BPhO Computational Challenge

Quantum, atoms, nuclear

Dr Andrew French.
December 2023.

BPhO British Physics Olympiad

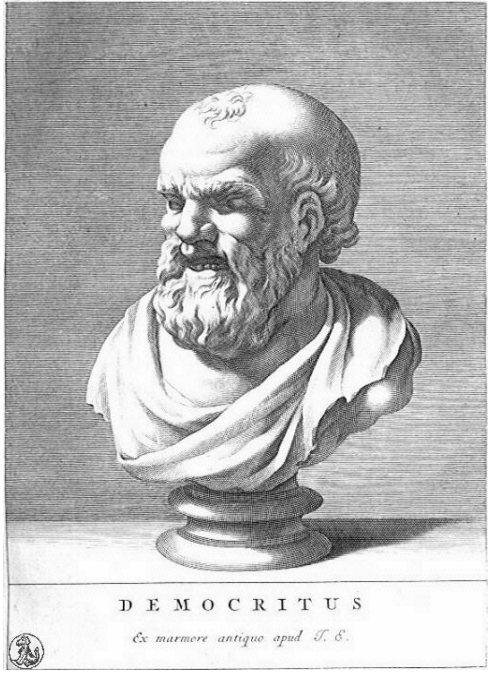
In ancient Greece, Democritus* proposed that matter is composed of ‘uncuttable’ *atomon* components. Today we call them **atoms**.

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

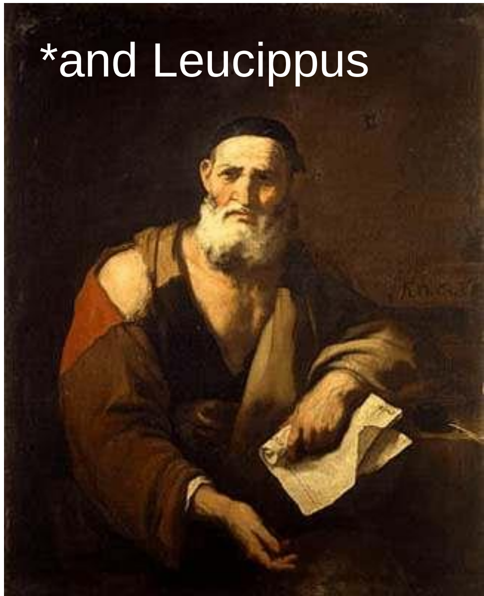
In the Standard Model of modern Physics, atoms are themselves composed of **fundamental particles**. **Quarks** are ‘glued’ together to form the **protons** and **neutrons** which comprise a tiny positively charged **atomic nucleus**, with radius 10^{-15}m (1femto-metre, fm). Around them is a cloud of 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.

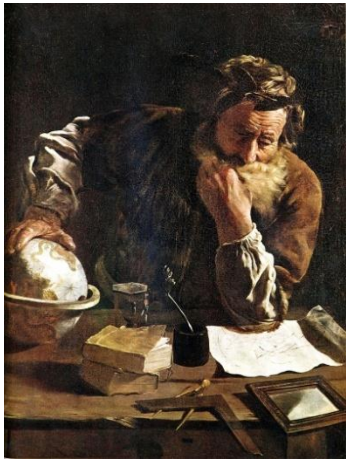
This theory is called **Quantum Mechanics**



Democritus
460 BC – 370BC

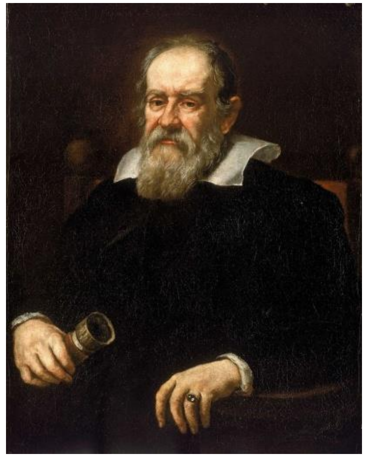


Mechanics



Archimedes
287BC - 212BC

Mechanics



Galileo Galilei
1564-1642

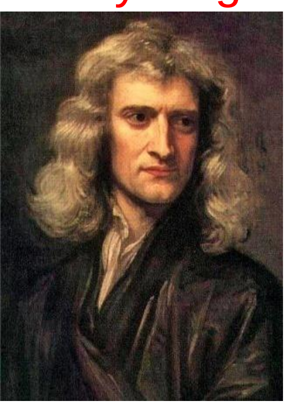
Orbits

Johannes Kepler
1571-1630

Waves

Christiaan Huygens
1629 - 1695

Everything!

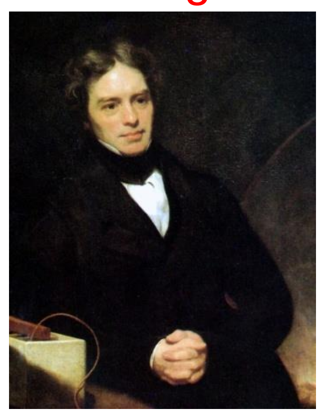


Isaac Newton
1642-1726

Waves, heat

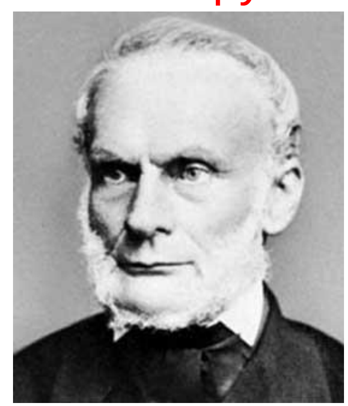
Joseph Fourier
1768-1830

Electromagnetism



Michael Faraday
1791-1867

Entropy



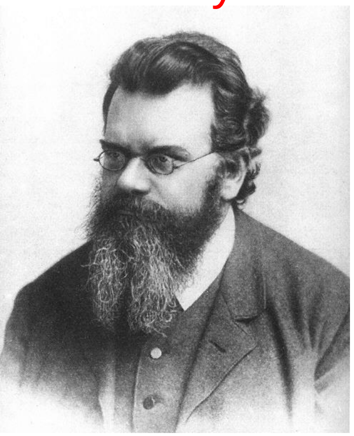
Rudolf Clausius
1822-1888

Electromagnetism

James Clerk Maxwell
1831-1879

A small selection of the **Pioneers of Classical Physics**

Thermodynamics

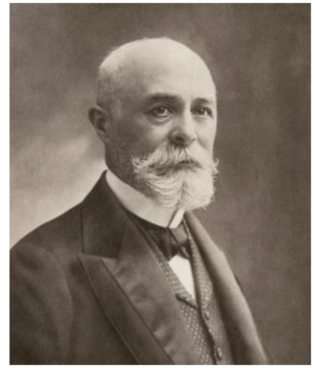


Ludwig Boltzmann
1844-1906

X-Rays

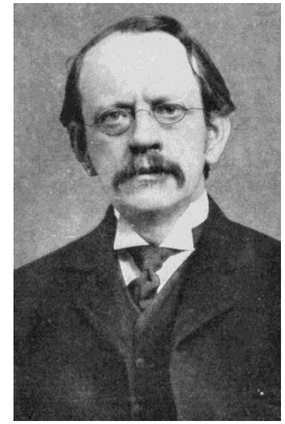
Wilhelm Röntgen
1845-1923

Radioactivity



Antoine Henri
Becquerel
1852-1908

Electron

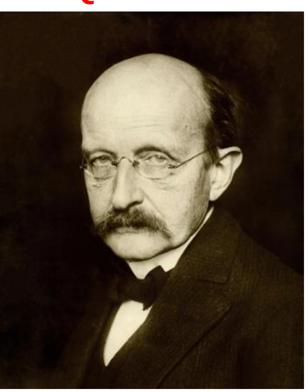


J.J.Thompson
1856-1940

Radio waves

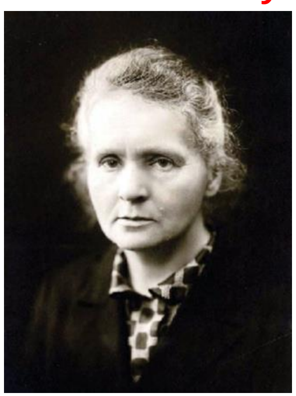
Heinrich Hertz
1857-1894

Quanta



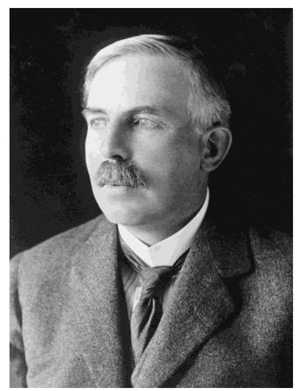
Max Planck
1858 – 1947

Radioactivity



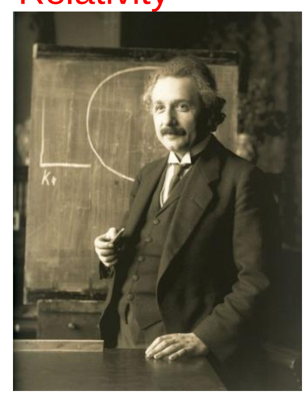
Marie Curie
1867-1934

Atomic nucleus



Ernest Rutherford
1871-1937

Quantum Theory
Relativity



Albert Einstein
1879-1955

Quantum
atom

Niels Bohr
1885-1962

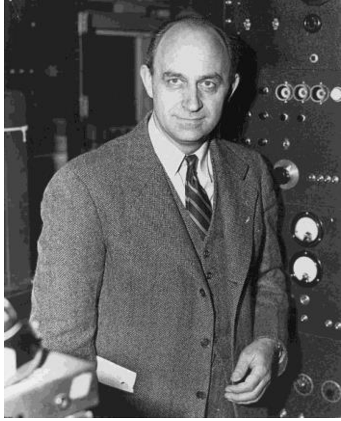
A small selection of the **Pioneers of Atomic & Quantum Physics**

Max Born
1882 –1970

Erwin Schrödinger
1887 –1961

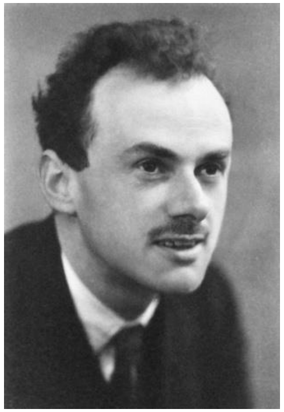
Louis de Broglie
1892 –1987

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**

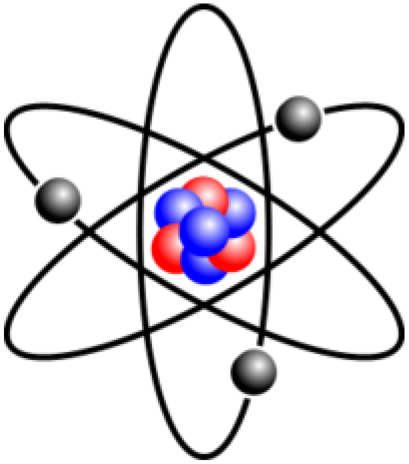
The development of Quantum Mechanics was a truly collaborative effort, and unprecedented in terms of the speed at which the theory was assembled.
The 1927 Solvay Conference in Brussels was devoted to Quantum Theory.
Many of the pioneers of the subject attended. Nine were eventually Nobel laureates.

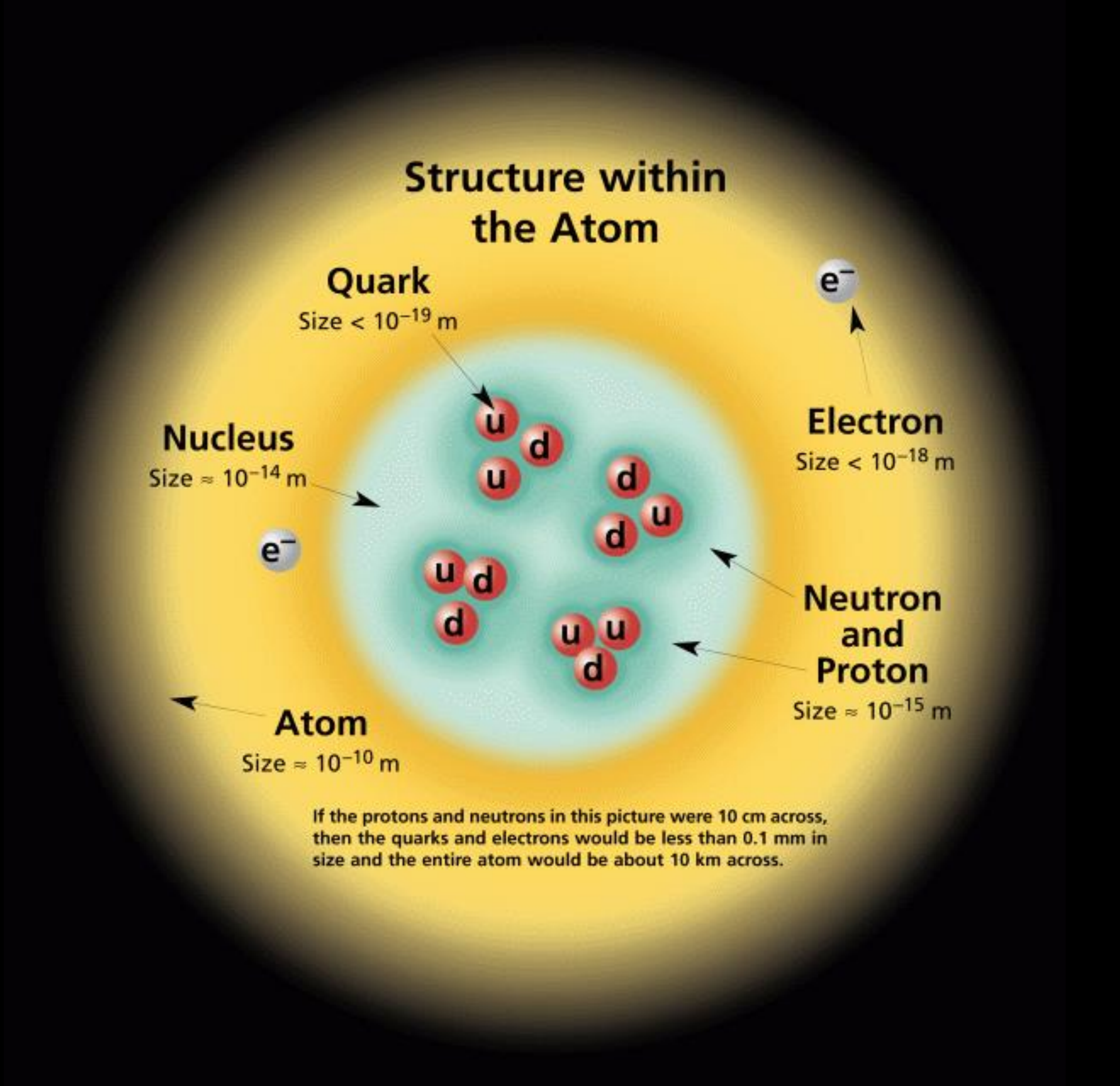
But first we must start with

ATOMS

and why they exist at all

This model has
a serious flaw!





Structure within the Atom
Quark
Size < 10^{-19} m
e⁻
Electron
Size < 10^{-18} m
Nucleus
Size ≈ 10^{-14} m
u
d
u
d
d
u
e⁻
u
d
d
u
u
d
Neutron and Proton
Size ≈ 10^{-15} m
Atom
Size ≈ 10^{-10} m
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.

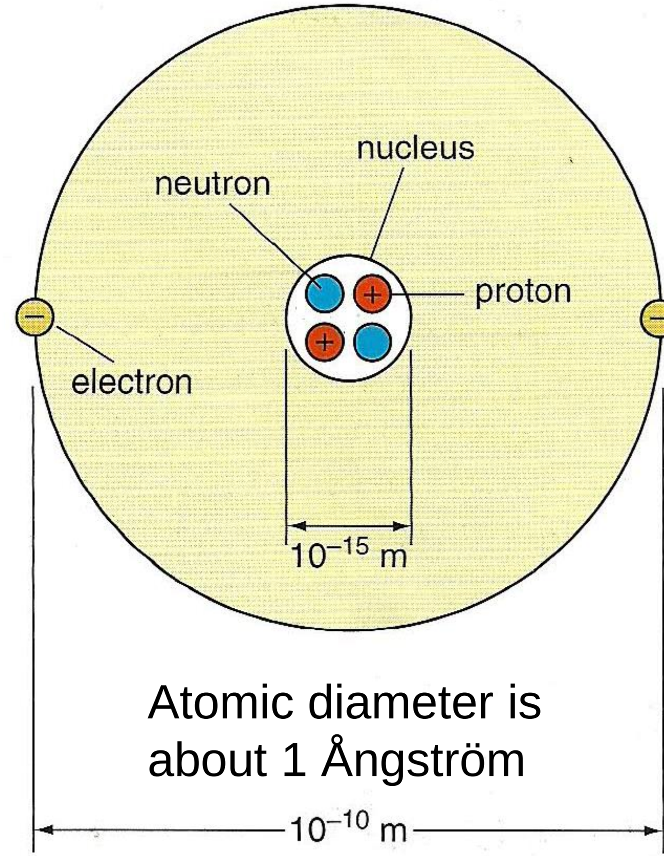
The size of an atom

Earth diameter
= 12,756km

Marble diameter =
3.6cm

$$\left(\frac{1.2756\times10^{7}}{3.6\times10^{-2}}\right)^{3}\approx 4.4\times10^{25}$$

Volume of Earth in marbles



Atomic diameter is
about 1 Ångström

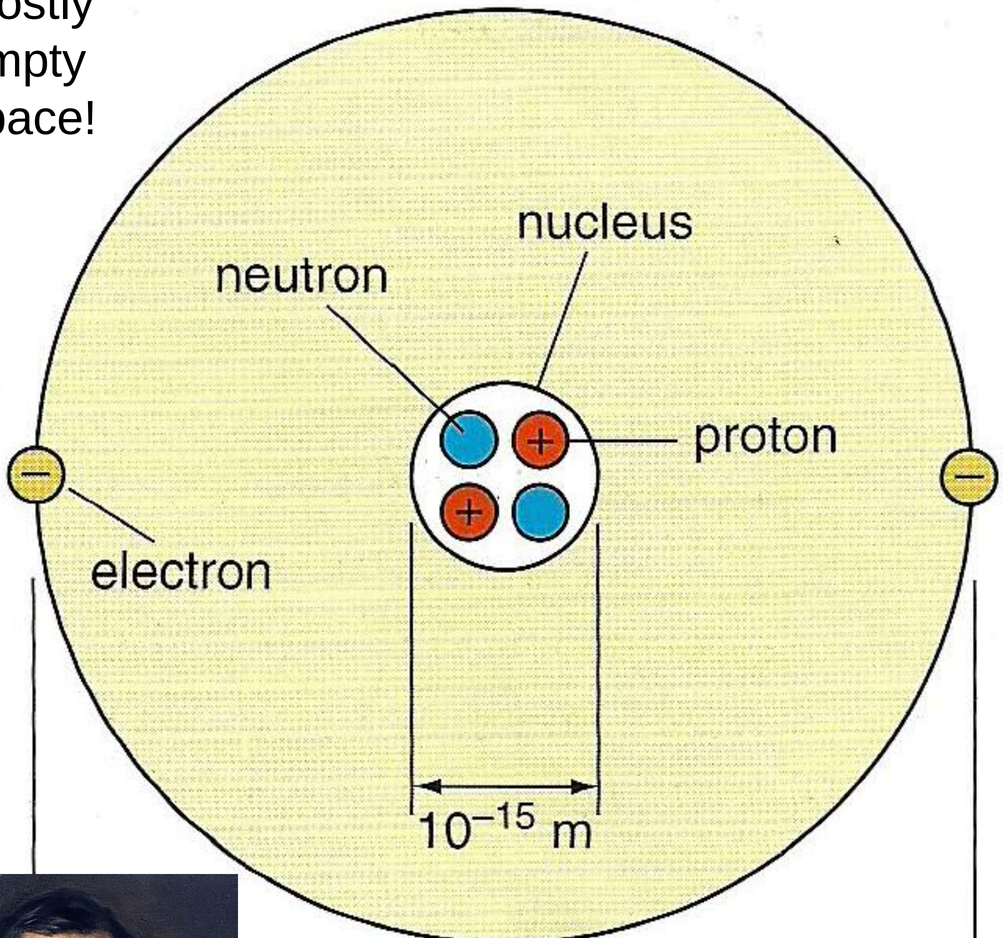
$$\left(\frac{3.6\times10^{-2}}{1\times10^{-10}}\right)^{3}\approx 4.7\times10^{25}$$

Number of atoms in a marble

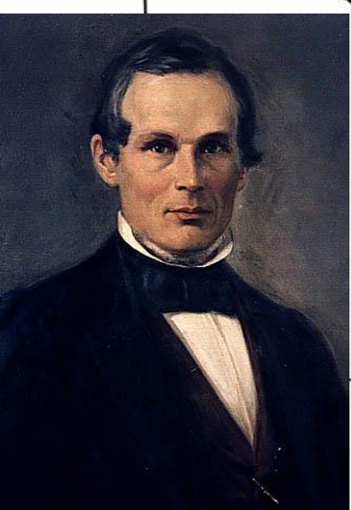
There are as many atoms in a marble as an Earth made of marbles!

