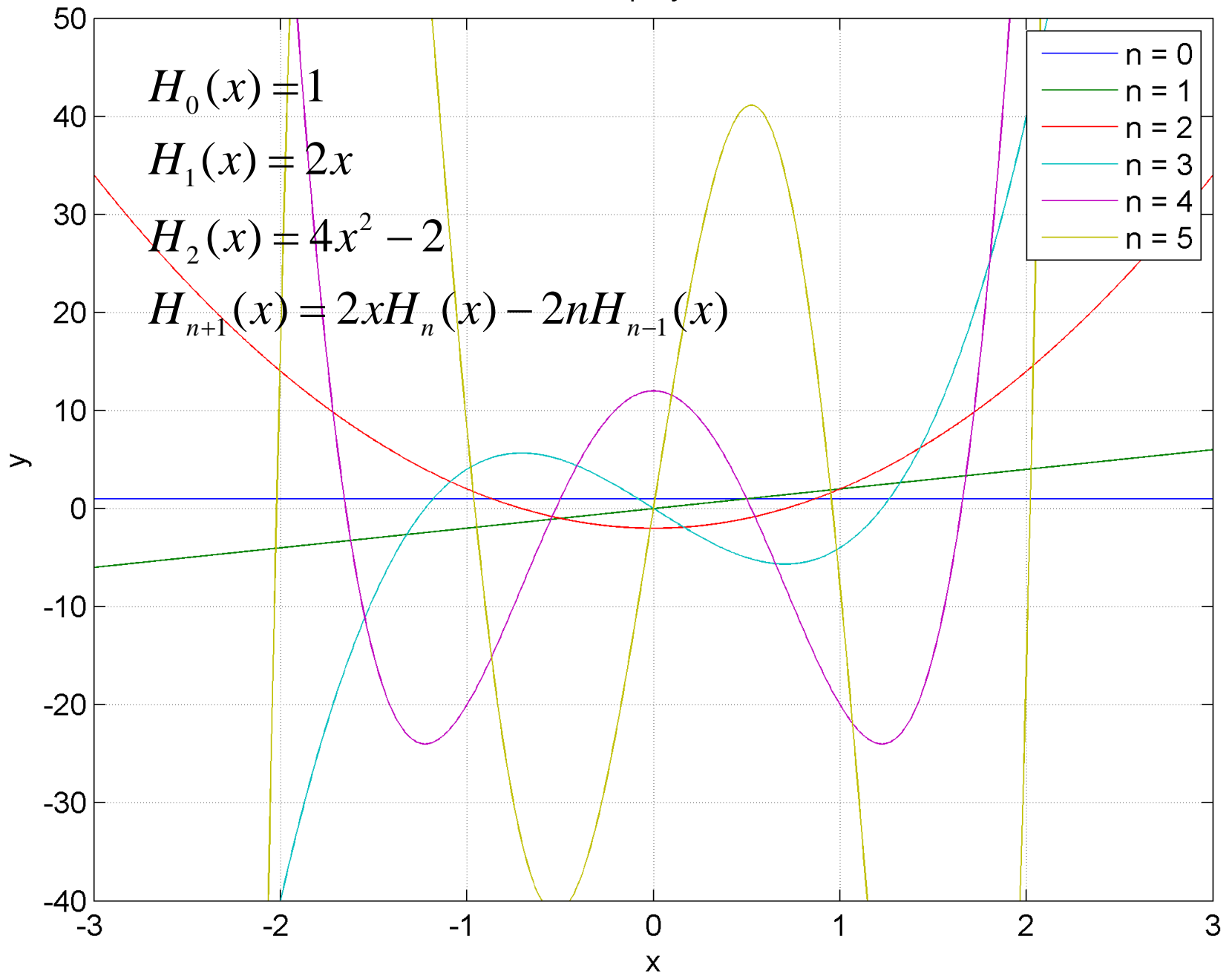
$H_0(z) = 1$ Hermite
 $H_1(z) = 2z$ polynomials

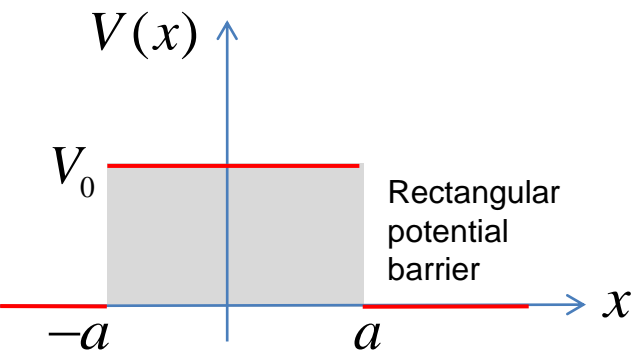
$$H_2(z) = 4z^2 - 2$$

$$H_{n+1}(z) = 2zH_n(z) - 2nH_{n-1}(z)$$



Hermite polynomials

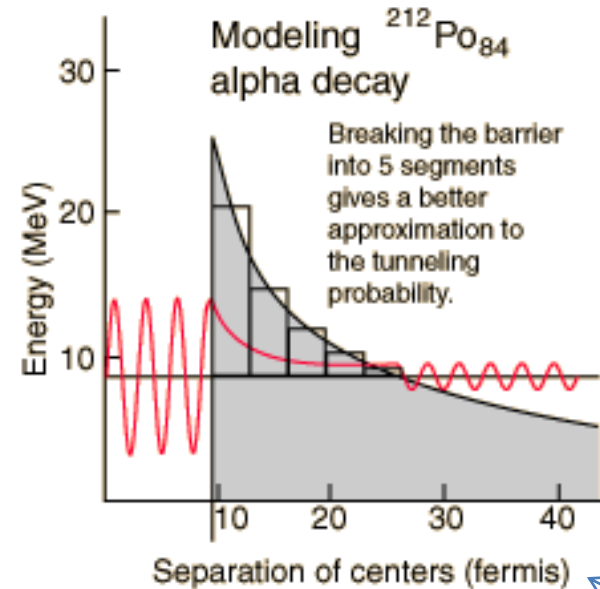




Gamow model of alpha decay



George Gamow
1904-1968



$$q = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

$$qa \ll 1$$

$$|t|^2 \approx e^{-2qa} \quad \text{Tunnelling probability}$$

“Lifetime of alpha particle =
time to traverse nucleus /
probability of alpha escaping”

$$P = \prod_n e^{-2q_n \delta r} \quad \text{let coulomb barrier be lots of thin rectangles}$$

