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Section 1: The Atom

1. Introduction Leucippus (~490BC \rightarrow ?) Democritos (~460BC \rightarrow 370BC) "By convention sweet and bitter, by convention hot and cold, by convention colour: in reality atoms and void." $\alpha \tau o \mu o \sigma$ (Atomos) \rightarrow atom. 1802, J. Dalton - "multiple proportions" 1811, L. Avogadro - "molecular theory of gases" 1815, W. Prout - everything was made of combinations of atom molecules. 1868, D. Mendeleev - set up periodic table. 1895, W. Rontgen - x-rays. 1896, H. Becquerel - Radioactivity & uranium. 1897, J. J. Thompson - first elementary particle, the Electron. 1900, Max Planck - E = hf1903, E. Rutherford - Nucleus. 1905, A. Einstein - $E = mc^2$ 1913, N. Bohr - Bohr model of the atom. 1926, Schrodinger - Wave Equation

1927, B. Heisengberg - $\Delta x \Delta p = \hbar$

Atomic physics == Quantum physics.

$$e = 1.602 \times 10^{-19} C R. A. Millikan 1911$$

 $N_A = 6.02 \times 10^{23} mol^{-1}$
 $\frac{1}{12} m_a ({}^{12}C) = 1u = 1.66 \times 10^{-24} g = 931.5 \frac{MeV}{c^2}$
 $m_e = 9.11 \times 10^{-26} g = 0.511 \frac{MeV}{c^2}$
 $m_p = 938 \frac{MeV}{c^2}$
 $\hbar = \frac{h}{2\pi} = 6.582 \times 10^{-22} MeVs$
 $a_o = 0.53A$

2. Hydrogen Atom 2.1 Schrödinger Equation in central field Reduced mass:

$$m_r = \frac{m_1 m_2}{m_1 + m_2}$$

For the mass of the proton and the electron, the reduced mass is approximately the same as the mass of the electron. $(m_r \approx m_p)$

Coordinates are spherical, (r, θ, ϕ) .

3D:

$$\nabla^{2}\Psi(r,\theta,\phi) + \frac{2m_{r}}{\hbar^{2}} (E - V(r))\Psi(r,\theta,\phi) = 0$$

$$\nabla^{2} = \frac{1}{r^{2}} \frac{\partial}{\partial r} \left(r^{2} \frac{\partial}{\partial r}\right) + \frac{1}{r^{2} \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta}\right) + \frac{1}{r^{2} \sin^{2} \theta} \frac{\partial^{2}}{\partial \phi^{2}}$$

$$\Psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$$

Solution $\ell(\ell+1)$. 1) Substitute $\Psi \to RY$ 2) Divide by RY3) Multiply by r^2 $\frac{1}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{2m_r r^2}{\hbar^2} (E - V) = -\frac{1}{Y} \left(\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} \right)$ $Y(\theta, \phi) = \Theta(\theta) \Phi(\phi)$ for RHS, simplify, rearrange. $\sin^2 \theta \left(\frac{1}{\Theta \sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + \ell (\ell + 1) \right) = -\frac{1}{\Phi} \frac{\partial^2 \Phi}{\partial \phi^2}$ Use *m* as constant. $\frac{d^2 \Phi}{d\phi^2} + m^2 \phi = 0$ (1) $\frac{1}{\Theta \sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + \ell (\ell + 1) - \frac{m^2}{\sin^2 \theta} = 0$ (2) $\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{2m_r}{\hbar} \left(E - V - \frac{\ell (\ell + 1)\hbar^2}{2m_r r} \right) = 0$ (3) Solution (there should be no ϕ -dependence): $\Phi(\phi) = \frac{1}{\sqrt{2\pi}} e^{\pm im\phi}$

$$\int_{0}^{2\pi} |\phi|^{2} d\phi = 1$$

 $\ell = 0, 1, 2, 3, ...$
 $|m| \le \ell$
 $m = -\ell(\ell + 1), ..., \ell$
 $m = 0$ Legendre polynomials
 $m \ne 0$ Associated Legendre Polynomials
 $P_{\ell}^{m}(\cos \theta) = \frac{(-1)^{m}}{2^{\ell} \ell !} (1 - \cos^{2} \theta)^{\frac{m}{2}} \frac{d^{\ell+m}(\cos^{2} \theta - 1)}{(d \cos \theta)^{\ell+m}}$
 $P_{1}^{1}(\cos \theta) = -\sin \theta$

 ϕ - dependence: equation 1 \rightarrow solution: $\Phi(\phi) = \frac{1}{\sqrt{2\pi}} e^{\pm im\phi}$

 θ -dependence: equation 2 \rightarrow solution: Associated Legendre Polynomials r-dependence: equation 3. \rightarrow solution not yet known. Work out this now.

If
$$\ell = m = 1$$
, $P_1^1(\cos\theta) = \frac{(-1)}{2}(1-\cos^2\theta)^{\frac{1}{2}}\frac{d^2(\cos^2\theta-1)}{d\cos\theta} = -\sin\theta$
 $Y_{\ell,m}(\theta,\phi) = \Theta_{\ell,m}(\theta)\Phi_m(\phi)$
 $Y_{\ell,m}(\theta,\phi) = \frac{N}{\sqrt{2\pi}}e^{\pm im\phi}P_\ell^m(\cos\theta)$
These are orthogonal. Integrate over the whole sphere.

These are orthogonal. Integrate over the whole sphere. $\int_{-\infty}^{\pi} \int_{-\infty}^{2\pi} dx = \int_{-\infty}^{2\pi} \int_{-\infty}^{2\pi} dx = \int_{-\infty}^{\infty} \int_{-\infty}^{2\pi} dx = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty}$

$$\int_{0}^{\pi} \int_{0}^{2\pi} \mathbf{Y}_{\ell,m} * (\theta, \phi) \mathbf{Y}_{\ell',m'} (\theta, \phi) \sin \theta d\theta d\phi = \delta_{\ell\ell'} \delta_{mm'}$$
$$\delta_{\ell\ell'} = 1 \text{ if } \ell = \ell' \cdot \delta \text{ is a Kroneker Delta.}$$
Replace $u(r) = rR(r)$.

$$P_{u\ell}(r)dr = r^2 \left| R(r) \right|^2 dr = u^2(r) dr$$

Take equation 3.

$$\frac{1}{r}\frac{d}{dr}\left(r^{2}\frac{d}{dr}\left(\frac{u(r)}{r}\right)\right) + \frac{2m_{r}}{\hbar^{2}}\left(E - V(r) - \frac{\ell(\ell+1)\hbar^{2}}{2m_{r}r^{2}}\right)u(r) = 0$$

$$\frac{d^{2}u(r)}{dr^{2}} + \frac{2m_{r}}{\hbar^{2}}\left(E - V(r) - \frac{\ell(\ell+1)\hbar^{2}}{2m_{r}r^{2}}\right)u(r) = 0$$

$$\frac{d^{2}u(r)}{dr^{2}} + \frac{2m_{r}}{\hbar^{2}}\left(E - V(r) - V_{\ell}(r)\right)u(r) = 0$$

 $V_{\ell}(r)$ is the "centrifugal potential".

$$L^2 = \ell \big(\ell + 1 \big) \hbar^2$$

2.2 Energy Levels and Eigenfunctions of the Hydrogen Atom

$$V(r) = -\frac{e^2}{4\pi\varepsilon_o r}$$
$$V_\ell(r) = \frac{\ell(\ell+1)\hbar^2}{2m_r r^2}$$
$$V_{eff}(r) = \frac{\ell(\ell+1)\hbar^2}{2m_r r^2} - \frac{e^2}{4\pi\varepsilon_o r}$$

To find the minimum,

$$\begin{split} \frac{dV_{\text{eff}}\left(r\right)}{dr} &= 0\\ r_{\text{min}} &= \frac{4\pi\varepsilon_{o}\ell\left(\ell+1\right)\hbar^{2}}{m_{r}e^{2}} = \ell\left(\ell+1\right)a_{o}' \end{split}$$

 a_o' is the Bohr radius, taking into account the reduced mass m_r .

$$a_{o}' = \frac{4\pi\varepsilon_{o}\hbar^{2}}{m_{r}e^{2}} = 0.53A$$

It is primed, as the reduced mass is used as opposed to the normal mass. (the difference is so small, it doesn't really matter whether a_{\circ} ' or a_{\circ} is used.)

$$V_{\text{eff}}(r_{\min}) = -\frac{E_R}{\ell(\ell+1)}$$
$$E_R = \frac{e^2}{8\pi\varepsilon_o a_o'} = \left(\frac{e^2}{4\pi\varepsilon_o}\right)^2 \frac{m_r}{2\hbar^2} = 13.6eV$$

This is known as the Rydberg energy.

The solution of (3) can only be given when we have an equation for potential, which we now do.

$$\frac{d^2u(r)}{dr^2} + \frac{2m_r}{\hbar^2} \left(E - \frac{e^2}{4\pi\varepsilon_o r} + \frac{\ell(\ell+1)\hbar^2}{2m_r r^2} \right) u(r) = 0$$

- (1) $u(r) \to 0$ as $r \to \infty$. Therefore solution should have a term $e^{-\frac{r}{na_o}}$.
- (2) $V_{\ell}(r)$ singular at r = 0. This should dominate the behaviour of the system at small r. $\rightarrow u(r) \sim r^{\ell+1}$.

(3) We need a polynomial to describe the nodes.

$$u(r) \sim P_{n_r}^{\ell}(r)$$
 where $n_r = n + \ell$.

Laguerre Polynomials.

$$u(r) = NP_{n_r}^{\ell}(r)r^{\ell+1}e^{-\frac{r}{na_o}}$$
$$R(r) = \frac{u(r)}{r}$$

So the final result; $\Psi_{n,\ell,m}(r,\theta,\phi) = R_{n,\ell}(r)Y_{\ell,m}(\theta,\phi)$ $Y_{\ell,m}(\theta,\phi) \sim P_{\ell}^{m}(\cos\theta)e^{im\phi}$

n	$\ell = 0$	$\ell = 1$	
	<i>m</i> = 0	<i>m</i> = 0	<i>m</i> = 1
1	-e ^{-^r/_{ao}}	-	-
2	$\left(1-\frac{r}{2a_{o}}\right)e^{-\frac{r}{2a_{o}}}$	$\frac{r}{2a_o}e^{-\frac{r}{2\alpha_o}}\cos\theta$	$\frac{r}{2a_o}e^{-\frac{r}{2a_o}}\sin\theta e^{i\phi}$

Energies:

$$E_n = -\frac{E_R}{n^2}$$

 $n = n_r + \ell$

n is the principle quantum number. Degeneracy: All states with the same value of $n = n_r + \ell$ have identical energies.