Atomic mass and density

Mostly empty space!



This is one Ångström



Anders Ångström
1814-1874

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

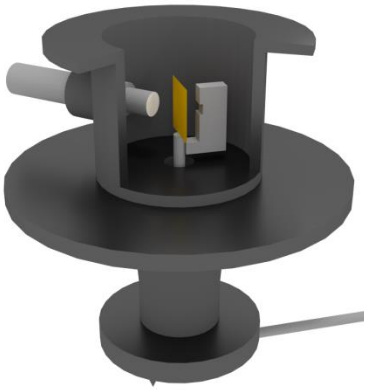
$$m_p = 1.673 \times 10^{-27}\,\mathrm{kg}$$

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

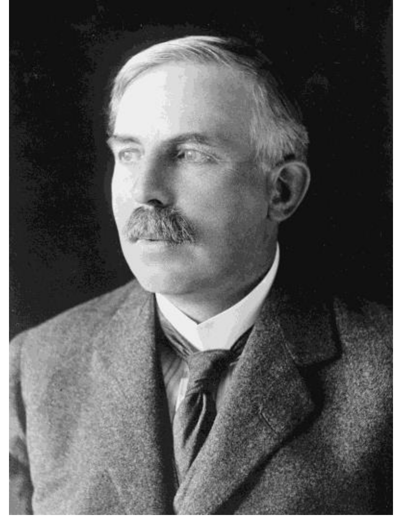
$$\rho \approx \frac{1.673 \times 10^{-27}\,\mathrm{kg}}{\frac{4}{3}\pi \times \left(\frac{1}{2} \times 10^{-10}\right)^3}$$

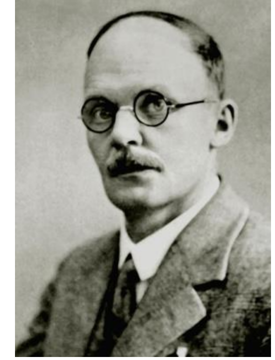
$$\rho \approx 3{,}200\,\mathrm{kgm^{-3}}$$

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



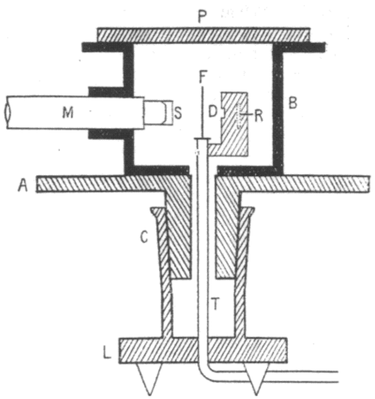
Ernest
Rutherford
1871-1937





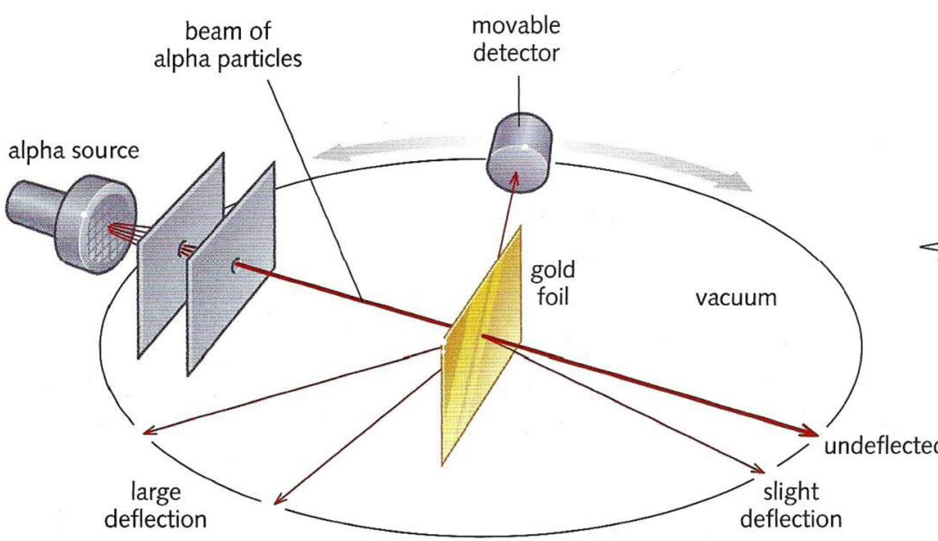
Hans
Geiger

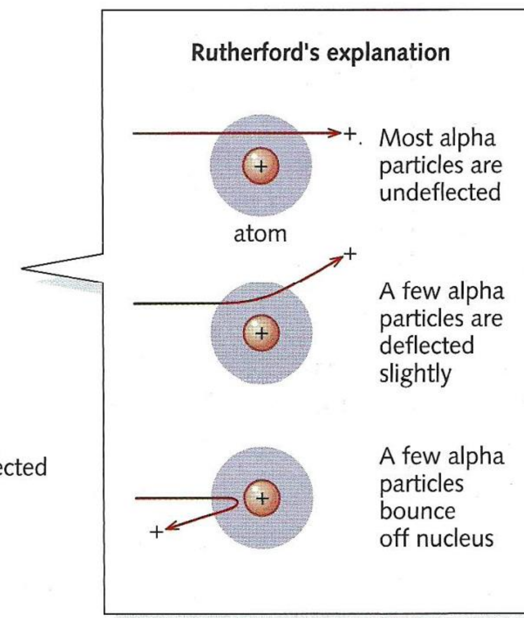
Ernest
Marsden



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





NUCLEAR BINDING ENERGY

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

$$B = a_V A - a_S A^{2/3} - a_C \frac{Z^2}{A^{1/3}} - a_A \frac{(A-2Z)^2}{A} + \delta(A,Z)$$

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

$$a_V = 15.76\,\text{MeV}$$

$$a_S = 17.81\,\text{MeV}$$

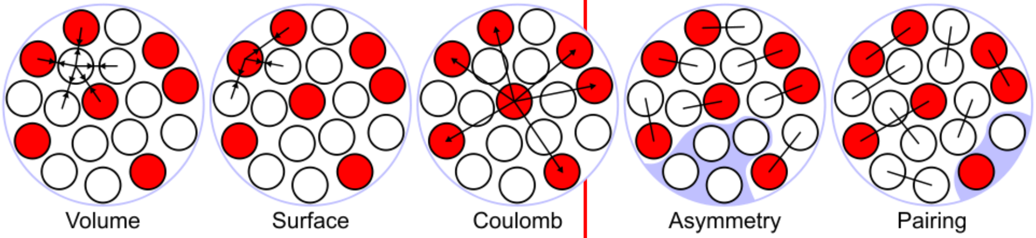
$$a_C = 0.711\,\text{MeV}$$

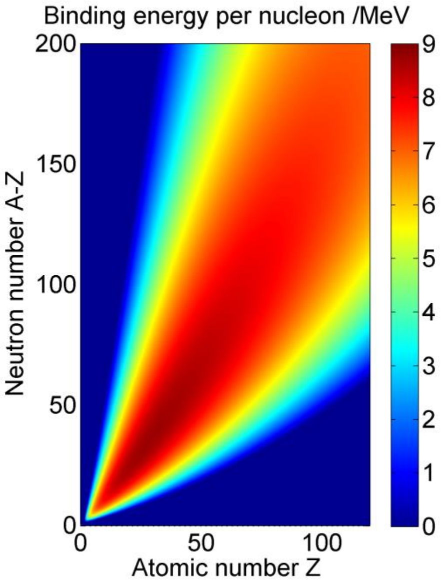
$$a_A = 23.702\,\text{MeV}$$

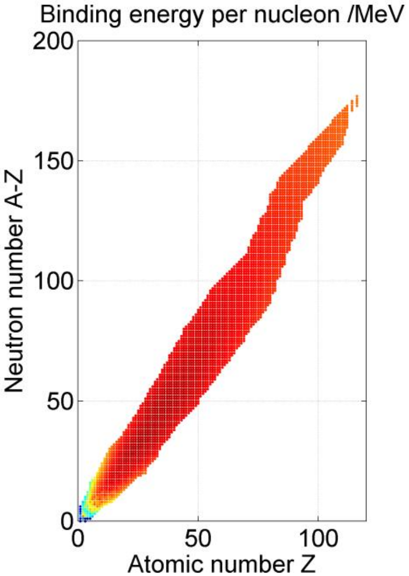
$$a_P = 34.0\,\text{MeV}$$

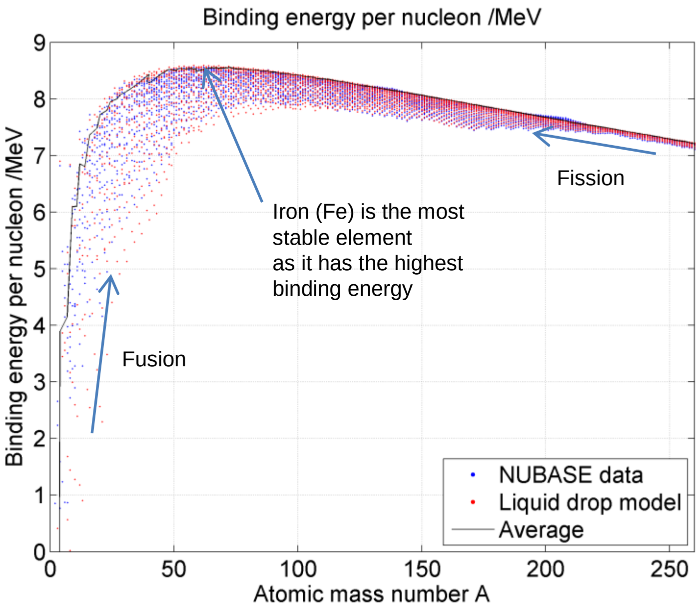
$${}^{A}_{Z}M \xrightarrow{B} Z \times \text{p} + (A-Z) \times \text{n}$$

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



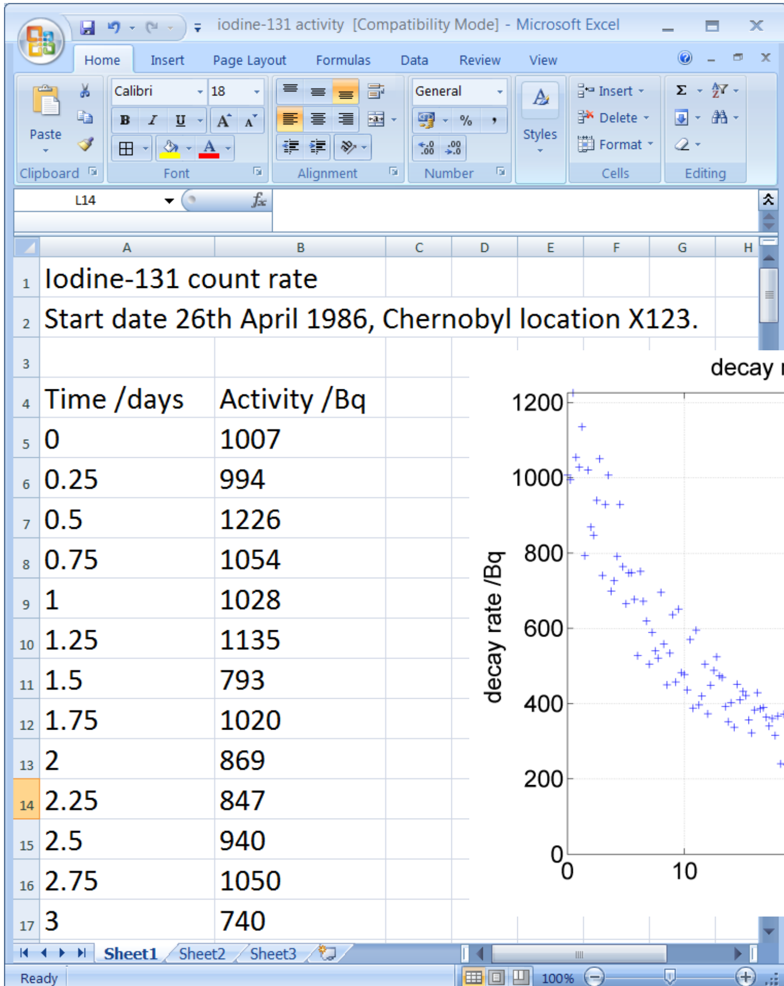






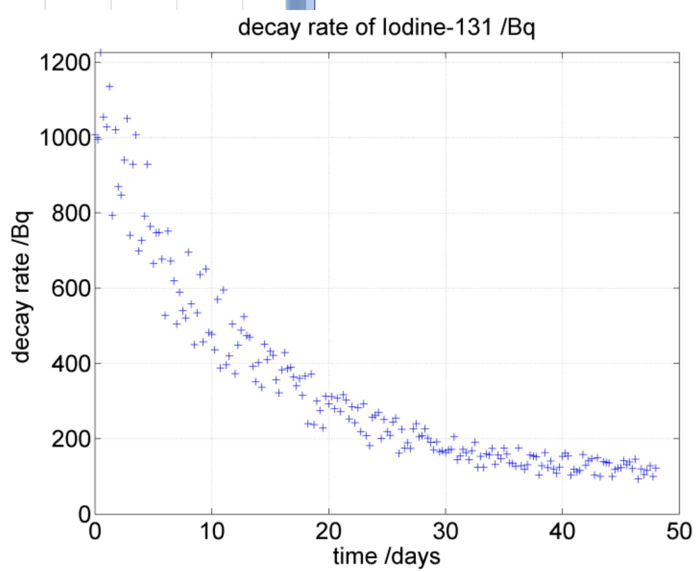
RADIOACTIVITY

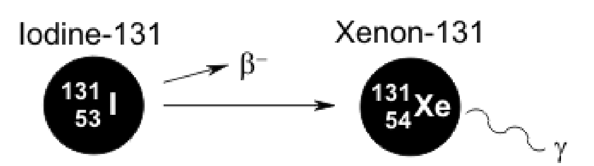
You are a soviet nuclear physicist sent to help with the Chernobyl disaster in 1986. You need to determine the presence of an isotope from its half life, but background levels are huge.... All you have is a text file of count rates. Your military commander demands results as soon as possible.



Iodine-131 count rate
Start date 26th April 1986, Chernobyl location X123.

Time /days	Activity /Bq
0	1007
0.25	994
0.5	1226
0.75	1054
1	1028
1.25	1135
1.5	793
1.75	1020
2	869
2.25	847
2.5	940
2.75	1050
3	740





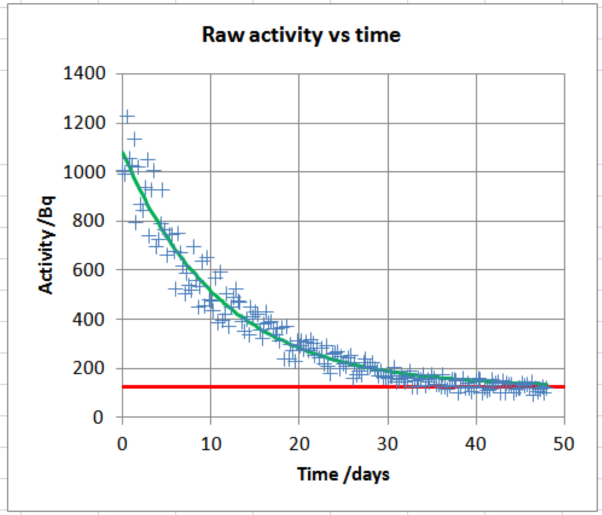
PERFORM ANALYSIS IN EXCEL

Iodine-131 count rate

Start date 26th April 1986, Chernobyl location X123.

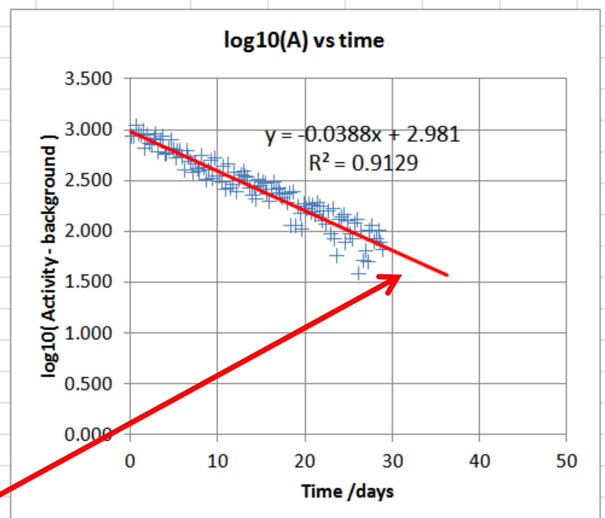
Time /days	Activity /Bq	A = Activity - Background	log10(A)	Model Activity /Bq
0	1007	884	2.946	1080.2
0.25	994	871	2.940	1059.1
0.5	1226	1103	3.043	1038.4
0.75	1054	931	2.969	1018.2
1	1028	905	2.957	998.39
1.25	1135	1012	3.005	979.05
1.5	793	670	2.826	960.14
1.75	1020	897	2.953	941.65
2	869	746	2.873	923.57
2.25	847	724	2.860	905.89
2.5	940	817	2.912	888.6
2.75	1050	927	2.967	871.69
3	740	617	2.790	855.15
3.25	929	806	2.906	838.98
3.5	1007	884	2.946	823.16
3.75	699	576	2.760	807.7
4	726	603	2.780	792.58
4.25	791	668	2.825	777.79
4.5	929	806	2.906	763.32
4.75	764	641	2.807	749.18
5	665	542	2.734	735.35
5.25	747	624	2.795	721.83
5.5	748	625	2.796	708.6
5.75	677	554	2.744	695.66
6	527	404	2.606	683.02
6.25	751	628	2.798	670.65
6.5	672	549	2.740	658.55
6.75	619	496	2.695	646.72
7	505	382	2.582	635.15
7.25	589	466	2.668	623.84
7.5	540	417	2.620	612.78
7.75	521	398		
8	695	572		
8.25	558	435		
8.5	450	327		
8.75	534	411		

NOTE IGNORE DATA AFTER 28.75 DAYS FOR BEST FIT



m	-0.039
c	2.981

Half life /days	7.759
A0 /Bq	957.2



Note this estimate is slightly different to the 100Bq used in the subsequent MATLAB analysis

Estimate background level /Bq

123

Time /days	Activity /Bq
0	123
50	123

$$A = \frac{A_0}{2^{t/t_{1/2}}}$$

$$\log_{10} A = \log_{10} A_0 - \log_{10}\left(2^{t/t_{1/2}}\right)$$

$$\log_{10} A = \log_{10} A_0 - \frac{t}{t_{1/2}}\log_{10} 2$$

$$y = \log_{10} A$$

$$x = t$$

$$y = mx + c$$

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

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

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

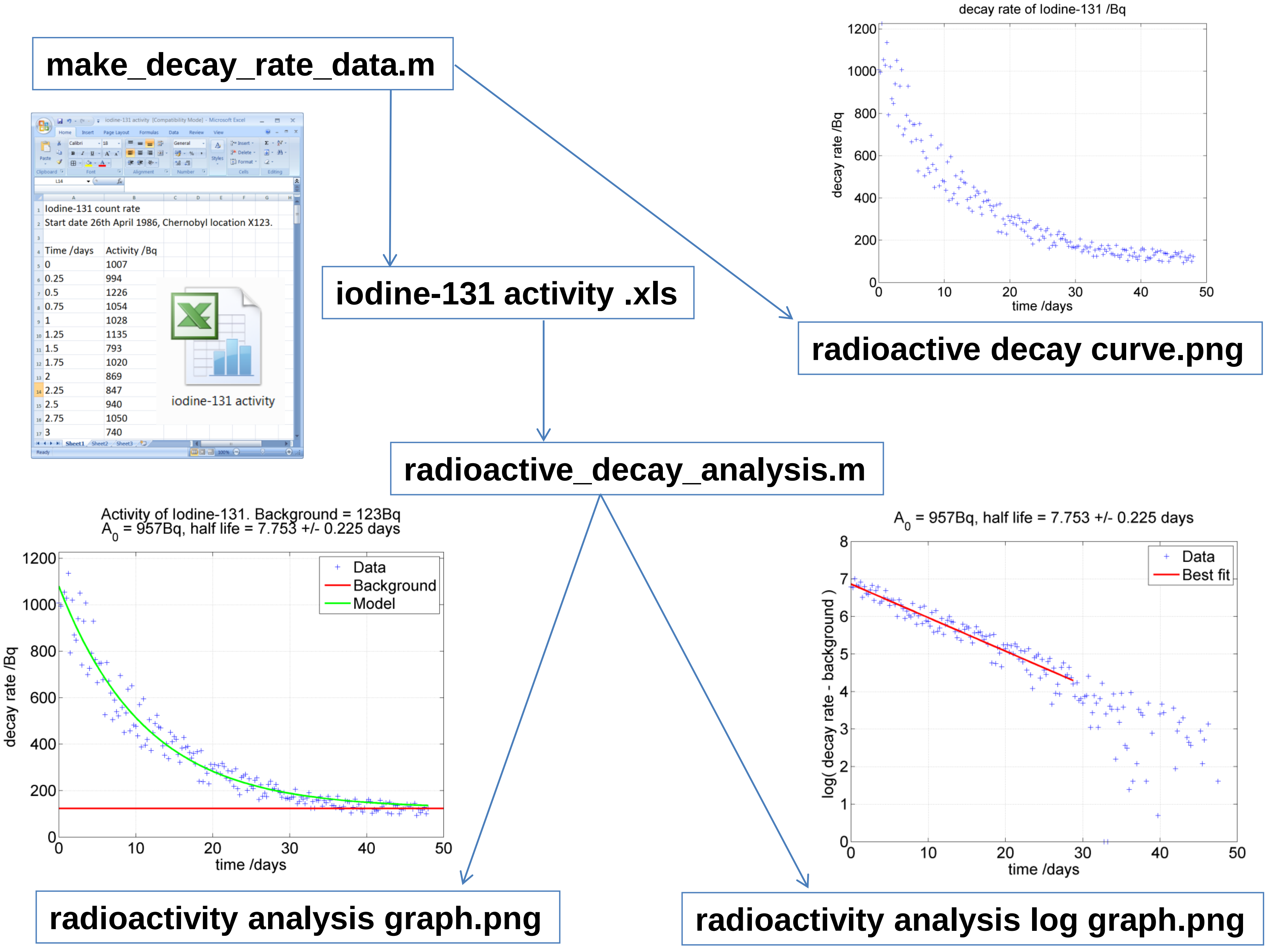
E:\Programming\A Course in Coding\2. MATLAB\Short Scientific Computing Course\1. The Signal and the Noise\radioactive_decay_analysis.m

