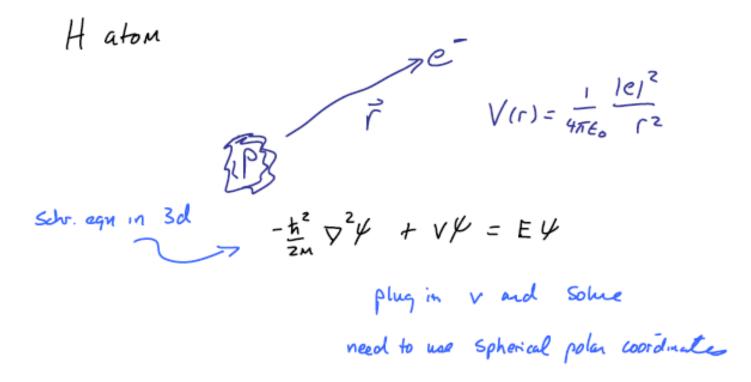
Physics 123 – April 22, 2013

Time Independent Schödinger equation (1d, nonrelativistic)

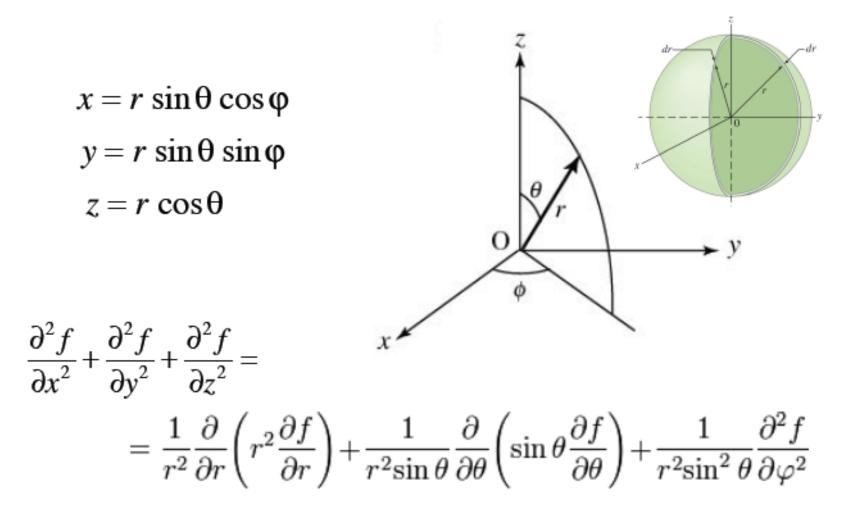
$$-\frac{\hbar^{2}}{2m} \frac{\partial^{2} \mathcal{H}_{(x)}}{\partial x^{2}} + V(x) \mathcal{H}(x) = E \mathcal{H}(x)$$

$$\frac{|\mathcal{H}_{(x)}|^{2} dv = \text{probability of finding particle in dv}$$

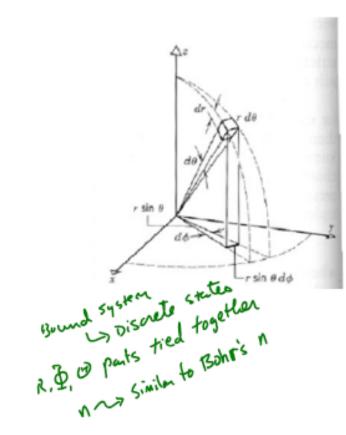
$$\int |\mathcal{H}_{(x)}|^{2} dv = 1 \qquad \text{Particle is Someplace}$$
all space