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

$$\ell = 0, 1, 2, \dots, n - 1$$

$$m = -\ell, (-\ell + 1), \dots, \ell$$

Degeneracy can be quantified:

$$\sum_{i=1}^{n-1} (2\ell + 1) = n^2$$

$$\ell = 0 = S(harp)$$

$$\ell = 1 = P(rinciple)$$

$$\ell = 2 = D(iffuse)$$

$$\ell = 3 = F(undamental)$$

 $\left|\Psi_{n,\ell,m}(r,\theta,\phi)\right|^2$ is the probability.

Ignore $\left|\Phi(\phi)\right|^2$ as it cancels out (Imaginary * complex conjugate)

$$\begin{split} & Y_{\ell,m}\left(\theta,\phi\right) = \Phi_m\left(\phi\right)\Theta_{\ell,m}\left(\theta\right) \\ & \left|\Theta_{\ell,m}\left(\theta\right)\right|^2 \text{ (Remembering that the answers to these are Legendre polynomials)} \\ & \text{For } \ell = 0 \text{, there is spherical symmetry.} \\ & \ell = 1, \ m = 0 \text{.} \\ & P_1\left(\cos\theta\right) = \cos\theta \\ & \ell = m = 1 \\ & P_1^1\left(\cos\theta\right) = \sin\theta \end{split}$$

 \rightarrow all others are nodes of superpositions of these.

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	n,	l	n
R ₃₀	3	0	3
R ₃₁	2	1	3
R ₃₂	1	2	3

Degenerate (Sum n)

$$P_{n,\ell}dr = r^2 \left| R(r) \right|^2 dr$$

The first maximum is at $r = a_0$. n = 1, $\ell = 0$.

In the Bohr model, the angular momentum was quantized. $L = pr = n\hbar$.

This means that for n = 1, L is greater than 0 - which is wrong. Hence the Bohr model is wrong here, although it does get a lot of other things right.

$$\langle r_{n\ell} \rangle = \int_{\Gamma}^{\infty} \Psi * r \Psi d\tau$$

gives the expectation value, where $d\tau$ is the infinitesimal volume.

$$\left\langle r_{n,\ell} \right\rangle = \int_0^\infty r \mathcal{P}_{n,\ell}\left(r\right) = \int_0^\infty r^3 \left| \mathcal{R}\left(r\right) \right|^2 dr = n^2 a_o \left(1 + \frac{1}{2} \left[1 - \frac{\ell\left(\ell + 1\right)}{n^2} \right] \right)$$

(The final solution is from the first examples sheet.)

The latter part of this equation can be considered to be a correction factor for a_0 . For n = 1. $\ell = 0$:

$$\left< r_{1,0} \right> = \frac{3}{2} a_{o}$$

This is not the Bohr radius - it is the corrected Bohr radius. It is due to the distribution of the probability not being symmetric - the expected value is not the maximum probability. The total waveform is

$$\left|\Psi_{n,\ell,m}\left(r,\theta,\phi\right)\right|^{2}=\left|\boldsymbol{R}\left(r\right)\right|^{2}\left|\boldsymbol{Y}_{\ell,m}\left(\theta,\phi\right)\right|^{2}.$$

What does the z-axis mean?

There should be no z-dependence, as it just depends on our choice of coordinate system. Superimpose the 3d levels from the handout - they will form a complete circle.

$$\sum_{m=-\ell}^{\ell} \left| \mathsf{Y}_{\ell,m} \left(\theta, \phi \right) \right|^2 = \frac{2\ell + 1}{4\pi}$$

This is constant - i.e. no dependence on the z-axis.

2.4 Angular Momentum

Classically:

$$\underline{L} = \underline{r} \underline{x} \underline{p}$$
.

With Quantum Mechanics, it is an operator.

$$P_{x} = -\hbar \frac{\partial}{\partial x}$$

$$\underline{L} = -\underline{r} \times i\hbar \nabla$$

$$\underline{\nabla} = \left(\frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}\right)$$

For spherical coordinate systems;

$$L_{z} = -i\hbar \frac{\partial}{\partial \phi}$$
$$L_{x} = i\hbar \left(\sin\phi \frac{\partial}{\partial \theta} + \cot\theta \cos\phi \frac{\partial}{\partial \phi}\right)$$

$$L_{y} = i\hbar \left(-\cos\phi \frac{\partial}{\partial\theta} + \cot\theta \sin\phi \frac{\partial}{\partial\phi} \right)$$

$$\underline{L}^{2} = L_{x}^{2} + L_{y}^{2} + L_{z}^{2} = -\hbar \left(\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^{2}\theta} \frac{\partial^{2}}{\partial\phi^{2}} \right)$$
From (2.1),
$$\underline{L}^{2}Y_{\ell,m}(\theta,\phi) = \ell \left(\ell + 1 \right) \hbar^{2}Y_{\ell,m}(\theta,\phi)$$

$$L_{z}^{2} = -\hbar^{2} \frac{\partial^{2}}{\partial\phi^{2}}$$

$$\Phi = \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

$$-\frac{L_{z}^{2}}{\hbar^{2}} \Phi = \frac{\partial^{2}\Phi}{\partial\phi^{2}} = -m^{2}\Phi$$

This confirms that m is just the z-component of L.

 $L_z = \hbar m$

$$L_{x}, L_{y} = ?$$

Commutation relation: $\left[\underline{L}^2, L_x\right] = \left[\underline{L}^2, L_y\right] = \left[\underline{L}^2, L_z\right] = 0$

But $[L_y, L_z] = i\hbar L_x \neq 0$, so the components can't be measured at the same time - just one component, and the squared total, i.e. $[L_y, L_z]$ does not commute.

By convention, the z-component is measured.

$$\begin{bmatrix} H, L_z \end{bmatrix} \Psi = 0$$

i.e. commutes with energy. $H\Psi = E\Psi$. Hammond operator.

$$\frac{\partial \langle \mathbf{0} \rangle}{\partial t} = \frac{1}{\hbar} \langle [H, \mathbf{0}] \rangle = \mathbf{0}$$

Constant of motion.

3. Magnetic Field and the spin of the electron

Electron: Greek word for amber. Amber is electric when you rub it against a jumper etc.

3.1 Magnetic Moments Magnetic dipole. Classically;

$$l = -\frac{e}{T} = -\frac{eV}{2\pi r}$$

The magnetic dipole moment is given by;

$$\mu = IA = \frac{ev}{2\pi r}\pi r^2 = -\frac{evr}{2}$$

We know $L = mrv$, so;
 $v = \frac{L}{mr}$

$$\underline{\mu} = \frac{e}{2m}\underline{L}$$

The magnetic moment is parallel to the angular momentum, which is perpendicular to r. It interacts with any magnetic field, where;

$$V_{mag} = -\mu \underline{B}$$

When Quantum Mechanics is used, we get "Quantum Magnets". Austaz: (means: assumption, starting point, ...)

$$V_{mag} = -\underline{\mu}\underline{B} = -(const.\underline{L})\underline{B}$$

$$\mu = cons.\underline{L} = \pm g_{\ell} \mu_{M} \, \frac{\underline{L}}{\hbar}$$

Where μ_{M} is called a magneton.

 \hbar is there as we measure angular momentum using it. We measure the magnetic moment in units of $\mu_{_M}$. Classically, $g_{_\ell} = 1$.

The "Bohr Magneton" is;

$$\mu_{\rm B} = \frac{e\hbar}{2m_{\rm e}} = 0.58 \, x 10^{-4} \, eV \, T^{-1} = 9.27 \, x 10^{-24} \, J \, T^{-1}$$

The magnitude of the magneton depends on the mass. For the nuclear magneton;

$$\mu_{N} = \frac{e\hbar}{2m_{p}} = 3.15 \times 10^{-8} \,\text{eV}\,\text{T}^{-1}$$

As the magnetic moment is parallel to the angular momentum, it can be assumed that it follows some of the same rules - i.e. only μ_z and μ^2 are observables at the same time.

 g_{ℓ} is the g-factor.

For now, assume $g_{\ell} = 1$.

Precession frequency (or the Larmor frequency):

As the electron tries to align itself with the magnetic field, which is the least-energy state, it starts to precess like a gyroscope with a certain frequency.

The torque $\underline{\tau} = \mu x \underline{B}$.

$$\tau = -\frac{e}{2m}LB\sin\alpha$$

It can be shown from trigonometry that;

$$\Delta L = (L \sin \alpha) (\omega_L \Delta t)$$
$$\frac{dL}{dt} = \omega_L L \sin \alpha = \tau .$$

Putting these together;

$$\omega_{L} = \frac{\mu B}{L}$$
$$\omega_{L} = \frac{g_{\ell} \mu_{B} B}{\hbar}$$

This is the Larmor frequency. It describes the frequency with which the electron precesses around the magnetic field vector, like a gyroscope.

3.2 The Spin of the Electron

This goes back to the experiment by Stern and Gerlach. They put an atomic beam through a inhomogenous magnetic field, so there is some field gradient in one direction. This results in two dots - up and down - on a screen. There is no way to explain this classically. When the field is inhomogenous in the z-direction;

$$F_{z} = -\frac{\partial V_{mag}}{\partial z} = \mu_{z} \frac{\partial B}{\partial z}$$

The reason is the spin of the electron. Why just two points? The only possibility is that the electron has an intrinsic angular momentum (intrinsic spin). This spin is;

$$s = \frac{1}{2}\hbar$$
$$(2s+1) = 2 \text{ states.}$$

But the electron is point-like - or of order 10^{-15} in the Bohr model. If you think of it as a ball rotating, then it is rotating with something like 200 times the speed of light... Once more;

$$\left[s_{z}, s^{2}\right] = 0$$
 etc.

$$s^{2} = \frac{1}{2} \left(\frac{1}{2} + 1 \right) \hbar^{2}$$
$$\left| s \right| = \frac{\sqrt{3}}{2} \hbar$$

Only the outermost shell is relevant here - the spin of all of the others cancel.

$$\mu_{s} = -g_{s} \frac{e}{2m}s$$

Classically, there would be evidence of all possible spin of the electron - not just the two... Experimental result:

 $\mu_{s} = \pm 1 \mu_{B}$ Define;

$$g_{s} = \frac{\mu}{s} = \frac{1}{\frac{1}{2}} = 2$$

This is part of the basis of modern quantum field theory.