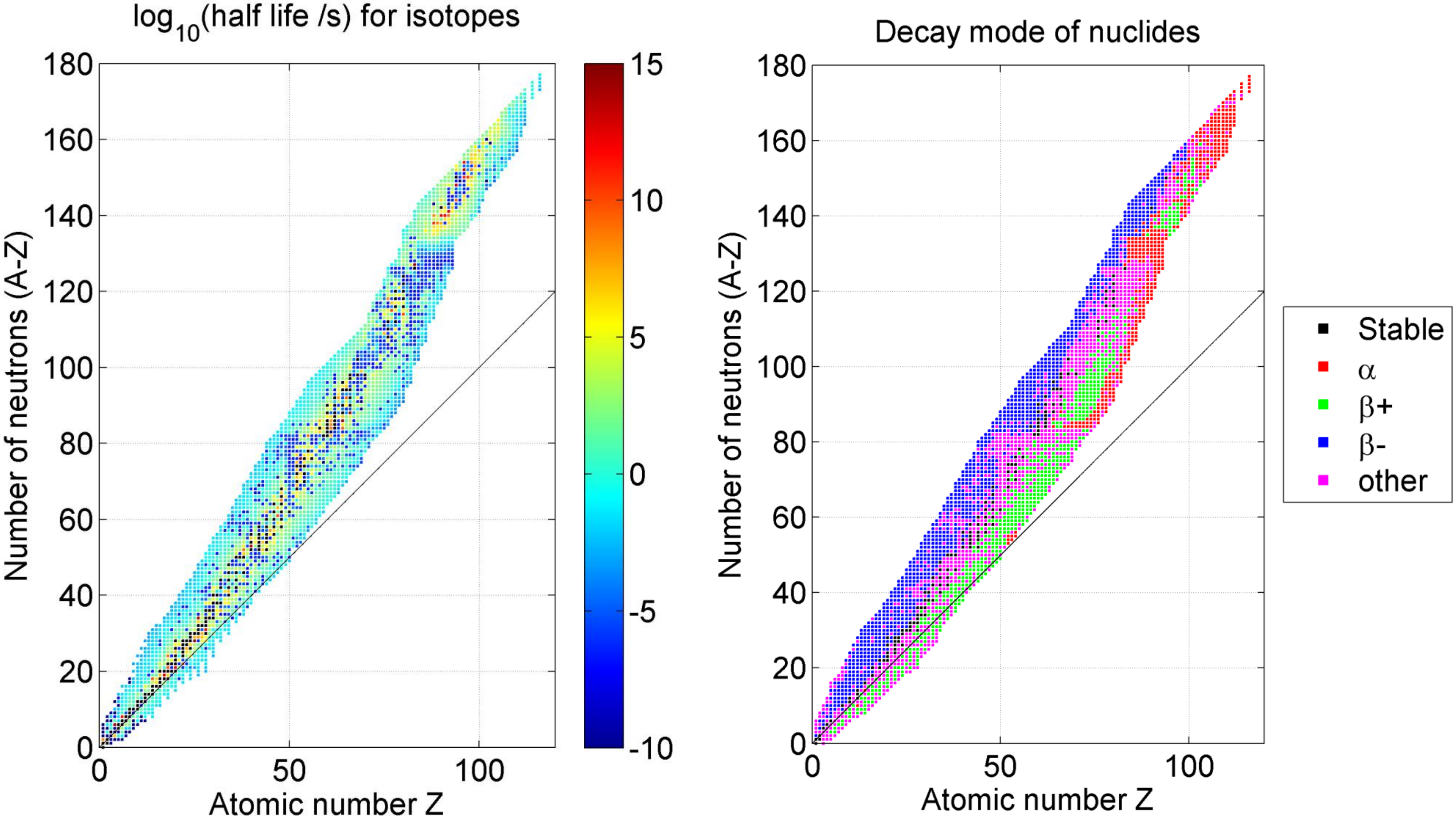
File Edit Text Go Cell Tools Debug Desktop Window Help

Stack: Base

```matlab
%radioactive_decay_analysis
% Analysis of Iodine-131 decay rate vs time data.
%
% LAST UPDATED by Andy French June 2019

function radioactive_decay_analysis

%Estimated background rate /Bq
B = 100;

%Fontsize for graphs
fsize = 18;

%

%Ingest Excel file of activity vs time
[num,txt,raw] = xlsread( 'iodine-131 activity.xls' );

%Extract vectors for time /days and activity /Bq
t = num(:,1); A = num(:,2);

%Plot activity vs time
fig1 = figure('color',[1 1 1],'name','radioactive decay curve');
plot(t,A,'+');
xlabel('time /days','fontsize',fsize);
ylabel('decay rate /Bq ','fontsize',fsize);
set(gca,'fontsize',fsize);
grid on; ylim([0,max(A)]);

%Overlay background level
xlimits = get( gca, 'xlim' ); hold on; plot( xlimits,[B,B],'r-' );

```

radioactive_decay_analysis.m

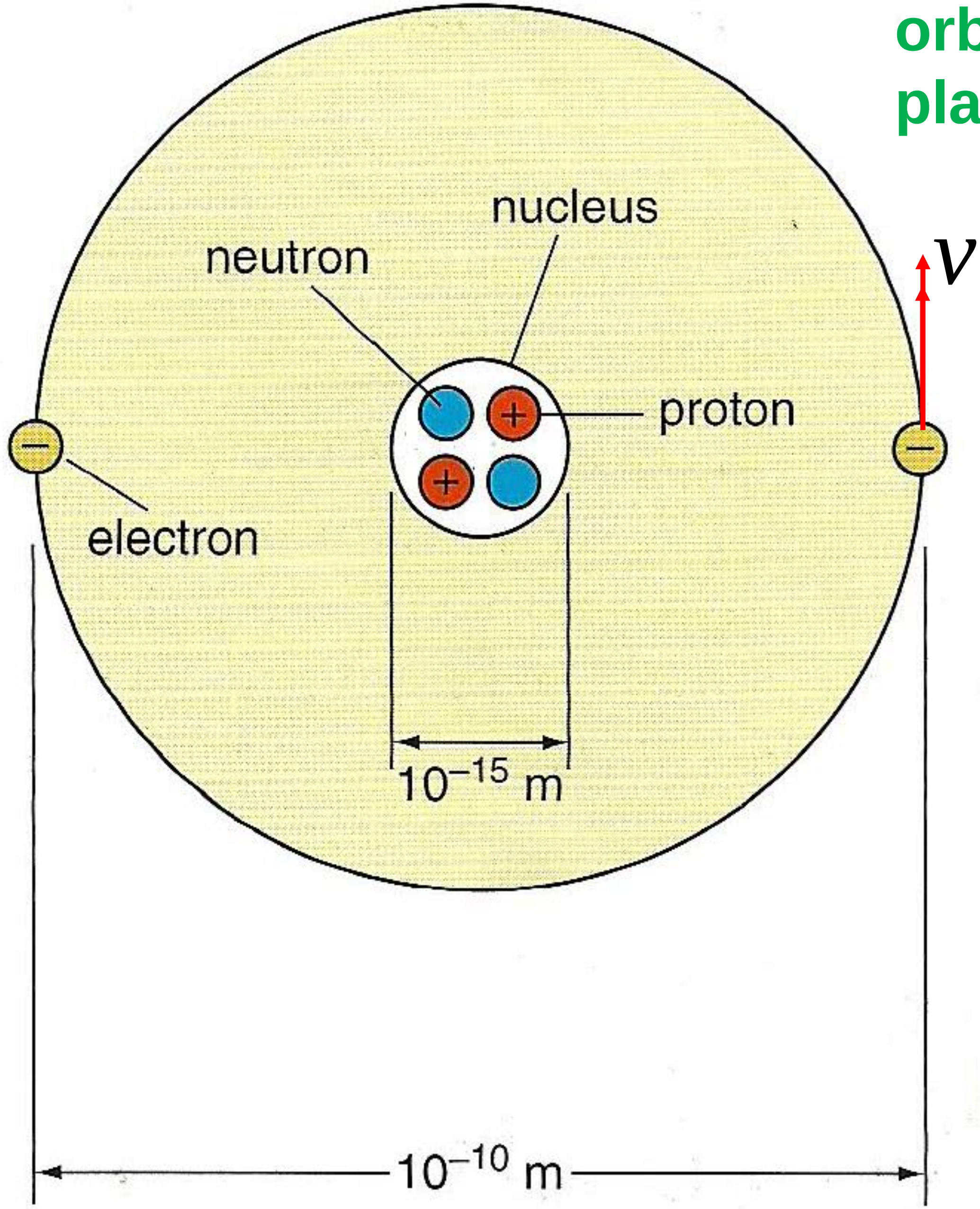

make_decay_rate_data.m
iodine-131 activity .xls
radioactive decay curve.png
radioactive_decay_analysis.m
radioactivity analysis graph.png
radioactivity analysis log graph.png
Iodine-131 count rate
Start date 26th April 1986, Chernobyl location X123.
Time /days Activity /Bq
0 1007
0.25 994
0.5 1226
0.75 1054
1 1028
1.25 1135
1.5 793
1.75 1020
2 869
2.25 847
2.5 940
2.75 1050
3 740
iodine-131 activity
decay rate of Iodine-131 /Bq
decay rate /Bq
time /days
Activity of Iodine-131. Background = 123Bq
A0 = 957Bq, half life = 7.753 +/- 0.225 days
Data
Background
Model
A0 = 957Bq, half life = 7.753 +/- 0.225 days
log(decay rate - background)
Best fit

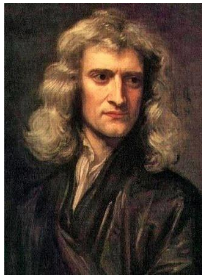


log10(half life /s) for isotopes
Number of neutrons (A-Z)
Atomic number Z
180
160
140
120
100
80
60
40
20
0
0
50
100
15
10
5
0
-5
-10
Decay mode of nuclides
Number of neutrons (A-Z)
Atomic number Z
Stable
α
β+
β-
other

… Back to the atom!

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





Gravity fields

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

$$F_E = \frac{Qq}{4\pi\varepsilon_0 r^2}$$

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!

$$\dot{E} = \frac{dE}{dt} = -\frac{e^2}{6\pi\varepsilon_0 c^3} a^2$$

Radiated power

$$\tau = \frac{\frac{1}{2} m_e v^2}{\left|\dot{E}\right|}$$

'electron lifetime'

$$\dot{E} = -\frac{e^2}{6\pi\varepsilon_0 c^3} \times \left(\frac{Ze^2}{4\pi\varepsilon_0 m_e r^2} \right)^2$$

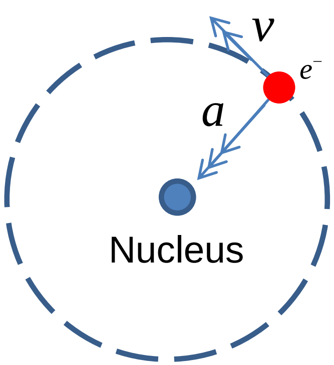
$$\therefore \dot{E} = -\frac{Z^2 e^6}{96\pi^3 \varepsilon_0^3 c^3 m_e^2 r^4}$$

$$\tau = \frac{Ze^2}{8\pi\varepsilon_0 r} \times \frac{96\pi^3 \varepsilon_0^3 c^3 m_e^2 r^4}{Z^2 e^6}$$

$$\tau = \frac{12\pi^2 \varepsilon_0^2 c^3 m_e^2 r^3}{Ze^4}$$

$$\tau \approx \boxed{4.7 \times 10^{-11}\,\mathrm{s}}$$

$$\varepsilon_0 = 8.854187817 \times 10^{-12}\,\mathrm{Fm}^{-1}$$
$$e = 1.6021766208(98) \times 10^{-19}\,\mathrm{C}$$
$$c = 2.99792458 \times 10^{8}\,\mathrm{ms}^{-1}$$
$$m_e = 9.10938356(11) \times 10^{-31}\,\mathrm{kg}$$



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

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

Radiation power per square metre → I

Emmisivity → ε

Stefan-Boltzmann constant → σ

Absolute temperature /K → T

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

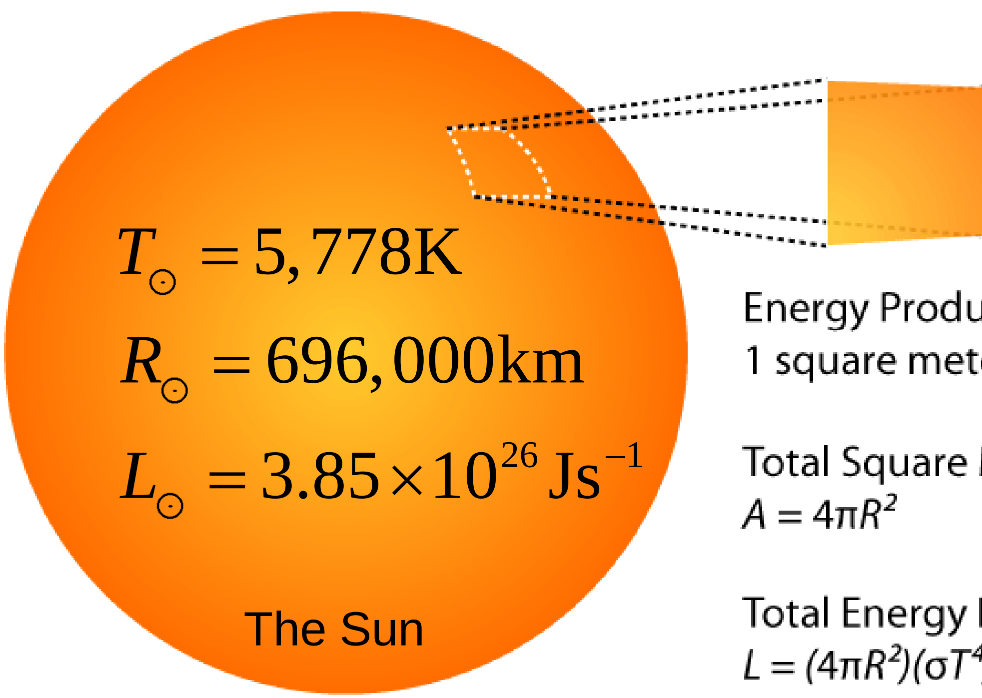
$$\varepsilon = 1$$

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

For a ‘Black Body’ at 20^{o}C = 293K

$$I = 418\,\mathrm{Wm^{-2}}$$

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



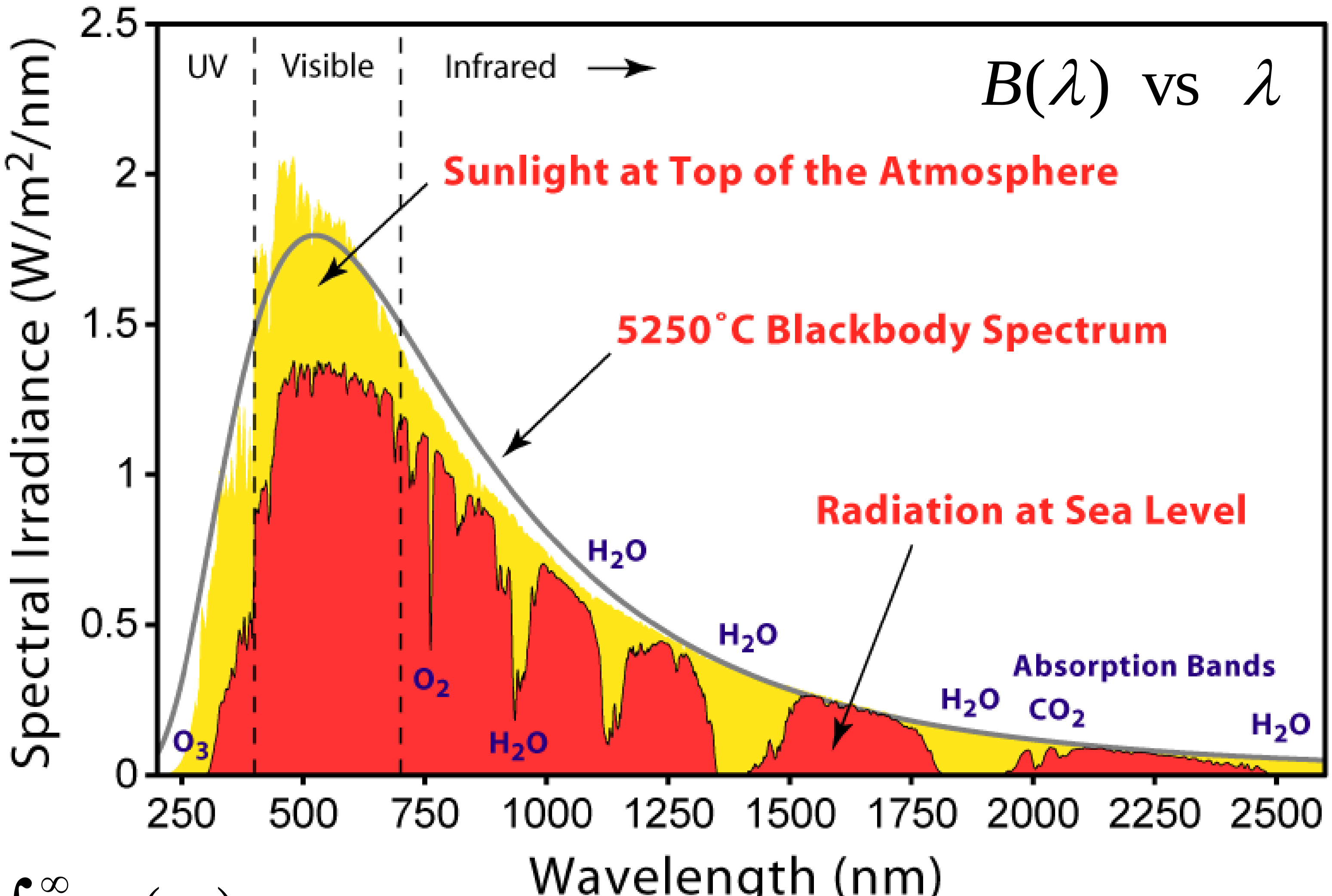
Energy Produced by 1 square meter = σT^4

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

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

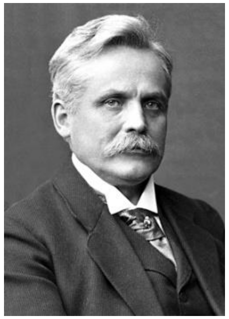
The measured solar irradiance (i.e. power received on Earth per square metre within a wavelength interval i.e. $\lambda \rightarrow \lambda + d\lambda$

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



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

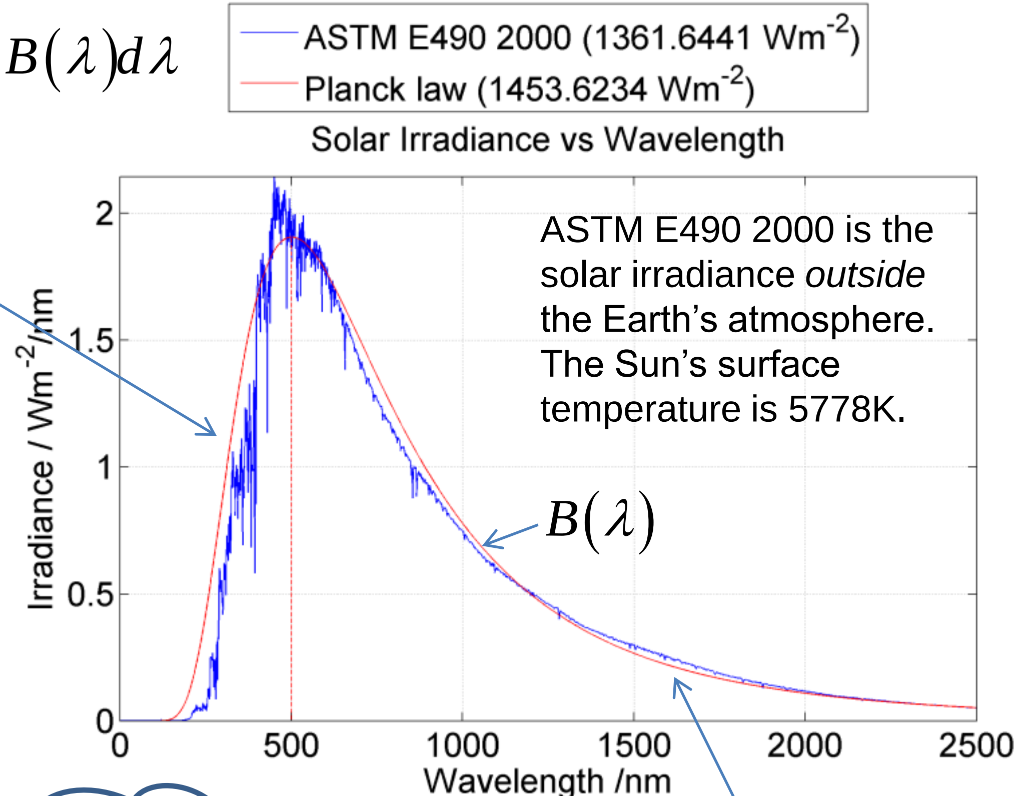
$$I = \int_0^\infty B(\lambda)d\lambda$$

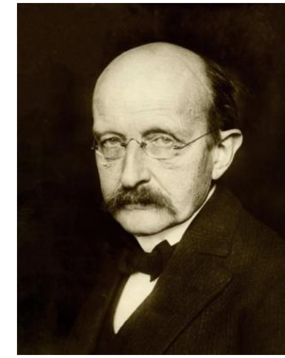


Wilhelm Wien
1864-1928

Predicted the short wavelength part well.....