$$q_n = \frac{\sqrt{2m}}{\hbar} \sqrt{\frac{2(Z-2)e^2}{r_n} - E}$$

$$E = \frac{1}{2}mv^2$$

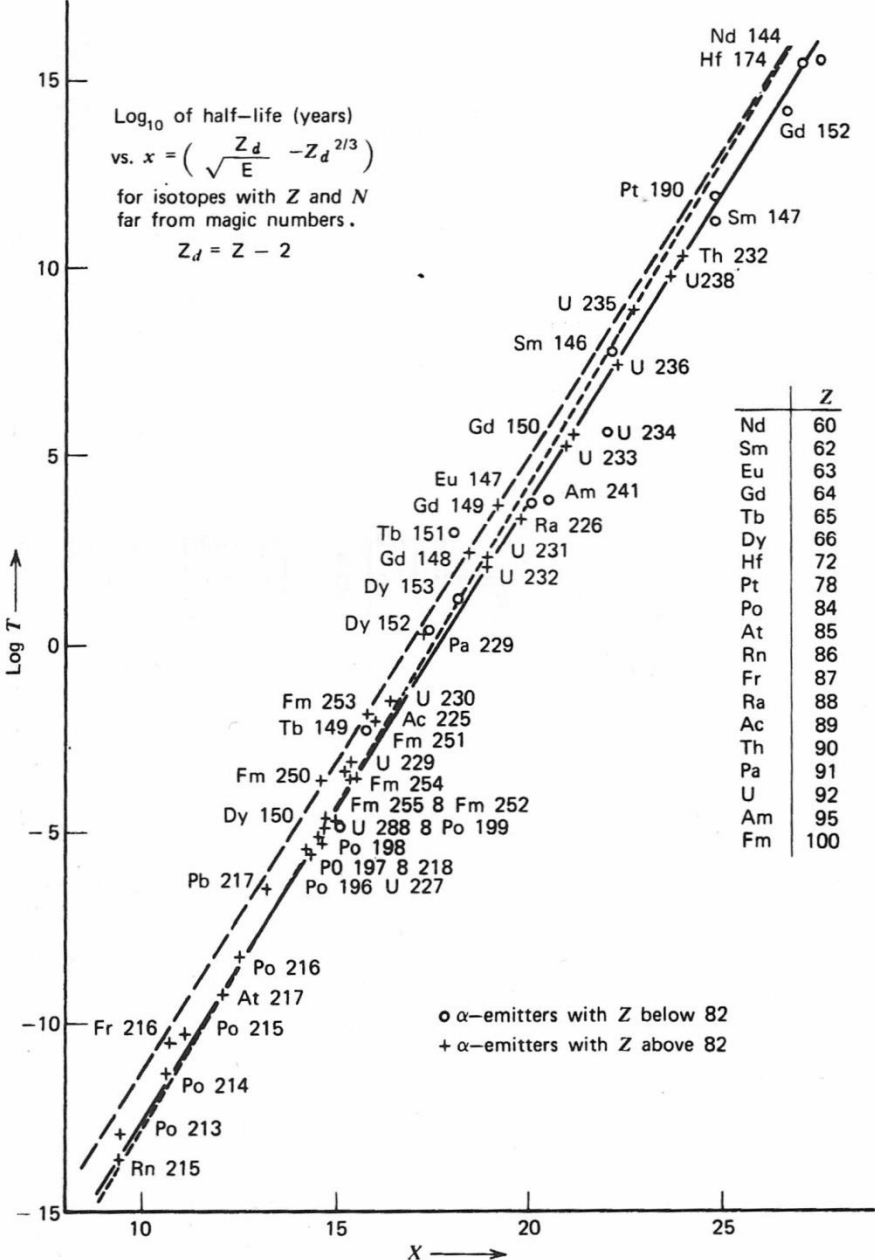
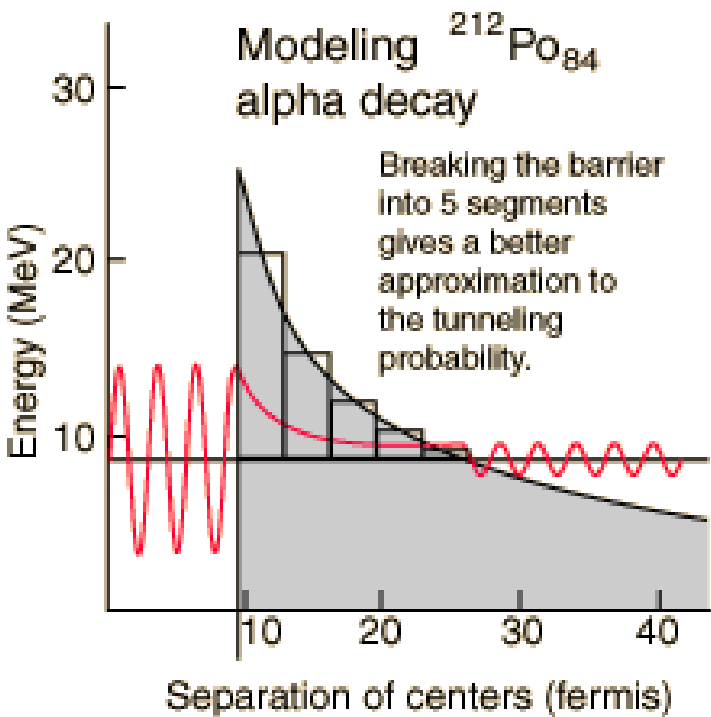
$$\tau \approx \frac{2R}{v} \div e^{-G} = 2R \sqrt{\frac{m}{2E}} e^G$$

$$G = 2 \left(\frac{2m}{\hbar^2} \right)^{1/2} \int_R^b \left(\frac{2(Z-2)e^2}{r} - E \right)^{1/2} dr$$

Half life of alpha-emmitter

$$\log_{10} T_{\frac{1}{2}} \approx 1.61 \times \frac{Z-2}{\sqrt{E_{\alpha}}} - 28.9 - 1.6(Z-2)^{\frac{2}{3}}$$

$$E_{\alpha} \approx 1\text{MeV}$$



Plot of $\log_{10} 1/\tau$ versus $C_2 - C_1 Z_1/\sqrt{E}$ with $C_1 = 1.61$ and a slowly varying $C_2 = 28.9 + 1.6Z_1^{2/3}$. From E. K. Hyde, I. Perlman, and G. T. Seaborg, *The Nuclear Properties of the Heavy Elements*, Vol. 1, Prentice-Hall, Englewood Cliffs, N.J. (1964)

Hydrogenic atom

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

Reduced mass $\mu = \frac{m_e M}{m_e + M} = \frac{m_e}{\frac{m_e}{M} + 1} \approx m_e$

Nucleus mass M

Electron mass m_e

$$-\frac{\hbar^2}{2\mu} \frac{\partial^2 \psi}{\partial x^2} + V\psi = i\hbar \frac{\partial \psi}{\partial t}$$

Schrödinger Equation

$$\psi_{nlm}(r, \theta, \phi) = R(r, n, l) \times \Omega(\theta, \phi, l, m) \quad \leftarrow \text{Angular wavefunction}$$

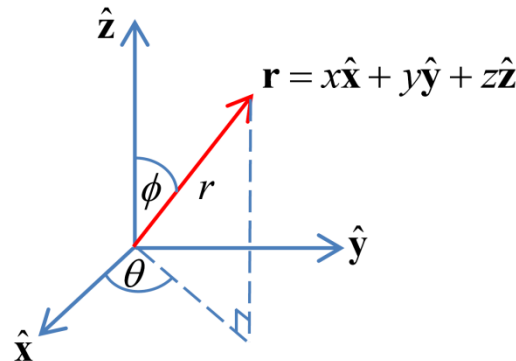
$$R(r, n, l) = \sqrt{\frac{(n-l-1)!}{2n(n+l)!}} \left(\frac{2}{an}\right)^{3/2} x^l e^{-x/2} \zeta(x, l, n) \quad \text{Radial wavefunction}$$

$$\zeta(x, l, n) = \sum_{k=0}^{n-l-1} \frac{(l+n)!(-x)^k}{(2l+1+k)!(n-l-1-k)!k!} \quad \text{Laguerre polynomial}$$