The Dirac equation also shows that $g_s = 2$.

Realistically, there is a small difference from 2. This is related to quantum electrodynamics - with this we can calculate the g-factor to great precision - one of the most precise tests of quantum mechanics.

3.3 Fine Structure and Spin Orbit Coupling

How can we see the effects of this magnetic moment stuff on our atoms? The angular momentum and the spin interact through the magnetic moments they create. (they "couple") This produces fine structure. Some rules:

 $j = \underline{\ell} + \underline{s}$

j is the total angular momentum.

$$\left|\underline{j}\right| = \left|\ell \pm \frac{1}{2}\right|$$

This is a new quantum number. Look at a p electron, which has;

$$\ell = 1, \ s = \frac{1}{2}$$

Two states are possible:

$$j = \frac{3}{2} \quad |\underline{j}| = \frac{\sqrt{15}}{2}\hbar$$
$$j = \frac{1}{2} \quad |\underline{j}| = \frac{\sqrt{3}}{2}\hbar$$

The difference happens because of the spin up and spin down. We need to work out the difference in energy between these two states.

The motion of the electrons around the nucleus generates a magnetic field. The spin interacts with this. $\rightarrow B_{e}$ interacts with the spin. It is best to work in the rest frame of the electron.

 \underline{r} changes to $-\underline{r}$. Use the Biot-Savart law.

$$B_{\ell} = \frac{Ze\mu_{o}}{4\pi r^{3}} \left(\underline{v} x \left(-\underline{r} \right) \right)$$

 B_{ℓ} is created by the moving charge Ze.

We know that the angular momentum:

$$\underline{L} = \underline{r} x m_e \underline{v}$$

$$B_{\ell} = \frac{Ze\mu_{o}}{4\pi r^{3}m_{o}}L$$

We have seen that the energy for the potential in a magnetic field is: V –

$$V_{\ell,s} = -\underline{\mu_s}\underline{B_\ell}$$
$$\underline{\mu_s} = g_s \frac{\underline{e}}{Zm_e} \underline{s}$$
$$g_s = z$$

$$V_{\ell,s} = \frac{Ze^2\mu_o}{4\pi r^3 m_e^2} \left(\underline{s}\underline{\ell}\right)$$

this is slightly wrong - in practice it is;

$$V_{\ell,s} = \frac{Ze^2\mu_o}{8\pi r^3 m_e^2} \left(\underline{s}\underline{\ell}\right)$$

Factor 2 off. Thomas factor. Back transformation to p rest frame.

For
$$z = 1$$
, $r = \begin{vmatrix} a \\ A \end{vmatrix}$

 $V_{\ell,s} = 10^{-4} eV$

 B_{ℓ} at the position of the electron ~ 1 Telsa.

$$\underline{j}^{2} = \underline{j}\underline{j} = (\underline{\ell} + \underline{s})(\underline{\ell} + \underline{s}) = \underline{\ell}^{2} + \underline{s}^{2} + 2\underline{\ell}\underline{s}$$

$$\underline{\ell}\underline{s} = \frac{1}{2}(\underline{j}^{2} - \underline{\ell}^{2} - \underline{s}^{2})$$

$$\langle \underline{\ell}\underline{s} \rangle = \frac{\hbar^{2}}{2}(j(j+1) - \ell(\ell+1) - s(s+1))$$

$$V_{\ell,s} = \frac{Ze^{2}\mu_{o}}{16\pi r^{3}m_{e}^{2}}(j(j+1) - \ell(\ell+1) - s(s+1))$$

Relativistic corrections;

To see what the effect of relativity is, we need to estimate the velocity of the electron. In the Bohr picture, we can just write;

$$\frac{e^2}{4\pi\varepsilon_o r^2} = \frac{mv^2}{r}$$
$$\frac{e^2}{4\pi\varepsilon_o} = rpv = \ell v = n\hbar v$$
Set $n = 1$
Velocity $v = \frac{e^2}{4\pi\varepsilon_o \hbar}$
$$\frac{v}{c} = \frac{e^2}{4\pi\varepsilon_o \hbar c} = \alpha = \frac{1}{137}$$

 α is known as the "fine structure constant". The relativistic changes of energies;

$$\frac{E_{rel}}{E_n} \sim \alpha^2 \sim 10^{-5}$$

The fine energy splittings is;

$$E_{FS} = E_{rel} + E_{ls} = -\frac{1}{2}m_{e}c^{2}(Z\alpha)^{4}\frac{1}{h^{3}}\left(\frac{1}{j-\frac{1}{2}}-\frac{3}{4n}\right)$$

1

$$j = \ell \pm \frac{1}{2}$$

Large Z, small $n \rightarrow$ not much effect on the hydrogen atom, but it is quite large for the higher Z atoms.



For the s-state, there is no ℓ hence no splitting.

Examples;

Atom	Wavelength	Splitting
H_{α}	6562 Angstrom	0.14 Angstrom i.e. very small
$Cs \ z = 55 \ n = 6$	8943 Angstrom	422 Angstrom - much bigger and noticeable.

 $n^{2s+1}\ell_i$

Hence;

$$2^{2} s_{\frac{1}{2}} \quad n = 2 \quad \ell = 0 \quad j = \frac{1}{2}$$
$$2^{2} P_{\frac{1}{2}} \quad n = 2 \quad \ell = 1 \quad j = \frac{1}{2}$$
$$2^{2} P_{\frac{3}{2}} \quad n = 2 \quad \ell = 1 \quad j = \frac{3}{2}$$

It is an unfortunate - but because of its' wide usage, unavoidable - inelegance that the same symbol μ is used both for the magnetic moments μ and μ_{B} , and for the induction or permeability constant of vacuum μ_{a} .

We now have j-degeneracy. All energy levels with the same j are identical, even if they have different ℓ and s.

Higher energy levels are pulled down to lower ones, as well as split up. (Not by a large amount, though)

All the levels for $j = \frac{1}{2}$ are at the same level, i.e. the same energy.

3.4 Hyperfine Structure

This is even smaller than fine structure, but is important as it shows a different element of the atom. Fine structure is due to the interaction between the angular momentum of the electron, and that of its' spin. i.e.:

 $E_{FS} \sim \underline{\ell} \cdot \underline{\mathbf{s}}$

Hyperfine structure is due to coupling of the magnetic moment resulting from the spin of the proton (and in general, the nucleus) with the magnetic field \underline{B}_j caused by the electron cloud. The proton and the neutron both also have;

$$s = \frac{1}{2}\hbar$$

 $g_{p} = 5.58$

This is something to do with the substructure of the proton, i.e. quarks. (See later).

$$\frac{\mu_{\rm e}}{\mu_{\rm p}} = \frac{\mu_{\rm B}}{2.79\mu_{\rm N}} \approx 658$$

Therefore we have a much smaller effect than that of fine structure, hence the name.

$$V_{HFS} = -\underline{\mu_P}B_J$$

It is $\underline{B_j}$ instead of $\underline{B_\ell}$ as there is some effect from the spin of the electron, in addition to the standard angular momentum.

 $\underline{F} = \mathbf{s}_{p} + \underline{j}$

F is the total angular momentum of the atom. This is now analogous to Fine Structure.

 $\Delta E_{HES} = 5.87 \times 10^{-6} eV$

This is 2 orders smaller than Fine Structure.

 $\lambda = 21 cm$ (this is an important line \rightarrow radio astronomy)

v = 1420.4 MHz (This is in the microwave range)

3.5 Lamb-Shift

$$v_{massured} = 1418.9 MHz$$

This is a big difference from that which was expected from Hyperfine Structure. At this point, we need QuantumElectroDynamics (QED) to explain this very important effect. Virtual contributions, e.g.:

Between the proton and the electrons, there is a binding force that can be shown by a photon, γ . As well as the standard one binding energy, there are a variety of permutations (see

diagrams). This is what QED predicts.

They are called virtual as they violate energy-momentum conservation. This can happen as it occurs within a very small amount of time given by Heisenberg

 $\Delta E \Delta t \sim \hbar$

Within this, the energy-momentum conservation can be violated.



These corrections are at the root of all modern quantum and particle physics. We can test these quantum corrections, and since energy and momentum are violated in here, anything can happen in here. The masses of the particles can be much bigger than "possible", briefly, etc.

For the electron, we can now calculate;

$$g_s = 2\left(1 + \frac{\alpha}{2\pi} - 0.328\frac{\alpha^2}{\pi^2} + \dots\right)$$

The electron is not the bare electron, but is the superposition of electrons. Similar things can be done for the muon, etc)



 ω_c is the cyclotron frequency.

$$\omega_c = \frac{eB}{m_c}$$

The spin of the electron should precess - this is $\omega_{\rm L}$, the Larmor frequency.

$$\omega_{\rm L} = g_{\rm s} \frac{\mu_{\rm B} B}{\hbar} = \frac{g_{\rm s} e B}{m_{\rm e}}$$

If $g_s = 2$, $\omega_L = \omega_c$.

We have to measure the difference between the precession frequency of the electron spin, and the cyclotron frequency, which means that if there is a difference the position of the spin, and hence the polarization, will change. In the ideal case, $g_s = 2$, the spin would always be orthogonal to the momentum.



The detector measures the angle between s and p to the precision of a billion or so.

4. Emission of Photons

4.1 Spin of the Photon

In a lithion atom, the transitions are governed by emitting photons. The transitions are similar to those of H due to 1 outer electron, however Li has two inner electrons causing a shifting effect (screening);

 $2p \rightarrow 2s$ is possible $(\Delta \ell = 1)$

 $3s \rightarrow 2p \Delta \ell = -1$

 $3s \rightarrow 2s$ is not possible. $\Delta \ell = 0$.

4d \rightarrow 3s. $\Delta \ell = 2$. Also not possible.

Only $\Delta \ell = \pm 1$ is allowed. By emitting a photon, the photon takes one unit of angular momentum with it. So, does the photon take orbital angular momentum? ~ 1 \hbar . Estimate:

If it were orbital angular momentum, it would have to be emitted at radius r.

$$r = \frac{\ell}{p} = \frac{h\lambda}{h} = \frac{\lambda}{2\pi}$$
$$p = \frac{h}{\lambda}$$

For Li; $2p \rightarrow 2s$ has $\lambda = 6708 \times 10^{-10} m$. So $r = 1068 \times 10^{-10} m$, which is not possible.