But not the spectrum at long wavelengths

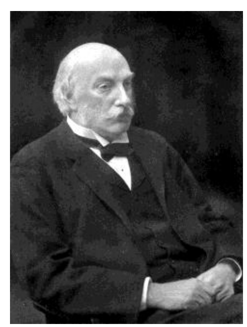




Max Planck 'guessed' what the law should be. But this led to a strange conclusion .....

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

Max Planck
1858 – 1947



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

Let's start from the Rayleigh-Jeans analysis

$$I = \sigma T^4 = \tfrac{1}{4} uc$$

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

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

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

$$f \to f + df$$

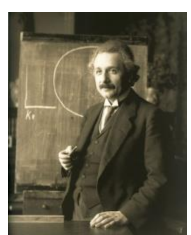
But $\bar{E} = \tfrac{3}{2} k_B T$ means

$$I = \infty$$

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

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

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



I worked this out!

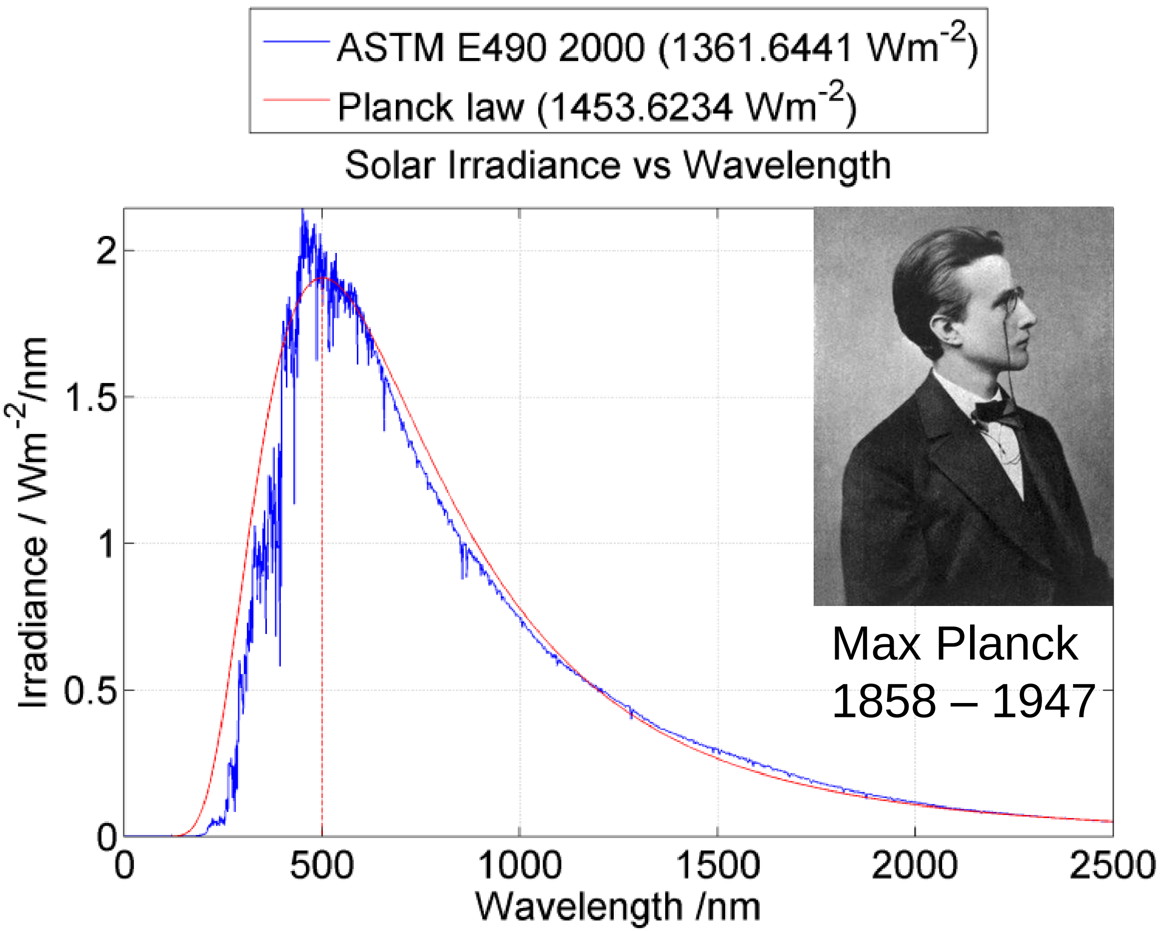
Ludwig
Boltzmann
1844-1906

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

Boltzmann's constant $k_B = 1.381\times10^{-23}\,\mathrm{m^2kgs^{-2}K^{-1}}$

Planck's constant $h = 6.626\times10^{-34}\,\mathrm{m^2kgs^{-1}}$

Speed of light $c = 2.998\times10^{8}\,\mathrm{ms^{-1}}$



Max Planck
1858 – 1947

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

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

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

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

$$E = hf$$

PHOTO ELECTRIC EFFECT

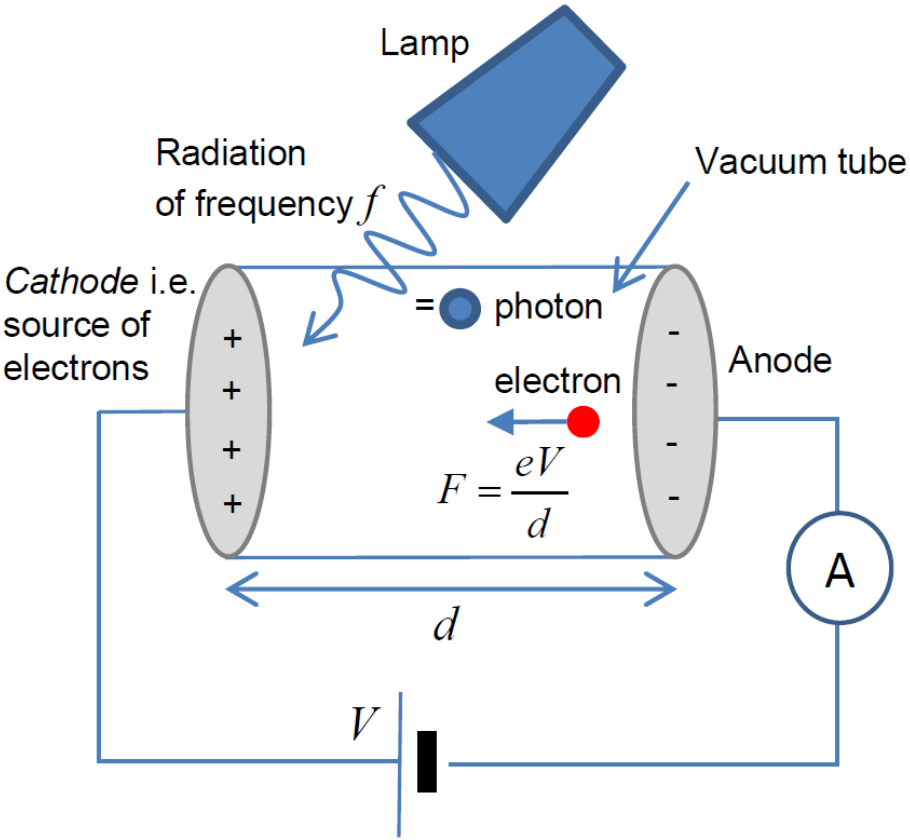
Maximum Kinetic energy of emitted electrons

$$E = hf - W$$

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 'cuttoff' frequency causes surfaces to emit electrons.

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

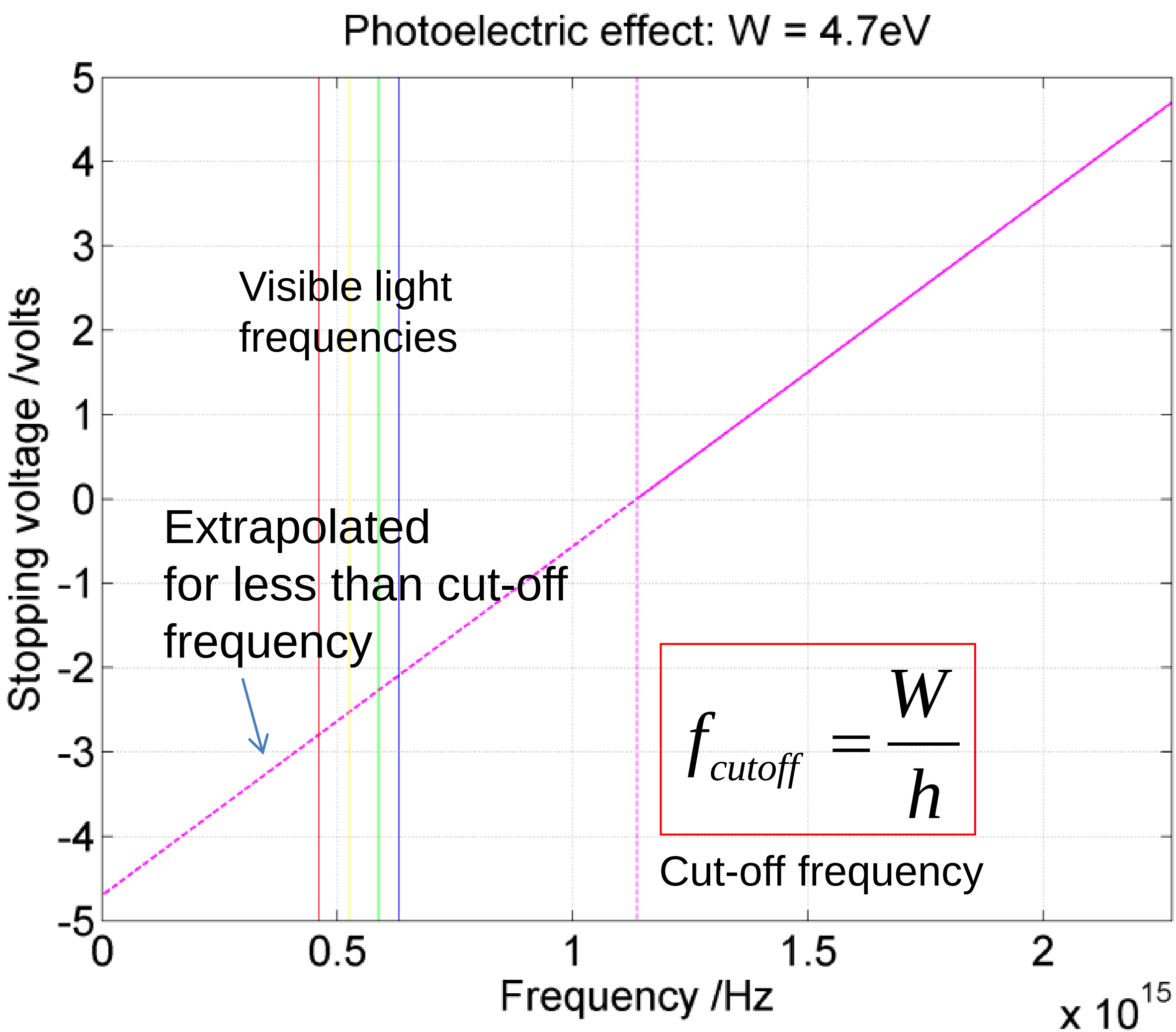
This is *not* a classical prediction!

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

$$eV = E = hf - W$$

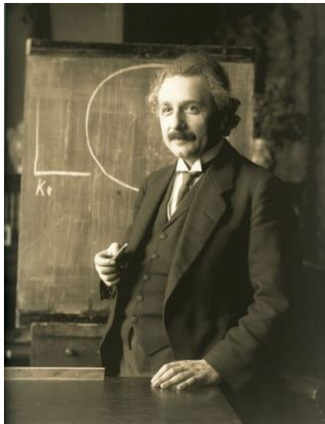
$$\therefore V = \frac{h}{e} f - \frac{W}{e}$$

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



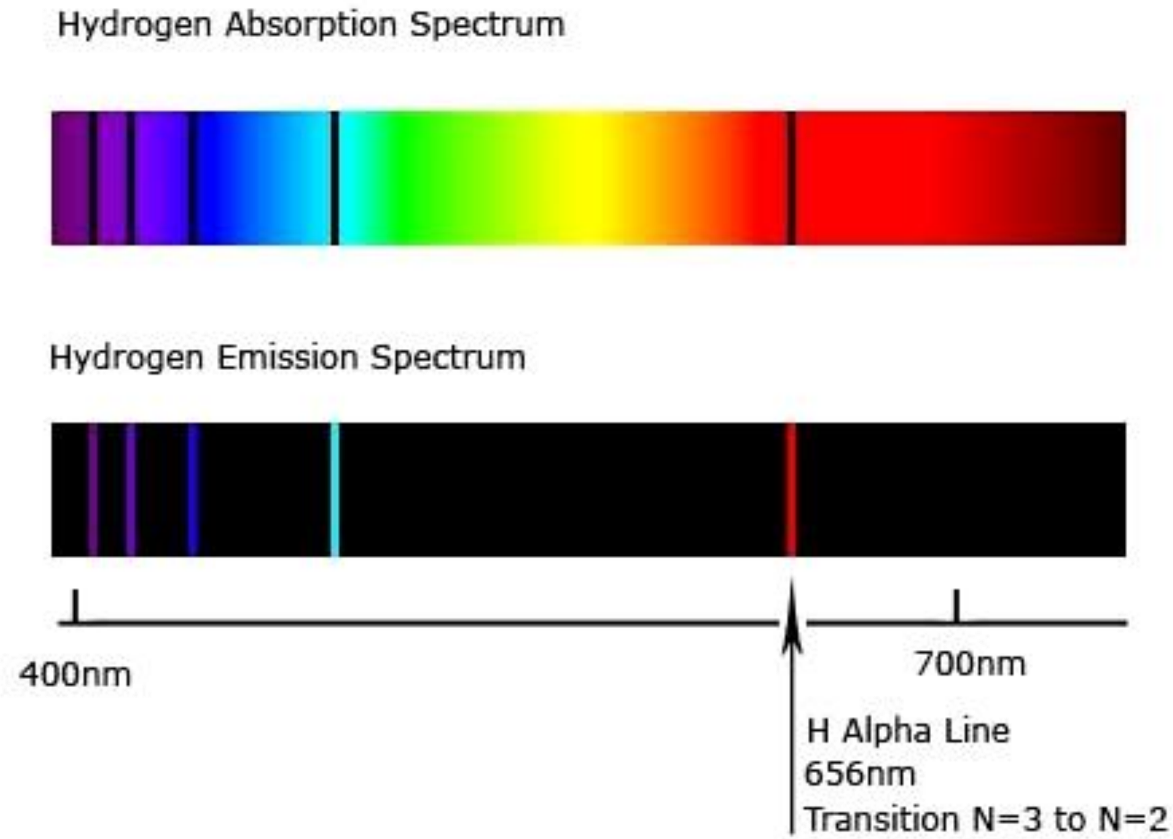
Material	Work function /eV
Silver (Ag)	4.3
Aluminium (Al)	4.3
Gold (Au)	5.1
Copper (Cu)	4.7
Tin (Sn)	4.4
Lead (Pb)	4.3
Tungsten (W)	4.5
Nickel (Ni)	4.6
Sodium (Na)	2.4

Albert Einstein 1879-1955



Yes, me again!

HYDROGEN SPECTRA

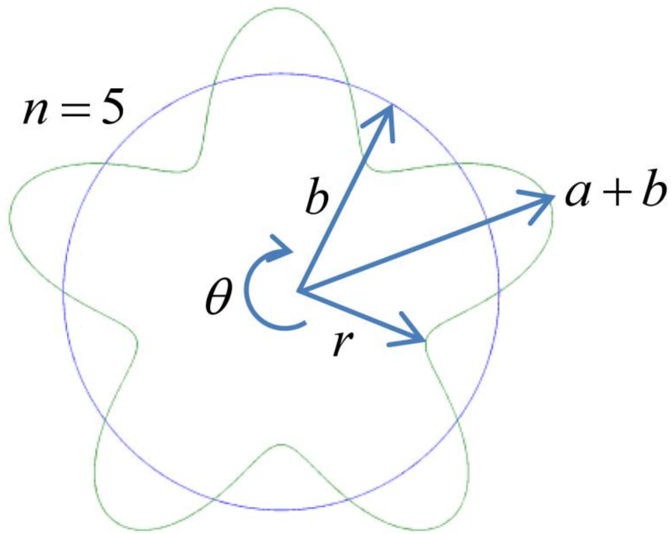


Johann Balmer
1825-1898

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

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

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



Louis de Broglie
1892 –1987

Niels Bohr
1885-1962

‘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**

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

$$E_n = -\frac{Ze^2}{8\pi\varepsilon_0 r_n}$$

Circular orbits, Coulomb force ...

$$\therefore E_n = -\frac{Ze^2}{8\pi\varepsilon_0} \times \frac{m_e Ze^2}{4\pi\varepsilon_0 n^2 \hbar^2}$$

for Hydrogen Z = 1

$$E_n = -\frac{m_e Z^2 e^4}{8\varepsilon_0^2 h^2}\frac{1}{n^2} \approx \frac{-13.6\text{eV}}{n^2}$$

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

$$hf_{nm} = \frac{m_e Z^2 e^4}{8\varepsilon_0^2 h^2}\left(\frac{1}{m^2} - \frac{1}{n^2}\right)$$

$$f_{nm} = \frac{m_e Z^2 e^4}{8\varepsilon_0^2 h^3}\left(\frac{1}{m^2} - \frac{1}{n^2}\right)$$