$$x = \frac{2r}{an}$$

$$E_n = -\frac{\mu e^4 Z^2}{8\epsilon_0^2 h^2 n^2}$$

Orbital energy



$$x = r \sin \phi \cos \theta$$

$$y = r \sin \phi \sin \theta$$

$$z = r \cos \phi$$

Conversion between Cartesian and polar coordinates

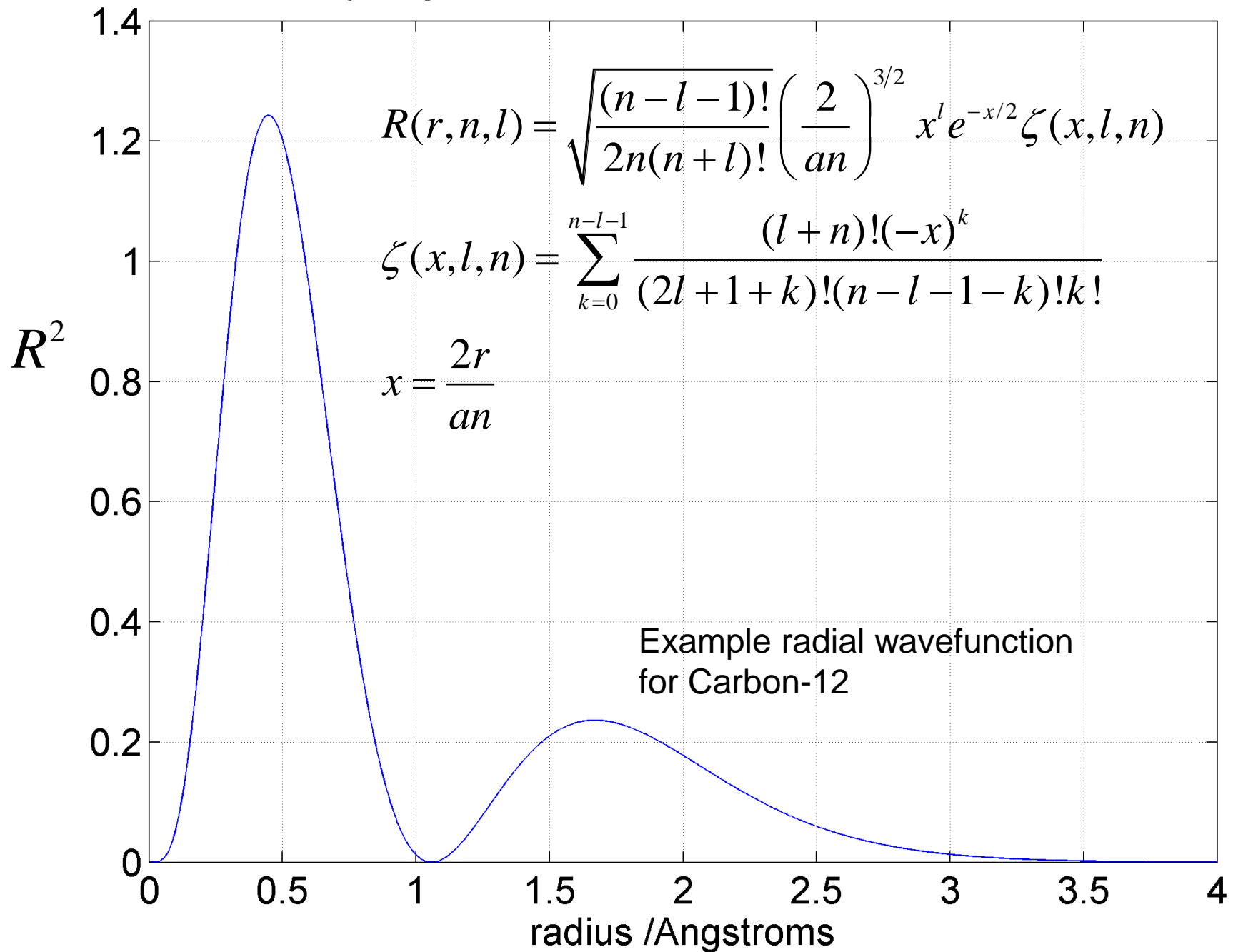
Polar coordinate unit vectors as Cartesian coordinates

$$\hat{\mathbf{r}} = \sin \phi \cos \theta \hat{\mathbf{x}} + \sin \phi \sin \theta \hat{\mathbf{y}} + \cos \phi \hat{\mathbf{z}}$$

$$\hat{\boldsymbol{\theta}} = -\sin \theta \hat{\mathbf{x}} + \cos \theta \hat{\mathbf{y}}$$

$$\hat{\boldsymbol{\phi}} = \cos \phi \cos \theta \hat{\mathbf{x}} + \cos \phi \sin \theta \hat{\mathbf{y}} - \sin \phi \hat{\mathbf{z}}$$

Hydrogenic atom: $Z=6$, $A=12.011$, $n=4$, $L=2$



Angular wavefunction

$$\Omega(\theta, \phi, l, m) = \begin{cases} Y_l^{-m}(\theta, \phi) - Y_l^m(\theta, \phi) & m < 0 \\ Y_l^0(\theta, \phi) & m = 0 \\ Y_l^m(\theta, \phi) + Y_l^{-m}(\theta, \phi) & m \geq 0 \end{cases}$$

Assume quantum numbers n, l, m are integers!

Spherical harmonics

$$Y_l^m(\theta, \phi) = (-1)^m \left[\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!} \right]^{1/2} P_l^m(\cos \theta) e^{im\phi} \quad m = -l, \dots, 0, \dots, l$$

$$\frac{d}{dx} \left[(1-x^2) \frac{dy}{dx} \right] + \left[l(l+1) - \frac{m^2}{1-x^2} \right] y = 0$$

$$y = P_l^m(x)$$

Legendre Polynomials can be evaluated using the MATLAB

`legendre(l,x)` function (which gives a vector of outputs for all possible m values).