Hence the photon also has intrinsic angular momentum \rightarrow spin.

The spin of the photon is $1\hbar$.

Thus spin is something that is beyond the classical interpretation of something rotating.

4.2 The Zeeman Effect

(He was a Dutch physicist who discovered in 1896 that the spectral lines are split when you put the electron in a magnetic field)

NB: whenever multiple electron are used, we use capital letters i.e. $s \rightarrow S$, $p \rightarrow P$, $d \rightarrow D$, $f \rightarrow F$, ... Atom is placed in an external field B. The energy levels are split up. Can we understand this in an intuitive way?

Think of the atom with an electron in the centre of the coordinate system. It will oscillate in the x, y and z directions, i.e. it is not always at (0,0,0). Apply a magnetic field in the z direction,

 B_{z} .

The electron will start to precess around the electric field vector due to its' magnetic moment. The electron in the x, y plane will go around on a circular orbit.

There is no reason to assume whether the electron will go around clockwise or anticlockwise - it just depends on the state the electron was in before the magnetic field was applied. It has equal probabilities of going either way (50%,50%). Call ω_1 when it is going anticlockwise, ω_2 when clockwise.

No effect in the z-direction.

 $\omega_1 = \omega_0 + \omega_p$

$$\omega_2 = \omega_o - \omega_p$$

When ω_{a} is the normal frequency when there is no magnetic field.

We know;

$$\omega_p = \frac{eB}{2m_p}$$

Be careful;

$$\omega_{L} = \frac{eB}{m_{e}}$$

due to $g_s = 2$ for the electron.

The B field slows down or increases ω depending on the direction. The difference;

 $\Delta \omega = \pm \frac{eB}{m_a}$

This is the normal Zeeman effect.

What do we observe?

Case (1): no B field.

We have 1 line.

Case (2): B field parallel to the z-direction.

We would expect 3 lines.

 $E \perp B$, $E \parallel B$, $E \perp B$

This is only observed if we look from the side. (a transverse observation)

If we look from the top (longitudinal observation), we only see two lines - only where $E \perp B$. The picture as drawn shows the motion of the electron in the z-direction as a Hertzian dipole. i.e. there is no emission along the dipole axis due to dipole radiation.

This is the Ordinary (or Normal) Zeeman effect, and is the exception not the rule. The anomalous Zeeman effect is what happens normally. (named this way for historical reasons). In the ordinary Zeeman effect, there is no net spin s = 0.

We assumed that the total spin is just the sum of all the spins.

In general, we want to calculate the energy splitting;

$$\Delta \boldsymbol{E} = \frac{\mu_{\scriptscriptstyle B}}{\hbar} \Delta \boldsymbol{m}_{j} \boldsymbol{B}$$

 Δm_i is the spin difference.

Remember;

 $\underline{j} = \underline{\ell} + \underline{s}$

Here, S is zero - $j = \underline{\ell}$.

$$\Delta \omega = \frac{\Delta E}{\hbar} = \pm \frac{eB}{2m}$$

The only values Δm_i can take are 0 or ± 1 .

The energy splitting is proportional to B.

For the ordinary Zeeman effect, all ΔE are the same.

What else can be learnt from this effect about the photon?

We choose the field axis, and hence the quantization axis, using the *B* field. We have observed that the photon cannot be emitted in this direction $(\Delta m_i = 0)$.

We know that $j = 1\hbar$. The photon has in principle 3 states. Up, down, or outwards. The outwards is not allowed, hence it can only have two states. These two states correspond to right or left-handed circular polarization. The light emitted is polarized.

In the anomalous Zeeman effect;

In general, $s \neq 0$, and we have to take into account s and ℓ (or S and L). The total angular momentum

 $j = \ell + s$

$$\mu_j = \mu_\ell + \mu_s$$

$$\Delta E = g_{i} \mu_{B} B$$

 $g_i = g_i = 1$ when it is only orbital.

 $g_i = g_s = 2$ when it only has spin.

If we only take into account one at once, then we can easily calculate g. If not, then;

$$g_{j} = 1 + \frac{j(j+1) + s(s+1) - \ell(\ell+1)}{2j(j+1)}$$

This can easily be checked for s = 0 or $\ell = 0$.

this is known as the Lande factor. It describes the anomalous Zeeman effect. The spacing is no longer equidistant, as is now depends on the angular momentum level you are in. Also, it always has $2\ell + 1$ states - more splittings as ℓ increases.

Normal	Anomalous	
$\Delta S = 0$ (net spin = 0)	<u>s</u> and $\underline{\ell}$ i.e. $\underline{S} \neq 0$	
∆E equidistant	ΔE	
2ℓ+1states	More states	
Exception	Rule	

5. Multi-Electron Systems

5.1 Helium Atom This has Z = 2. The binding energy;

 $E_{_B} = -\frac{Ze^2}{4\pi\varepsilon_{_o}r_{_1}} - \frac{Ze^2}{4\pi\varepsilon_{_o}r_{_2}}$

The first part of this corresponds to the first electron; the second to the second electron.

 $E_{_B} = -108.8 eV$

Experiments show that the binding energy is;

 $E_{B(exp)} = -24.6eV - 54.4eV = -79eV$

This is quite different to the experimental one. This is due to the electrostatic forces between the electrons.

$$E_{\scriptscriptstyle B} = -\frac{Ze^2}{4\pi\varepsilon_{\scriptscriptstyle o}r_{\scriptscriptstyle 1}} - \frac{Ze^2}{4\pi\varepsilon_{\scriptscriptstyle o}r_{\scriptscriptstyle 2}} + \frac{e^2}{4\pi\varepsilon_{\scriptscriptstyle o}r_{\scriptscriptstyle 12}}$$

The last part is the repulsive force between the electrons. r_{12} is the distance between the electrons.

This is a non-central force. There is no exact solution to the Schrödinger equation for this. However we can estimate the size and importance of this term by estimating r_{12} .

$$r_1 \sim \frac{a_o}{Z}, r_2 \sim \frac{a_o}{Z}$$

So *r* ~ *a*_o.

Hence the last term is;

$$\frac{e^2}{4\pi\varepsilon_o a_o} = 27.2eV$$

Hence the total binding energy is $E_{_{B}} = -81.6 eV$.

Qualitatively, this picture is OK.

What else do we need to take into account?

When people looked at Helium, they found there were two types - the singlet, and the triplet helium. The latter has no ground state, and also each energy level is split up into 3 - hence the name. The energy levels themselves are also different between the two.

In one case, $S = 0 \uparrow \downarrow$, and in the other $S = 1 \uparrow \uparrow$. The latter has no ground state, while the first does.

The reason for this is the Pauli principle: no two electrons have exactly the same quantum numbers in an atom.

We can generalise this from electrons to fermions. Fermions are spin $\frac{1}{2}\hbar$ particles.

(Bosons have integer spin, and have symmetric wavefunctions)

Fermion wavefunctions are antisymmetric.

In general, you can say that all fundamental particles are fermions. All particles that exchange photons are bosons.

5.2 Angular Momentum Coupling

Things are starting to get complicated, with lots of electrons, each with their own spin and angular momentum. You need to couple the electrons.

(Check which couple strongly, which don't)

For the one-electron system, it was simple, $\underline{j} = \underline{\ell} + \underline{s}$.

Now for Helium we have ℓ_1 , ℓ_2 and s_1 , s_2 .

It turns out that in most cases, ℓ_1 , ℓ_2 and s_1 , s_2 coupling is more important than ℓ_1 , s_1 and

 ℓ_2 , \mathbf{S}_2 .

 $\underline{S} = \underline{S}_1 + \underline{S}_2$

 $\underline{L} = \underline{\ell_1} + \underline{\ell_2}$

 $\underline{J} + \underline{L} + \underline{S}$

This $\underline{L}, \underline{S}$ coupling is called the Russell-Saunders coupling.

The second type of coupling is jj coupling. $\underline{j}_i = \underline{s}_i + \underline{\ell}_i$. This is important for high Z atoms. This explains the term scheme.

5.3 ShellsOnce again, take the Helium atom. Look at the magnitudes of the quantum numbers.(i) Ground state.

Principle quantum number;

$$n_1 = 1$$
 $n_2 = 1$
 $\ell_1 = 0$ $\ell_2 = 0$

 $s_{1} = \frac{1}{2} \quad s_{2} = \frac{1}{2}$ The configuration is (1s)(1s) (ii) Excited state (First shell) $n_{1} = 1 \quad n_{2} = 2$ $\ell_{1} = 0 \quad \ell_{2} = 0$ $s_{1} = \frac{1}{2} \quad s_{2} = \frac{1}{2}$ (1s)(2s)

Closed shells have $\underline{L} = 0$.

 $\sum_{m=-\ell}^{\ell} \left| \mathsf{Y}_{\ell,m} \left(\theta, \phi \right) \right|^2 = const.$

 \rightarrow Only the valence electrons are really relevant in most considerations of the atoms, This is convenient for many observations.

Beyond Helium

Multi-electron problems can be solved by using an effective potential $V_{eff}(r)$, and then solving

the Schrödinger equation.

This is an iterative procedure; go through it and see if you get a reasonable answer, then modify and repeat.

If the electron is moved close to the nucleus, it will see the whole charge of the nucleus. So the potential will look like

$$2e^2$$

Further away, the electrons will do some shielding of the nucleus and the potential will look like

$$-\frac{\mathbf{e}^2}{r}$$
.

e.g. for Helium;

Small r: e^- sees $Z_{eff} = 2$. For large r, e^- sees $Z_{eff} = 1$.

We now have a central potential again. We can now solve the Schrödinger equation through separation of variables, etc.

 $\Psi_{n,\ell,m} = R_{n,\ell}(r) Y_{\ell,m}(\theta,\phi)$

 \rightarrow Eigenfunction solutions should look H-like.

We now expect that the solutions have the same quantum numbers as the Hydrogen atom; n = (-0, n-1, m-0, +1, +1)/(1-1)

$$n, \ell = 0, ..., n-1, m_{\ell} = 0, \pm 1, ..., \pm \ell, m_{s} = \pm \frac{1}{2}$$

NB: m stands for magnetic.