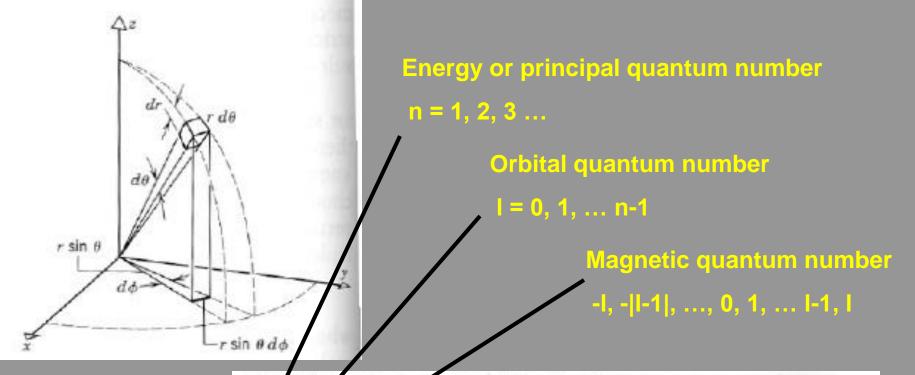
Spherical Coordinates



$$\begin{array}{c}
\psi \longrightarrow \psi(r,\theta,\theta) \\
\psi(r) = -\frac{1}{4\pi\epsilon_{0}}\frac{|e|^{2}}{r^{2}} \\
\frac{1}{2m}\left[\frac{1}{r^{2}}\frac{\partial}{\partial r}\frac{r^{2}}{\partial r}\frac{\partial \psi}{\partial r} + \frac{1}{r^{2}sin^{2}\theta}\frac{\partial^{2}\psi}{\partial \theta^{2}} + \frac{1}{r^{2}sin\theta}\frac{\partial}{\partial \theta}sin\theta\frac{\partial \psi}{\partial \theta}\right] - \frac{1}{4\pi\epsilon_{0}}\frac{|e|^{2}}{r^{2}}\psi = E\psi$$
Now solve



Can be solved exactly ... YIG, Q, Q) -> YIR) YIO) YID) Can separate Schr. equation into equis for YIR, YO, MEDI + Some Energy" or "principle" quantum # n=1, 2, 3 ... "orbital" quantum # l= 0,1,...n-1 - "Magnetic" quantum # -L, -12-11, ... 9, 1, ... , L-1, 1 ble 7.1 Some Hydrogen Atom Wave Functions R[r] $\Theta(\theta)$ $\Phi(\phi)$ m, $0 = \frac{2}{\sigma_{\pi}^{3/2}} e^{-r i \alpha_0}$ 0 $0 = \frac{1}{|2a_{*}|^{3/2}} \left(2 - \frac{r}{a_{*}}\right) e^{-r/2a_{*}}$ 2 0 1/2= $0 \qquad \frac{1}{\sqrt{3}(2\sigma_{*})^{n_{2}}} \frac{r}{\sigma_{*}} e^{-r\Delta n_{*}} \qquad \sqrt{\frac{3}{2}}\cos\theta$ $\frac{1}{\sqrt{2-1}}$ 2 $\pm 1 \qquad \frac{1}{\sqrt{3}(2\sigma_a)^{3/2}} \frac{r}{\sigma_a} e^{-r/2s_a} \qquad \frac{\sqrt{3}}{2}\sin\theta$ 2 1



n	l	m_l	R(r)	$\Theta(\theta)$	$\Phi(\phi)$		
1	t 0 0 ,		$\frac{2}{a_0^{3/2}}e^{-r/a_0}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2\pi}}$		
2	0	0	$\frac{1}{(2a_0)^{3/2}} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2\pi}}$		
2	1	0	$\frac{1}{\sqrt{3}(2a_0)^{3/2}} \frac{r}{a_0} e^{-r/2a_0}$	$\sqrt{\frac{3}{2}}\cos\theta$	$\frac{1}{\sqrt{2\pi}}$		
2	1	± 1	$\frac{1}{\sqrt{3}(2a_0)^{3/2}}\frac{r}{a_0}e^{-r/2a_0}$	$\frac{\sqrt{3}}{2}\sin\theta$	$\frac{1}{\sqrt{2\pi}}e$		

$$\Psi_{n,l,m_l}(\mathbf{r}) = R_{n,l}(r)Y_{l,m_l}(\theta,\phi)$$

$$n = 1 \qquad l = 0 \qquad m_l = 0 \qquad \psi_{100} = \frac{2}{\sqrt{r_0^3}} e^{-r/r_0} \sqrt{\frac{1}{4\pi}}$$

$$n = 2 \qquad l = 0 \qquad m_l = 0 \qquad \psi_{200} = \frac{1}{\sqrt{2r_0^3}} \left(1 - \frac{r}{2r_0}\right) e^{-r/2r_0} \sqrt{\frac{1}{4\pi}}$$