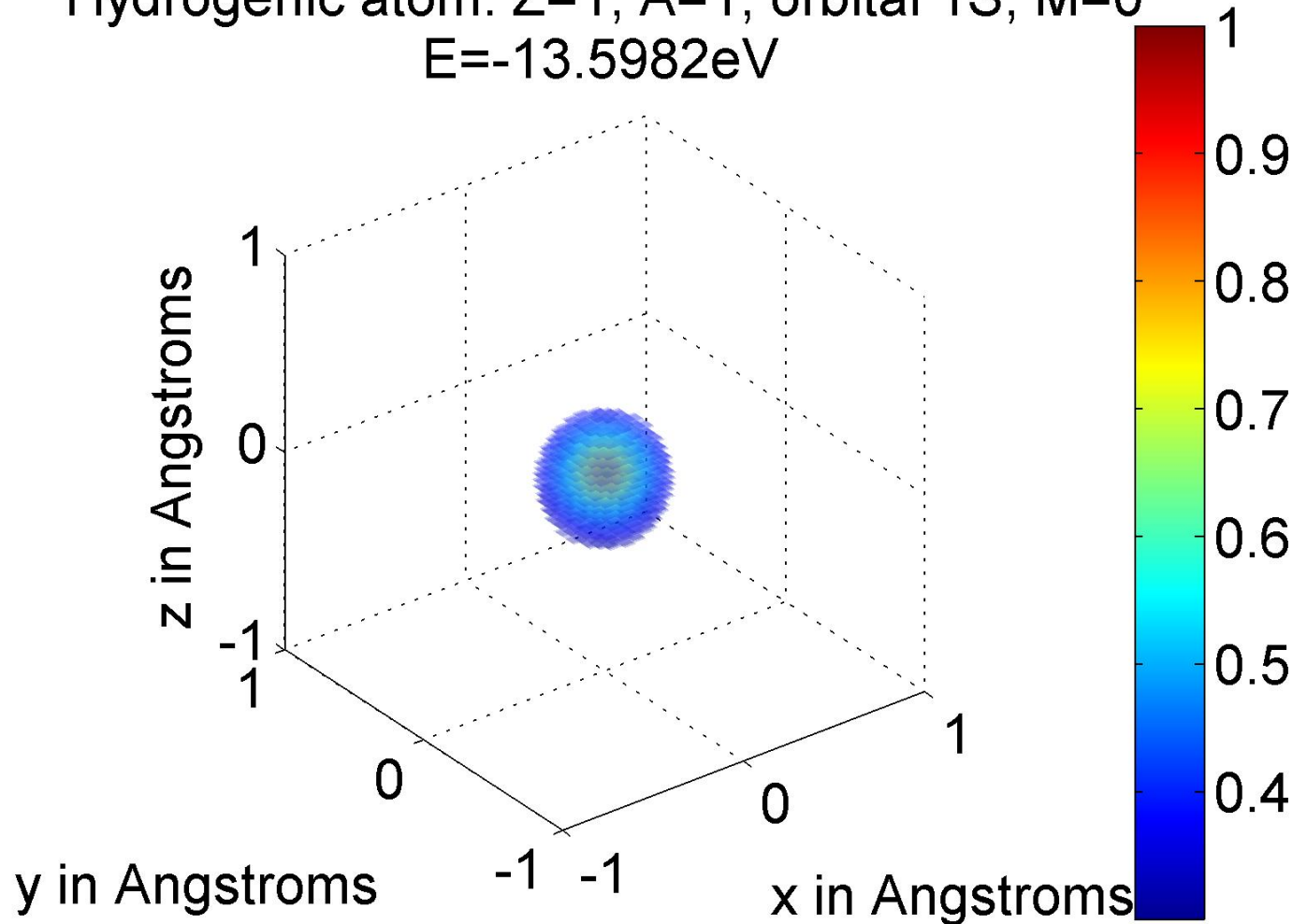
S

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

$l = 0$

$m = 0$

Hydrogenic atom: $Z=1$, $A=1$, orbital $1S$, $M=0$
 $E=-13.5982\text{eV}$



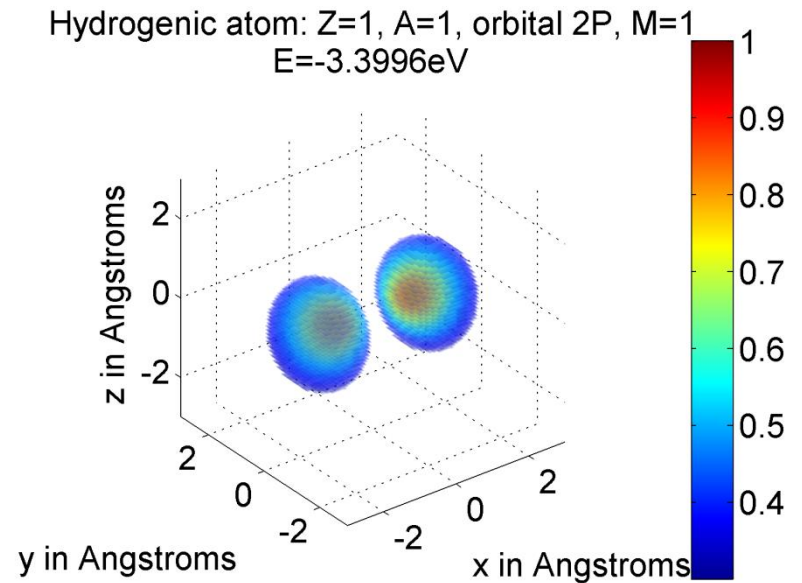
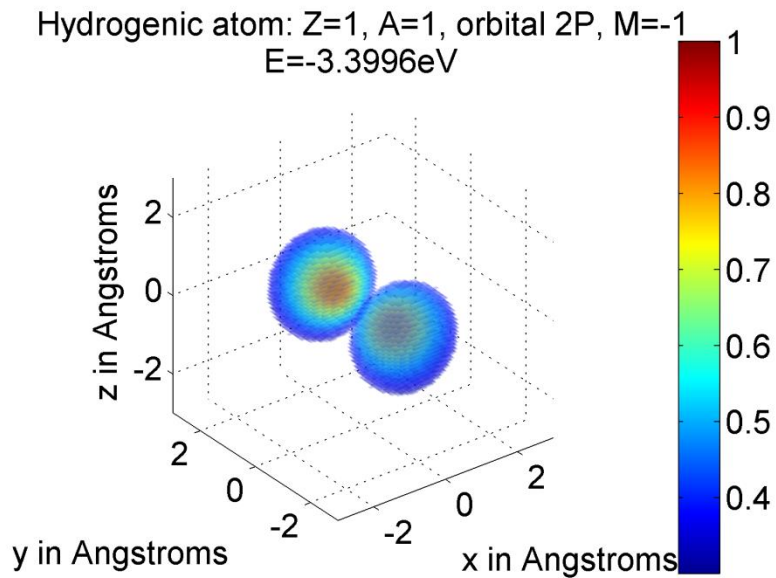
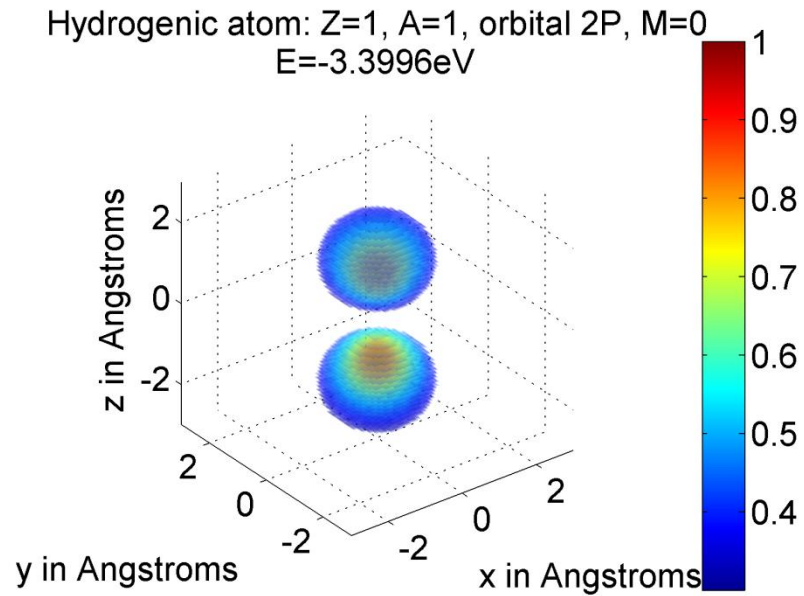
$1\text{\AA} = 10^{-10}\text{ m}$

P

$n = 2, 3, 4, \dots$

$l = 1$

$m = -1, 0, 1$



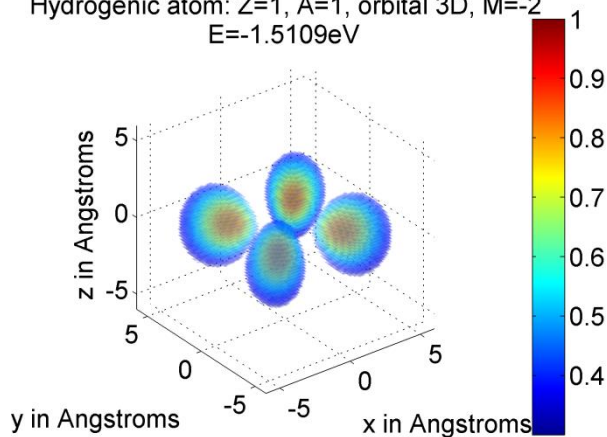
D

$$n = 3, 4, 5, \dots$$

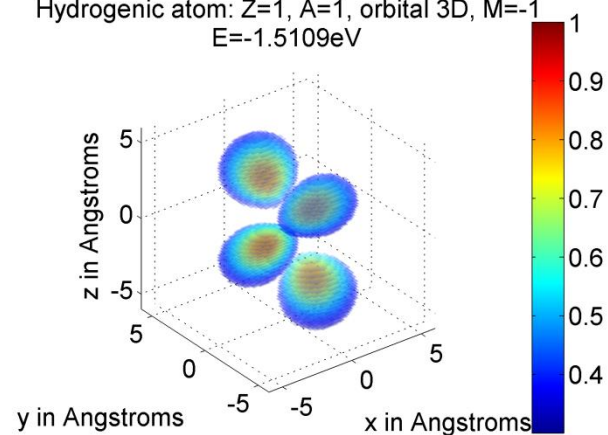
$$l = 2$$

$$m = -2, -1, 0, 1, 2$$

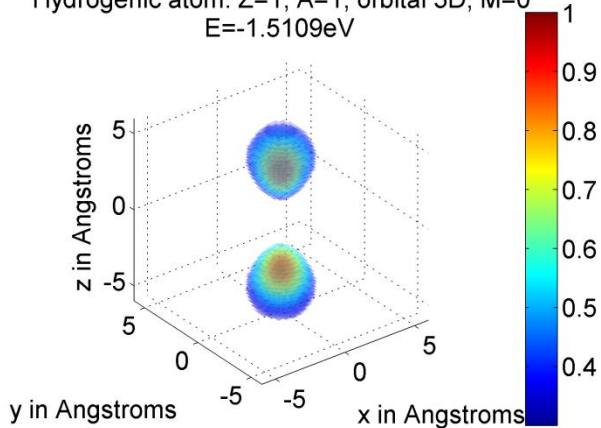
Hydrogenic atom: Z=1, A=1, orbital 3D, M=-2
E=-1.5109eV



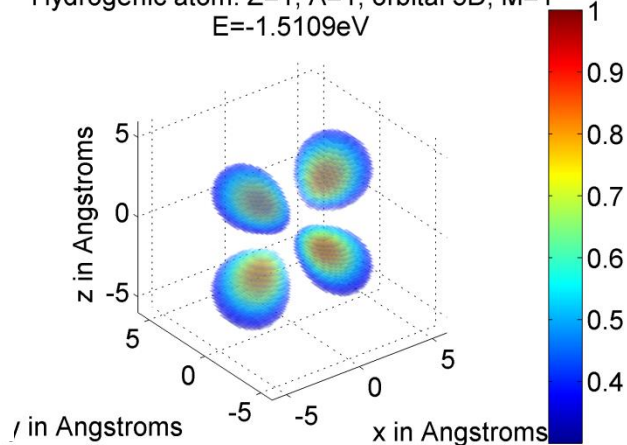
Hydrogenic atom: Z=1, A=1, orbital 3D, M=-1
E=-1.5109eV