Remember that the hydrogen atom has ℓ degeneracy. In Lithium, energy levels with the same quantum number ℓ are at different energy levels. This means that for multi-electron atoms in general, this degeneracy is no longer there. This is because Z_{eff} (the effective

charge that the electron sees) depends on r. Different ℓ have different R(r).

The order of energy levels can change.

(e.g.: 1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f, 6d, 7p)



When we now count the number of possible states, we can use the current set of quantum numbers. For example;

	S	р	d
$\ell =$	0	1	2
2ℓ+1=	1	3	5
$2(2\ell + 1)$	2	6	10

For any shell,;

$$\sum_{\ell=0}^{n-1} 2(2\ell+1) = 2n^2$$

For Helium;

$$n_1 = n_2 = 1$$

$$\ell_1 = \ell_2 = 0$$

Electron configuration;

MshMsh " Msh²

Full shells are stable configurations. They are difficult to ionize.

n	2 <i>n</i> ²	Ζ	Element	$E_{ion}(\mathbf{eV})$	Shell
1	2	2	Не	24.6	K
2	8	10	Ne		L
3	18	18	Ar		М
4	32	36	Kr		Ν

He, Ne, Ar, Kr, Xe and Ru are noble gases.

These are where the outer shells are filled up.

We can see that if we look at the ionization energy plotted against $\, Z \, . \,$

Shells are not filled sequentially hue to changes in energy ordering. This is especially important for heavier things.

Subshells, which are stable shells that are not completely filled, can happen. An example in Krypton, which has n = 4.

 $(4s)^{2}(3d)^{10}(4p)^{6}$

For Krypton, we have to get Z = 36. We have 18 electrons (2+10+6). The other electrons

are in the lower shells. We aren't interested in these lower shells, as the chemical properties of the atoms are only reliant on the outer shells. The inner shells are "invisible" to these chemical properties.

The angular momentum and the spin of all those closed shells add up to zero.

The nomenclature which we use to label these states is;

 $n^{2s+1}L_i$

Lithium is n = 2 ground state. Z = 3, L = 0, $S = \frac{1}{2}$, 2s + 1 = 2.

$$J = L + S = \frac{1}{2}$$
$$2^2 S_{\frac{1}{2}}.$$

6. X-Rays

W. Röntgen

Until now we mainly looked at the outer (valence) electrons. Now, we look at the inner shell where the energy levels are the highest.

X-rays were discovered by W. Röntgen



X-rays are where the wavelength is less than those for UV. So the wavelengths are in the range of $1x10^{-9} < 100x10^{-9}$.

1<*E*<100*K*eV.

Remember $\Delta E = hv = E_1 - E_2$.

The inner electrons will see the whole nucleus, so it is similar to the hydrogen atom except the charge is increased by a factor Z. So;

$$\Delta \boldsymbol{E} = \boldsymbol{E}_{R} \boldsymbol{Z}^{2} \left(\frac{1}{n_{1}^{2}} - \frac{1}{n_{2}^{2}} \right)$$

(as for the hydrogen atom) For a lot of energy, we want high Z. There are two effects that lead to X-ray emission.

1) Bremsstrahlung ("Braking radiation")

This is the energy emitted from a decelerating or accelerating charge.

The electron passing by a nucleus changes direction, and looses energy. It will emit a photon of energy h_V .

2) Inner shell transitions

This is sometimes call characteristic radiation. This depends on the accelerating voltage, i.e. the energy of the electrons.

The characteristic energies are;

$$E_{k_{\alpha}} = E_{R} \left(Z - 1 \right)^{2} \left(\frac{1}{1^{2}} - \frac{1}{2^{2}} \right)$$

There is a correction factor, the "screening factor", due to the second electron (i.e. the position that the electron moves into) not seeing the full charge. That is the Z-1 part. The one is not fixed, and can be around 1-2.

This is known as the K_{α} line, due to it being the first transition in the k-shell.

Another energy is;

$$E_{L_{\alpha}} = E_{R} \left(Z - 7.4 \right)^{2} \left(\frac{1}{2^{2}} - \frac{1}{3^{2}} \right)$$

This is the first transition in the L shell.

$$v_{k_{\alpha}} = \frac{E_{\kappa_{\alpha}}}{h} = const.(Z-1)^2 Hz$$

Plotting the energy of the X-rays against the Z of the atom they came from, straight lines will be in evidence. This is the Moseley diagram. (Henry Moseley) These frequencies agreed with the Bohr model.

By bombarding the atoms with electrons, it is possible to identify the elements. For high Z, the inner shells' *l*-degeneracy is lifted. This is due to different Coulomb screening. This will lead to fine structure in the X-rays that can be observed.

Absorption;

When plotting the absorption cross-section as a function of the energy, you get a characteristic structure.



Electrons are moved into a higher energy state. However this state is usually occupied, hence you often get ionisation. Also, due to the fact that the energy is guantized, when the energy of the radiation increases to a sufficiently high energy, transitions from a lower shell can occur. it is much more probable that these will occur than others.

(Ionization is what basically causes cancer)

Section 2: The Nucleus

The radius of the nucleus is of the order of 1 fermi, i.e. $10^{-15}m$. That of the atom is of the order of $5.3 \times 10^{-9} m$.

The nucleus is basically made of two particles - protons and neutrons. These are fermions,

like the electron, so they also have spin of $\frac{1}{2}\hbar$.

They consist of guarks. We now move from QED to strong interactions, which are much more difficult to treat theoretically.

1) Introduction

Rutherford demonstrated that the atom consists of a nucleus at the centre by scattering alpha particles (helium nuclei) on gold foil. By measuring the angular distribution of the deflected particles, he was able to deduct that the nucleus was much smaller than the atom. The basic constituents of the nucleus are protons and neutrons. These are very similar, but not quite the same.

	Proton	Neutron
Charge	+ e	0
Spin	<i>ħ</i> ∕∕2	<i>ħ</i> ∕∕2
Mass	938.272 <i>MeV</i> /c ²	939.566 <i>MeV</i>

Consequences from these numbers:

- Charge exactly balances with the electron charge

- Number of protons determines the Z of the atom.

- Different isotopes, where the atoms have different amounts of neutrons, can be formed.

- Both protons and neutrons are fermions, i.e. spin $\frac{1}{2}\hbar$. So the Pauli principle applies.

- Free neutrons decay into protons, but not vice versa.

- It is possible that the proton will decay. But the lifetime of the proton is greater than 10³³ years - many times the age of the universe. So take 10³³ protons, and wait for one to decay in a year.

The Atom

The atom is described by electromagnetic interactions. The theory behind these interactions is described by QuantumElectroDynamics (QED). This has almost arbitrary precision - it is the best theory we know.

The Nucleus

This is more complex, in a way. Nucleons have structure - the proton and the neutron together are a nucleon. The electron that governs the properties of the atom is point-like. Protons and neutrons are spread out more, and have substructures. Also, there is a strong force interaction that holds the nucleus together that is much more difficult to handle theoretically, as it is strong. Thus, we have to use more models than exact calculations for some things.

The strong force must obviously be much stronger than the coulomb repulsion, as it holds the nucleus (an entirely positively charged object) together. It is not really a fundamental force, as the protons consist of something else. It is a residual force, similar to the Van der Waal forces in chemistry. The proton consists of uud quarks, while the nucleus is udd. u stands for

up (charge is $+\frac{2}{3}e$), while d is down (charge $-\frac{1}{3}e$).

(Quark = cottage cheese in german!)

There are also gluons in the nucleus, which hold the guarks together. (Think of a triangle: quarks at corners, gluons are the edges.)

Residual force is a short-range force. This has a range of around one Fermi $(10^{-15} m)$. For

comparison, the size of the atom is around $10^{-10} m$.

The simplest nucleus is the deuteron, from deuterium. This is an isotope of the hydrogen atom, and consists of one proton and one neutron.

	Hydrogen	Deuteron
Constituents	e ⁻ + p	p+n
Range of Force	$\frac{1}{r} \to \infty$	1fm
Size	10 ⁻¹⁰	1fm

The nucleus is a compact accumulation of little balls. They don't overlap. Potential





 $R_1 \sim 0.5 fm$, $R_2 \sim 1 - 2 fm$

We can simplify this even more by shifting the 0 point so it is at R_1 . Hence we have a line at

 $-V_{o}$ at *R*. Outside this, it is 0.

 $V(r) \rightarrow$ factorization is now possible for the central potential. (already exploited for Hydrogen).

We can now write the Schrödinger equation just as a function of R.

$$\frac{d^2 u}{dr^2} + \frac{2m}{\hbar^2} \left(E - V(r) \right) u = 0$$

For this, we have used;

$$u(r) = r\psi(r)$$

Here, use the reduced mass.

$$m_r = \frac{m_p m_n}{m_p + m_p}$$

which is approximately the mass of the nucleon divided by 2. So we now have;

$$\frac{d^2u}{dr^2} + \frac{m_n}{\hbar^2} \left(E - V(r) \right) u = 0$$

Where m_n is the nucleon mass.

For
$$r < R$$
, we know that;
 $E = -E_{binding}$
 $V(r) = -V_o$
 $\frac{d^2u}{dr^2} + \frac{m_n}{\hbar^2} (V_o - E_B)u = 0$

For *r* > *R* ;

$$\frac{d^2 u}{dr^2} - \frac{m_n E_B}{\hbar^2} u = 0$$

These are the equations for inside and outside the radius R. We can now write down a general solution;

$$u(r) = Ae^{ikr} + Be^{-ikr}$$

where A and B are constants, and

$$\begin{aligned} &k = \frac{1}{\hbar} \sqrt{m_n (E - V)} \\ &\text{So for } r < R ; \\ &k_1 = \frac{1}{\hbar} \sqrt{m_n (E_B + V_o)} \\ &\text{And for } r > R ; \\ &k_2 = \frac{i}{\hbar} \sqrt{m_n E_B} \\ &\text{Now, input the boundary conditions.} \\ &\text{For } r < R ; \\ &u(r = 0) = 0 \\ &\text{Remember that} \\ &u(r) = r\psi(r) \\ &\text{So } \psi(r) \text{ would diverge at } r = 0 \text{ otherwise.} \\ &\text{For } r > R \text{, the wave function has to disappear for } r \to \infty . \end{aligned}$$

The solution for
$$r < R$$
 is;
 $u_1(r) = 2iA\sin(k_1r)$
Solution for $r > R$;

$$\begin{split} & u_2(r) = A_2 e^{ik_2 r} \\ & \text{Now we just need to add the continuity condition, i.e. when } r = R \, . \\ & u_1(R) = u_2(R) \\ & \frac{du_1(R)}{dr} = \frac{du_2(R)}{dr} \\ & \text{The result is;} \\ & k_1 \cot(k_1 r) = -ik_2 \end{split}$$

 $\frac{1}{\tan\theta} = \cot\theta$

This depends only on three things; V_o (depends on the form of potential - this is calculable), E_B and R (which are measurable).