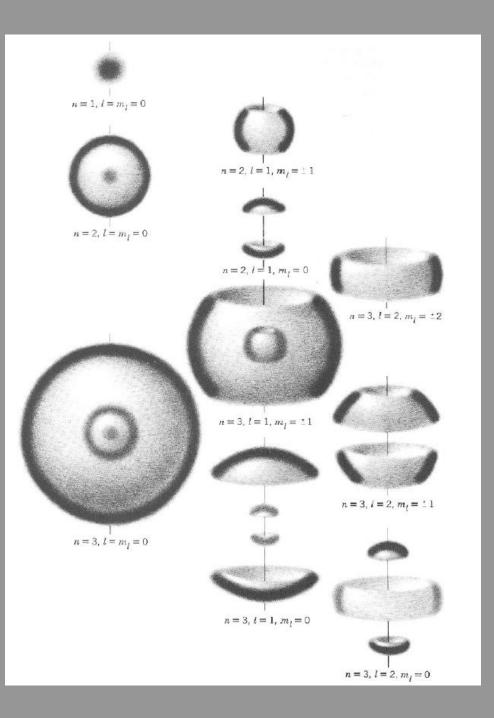
$$n = 2 \qquad l = 1 \qquad m_l = +1 \qquad \psi_{211} = \frac{1}{2\sqrt{6r_0^3}} \left(\frac{r}{r_0}\right) e^{-r/2r_0} \sqrt{\frac{3}{8\pi}} \sin \theta \ e^{i\phi}$$

$$n = 2 \qquad l = 1 \qquad m_l = 0 \qquad \psi_{210} = \frac{1}{2\sqrt{6r_0^3}} \left(\frac{r}{r_0}\right) e^{-r/2r_0} \sqrt{\frac{3}{4\pi}} \cos \theta$$

$$n = 2 \qquad l = 1 \qquad m_l = -1 \qquad \psi_{21-1} = \frac{1}{2\sqrt{6r_0^3}} \left(\frac{r}{r_0}\right) e^{-r/2r_0} \sqrt{\frac{3}{8\pi}} \sin \theta \ e^{-i\phi}$$

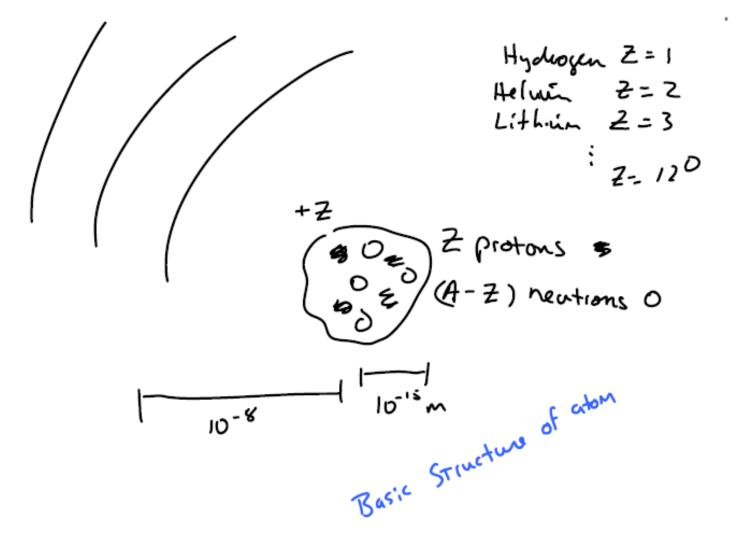
Probability distributions for several allowed atomic states for the 1-electron atom