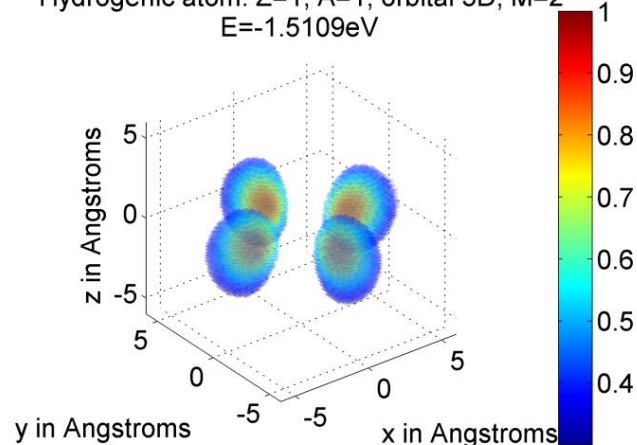
Hydrogenic atom: Z=1, A=1, orbital 3D, M=0
E=-1.5109eV

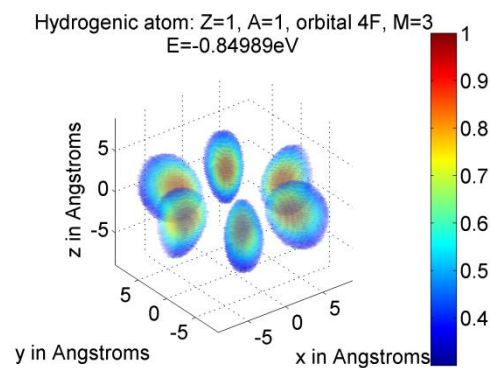
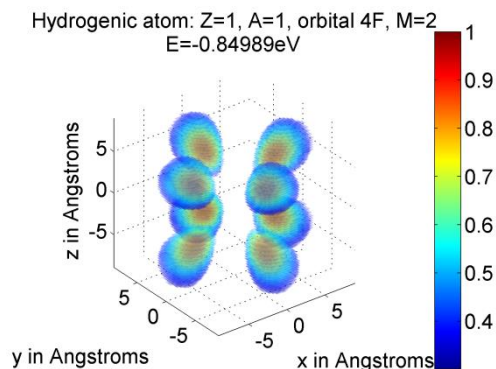
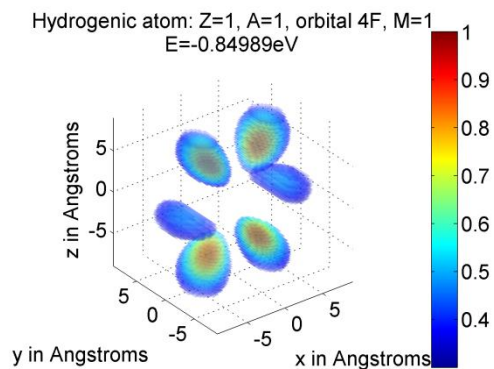
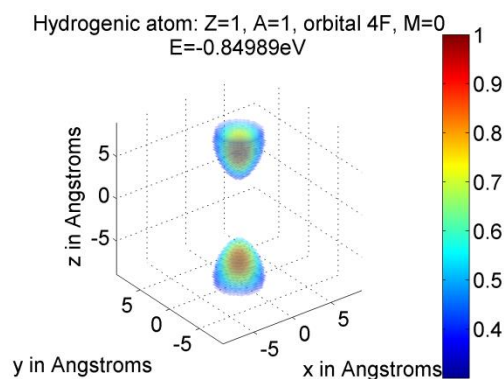
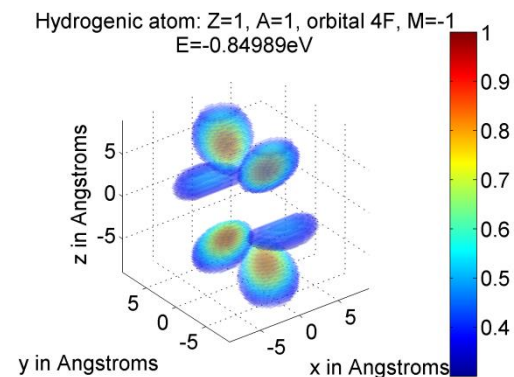
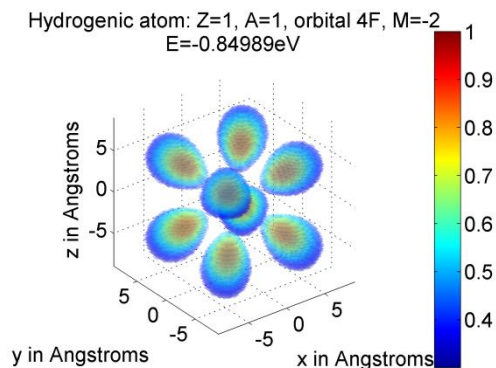
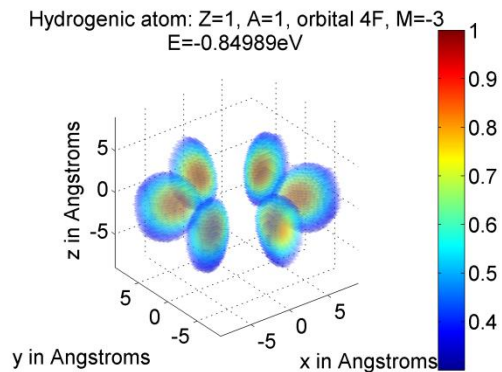