NB: $E_{B} = 2.2 MeV$ $m_{n} = 938 \frac{MeV}{c^{2}}$ We don't know V_{o} or R.

There is a unique relationship between V_o (the depth of the potential) and R (the radius). The size of the potential depends on the radius it goes out to, and vice versa. For R = 1 - 2fm we get $V_o \approx 30 - 50 MeV$.

We can also sketch the wave function u(r).



Before *R*, the line follows $\sin(k_1 r)$. After, $e^{ik_2 r}$.

So there is a significant probability to find the nucleon outside R. Comparing the potential with the binding energy, it can be seen that the nucleon is fairly loosely bound.





How does this compare to the Coulomb potential for the same typical radius of 1 fermi?

$$V_c = \frac{e^2}{4\pi\varepsilon_o r}$$

So for 1 fermi, we get $V_c = 1.4 MeV$. This is much weaker.

How do we know E_{B} ?

Possible way: take a photon, apply it to deuterium. You get hydrogen plus a neutron. $\gamma + {}_{1}^{2}D \rightarrow {}_{1}^{1}H + {}_{0}^{1}n$

the photon has to have an energy greater that 2.2 MeV (from experiments). This is equal to the binding energy.

For other nuclei, $E_{B} \sim 8MeV$ so the binding energy for deuterium is atypical.

Spin and orbital angular momentum of deuterium

The total spin is usually given by I.

 $\underline{I} = \mathbf{S}_p + \underline{\mathbf{S}_n} + \underline{\ell}$

where s_p is the spin of the proton, s_n that of the neutron, and ℓ the relative angular momentum.

Ground state is l = 1. $\rightarrow \underline{\ell} = 0$

$$\underline{\mathbf{s}_{p}} + \underline{\mathbf{s}_{n}} = \frac{1}{2}\hbar$$

(in principle, always add \hbar 's - this is just the unit, so is quite often dropped in calculations.) i.e.

 $\uparrow\uparrow$

рn

which is bound. The arrows indicate the spin direction. But

 $\uparrow \downarrow$

рn

is not bound (this is an experimental fact.) \rightarrow nuclear force must depend on the spin. Experiments also show that nuclear force is independent of nucleon types (*nn*, *np*, *pp*) \rightarrow bound states of *pp* or *nn* must look like this;

 $\uparrow\uparrow$

рр

n n

This contradicts the Pauli principle for fermions \rightarrow no bound *pp* or *nn* can exist. This is because, so far, our model is over simplified. We neglected the spin dependence of the nuclear force.

 $V(\underline{s}_1,\underline{s}_2)$

and the assumption of a radially symmetric potential is clearly wrong - the neutrons and protons are in a dumbbell shape - but this was needed for the Schrödinger equation.

3. Basic properties of Nuclei

- Size, mass, binding energy, shapes, ...

3.1 Nuclear size

How do we define nuclear size? It depends on the probe used - i.e. whether the particle used to see the effect on the atom is affected by the strong interaction (e.g. alpha particle), or EM interaction (alpha particle, electron, ...).

There is no abrupt boundary for the nucleus.

Rutherford scattering

Rutherford used alpha particles aimed at a gold foil to find out about the atom, and hence the nuclei. This particle is affected by both the strong and EM force.





The max point is $V_{c, max}$.

The alpha particle needs to penetrate the Coulomb barrier. Typical $E_{\alpha} \sim 5 \rightarrow 8 MeV$ (from radioactive decay).

$$V_{c}(r) = \frac{2Z_{r}e^{2}}{4\pi\varepsilon_{o}r} = \frac{2Z_{N}.1.44}{r/1fm}MeV$$

The 2 has arisen from the Z of the alpha particle. Z_N is the Z of the nucleus. Rutherford used gold (Aureum) as the nucleus.

$$Z_{N} = 79$$

$$\rightarrow V_{c}(r) = \frac{228MeV}{r/1fm}$$

We want $V_c = E_a$.

$$r = \frac{228}{8} = 28.5 fm$$

The real radius is significantly smaller $(\sim 5 fm)$.

If $E_{\alpha} \ge V_{c}^{\max}$ then the alpha particle will be absorbed into the nucleus (strong interaction). For $E_{\alpha} < V_{c}^{\max}$, it only feels the Coulomb repulsion. For the Rutherford scattering, only EM interaction is seen, not the strong interaction.

The alpha particles scatter elastically i.e. no change in the magnitude of the momentum. The impact parameter is defined as the minimum separation of the particles. The particles are scattered at angle θ .

$$b \propto \cot \frac{\theta}{2} = \frac{\cos \frac{\theta}{2}}{\sin \frac{\theta}{2}}$$

If $\theta = 0$, $b \to \infty$. If $\theta = 180^{\circ}$, b = 0. From the angular distribution, you can infer the nuclear size. $I(E_{\alpha})$ vs E_{α} the alpha particle energy:



Scattered intensity $I(E_{\alpha})$ is at $\theta = 60^{\circ}$.

The dotted line is the Rutherford formula. This breaks down when the strong interaction takes effect.

We have another probe that does not have these problems - the electron. This has the advantage that it is unaffected by the strong force. Electrons will scatter off the 3D charge distribution of the nucleus. It "sees" the whole nucleus.



Electron scattering on the nucleus I similar to light scattering on a disk (wave particle duality). $I(\theta)$ looks similar to diffraction.

Energies of the electrons;

$$E_e = p_e c$$

$$\lambda = \frac{\hbar}{p} = \frac{\hbar c}{pc} = \frac{\hbar c}{E_e}$$

$$E_e = \frac{\hbar c}{\lambda}$$

Remember $\lambda = \frac{h}{n}$.

We probe length scales $\hat{\lambda}$ with this energy.

$$\lambda = 1 fm \rightarrow E_{\rho} = 2 GeV$$

The highest energy EP Collider is HERA at DESY (Hamburg), with $E_p = 820 GeV$ and

 $E_e = 30 GeV$. Length scales ~ 0.001 fm .

Measure distribution of scattering angles

- \rightarrow form factor.
- \rightarrow Fourier transform of form factor
- → radial charge density $\rho(r)$

Observation: $\rho(r) \sim const.$ for r < R.

Uniformly charged sphere. No abrupt radius. Typical size $\sim 5 fm$

$$\langle r^2 \rangle = \frac{3}{5}R^2$$

 $A = const. \frac{4}{3}\pi R^3$

Volume of densely packed nucleons;

$$R = R_o A^{\frac{1}{3}}$$
$$\sqrt{\langle r^2 \rangle} \propto A^{\frac{1}{3}}$$
$$R_o \simeq 1.23 \, fm$$

3.2 Binding Energy

$$M(Z,A) = Zm_{H} + Nm_{n} - \frac{B(Z,A)}{c^{2}}$$

Total mass = number of protons x mass of hydrogen (= mass of proton plus effects from atom) + number of neutrons x neutron mass - binding energy.

We actually measure atomic masses not nuclear masses, but the effect is negligible.

$$M(Z,A) < Zm_{H} + Nm_{n}$$
for a bound system.
1) which nuclei are bound?

$$Z = \frac{N=2}{Stable}$$
More neutrons

This predicts that when Z is less than 83, the particle is bound / stable. The last stable nucleus is $\frac{209}{83}Bi$.

2) how does B(Z,A) change with A and Z?

N

B(A,Z) vs. A;



Remember binding energy of Deuterium is 2.22MeV .

 $\frac{B}{A} \sim const \sim 8MeV$ (at first approximation).

4. The liquid drop model and the semi-empirical mass formula

This model goes back to 1935, when it was discovered by C. F. von Weizsacker, and describes the properties of the nucleus in terms of macroscopic effects. Consider the nucleus to be a liquid drop, with 2 complications. First, we have two types of constituents - the protons and the neutrons. Second, the protons are charged. We have three forces - the nuclear force, the coulomb repulsion, and the surface tension.

1. Volume term

This is the nuclear force that keeps everything together, and is proportional to the number of nucleons in the nucleus.

$B_{V} = a_{V}A$,

where a_{v} is a proportionality constant, and is a consequence of the fact that the nuclear force is a short-range force - and only the nearest neighbours interact.

2. Coulomb term

This is due to protons repelling each other and is a long range force. It must depend on the number of proton pairs, as well as the radius.

$$B_c \propto \frac{Z(Z-1)}{R}$$

But $R \propto A^{\frac{1}{3}}$.

$$B_c = -a_c \frac{Z(Z-1)}{A^{\frac{1}{3}}}.$$

The negative sign is because this is a repulsive force.

3. Surface term

This is due to the analogy to the liquid drop. When a nucleon is on the outside of the nucleus, it will not be interacting closely with nucleons all around it - just those inside the drop ("missing" nucleons). This will reduce the binding energy, and is proportional to the surface of

the sphere, ~ $A^{2/3}$.

$$B_{\rm s}-a_{\rm s}A^{2/3}$$

4. Asymmetry term

Until now, we haven't used much quantum mechanics. However, there are terms that are rather more complicated. We know that the atom has shells which are due to the different energy levels and the Pauli exclusion principle. For a nucleus, there is something rather similar - the protons and neutrons are fermions, so also obey the Pauli exclusion principle. Hence they also have shells.

If we have a lower shell, we can have 4 particles in this level - both protons and neutrons, each with either spin up or spin down. Place 2 neutrons, 0 protons, into the second level (max of 4 also).



If we then want to add another neutron, it will have to go into level 3. If we want to then add a proton, it can be added to level 2.

It is preferred that the levels are filled one after the other, as the neutrons have to go into higher energy levels if there are more neutrons than protons. (Hence there is a "penalty" for putting in neutrons instead of protons. ?)

$$\rightarrow \left(Z - \frac{A}{2}\right)^2$$
 must be small.

Empirically (using data);

$$B_a = -a_a \frac{\left(Z - \frac{A}{2}\right)^2}{A}$$

The asymmetry becomes less important as the nucleus gets heavier.