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

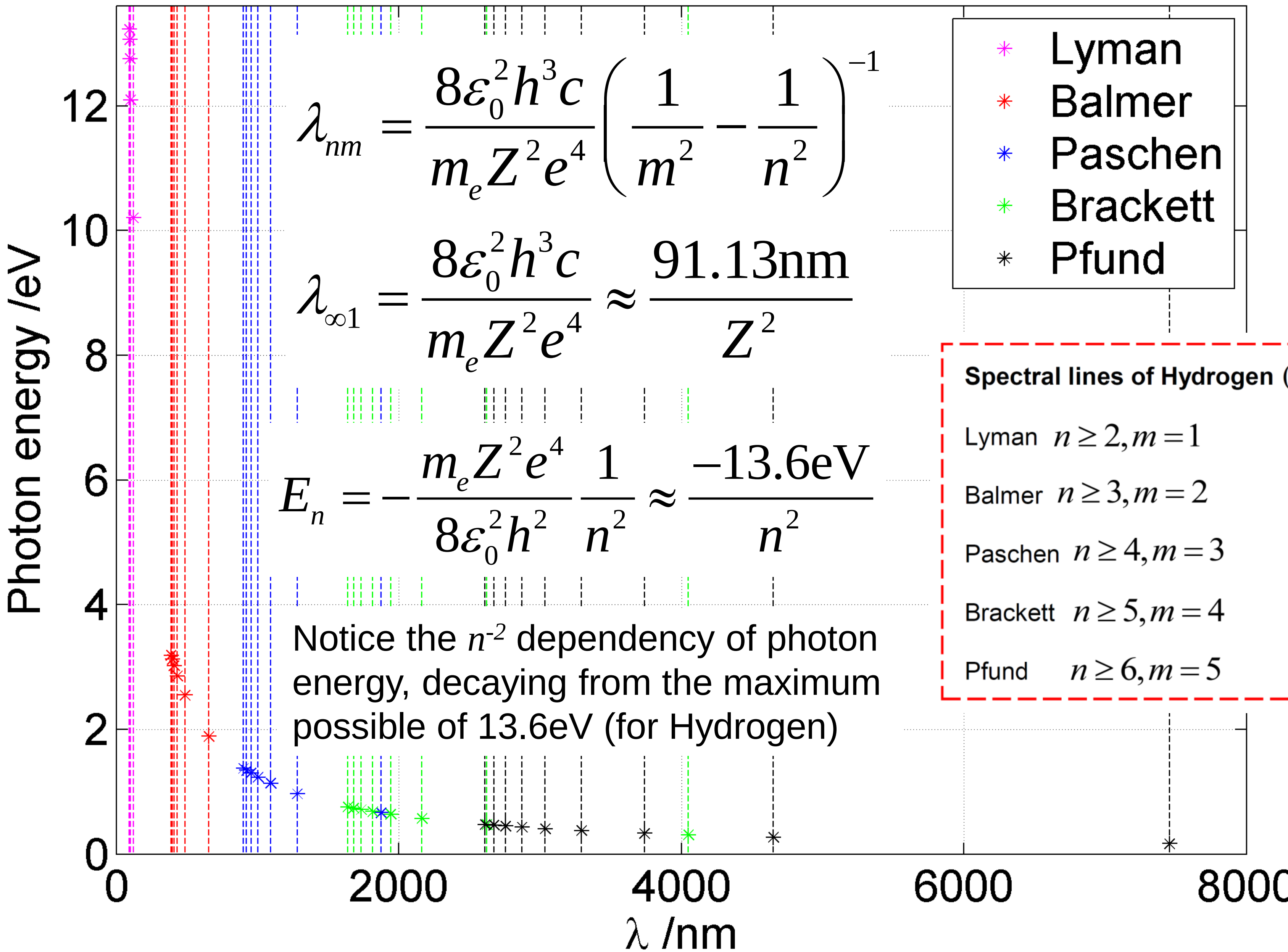
$$c = f_{nm}\lambda_{nm}$$

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

$$\lambda_{nm} = \frac{8\varepsilon_0^2 h^3 c}{m_e Z^2 e^4}\left(\frac{1}{m^2} - \frac{1}{n^2}\right)^{-1}$$

$$\lambda_{\infty 1} = \frac{8\varepsilon_0^2 h^3 c}{m_e Z^2 e^4} \approx \frac{91.13\text{nm}}{Z^2}$$

Bohr model of Hydrogenic atom photon emissions: Z = 1



$$\lambda_{nm} = \frac{8\varepsilon_0^2 h^3 c}{m_e Z^2 e^4}\left(\frac{1}{m^2} - \frac{1}{n^2}\right)^{-1}$$

$$\lambda_{\infty 1} = \frac{8\varepsilon_0^2 h^3 c}{m_e Z^2 e^4} \approx \frac{91.13\text{nm}}{Z^2}$$

$$E_n = -\frac{m_e Z^2 e^4}{8\varepsilon_0^2 h^2}\frac{1}{n^2} \approx \frac{-13.6\text{eV}}{n^2}$$

Notice the n^{-2} dependency of photon energy, decaying from the maximum possible of 13.6eV (for Hydrogen)

Spectral lines of Hydrogen $(Z=1)$

Lyman $n \geq 2, m = 1$

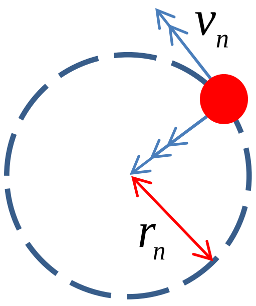
Balmer $n \geq 3, m = 2$

Paschen $n \geq 4, m = 3$

Brackett $n \geq 5, m = 4$

Pfund $n \geq 6, m = 5$

Orbital velocity



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

$$v_n = \frac{1}{n}\frac{\hbar m_e Z e^2}{m_e 4\pi\varepsilon_0 \hbar^2} = \frac{Ze^2}{4\pi\varepsilon_0\hbar}\frac{1}{n}$$

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

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

$$\alpha = \frac{e^2}{4\pi\varepsilon_0 \hbar c} \approx \frac{1}{137}$$

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

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

$$p = m_e v$$

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

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

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

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

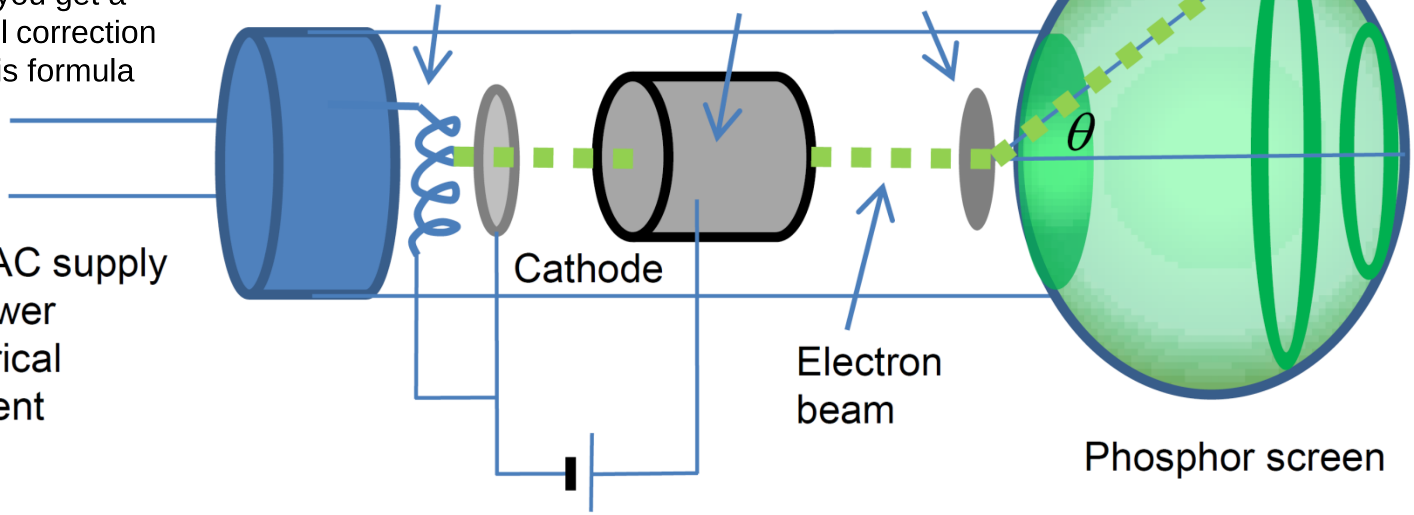
Louis de Broglie
1892 –1987

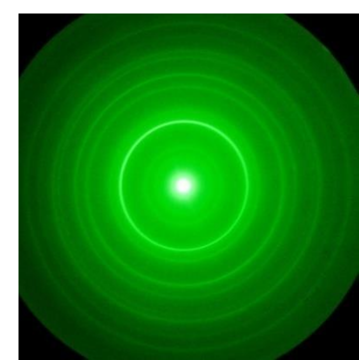
All particles have an associated wave

Lester Germer (right) with Clinton Davisson in 1927

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

wavelength (λ), Planck's constant (h), momentum (p)

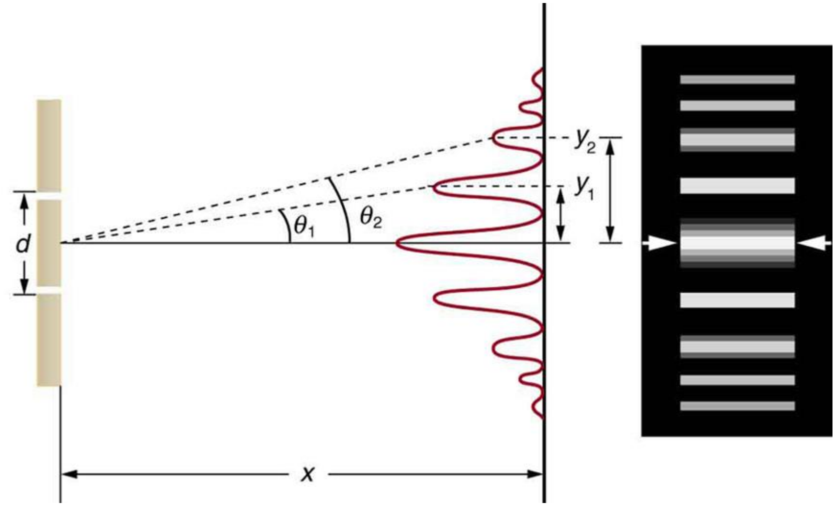




Thomas Young
1773-1829

Young's slits and photons

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



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

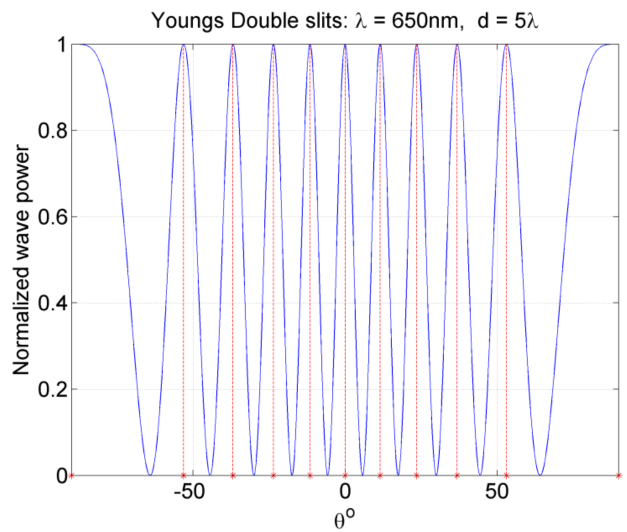
$$\psi(r,t) \approx \frac{2Ae^{i(kr-\omega t)}}{r}\cos\left(\tfrac{1}{2}kd\sin\theta\right)$$

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

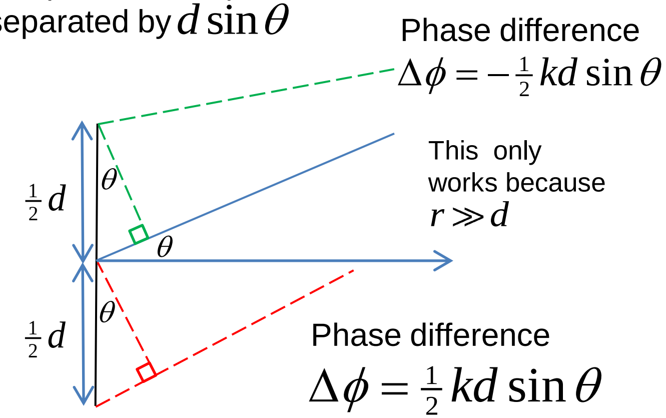
Hence *maxima* when

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

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



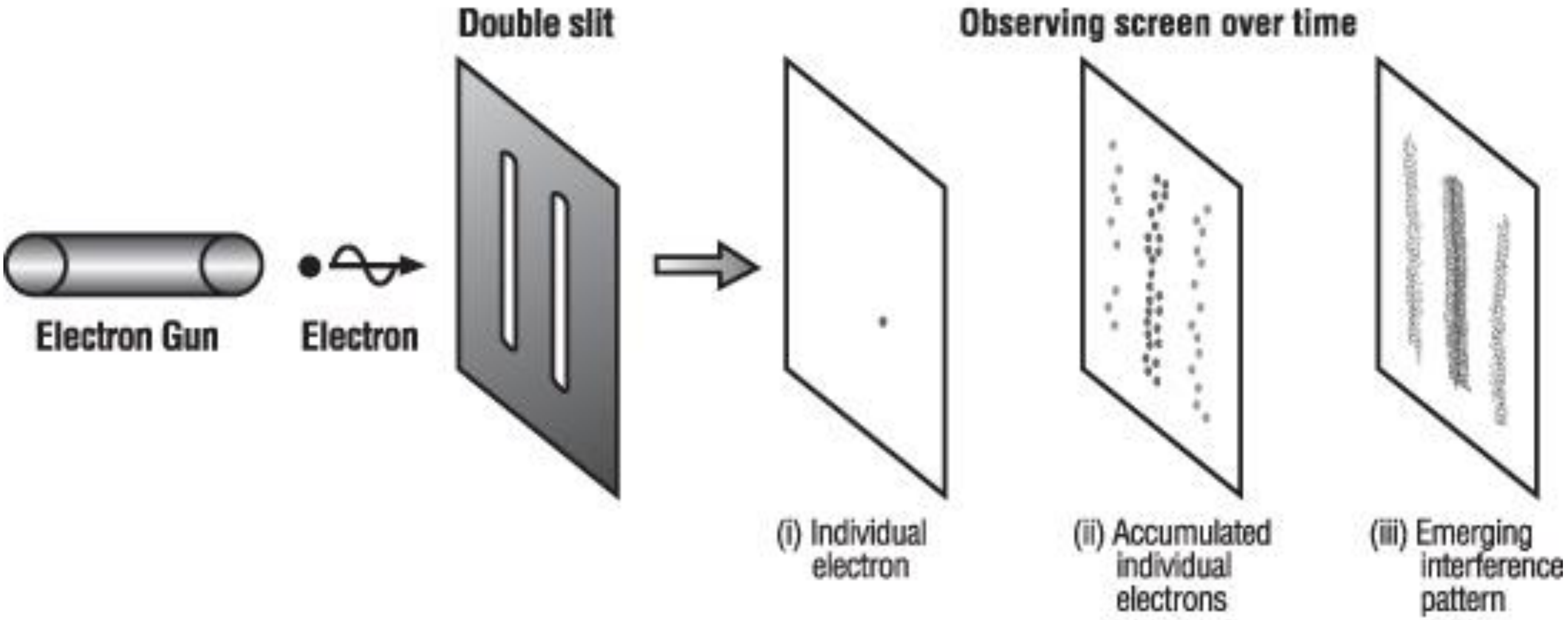
Equivalent geometry is wavelet sources are at the same angle (i.e. *plane waves*) but separated by $d\sin\theta$



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

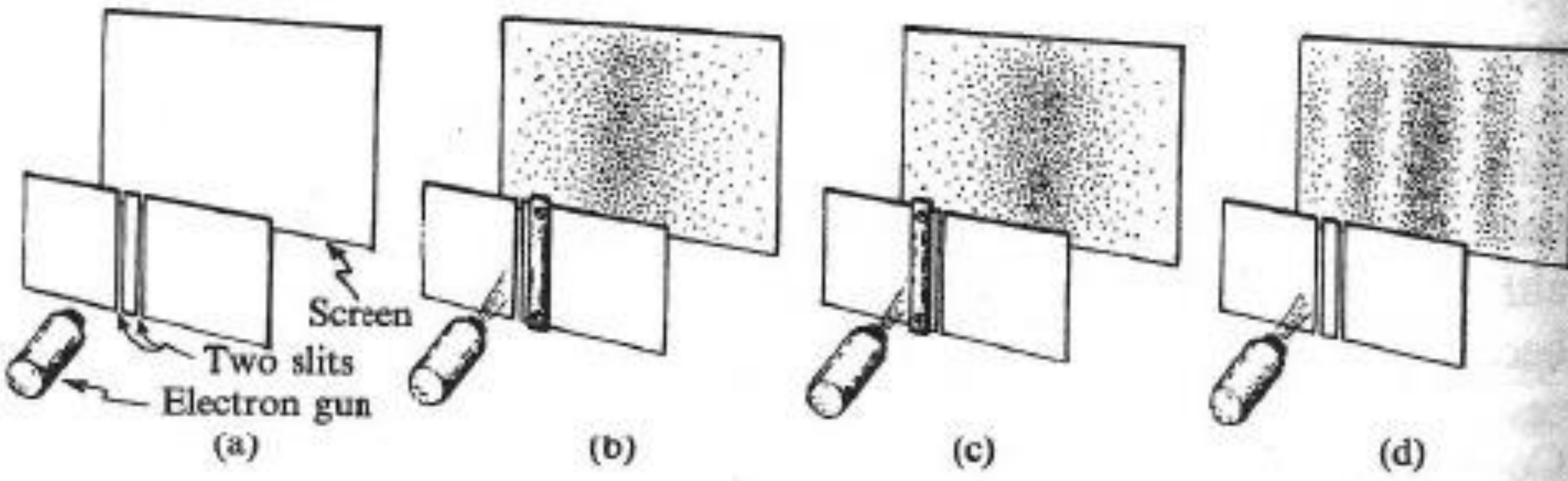
$$\lambda = \frac{h}{p}$$



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:

Wave amplitude

The wave equation

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

Conservation of energy

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

de-Broglie relation

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

Erwin Schrödinger
1887 – 1961

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

Erwin Schrödinger
1887 – 1961

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

Schrödinger Equation

Max Born
1882 – 1970

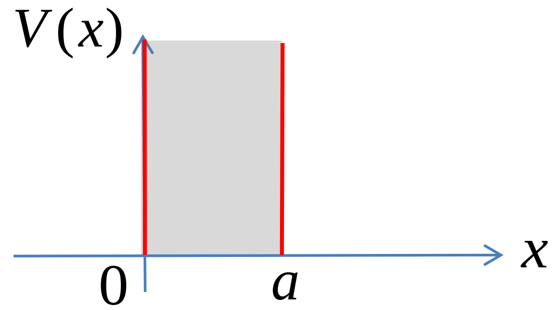
Born interpretation

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

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

Particle in a box

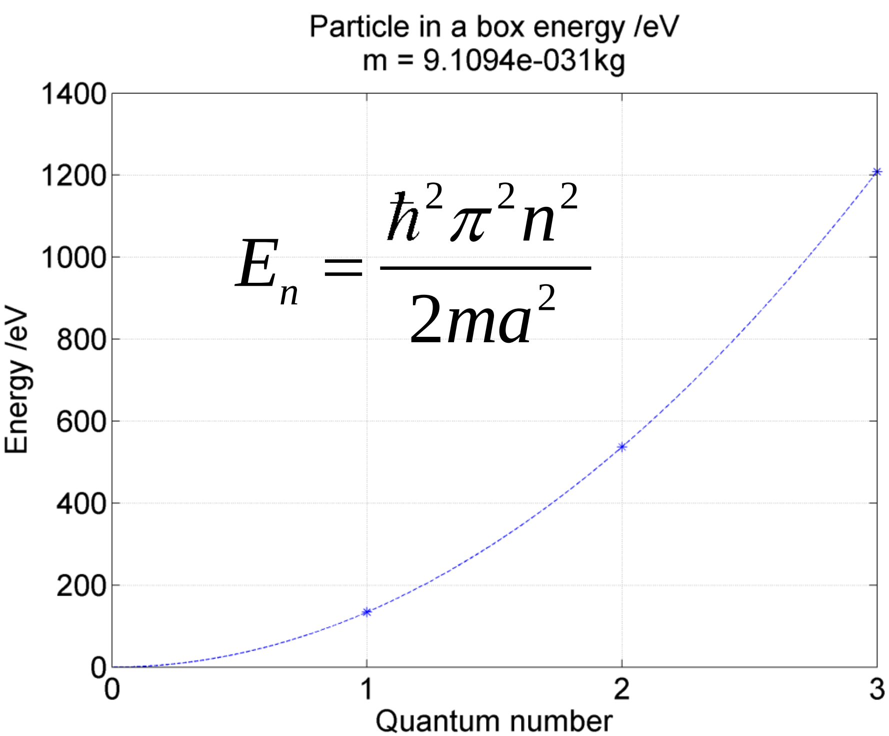
$$V(x) = \begin{cases} \infty & x \le 0,\ x \ge a \\ 0 & 0 < x < a \end{cases}$$