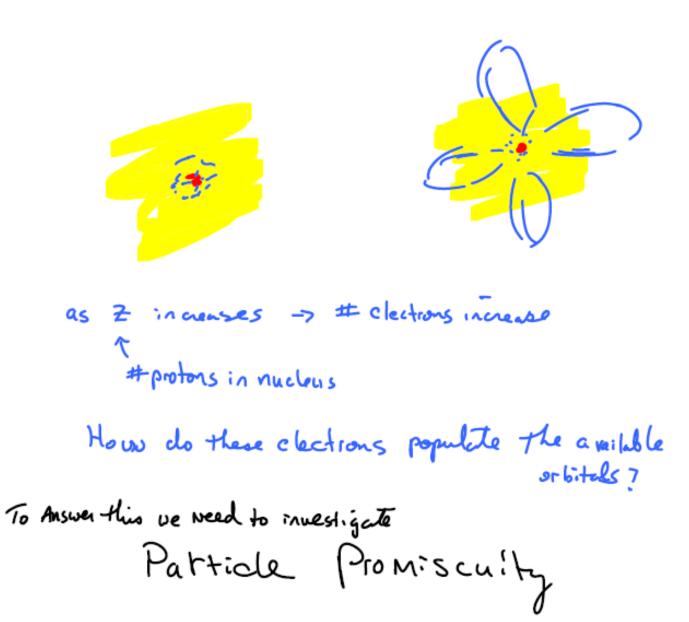
Increasing n adds new radial layers, I=0 give spherical symmetry, I not 0 brings in angular dependence



only discrete energies and spatial states allowed for the electron to occupy -> orbital Higher Hydrogen Wave Function 0 $\mathbb{S}_{nlm}(r, \vartheta, \varphi) = \sqrt{\left(\frac{2}{na_{0}}\right)^{2} \frac{(r-l-1)!}{2n[(r+l)!]}} r^{-\mu/2} d\mathbf{E}_{n-l-1}^{2l+1}(\rho) \cdot Y_{lw}(\vartheta, \varphi)$ (2,0.0) (3,0,0) 100 + (2,1,0) (3,1,0) (3,1,1)(2,1,1)(3, 2, 1)(3,2,0)(3,2,2) 0 (4,0,0) (4,1,0)(4,1,1)4.2.1) (4.2.2) 43.2) (4.3.3)

figure from http://en.wikipedia.org/wiki/File:Hydrogen_Density_Plots.png

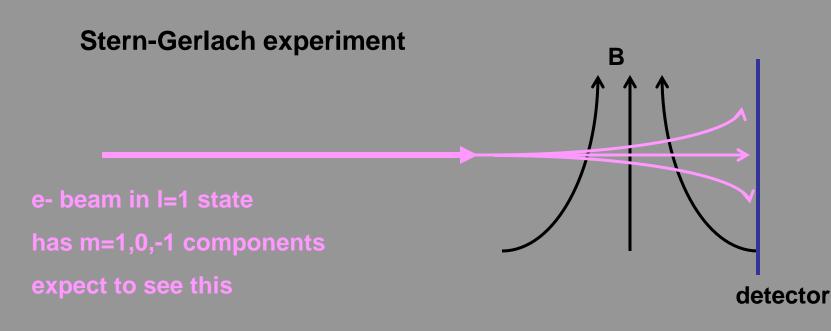




Siern-Gerlach experiment - 1922 -> Discovery that electrons have spin Classical prediction What was Silver atoms actually observed Furnace Diagram From Inhomogeneous magnetic field Willipedia "If this nonsense from Bohr will OTTO STERM Prove to be right we will quit physics." (Stem vowed in 1913) -Willipedic asquoted in Phys. Today Dec 03 Walther Gerlach from phys Today art. ele (Dec. 03)