Hydrogenic atom: Z=1, A=1, orbital 3D, M=1
E=-1.5109eV

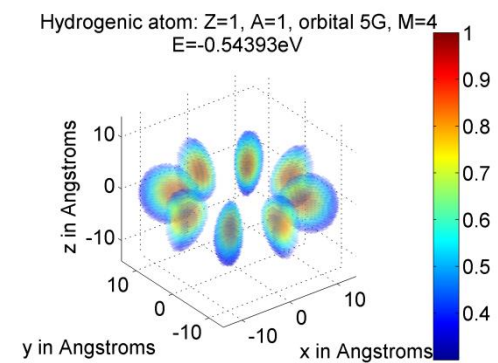
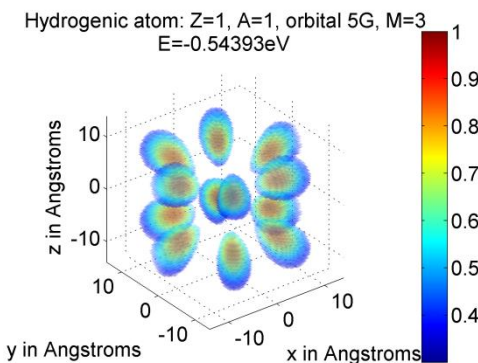
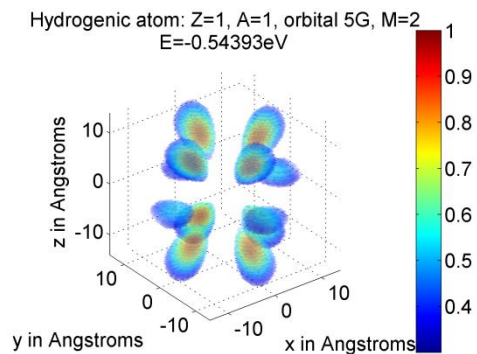
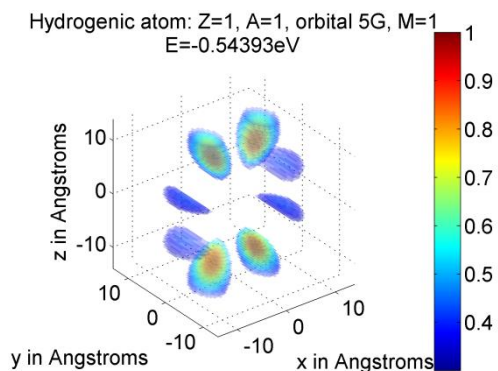
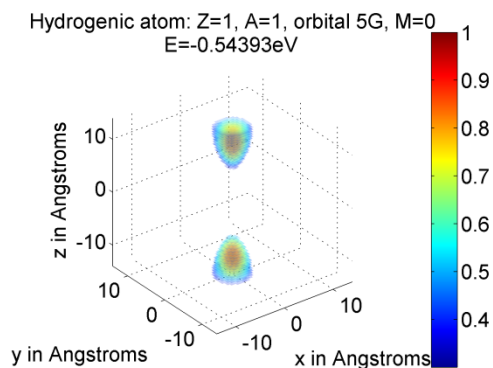
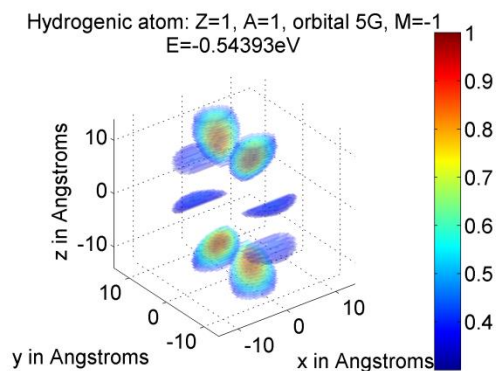
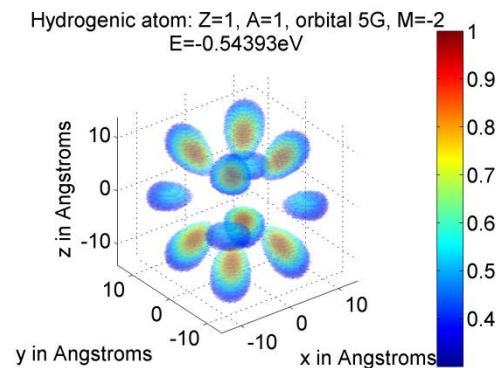
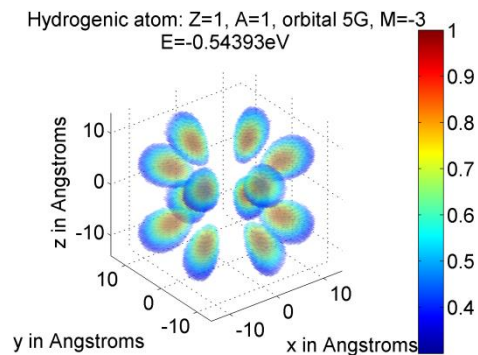
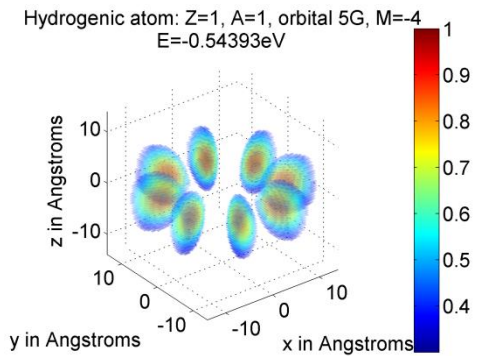


Hydrogenic atom: Z=1, A=1, orbital 3D, M=2
E=-1.5109eV





$$F \quad n = 4, 5, 6, \dots \quad l = 3 \quad m = -3, -2, -1, 0, 1, 2, 3$$



$$G \quad n=5,6,7,\dots \quad l=4 \quad m=-4,-3,-2,-1,0,1,2,3,4$$

Heisenberg Uncertainty Principle

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

In other words, we have a *limit* upon how precisely we can measure **position** and **momentum** of a particle

$$\Delta E \Delta t \geq \frac{1}{2} \hbar$$

A similar relationship exists between **energy** and **time**



Werner
Heisenberg
1901 – 1976



Not this one!

THE COPENHAGEN INTERPRETATION

The Copenhagen Interpretation of Quantum Mechanics

(Bohr, Heisenberg, Born et al 1925-1927)

“Physical systems generally do not have definite properties prior to being measured, and quantum mechanics can only predict the **probabilities** that measurements will produce certain results.

↖ $|\psi|^2$

The act of measurement affects the system, causing the set of probabilities to reduce to only one of the possible values immediately after the measurement. This feature is known as wavefunction collapse.”

An electron therefore has a wavefunction which incorporates *both* spin states, until it is measured.

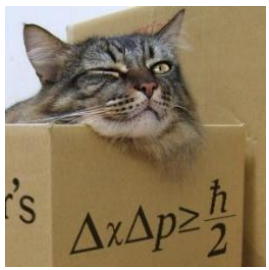
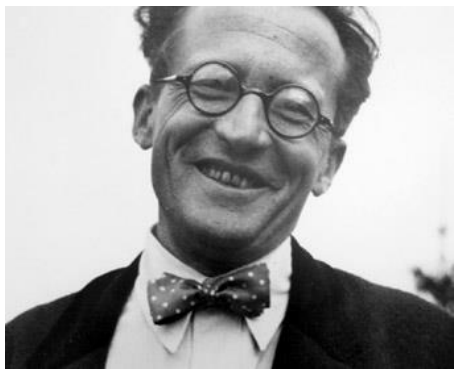
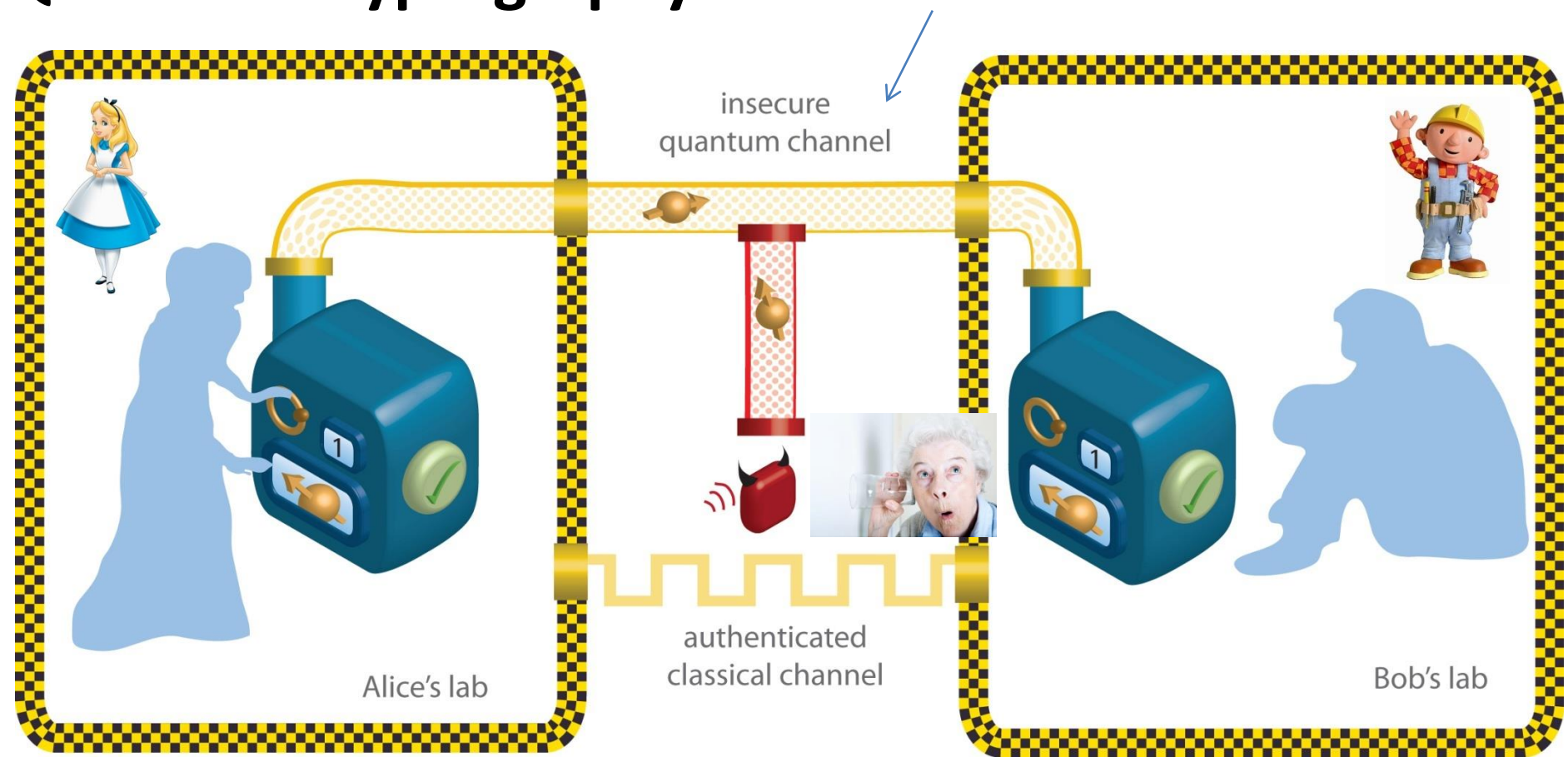
An electron in a hydrogen atom has wavefunction which is a *superposition of all possible quantum numbers*. Only when you measure it, does it collapse to one particular ‘eigenstate.’