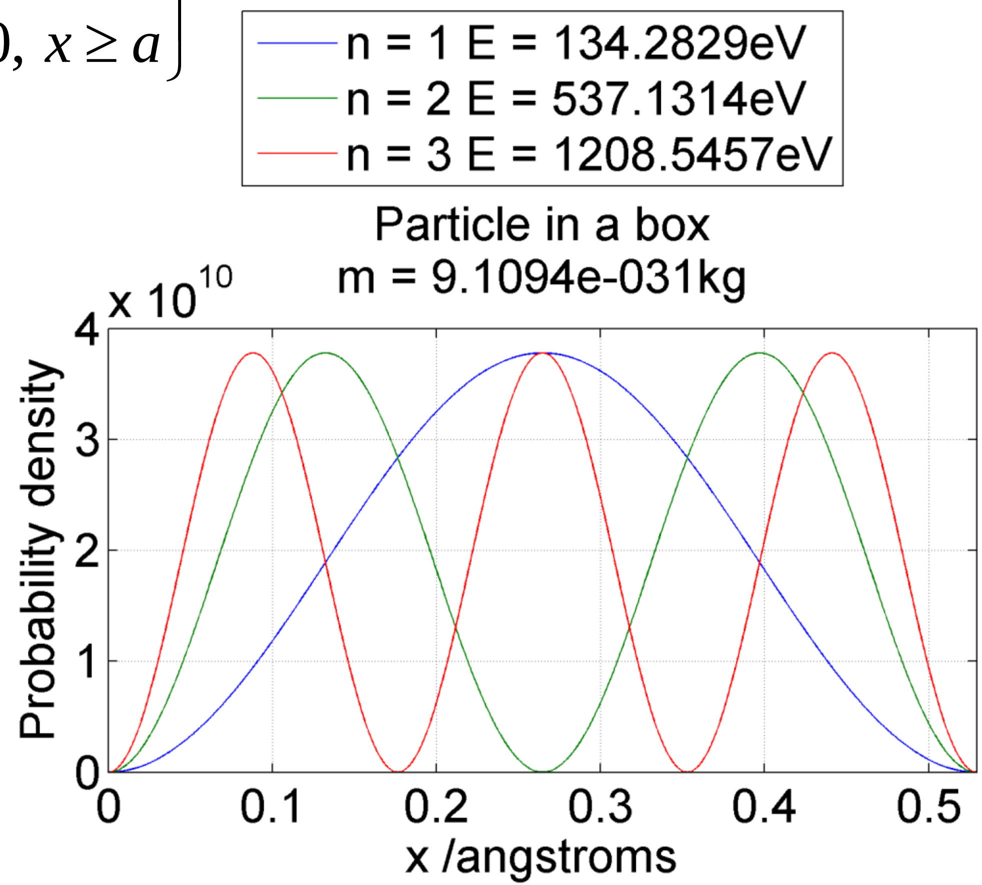
$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi = i\hbar\frac{\partial \psi}{\partial t}$$

Schrödinger Equation

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



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



Harmonic oscillator

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

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

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

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

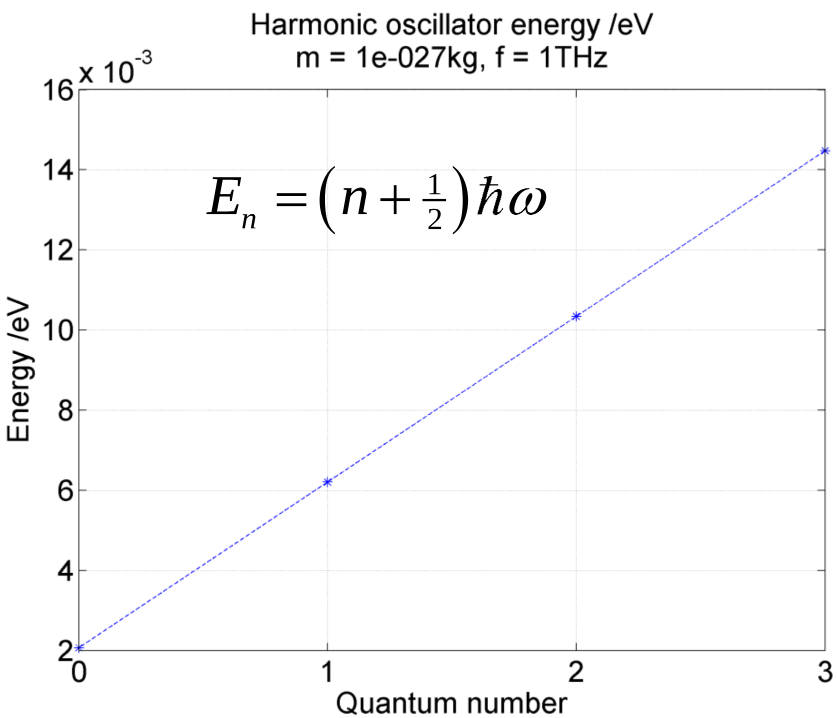
Hermite polynomials

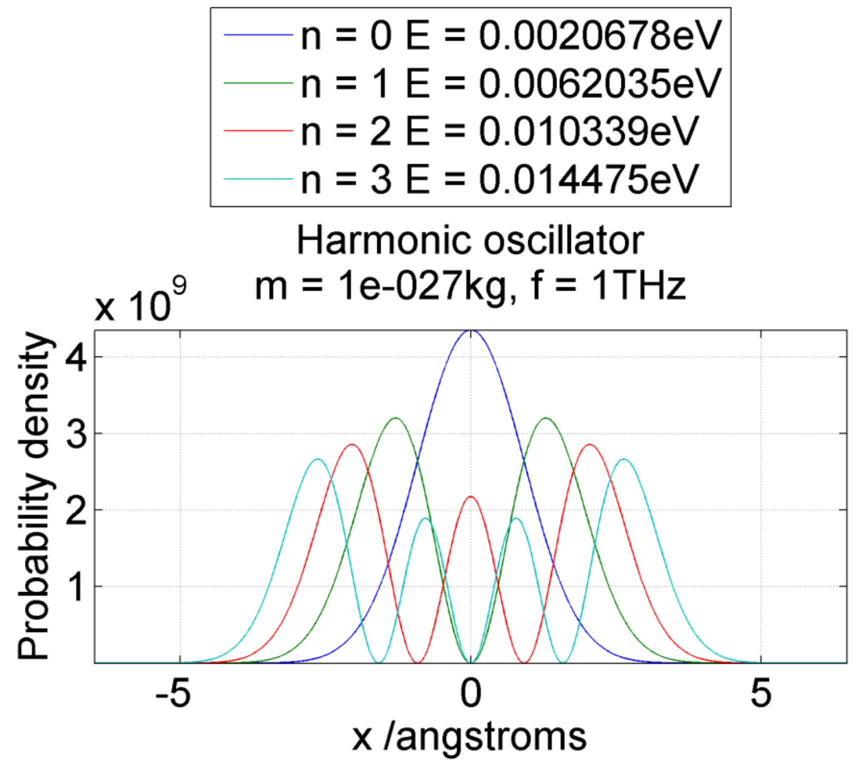
$$H_0(z) = 1$$

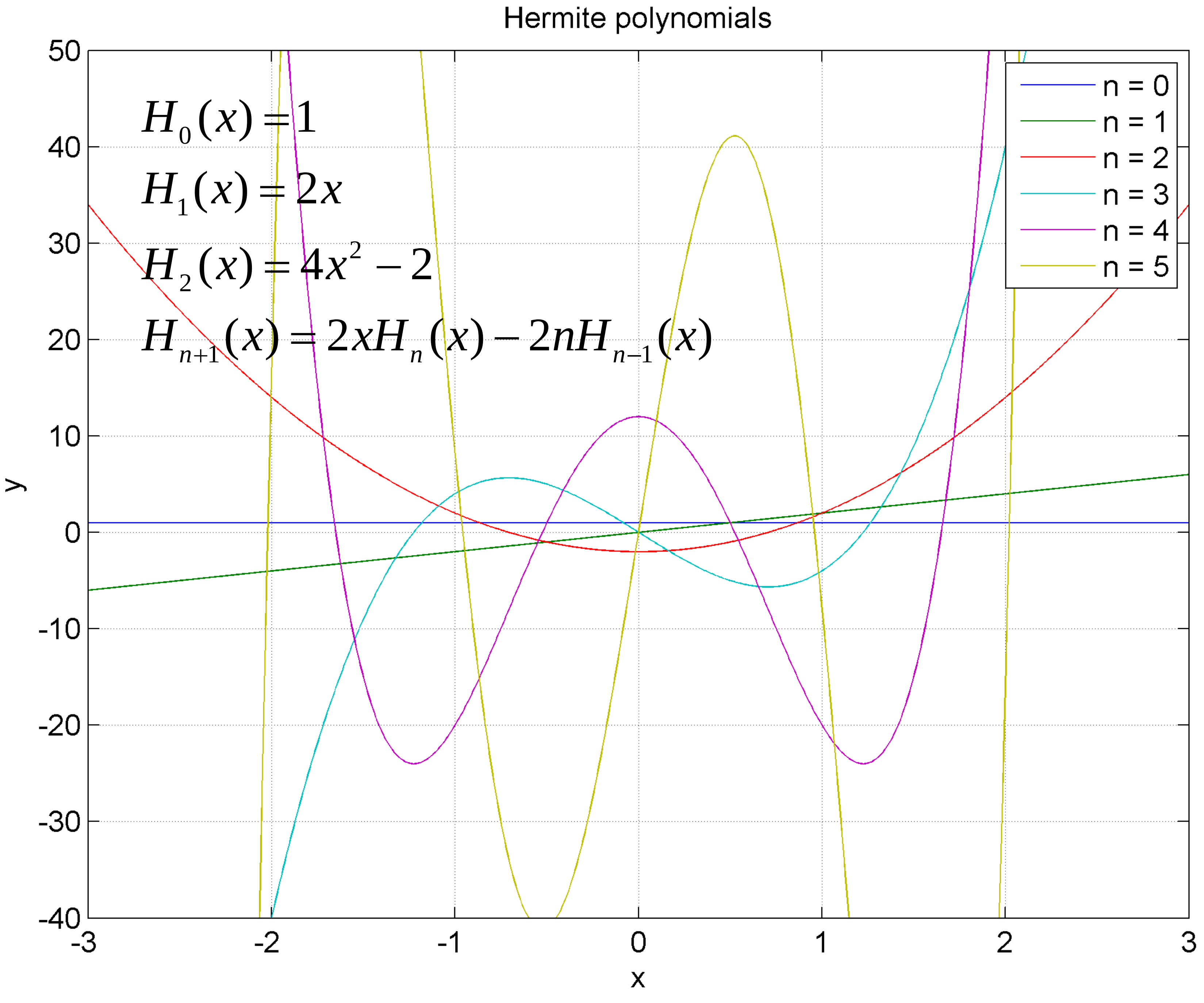
$$H_1(z) = 2z$$

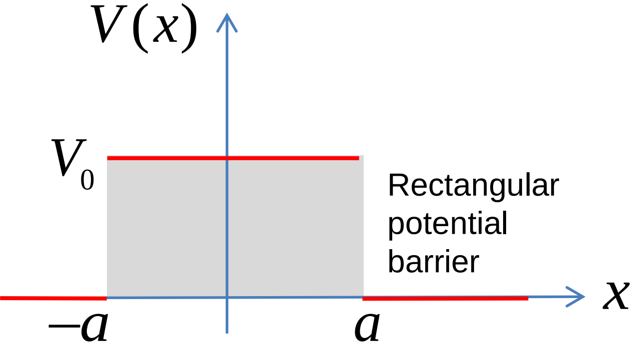
$$H_2(z) = 4z^2 - 2$$

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



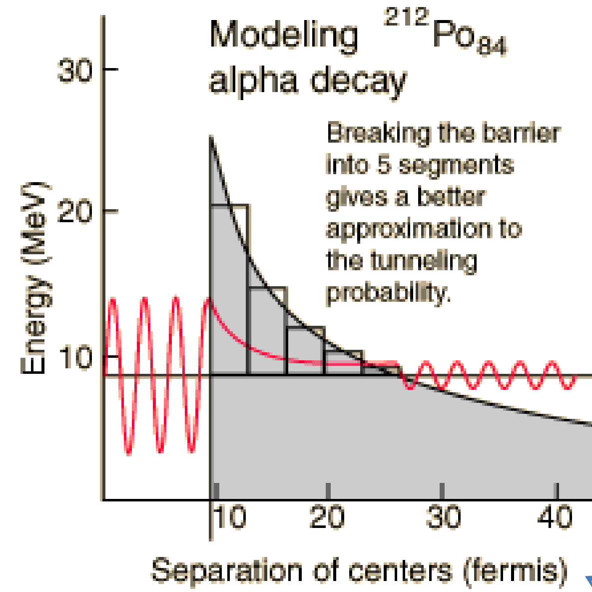



Hermite polynomials
$H_0(x) = 1$
$H_1(x) = 2x$
$H_2(x) = 4x^2 - 2$
$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$
n = 0
n = 1
n = 2
n = 3
n = 4
n = 5
50
40
30
20
10
0
-10
-20
-30
-40
-3
-2
-1
0
1
2
3
x
y



Gamow model of alpha decay

Gasiorowicz, *Quantum Physics*



10^{-15} m

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

$$qa \ll 1$$

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

George Gamow 1904-1968

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

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

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

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

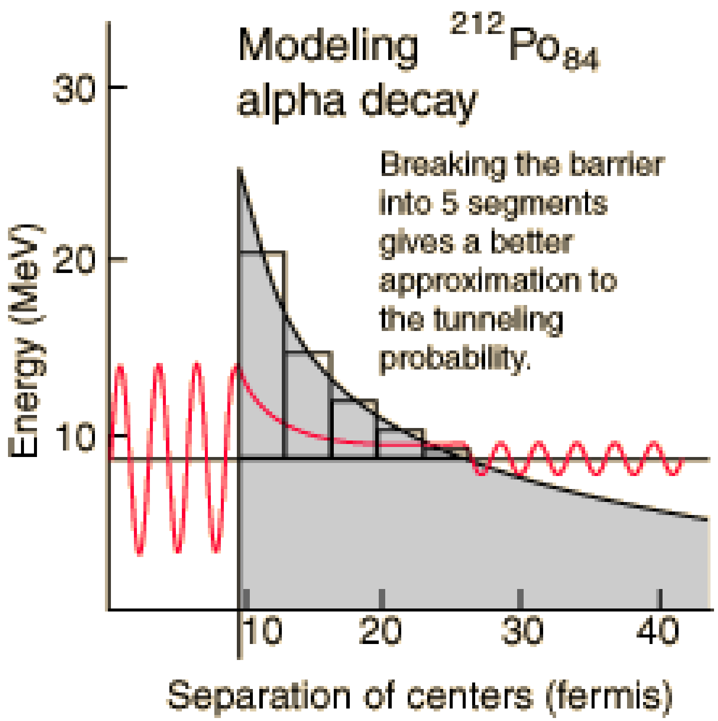
$$\tau \approx \frac{2R}{v} \div e^{-G} = 2R\sqrt{\frac{m}{2E}}\,e^{G}$$

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

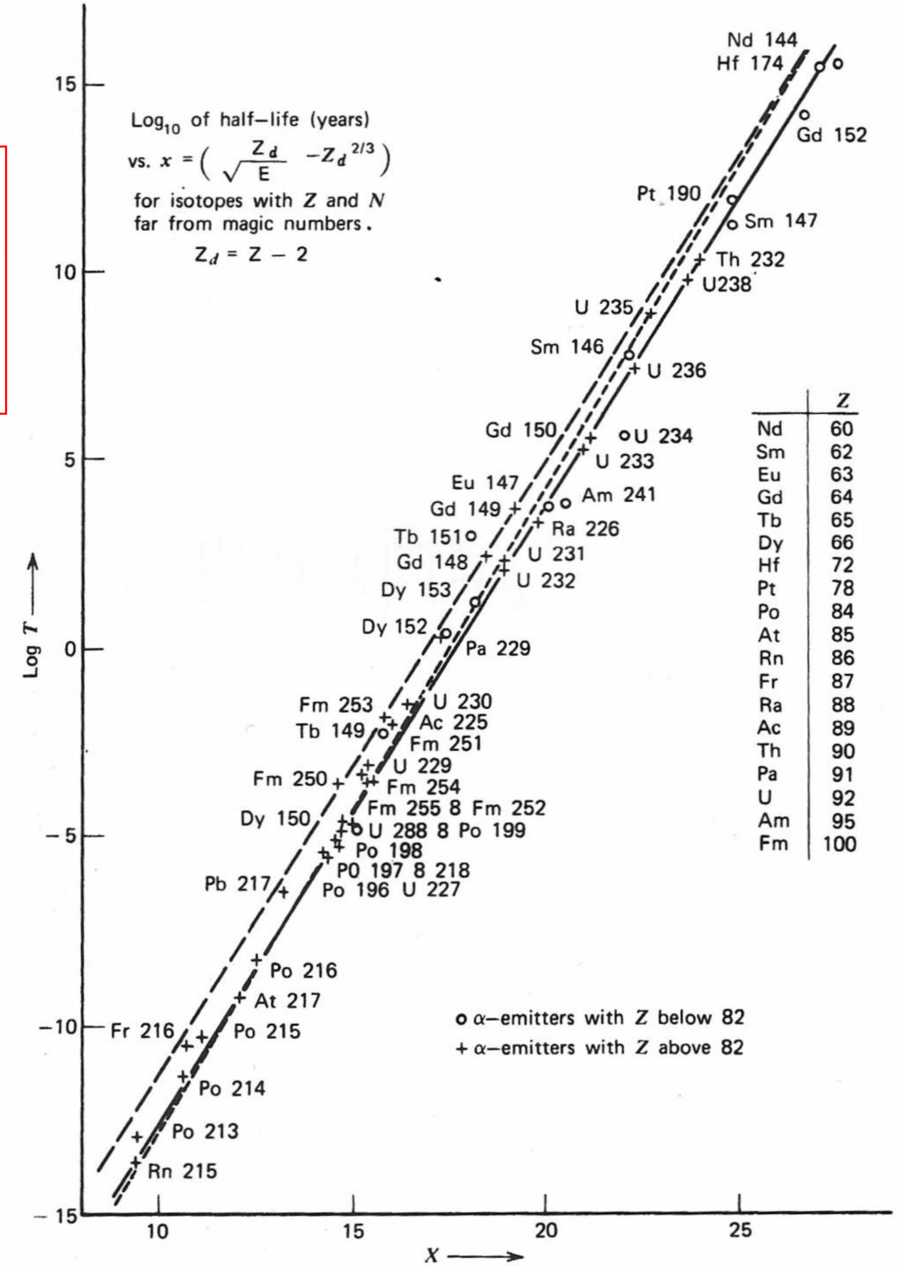
Half life of alpha-emmitter

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

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



Gasiorowicz, *Quantum Physics* pp87



Plot of $\log_{10} 1/\tau$ versus $C_2 - C_1 Z_1/\sqrt{E}$ with $C_1 = 1.61$ and a slowly varying $C_2 = 28.9 + 1.6 Z_1^{2/3}$. 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

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

$$V(r) = -\frac{Ze^2}{4\pi\varepsilon_0 r}$$

$$\psi_{nlm}(r,\theta,\phi) = R(r,n,l) \times \Omega(\theta,\phi,l,m)$$

← **Angular wavefunction**

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

Radial wavefunction

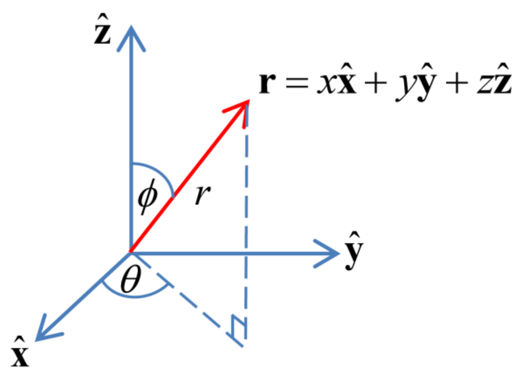
$$\zeta(x,l,n) = \sum_{k=0}^{n-l-1}\frac{(l+n)!(-x)^k}{(2l+1+k)!(n-l-1-k)!k!}$$