The total mass of any nucleus is;

$$M(A,Z) = Zm_{H} + (A - Z)m_{n} - \frac{B}{c^{2}}$$
$$= Zm_{H} + (A - Z)m_{n} - a_{v}A + a_{s}A^{\frac{2}{3}} + a_{c}\frac{Z(Z - 1)}{A^{\frac{1}{3}}} + a_{a}\frac{\left(Z - \frac{A}{2}\right)^{2}}{A}$$

the c^2 is often neglected, as long as the energy and mass is measured in the same units so it is the equivalent of c = 1. Plus, it can be hidden with the different values for a. The constants vary between books, depending on how the derivations have been done, and what is included in them.

 $a_v = 15.85 \ MeV$ $a_s = 18.34 \ MeV$ $a_c = 0.71 \ MeV$ $a_a = 92.86 \ MeV$

4.1 Most Bound nucleus for fixed A

A = N + Z We are talking about isobars, which is when A is fixed but Z varies.

The most bound nucleus for a given A must have the maximum binding energy or the minimum mass.

$$\frac{\partial B(A,Z)}{\partial Z}\Big|_{A=const} = 0$$

In the mass formula, there are only two terms that depend on Z - the Coulomb term and the asymmetry term.

$$\frac{\partial}{\partial Z}\left(-a_{c}\frac{Z(Z-1)}{A^{\frac{1}{3}}}-a_{a}\frac{\left(Z-\frac{A}{2}\right)^{2}}{A}\right)=0$$

We can immediately see that this is quadratic in Z.

Simplify this slightly;

$$2Z - 1 \approx 2Z$$
$$Z_o = \frac{A}{2} \left(\frac{a_a}{a_c A^{2/3} + a_a} \right)$$

This is the minimum Z.

$$Z_{o} \approx \frac{A}{2 + 0.015 A^{2/3}}$$

e.g. $A = 111 \rightarrow Z_{o} = 47.3$. This needs to be an integer $\rightarrow 48$ here.

This corresponds to $^{111}_{48}Cd$

This is the most stable nucleus for A = 111. \rightarrow the formula is OK.

Particles will decay down to this state - Z will either increase $(Z < Z_o)$ through β^- decay

 $(n \rightarrow p + e^- + v_e)$, or decrease $(Z > Z_o)$ through β^+ decay $(p \rightarrow n + e^+ + v_e)$. β^+ decay can only happen if the neutron is bound in the nucleus, as the neutron is heavier than the proton.

Another possible process is Electron Capture (EC). This is the reverse of β^- decay. $e^- + p \rightarrow n + v_a$.



A = 111 is odd, so you get a good fit with a parabola. When A is even, the parabola doesn't seem as good a fit as before - you get two parabolas. This is an effect that cannot be simply explained by the microscopic model as it is here. It is linked to the detailed structure of the nucleon \rightarrow nucleon force. The nucleons prefer to have an even number of protons and neutrons, i.e. they prefer to pair into proton-neutron or neutron-neutron sets, related to the spin. (note that *nn* sets weren't allowed separately due to the Pauli principle. but they are allowed within the nucleus.) Pairing term;

$$B = \delta$$

 $\delta > 0$ if N is even and Z is even.

 $\delta < 0$ if N is odd and Z is odd.

 $\delta = 0$ if one is odd, and one is even.

$$\delta = a_{p}A^{-1}$$

This is parameterized, not derived. It does change between books. a_{p} is the fitted parameter,

and is
$$a_p = 11.5 MeV$$

There are only 4 stable odd-odd nuclei. ${}^{2}H_{1}$, ${}^{6}Li$, ${}^{10}B$, ${}^{14}N$. However, there are 167 eveneven stable nuclei.

4.2 Alpha Decay and Instability

 ${}^{A}_{z}X \rightarrow {}^{A-4}_{z-2}X' + {}^{4}_{2}He^{++}$ Energy conservation (assuming that X is at rest); $M_{x}c^{2} = M_{x}c^{2} + E_{x} + M_{\alpha}c^{2} + E_{\alpha}$

 $E_{x'}$ is the kinetic energy of the recall, and E_{α} the kinetic energy of the alpha particle.

$$\boldsymbol{E}_{X'} + \boldsymbol{E}_{\alpha} = \left(\boldsymbol{M}_{X} - \boldsymbol{M}_{X'} - \boldsymbol{M}_{\alpha}\right)\boldsymbol{c}^{2} = \boldsymbol{Q}_{\alpha}$$

Alpha decay is only possible if $Q_{\alpha} > 0$. This is often called the "Q-value" of a reaction.

$$Q_{\alpha} = B(4,2) + B(A-4,Z-2) - B(A,Z)$$

 $B_{\alpha} = B(4,2) = 28.3 MeV$

This has to be greater than B(A,Z) - B(A-4,Z-2). This is fulfilled for $A \ge 140$.

this means that atoms above A=140 should not exist, as they should have decayed. This is obviously not the case - the reason for this will be explained shortly.

How much kinetic energy E_{α} is taken by the alpha particle?

(i) applying momentum conservation

$$P_{\alpha} = P_{x},$$

$$m_{\alpha}v_{\alpha} = m_{x}v_{x},$$

(ii) Energy conservation

$$Q_{\alpha} = \frac{1}{2}m_{\alpha}v_{\alpha}^{2} + \frac{1}{2}m_{\chi}v_{\chi}^{2}$$

So;

$$E_{\alpha} = \frac{Q_{\alpha}}{1 + \frac{m_{\alpha}}{m_{x'}}}$$

The factor $\frac{m_{\alpha}}{m_{\chi^{*}}}$ is very small (e.g. $\frac{4}{200}$), so the particle takes a large amount of the E_{κ} from

the reaction. The typical Q values vary between 5 and 10MeV. this has a very large influence on the half-life.

It is called the Geiger-Nuttall rule.

$$2^{32}Th$$
, Q = 4MeV . $t_{1/2}$ = 1.4x10¹⁰ years
 $2^{18}Th$. Q = 9.85MeV . $t_{1/2}$ = 1.0x10⁻⁷ vears

$$^{210}Th$$
, Q = 9.85MeV . $t_{\frac{1}{2}} = 1.0 \times 10^{-7}$ year

"Theory" of alpha-decay;

-V(o)



40MeV

the Q value is above the 0 point, but below the maximum of the EM force. Thus, in order to get out of the neutron the atom has to "jump" over the EM force. This is not possible classically, but can occur rarely with quantum mechanics.

b-a is the thickness of the wall.

$$b = \frac{1}{4\pi\varepsilon_{a}} \frac{2Ze^{2}}{Q}$$

Let Q = 6MeV and b = 42fm.

The alpha particle can only get out by tunneling.

Decay constant $\lambda = \frac{\ln 2}{t_{\frac{1}{2}}} = fp$

This is semi-classical.

f is the frequency of how often the alpha particle presents itself at the wall. p is the transmission probability, i.e. the probability that it will go through the wall.

$$E_{\alpha} = \frac{1}{2} m_{\alpha} v_{\alpha}^{2} \approx |V_{o}| + Q_{\alpha} \approx 40 - 50 MeV$$
$$f = \frac{v_{\alpha}}{2R} \approx 6 \times 10^{21} s^{-1} \text{ for } Q = 5 MeV.$$
$$P \approx e^{-k(b-a)}$$

The probability for ²³⁸*U* is around 10^{-39} . For ²¹⁸*Th* it is around 10^{-15} . $\rightarrow Q_{\alpha} > 0$ still can mean a long lifetime.

4.3 Fission $A \rightarrow X + Y$ $M_x \approx M_y$ Semi-Empirical mass formula.

Symmetric case.

Plus very small pairing terms. The first and last terms cancel. Only the surface and Coulomb terms are important.

$$E_{f} = -0.26a_{s}A^{\frac{2}{3}} + 0.37a_{c}\frac{Z(Z-1)}{A^{\frac{1}{3}}}$$

The energy given out from the reaction only depends on the surface (negative) and coulomb (positive) terms - so the energy given out is coulomb energy rather than nuclear energy. Example;

$$^{238}_{92}U$$
, $E_f = 180 MeV$.

 $E_f > 0$ must be true, so $\frac{Z^2}{A} \ge 18$. This is fulfilled for $A \approx 90$. e.g. $\frac{^{116}Su}{^{50}}Su$ should decay, but it doesn't. These nuclei are still stable. Is this a failure of the SIMF? No - the same happens here as with the alpha particle.

When the nucleus starts to fall apart, it starts as a circle before changing into an ellipsoid. This means that the surface term increases, while the volume stays the same. When the two particles split, the surface still increases. Thus the potential energy increases until the particles are far enough apart for coulomb repulsion to take place, and then the potential energy decreases.



$$B_{s} = a_{s} A^{\frac{2}{3}} \left(1 + \frac{2}{3} \varepsilon^{2} \right)$$
$$B_{c} = a_{c} \frac{Z(Z-1)}{A^{\frac{1}{3}}} \left(1 - \frac{1}{5} \varepsilon^{2} \right)$$

Calculate the energy difference between the sphere and the ellipsoid.

$$\Delta B = \varepsilon^2 \left(\frac{7.34A^{\frac{2}{3}} - 0.142 \frac{Z(Z-1)}{A^{\frac{1}{3}}}}{\sum_{=0}} \right)$$

for $\frac{Z^2}{A} \ge 50$

 $\rightarrow Z \approx 100$

5) Radioactive decay

There are four different types of nuclear decay.

- \rightarrow Alpha decay
- → Beta decay
- \rightarrow Fission
- \rightarrow Gamma decay

N radioactive nuclei at a given time t.

$$-\frac{dN}{dt} = \lambda N$$

where λ is called the decay constant.

This implies that the rate of decay is constant - this is true for nuclei, but not often for other systems (e.g. human lifespan)

$$\lambda = \frac{-\frac{dN}{dt}}{N}$$
$$N(t) = N_{o}e^{-\lambda t}$$

 N_o is the original number of nuclei at t = 0.

The half-life is when half of the original nuclei have decayed.

$$N(t) = \frac{N_o}{2} = N_o e^{-\lambda t}$$
$$e^{\lambda t} = 2$$

$$t = \frac{\ln 2}{\lambda} = t_{\frac{1}{2}}$$

The (mean) lifetime τ is the average time a nuclei survives before it decays.

$$\tau = \frac{\int_{0}^{\infty} t \left| \frac{dN}{dt} \right| dt}{\int_{0}^{\infty} \left| \frac{dN}{dt} \right| dt} = \frac{1}{\lambda}$$

Activity A is;

$$A = -\frac{dN}{dt} = \lambda N$$

Activity at $t = 0$ is;

$$A_{o} = \lambda N_{o}$$

Units are decays / second.