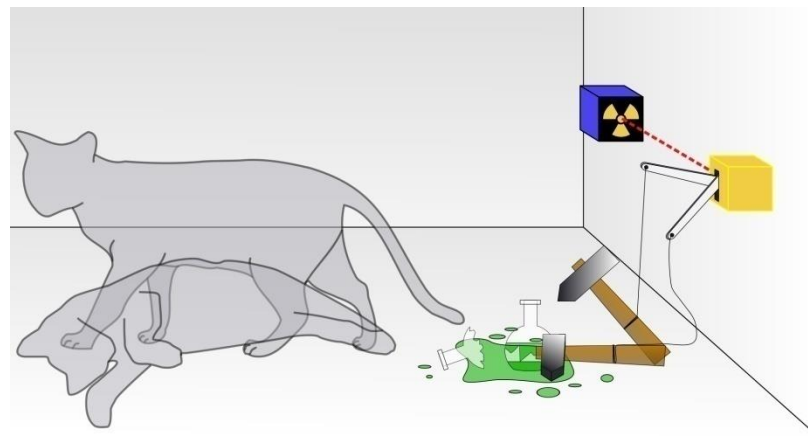
https://en.wikipedia.org/wiki/Copenhagen_interpretation

Quantum Cryptography

Here you can tell whether Eve has been listening!



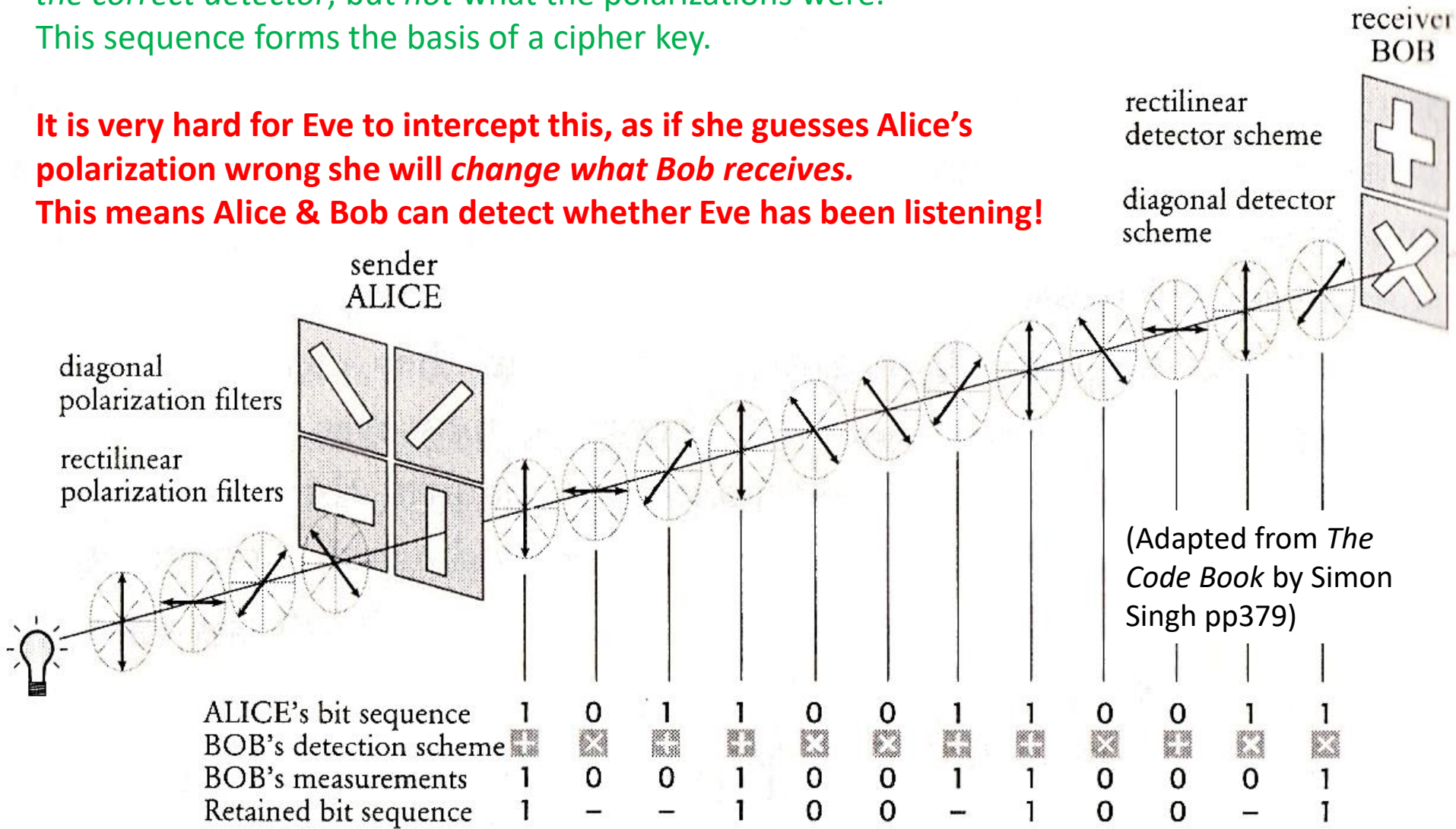
Erwin
Schrödinger
(1887-1961)

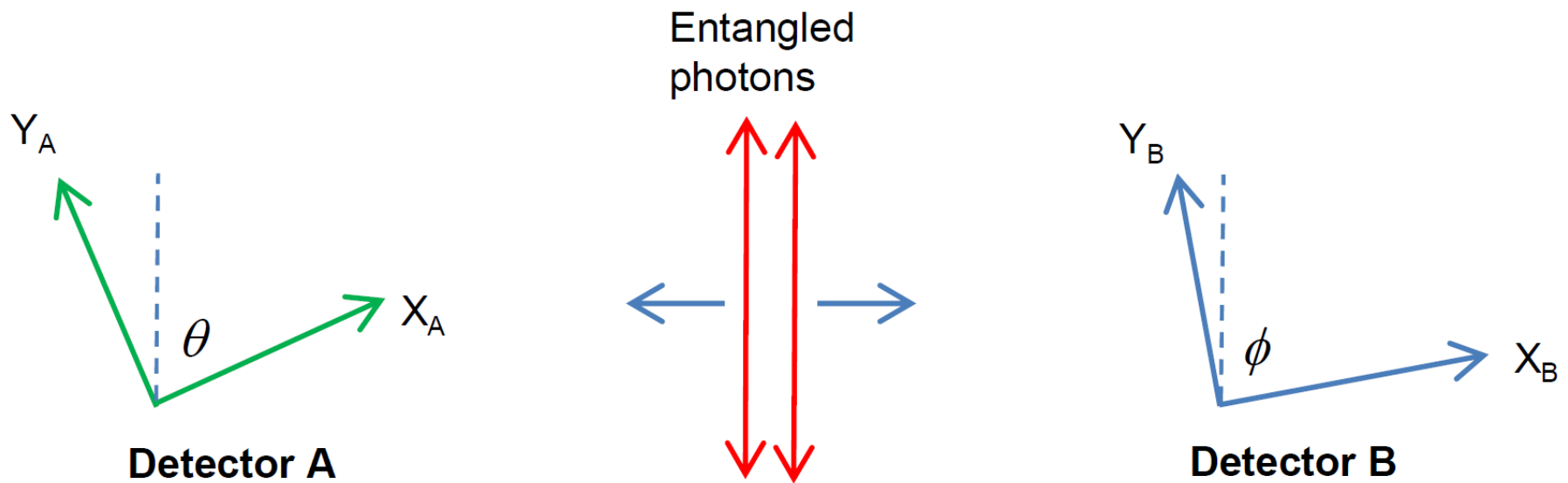


If you intercept a photon, you will force its polarization to be that of the detector.
In Quantum Mechanics your *act of measurement collapses the wavefunction*.