Lageurre polynomial

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

$$E_n = -\frac{\mu e^4 Z^2}{8\varepsilon_0^2 h^2 n^2}$$

Orbital energy



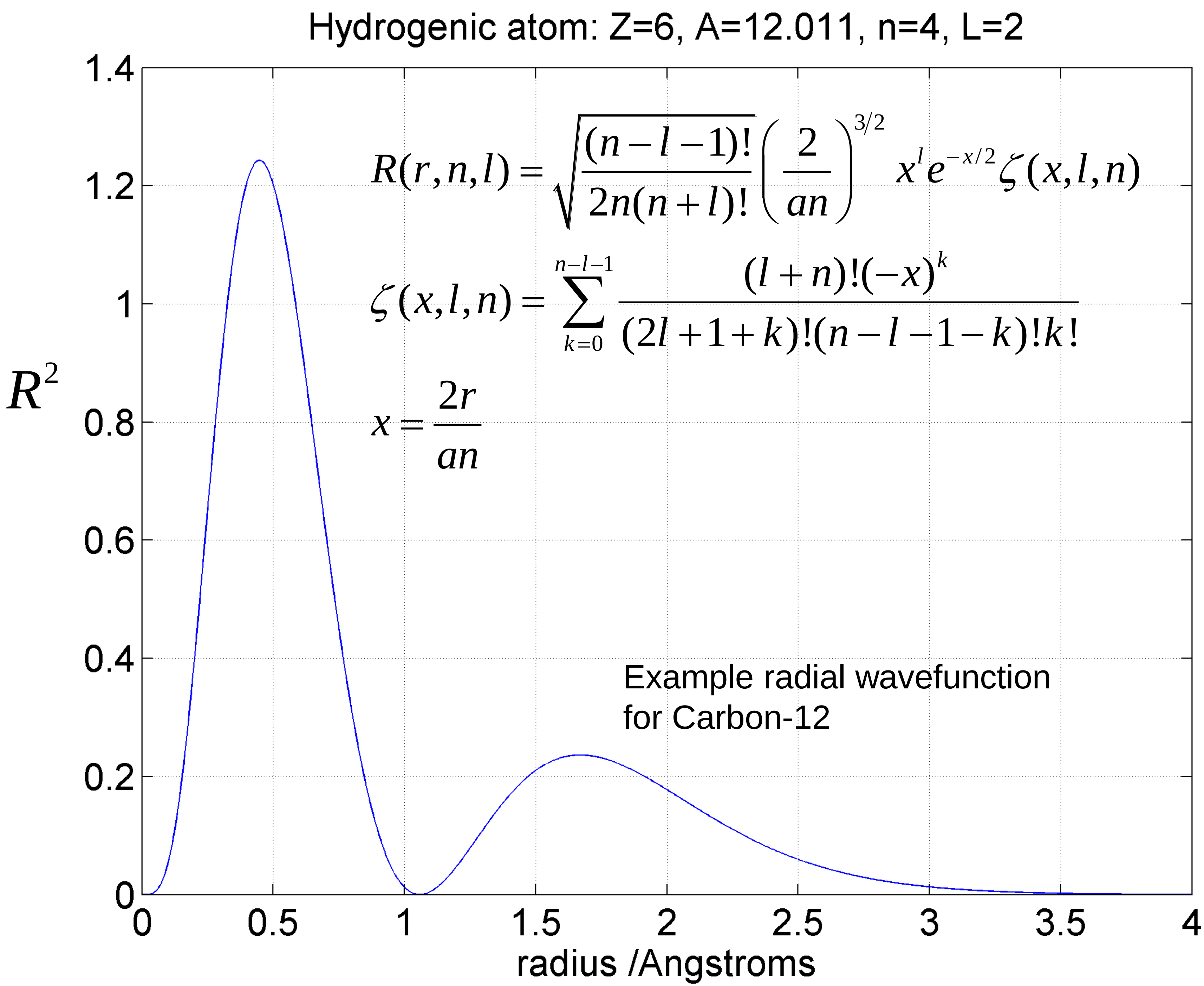
$$x = r\sin\phi\cos\theta$$
$$y = r\sin\phi\sin\theta$$
$$z = r\cos\phi$$

Conversion between Cartesian and polar coordinates

Polar coordinate unit vectors as Cartesian coordinates

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

Woan, *The Cambridge Handbook of Physics Formulas*


Hydrogenic atom: Z=6, A=12.011, n=4, L=2
$$R(r,n,l)=\sqrt{\frac{(n-l-1)!}{2n(n+l)!}}\left(\frac{2}{an}\right)^{3/2}x^l e^{-x/2}\zeta(x,l,n)$$
$$\zeta(x,l,n)=\sum_{k=0}^{n-l-1}\frac{(l+n)!(-x)^k}{(2l+1+k)!(n-l-1-k)!k!}$$
$$x=\frac{2r}{an}$$
Example radial wavefunction
for Carbon-12
R^2
radius /Angstroms
0
0.2
0.4
0.6
0.8
1
1.2
1.4
0
0.5
1
1.5
2
2.5
3
3.5
4

Angular wavefunction

Assume quantum numbers n, l, m are integers!

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

Spherical harmonics

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

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

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

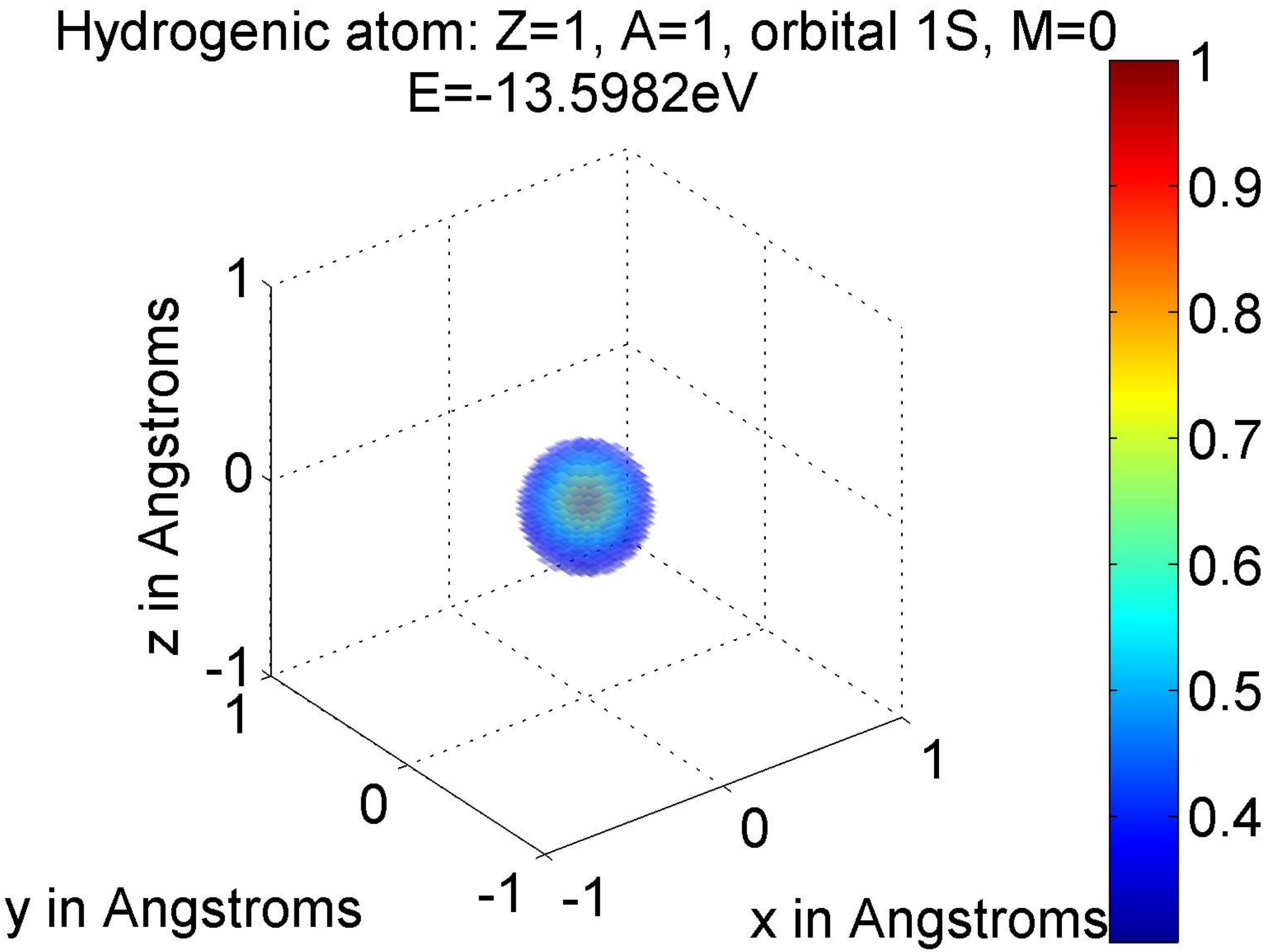
Legendre Polynomials can be evaluated using the MATLAB `legendre(`l,x`)` function (which gives a vector of outputs for all possible m values).