1 Curie = $1Ci = 3.7 \times 10^{10} decays s^{-1}$

The SI unit is the Becquerel $1Bq = 1decay s^{-1}$

Decay width From Heisenberg; $\Delta E \Delta t \approx \hbar$

$$\Gamma = \Delta E = \frac{\hbar}{\tau} = \hbar \lambda$$

Long lifetime, little energy uncertainty. Short lifetime, big energy uncertainty.

Natural radioactivity;

There are two main sources of natural activity. The first is heavy elements created in supernovae, for example Thorium and Uranium (these have long lifetimes, hence have not decayed yet). The second source is radioactive isotopes, for example ${}^{40}k$, ${}^{113}Cd$, ${}^{14}C$. These are normally stable, but can be excited by gamma rays for example. These are continuously produced, and generally have a shorter lifetime.

Dating methods;

(i) how do we determine the age of the Earth?

The problem is that we have to know the number of nuclei available at t = 0. We have to derive this indirectly.

Call D the daughter nuclei. One example is ²⁰⁸Pb.

Call P the parent nuclei, ²³²Th.

We can now measure the percentage of Pb and Th in a rock, and we can assume that;

$$N_{D}(t) + N_{p}(t) = N_{p}(t=0)$$

Here we assume that all daughter nuclei have come from the decay of the same parent nuclei, and that no daughter nuclei were present at t = 0.

$$N_{p}(t) = \left(N_{D}(t) + N_{p}(t)\right)e^{-\lambda t}$$
$$t = \frac{1}{\lambda}\ln\left(1 + \frac{N_{D}(t)}{N_{p}(t)}\right)$$

 $t = 4.5 x 10^9 yrs$

Carbon dating;

¹⁴*C* nuclei are produced at a constant (?) rate through cosmic rays.

$$\frac{N(^{14}C)}{N(^{12}C)} \sim 1.5 \times 10^{-12}$$

The assumption that the decay rate is constant is not correct after 1900. This is due to using fossil fuels - $N({}^{14}C)$ will be less common than supposed, hence the ratio decreases. Also, nuclear bombs increases the ratio by around a factor of 2. The lifetime of ${}^{14}C$ is around 5700 years.

t < 50000*yrs*

6. Power generation from nuclear physics

SEMF: ~ 200MeV per fission for heavy element. 1938; Otto Hahn, F. Strassmann. 1942; Enrico Fermi; first controlled fission. 1945; Hiroshima

Naturally occurring uranium has a long lifetime. Hence by itself it isn't a good material to build a power source from. The reaction needs to be sped up.

Fission: splitting into $\frac{A}{2}$, $\frac{Z}{2}$ nuclei. The actual situation is more complex.

$$^{236}U \rightarrow A_1 \sim 140$$
, $A_2 \sim 96$

Typical process; ${}^{236}U \rightarrow {}^{148}_{57}La + {}^{88}_{35}Br$ Charge; 92 = 57 + 35

E_f ~ 170*MeV*

Decay nuclei are highly excited and they have many more neutrons than their stable isotopes - ${}^{139}_{57}La$ and ${}^{79,81}_{35}Br$.

On average, 2 or 3 neutrons are "evaporated" i.e. they exit the nuclei. The average kinetic energy of these neutrons is $\langle E_n \rangle \sim 2MeV$. These excited states decay through gamma emission. \rightarrow prompt energy. This is the energy emitted immediately after the reaction.

(i) fission fragments.

(ii) neutrons from fission

(iii) Gamma rays

We now have ${}^{87}_{35}Br$, which is β unstable. So it will decay through emission of a β particle.

$${}^{87}Br \xrightarrow{\beta^{-}} {}^{87}Kr \xrightarrow{\beta^{-}} {}^{87}Rb \xrightarrow{\beta^{-}} {}^{87}Sr$$

 $t_{1/2}$ 56s 76m 5x10¹⁰ years

⁸⁷Sr is stable. However, Rb has a long half-life, hence it is a long-term problem.

Radioactive decays;

 $(n \rightarrow p + e^- + v_e)$

(i) electrons

(ii) neutrinos

(iii) Gamma rays

⁸⁷*Br* very high on quadratic curve.

 \rightarrow energy is so large that it can produce neutrons in the decay chain.

Delayed neutrons are only about 1% of the total amount of neutrons (important for regulating reactor). Most energy is transformed into heat by scattering processes. Energy lost;

 \rightarrow neutrinos

→ high energy gamma rays

Let's say that we have 1 fission per second. $\approx 200 MeV / s \approx 3 \times 10^{-11} Watts$

We need to induce fission. Need thermal neutrons.

$$E_{k}\approx\frac{3}{2}kT\sim0.026eV\approx\frac{1}{40}eV$$

Cross-section

 $\overline{\sigma}$ = number of interactions per scattering centre / flux of incoming particles.

Units;
$$\frac{s^{-1}}{s^{-1}cm^{-2}} = cm^2$$
 or area. 1 barn $(10^{-28}m^2 = 100fm^2)$

Cross-section for pp scattering; $R_p \approx 1 fm$. Area $\approx 3 fm^2$

 $\sigma_{_{pp}} \approx 0.03 barns = 30 mb$

Simple geometric model, good approximation!

We define two cross-sections;

(i) σ_f : fission cross-section for neutrons (i.e. $U + n \rightarrow X + Y + vn$ where v is the number of produced neutrons.

(ii) σ_a : absorption cross-section of neutrons with subsequent γ radiation.

	$\sigma_{_{f}}[b]$	$\sigma_{a}[b]$
²³⁵ U	584	97
²³⁸ U	0	2.7

- More stable

- Related to probability of hitting U and cause fission (σ_f) & probability of hitting U and absorbing v_a .

$$\sigma_{\epsilon}$$

$$\eta = v \frac{\tau}{\sigma_f + \sigma_a}$$

This is the number of fast neutrons produced per thermal neutron.

$$\eta < v \quad v \approx 2.6$$

 $\eta \left({}^{235}U \right) = 2.23$

 $\eta(^{238}U) = 0$

We need at least one neutron out of every process so the next process can begin.

Natural Uranium consists of 99.28% ^{238}U and 0.72% ^{235}U . So we have to enrich the Uranium, i.e. increase the percentage of ^{235}U .

For natural uranium, $\eta = 1.33$. This could be enough, but geometric effects etc. mean that more neutrons are lost than just in reactions. (e.g. neutron hitting wall of reactor).

To take advantage of high fission cross-section at lower neutron energies, we need to slow down the neutrons. To do this, we can use scattering with a moderator - but we can't scatter them using uranium due to resonance regions where the neutron will be absorbed at higher energies.



The moderator has to have the following conditions; (i) Small nucleon mass (i.e. $\approx m_n$) \rightarrow rapid energy loss. (ii) Low cross-section for capturing neutrons.

	$\sigma_a[b]$
H ₂ O	0.664
D ₂ O	0.001
Graphite (Carbon)	0.0045



We also want to be able to lift or lower the fuel rods, to be able to control the reaction speeds.

 H_2O and D_2O can also transport heat - another benefit.

There was a natural reactor around a billion years ago in Oklo (Gabun). At that time, the percentage of ^{235}U was higher (around 2% - so already "enriched"), and it was surrounded with water. It ran for around 50,000 years.

The geometry of the reactor is also important. Let k_{eff} be the neutron reproduction factor. $k_{eff} = \eta \varepsilon \rho f P_f P_{th}$



 $K_{\infty} = N\eta\varepsilon pf$ (for ideal geometry $P_{th} = P_f = 1$) We need K = 1 "critical".

Neutron density ρ ;

$$\frac{\Delta \rho}{\Delta t} = \frac{k\rho - \rho}{t_{o}}$$

 t_o is the time for one neutron generation, i.e. to go through the above process once.

$$\frac{d\rho}{dt} = \rho \frac{(k-1)}{t_o}$$
$$\rho = \rho_o e^{\frac{(k-1)t}{t_o}}$$

Exponential growth Typical factors for the reactor are k = 1.007, $t_o = 1ms$

$$\tau = \frac{t_o}{k-1} \approx 0.15$$

This defines the time needed to regulate the reactor.

(NB; second type of reactor; Breeding reactors are reactors that breed their own fuel.)



For the Plutonium breeder, the energy density is very high and we need sodium as a coolant. This is chemically dangerous, hence being a problem with this type of reactor.

The Thorium breeder has an advantage in that it is safer as its' reactivity R

$$R = \frac{k_{eff} - 1}{k_{eff}}$$

decreases with temperature. "This is a very nice thing." - if it overheats, then it shuts itself down chemically.

6.2 Fusion

This is the source of energy for a star, and was also used in the Hydrogen bomb. Problem; before fusion we have to overcome the Coulomb barrier. In order to do this, we need high temperatures e.g. a plasma, and also a high density. In the sun;

 $\rho = 100 g.cm^{-3}$, $T = 1.5 x 10^7 k$.

Key topics - Atoms;

2) Hydrogen Atom

- Reduced Mass
- Central potential
- Schrödinger equation
- Energy levels
- Degeneracy
- Rydberg Energy
- Bohr radius
- Wavefunctions

3. Magnetic Field and the spin of the electron

- Magnetic moment
- Larmor frequency
- Spin (Stern-Gerlach)
- Fine structure (<u>*l*</u>,<u>s</u>, relativistic effects, magnitudes)
- Hyper-Fine structure
- 4. Emission of Photons
- Ordinary vs. Anomalous
- Energy splitting

5. Multi-Electron Systems

- Helium
- Shell

6. X-Rays

- Energy
- Absorption
- Mosely

Key topics - Nucleus;

- 2) Deuteron
- Potential
- Binding energy
- Pauli principle

3) Basic Properties

- Size $R = R_{a} A^{\frac{1}{3}}$

- Rutherford scattering (which size does the α measure?)

4. Semi-Empirical Mass Formula

- Different terms, and what they mean

- B(A,Z) for fixed A

- α , $\beta \, {\rm and} \, \, \gamma \, \, {\rm decay}$

- Apply SEMF to determine energy in fission, α -decay etc.

5. Lifetimes

- ¹⁴C dating
- Geological dating

6. Fission

- Principle of reactor

- Neutron cycle