Alice sends Bob a message based upon photons of different polarizations.
Alice & Bob communicate to agree *which photons were intercepted with the correct detector*, but *not* what the polarizations were.
This sequence forms the basis of a cipher key.

It is very hard for Eve to intercept this, as if she guesses Alice's polarization wrong she will *change what Bob receives*.
This means Alice & Bob can detect whether Eve has been listening!

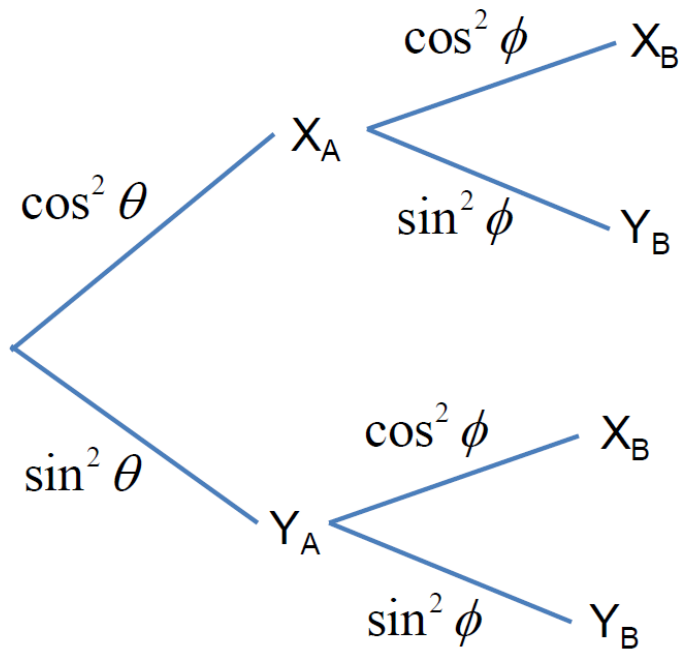




$$P(X_A) = \cos^2 \theta, \quad P(Y_A) = \sin^2 \theta$$

$$P(X_B) = \cos^2 \phi, \quad P(Y_B) = \sin^2 \phi$$

We shall assign probabilities for each detector's eigenstate to be based upon the statistics of the **classical limit** i.e. billions and billions of photons! In this case we expect Malus' Law to hold i.e. the square of the projection of the polarization yields transmitted power.

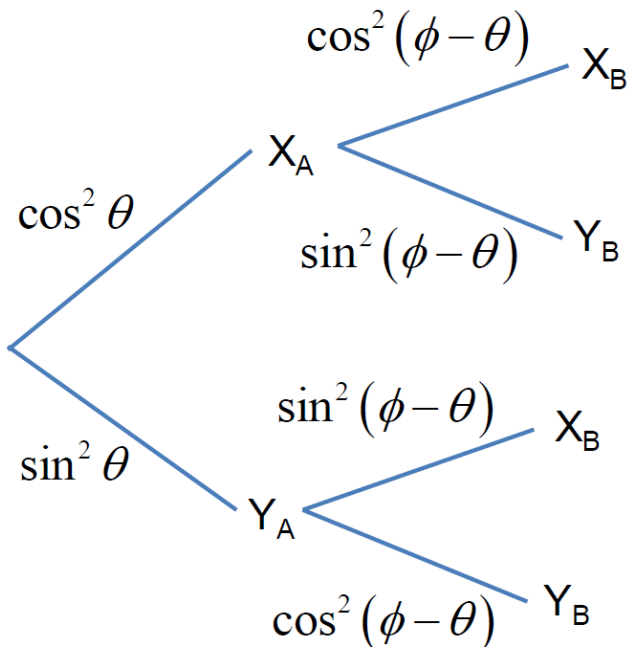
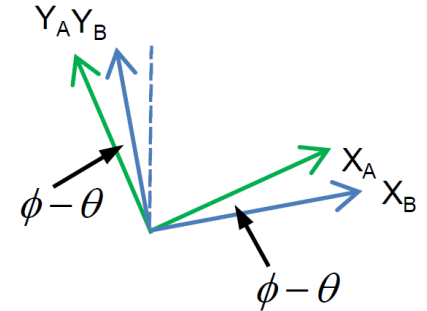


Classical scenario

$$P(\text{match}) = P(X_A, X_B) + P(Y_A, Y_B)$$

$$P(\text{match}) = \cos^2 \theta \cos^2 \phi + \sin^2 \theta \sin^2 \phi$$

$$P(\text{mismatch}) = 1 - \cos^2 \theta \cos^2 \phi - \sin^2 \theta \sin^2 \phi$$



Quantum scenario

$$P(\text{match}) = P(X_A, X_B) + P(Y_A, Y_B)$$

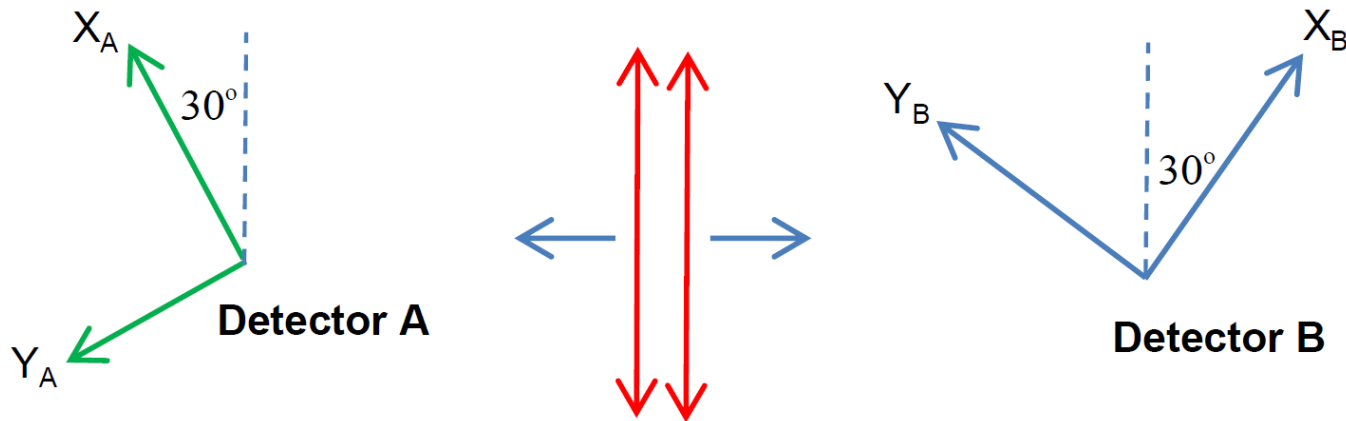
$$P(\text{match}) = \cos^2 \theta \cos^2(\phi - \theta) + \sin^2 \theta \cos^2(\phi - \theta)$$

$$P(\text{match}) = (\cos^2 \theta + \sin^2 \theta) \cos^2(\phi - \theta)$$

$$P(\text{match}) = \cos^2(\phi - \theta)$$

$$P(\text{mismatch}) = 1 - \cos^2(\phi - \theta)$$

$$P(\text{mismatch}) = \sin^2(\phi - \theta)$$



Example:
Classical

$$\theta = -30^\circ, \phi = 30^\circ$$

$$P(\text{mismatch}) = 1 - \cos^2 \theta \cos^2 \phi - \sin^2 \theta \sin^2 \phi$$

$$P(\text{mismatch}) = 1 - \left(\frac{\sqrt{3}}{2}\right)^2 \left(\frac{\sqrt{3}}{2}\right)^2 - \left(-\frac{1}{2}\right)^2 \left(\frac{1}{2}\right)^2$$

$$P(\text{mismatch}) = 1 - \frac{9}{16} - \frac{1}{16} = \frac{16-10}{16} = \frac{3}{8}$$

Example:
QM

$$\theta = -30^\circ, \phi = 30^\circ$$

$$P(\text{mismatch}) = \sin^2(\phi - \theta)$$

$$P(\text{mismatch}) = \sin^2(60^\circ) = \frac{3}{4} = \frac{6}{8}$$