S

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

$l = 0$

$m = 0$



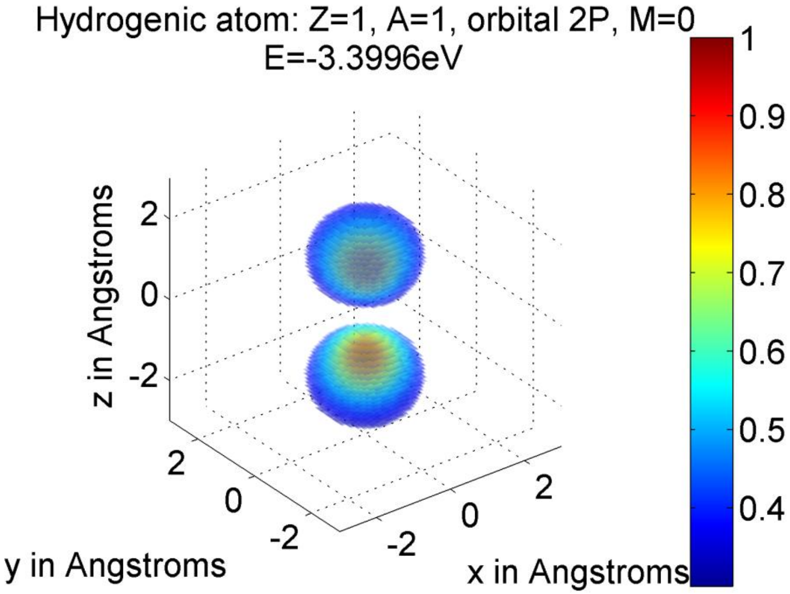
1Å = 10^{-10} m

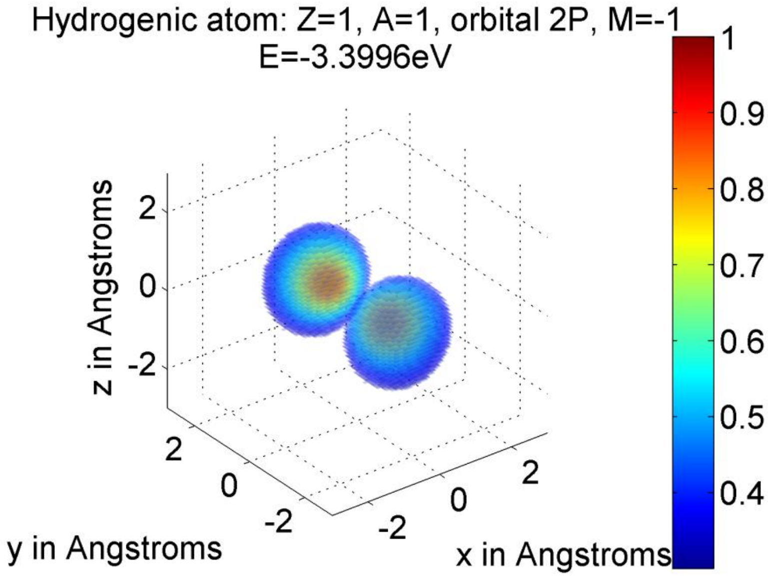
P

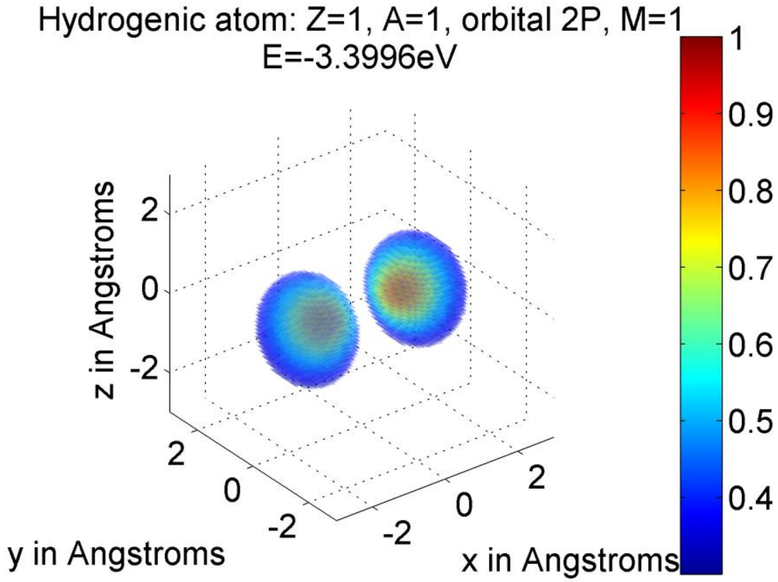
$n = 2, 3, 4, ...$

$l = 1$

$m = -1, 0, 1$





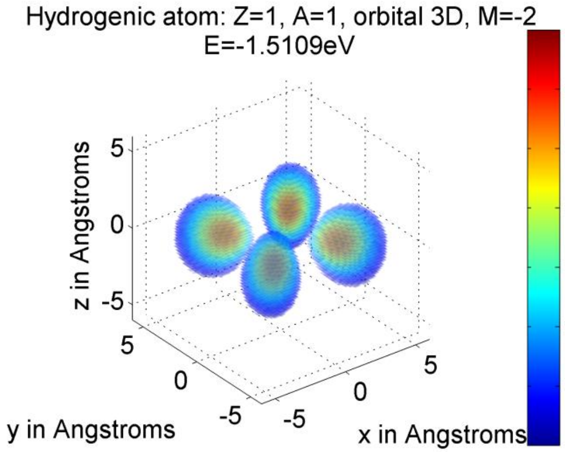


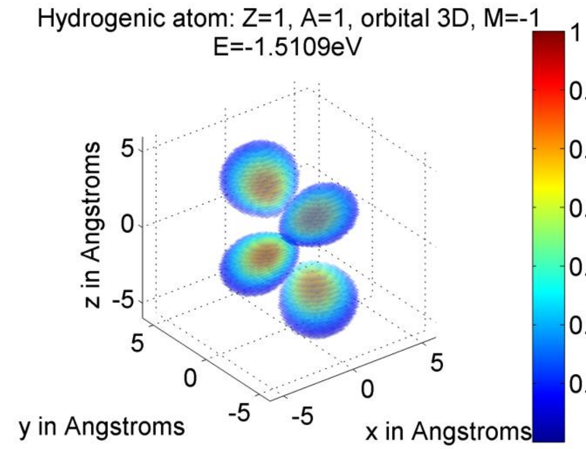
D

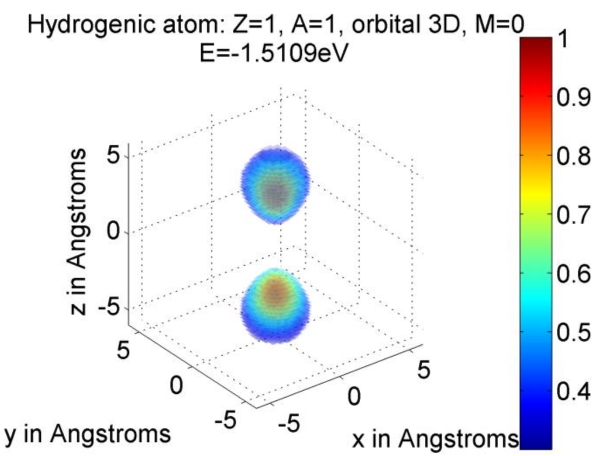
$n = 3, 4, 5, \ldots.$

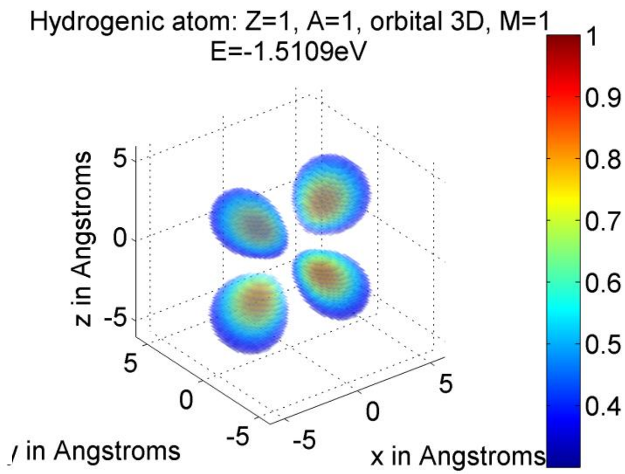
$l = 2$

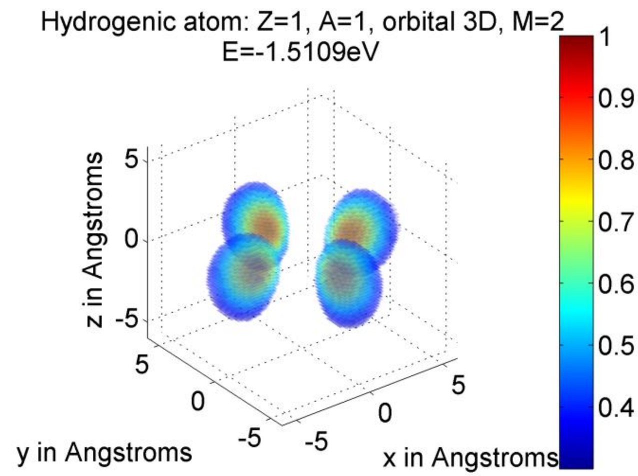
$m = -2, -1, 0, 1, 2$

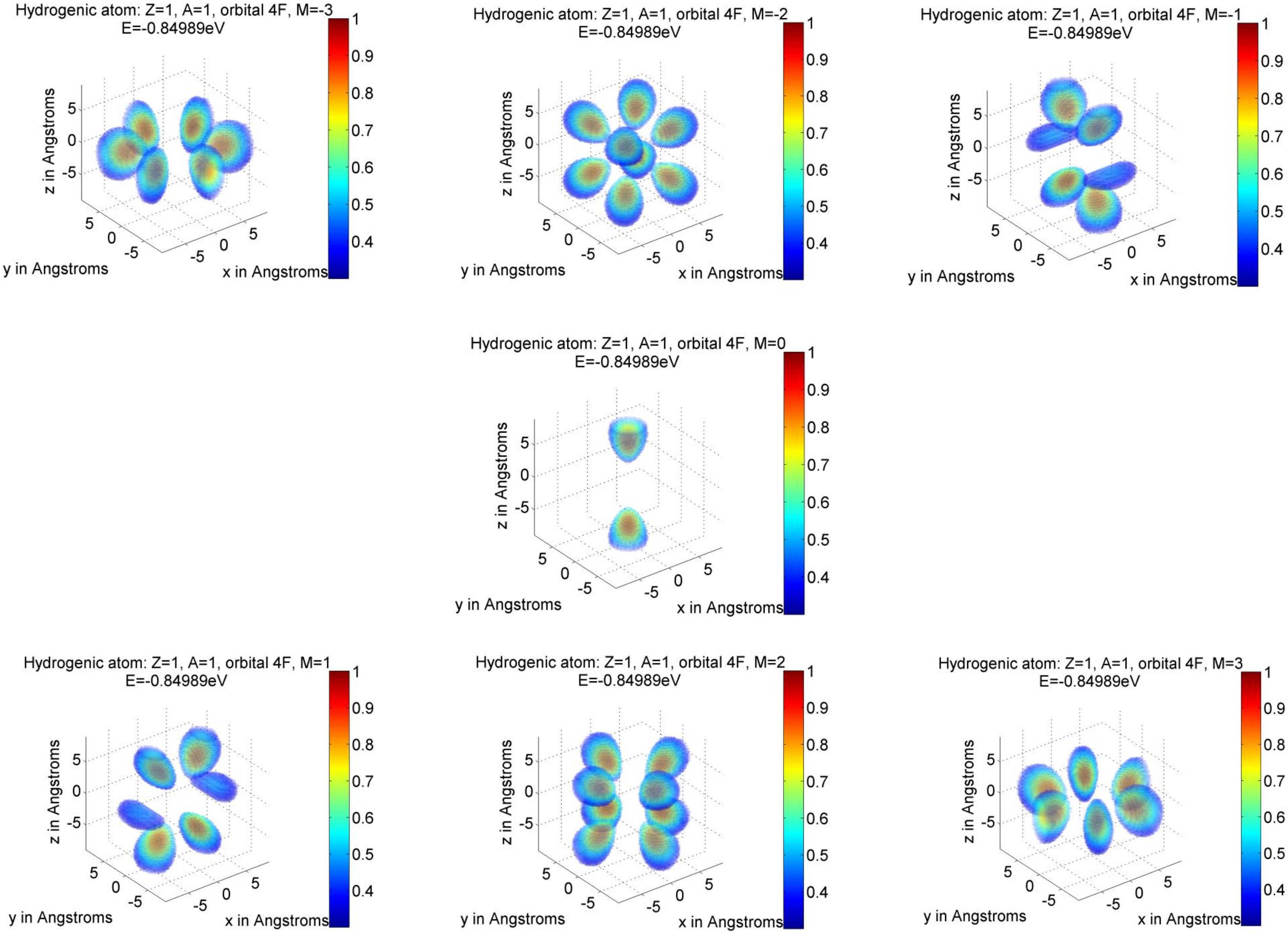




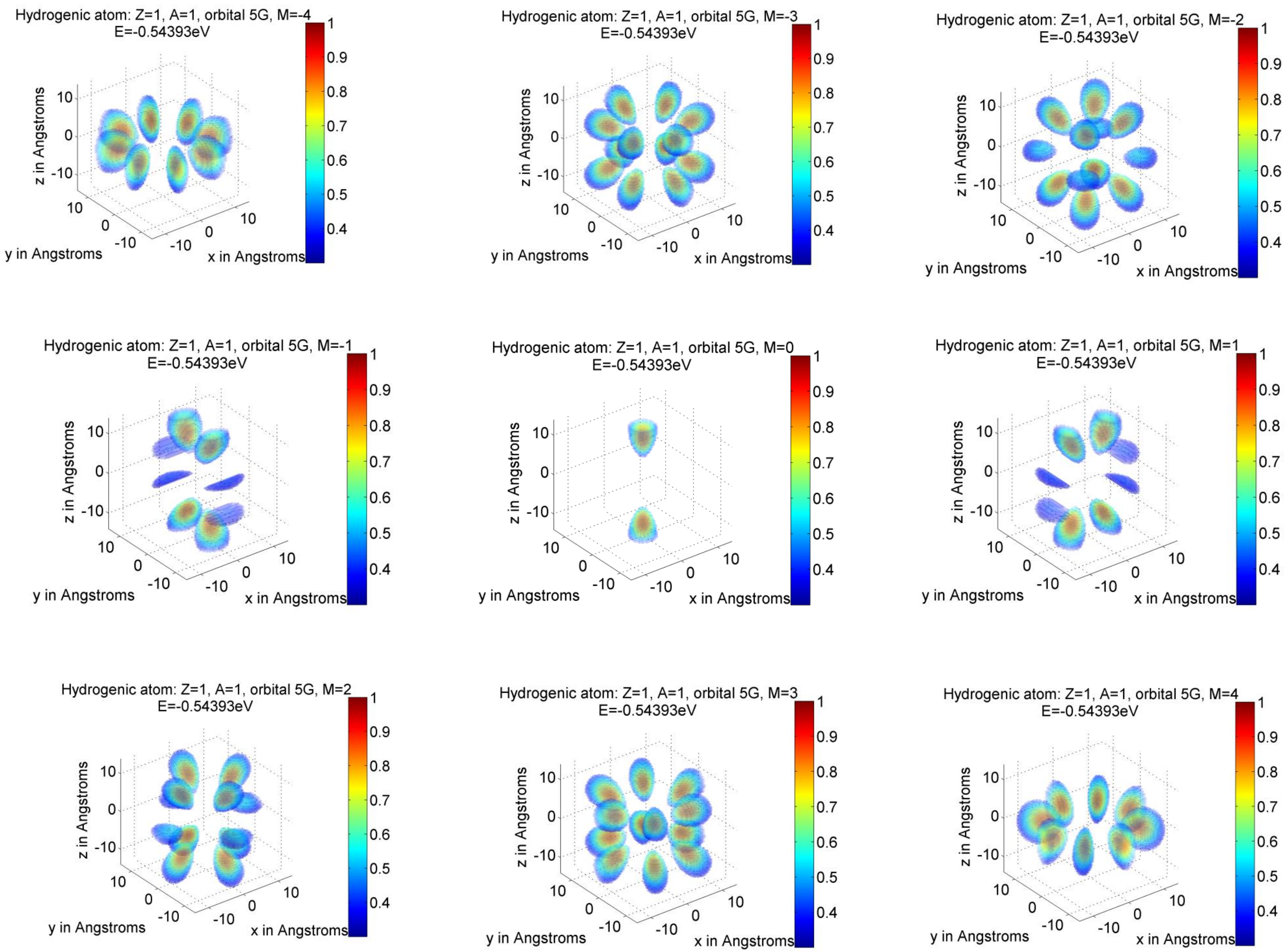








$$F \quad n = 4, 5, 6, \ldots \quad l = 3 \quad m = -3, -2, -1, 0, 1, 2, 3$$



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

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.”

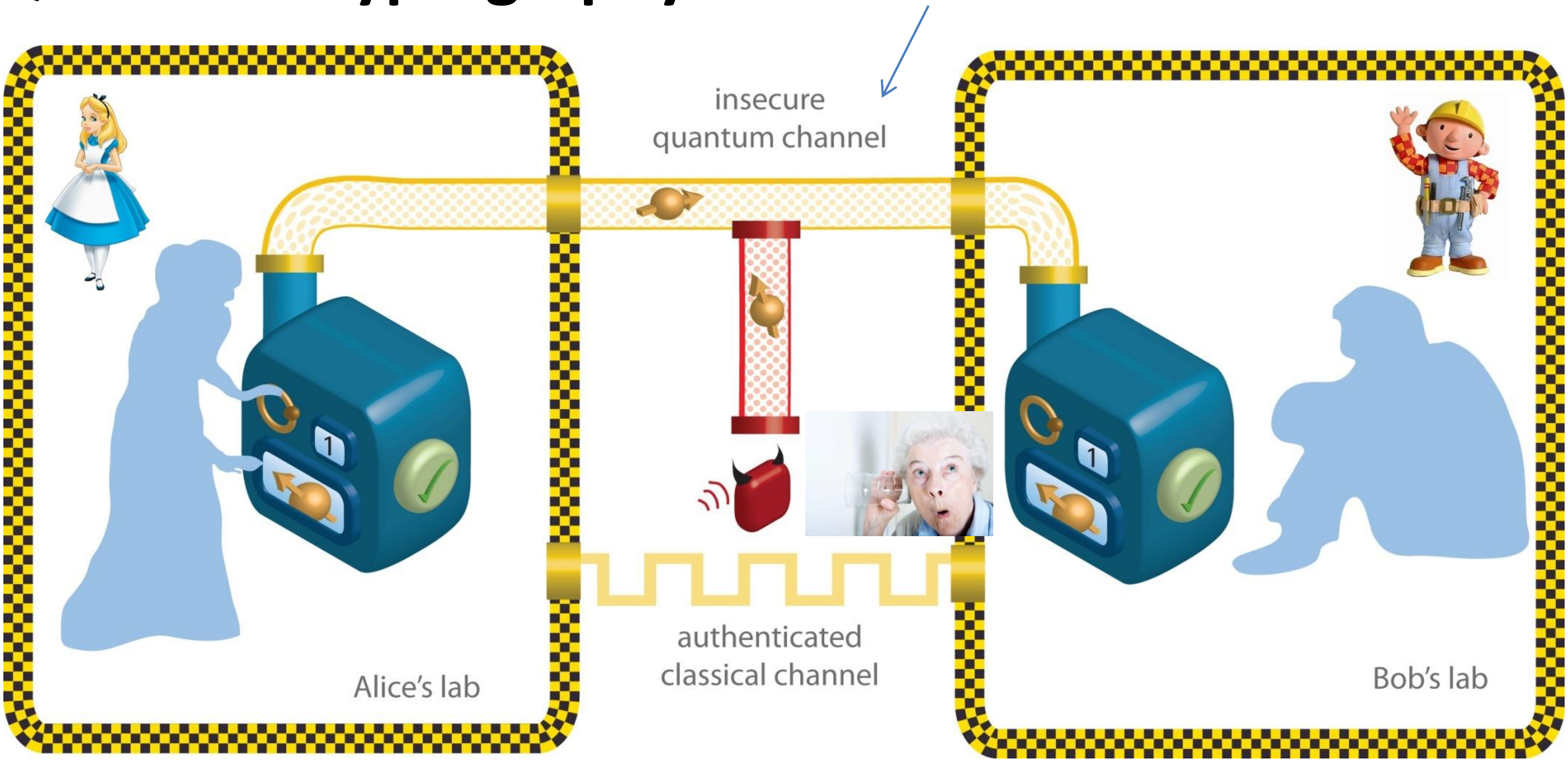
An electron therefore has a wavefunction which incorporates *both* spin states, until it is measured.

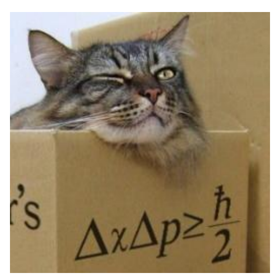
An electron in a hydrogen atom has wavefunction which is a *superposition of all possible quantum numbers*. Only when you measure it, does it collapse to one particular ‘eigenstate.’

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

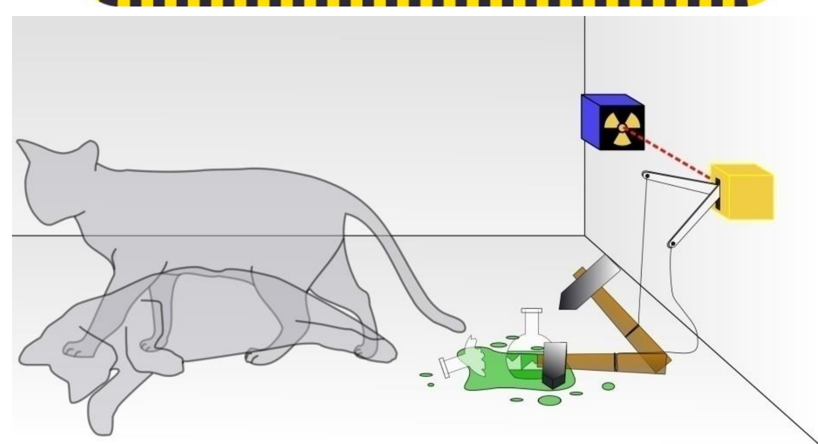
Quantum Cryptography

Here you can tell whether Eve has been listening!





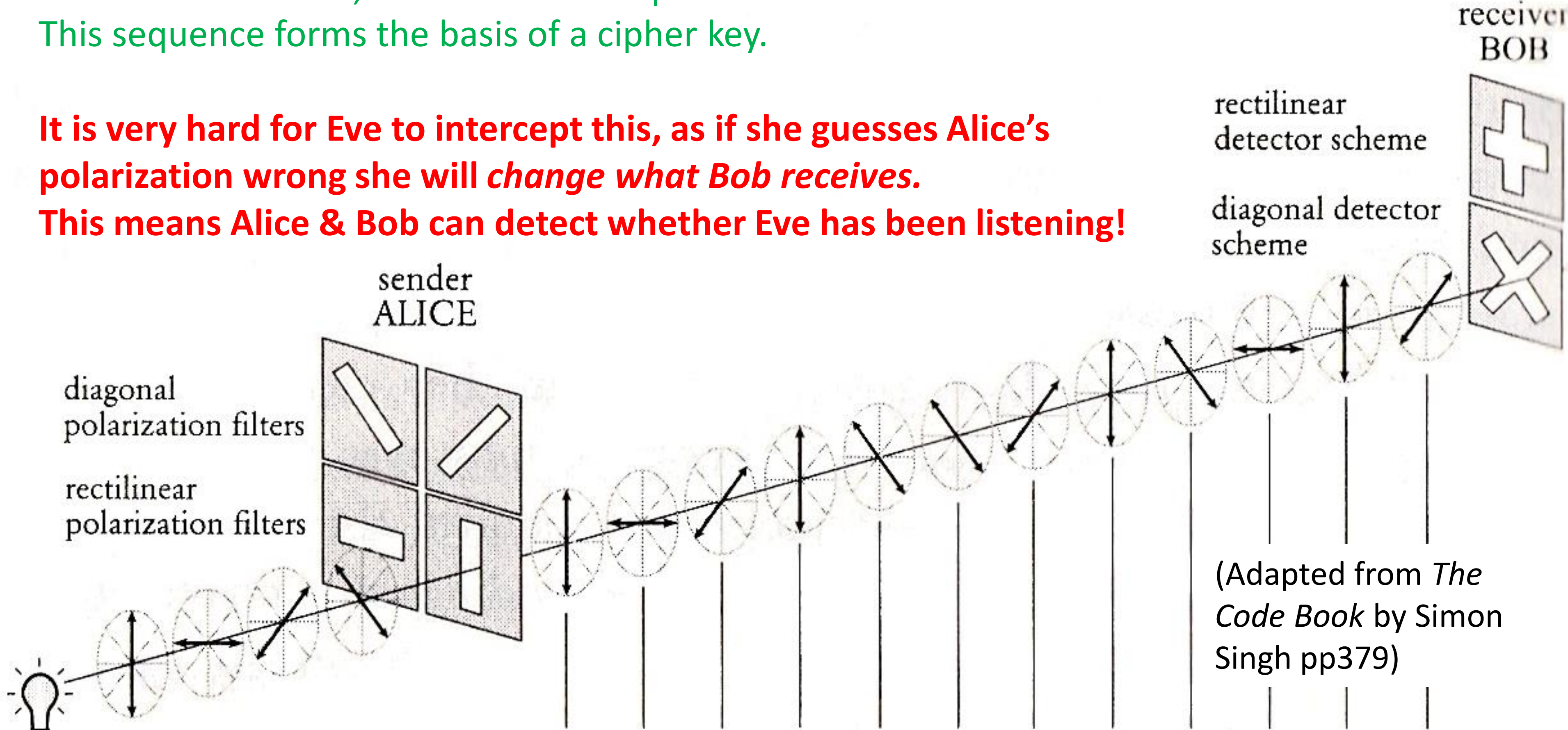
Erwin
Schrödinger
(1887-1961)



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.***

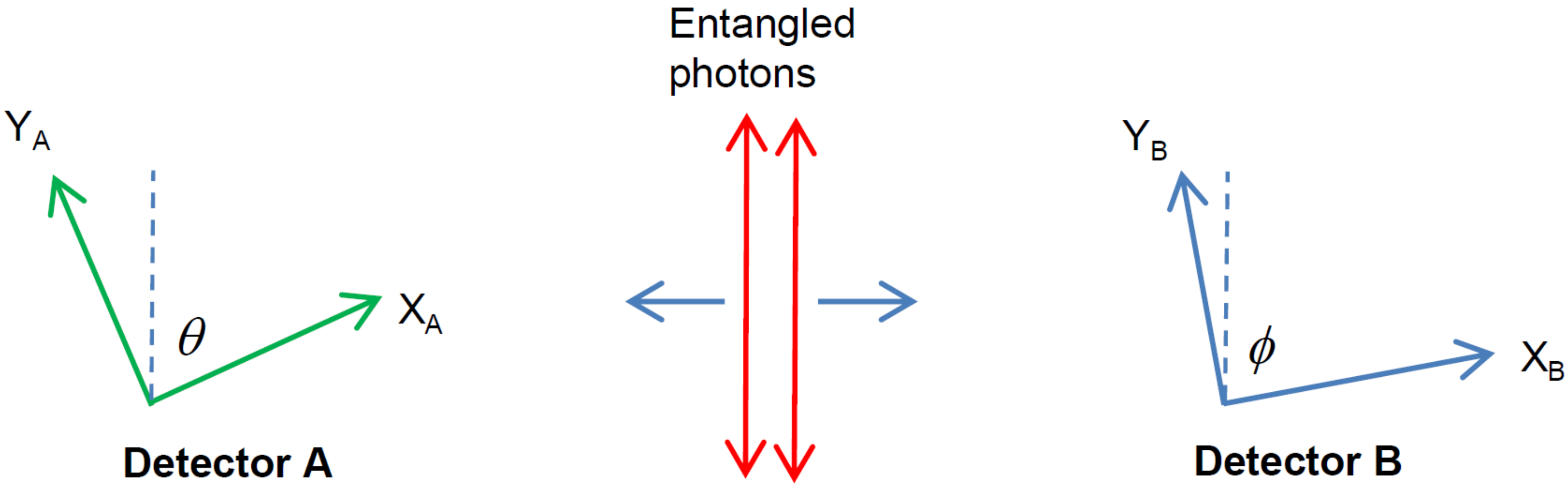
Alice sends Bob a message based upon photons of different polarizations.
Alice & Bob communicate to agree *which photons were intercepted with the correct detector*, but *not* what the polarizations were.
This sequence forms the basis of a cipher key.

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!



(Adapted from *The Code Book* by Simon Singh pp379)

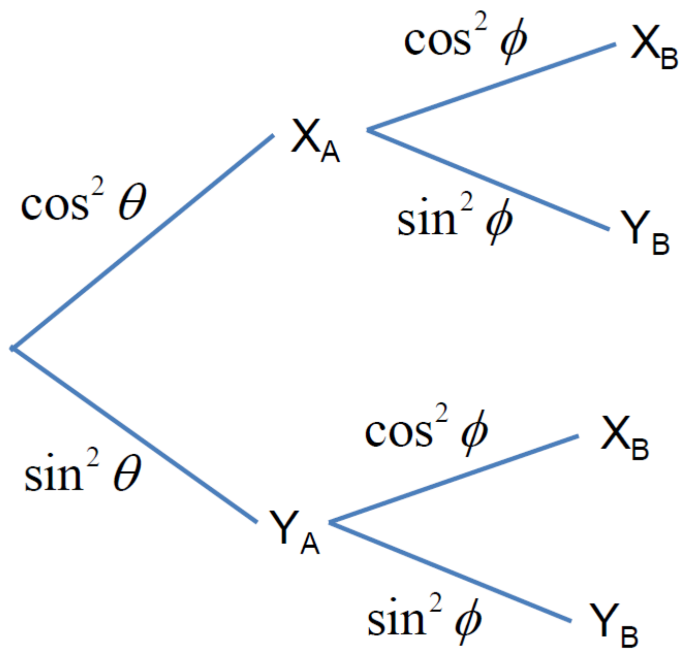
ALICE's bit sequence	1	0	1	1	0	0	1	1	0	0	1	1
BOB's detection scheme	+	×	+	+	×	×	+	+	×	+	×	×
BOB's measurements	1	0	0	1	0	0	1	1	0	0	0	1
Retained bit sequence	1	–	–	1	0	0	–	1	0	0	–	1



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

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

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.

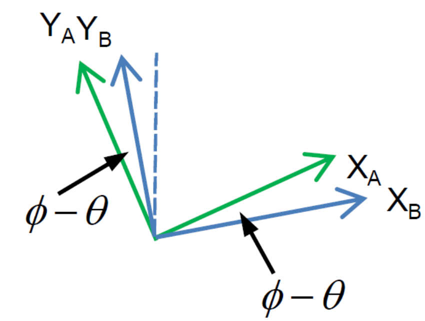


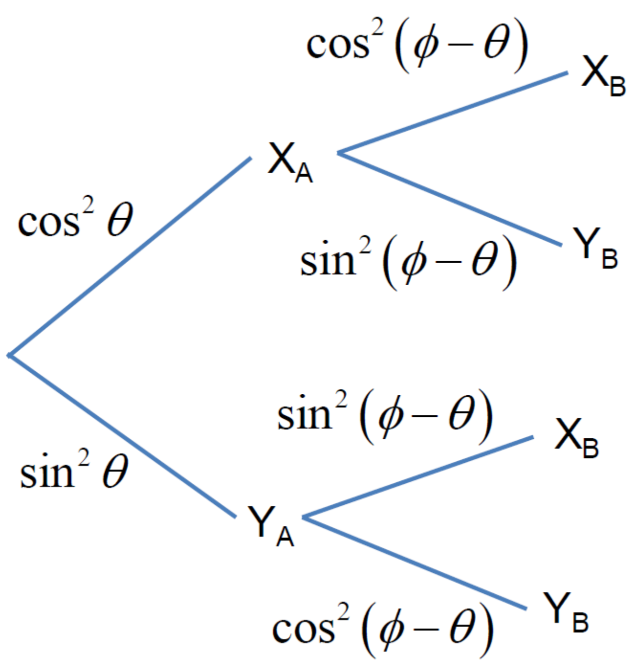
Classical scenario

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

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

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





Quantum scenario

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

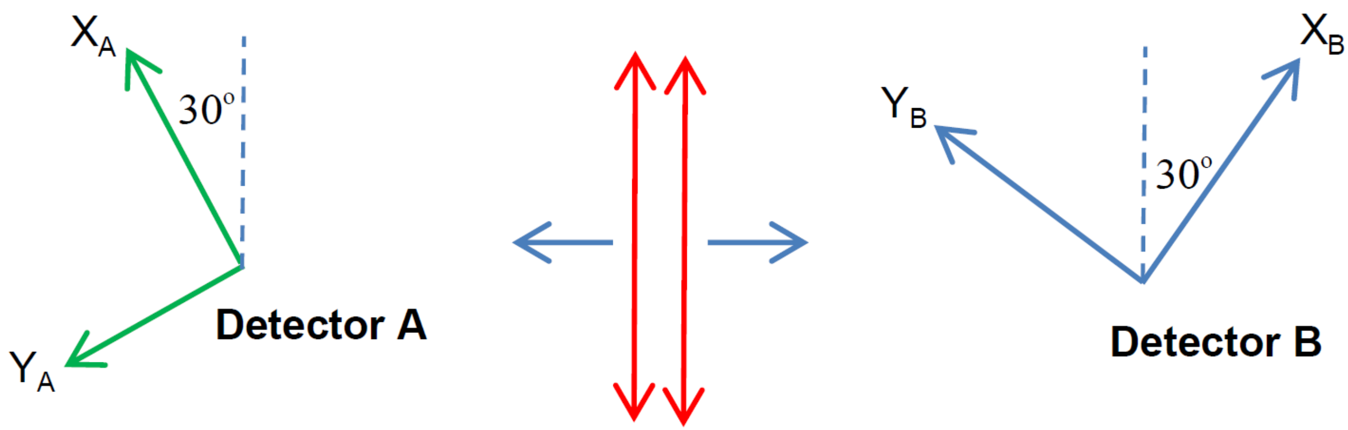
$$P(\text{match}) = \cos^2\theta\cos^2(\phi-\theta) + \sin^2\theta\cos^2(\phi-\theta)$$

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

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

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

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



Example:
Classical

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

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

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

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

Example:
QM

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

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

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