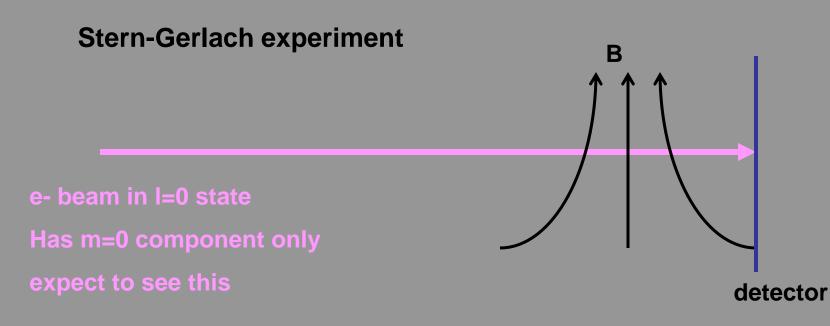
General Quant. Mech. result regarding force on magnetic dipole in a non-uniform magnetic field

$$\vec{F}_z = \frac{\partial B_z}{\partial z} \mid \vec{\mu}_z \mid = \frac{\partial B_z}{\partial z} m$$



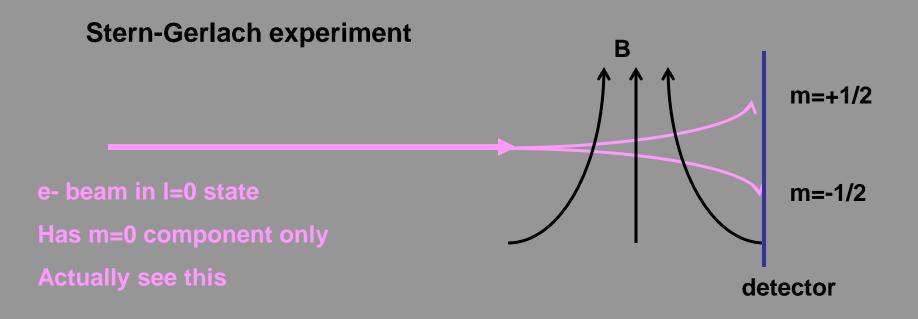
General Quant. Mech. result regarding force on magnetic dipole in a non-uniform magnetic field

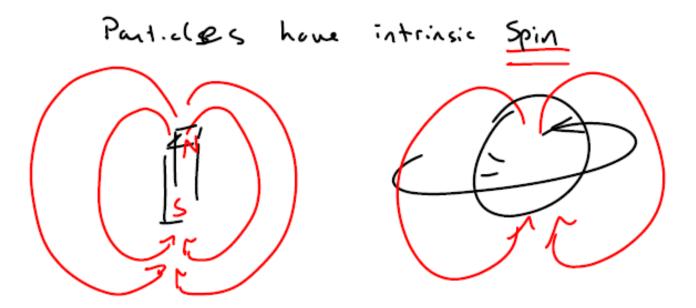
$$\vec{F}_{z} = \frac{\partial B_{z}}{\partial z} \mid \vec{\mu}_{z} \mid = \frac{\partial B_{z}}{\partial z} m$$



SURPRISE! ... fundamental particle have an intrinsic magnetic moment. Call it spin.

$$\vec{F}_{z} = \frac{\partial B_{z}}{\partial z} | \vec{\mu}_{z} | = \frac{\partial B_{z}}{\partial z} m$$





Spin is quantized 0, 1/2, 1, 3/2, 2, 5/2

Intrinsic spin - two varieties

Huge effect on multi-electron atoms

Fermions = half integral spin, such as 1/2, 3/2, 5/2, ..., 73/2 ... protons, neutrons, electrons are all fermions (s=1/2) no two fermions can occupy the same exact quantum state

Bosons = integral spin, such as 0, 1, 2 ...

photons (s=1) and pions (s=0) are examples of bosons

bosons can occupy the same exact quantum state

Rules for Filling of state for multi-electron atom n, l, m_l, m_s

Spectroscopic notation - s: I=0, p: I=1, d: I=2, f: I=3, ...

> No two electrons in same state (Pauli exclusion)

Electrons go into the state with the lowest possible energy (Aufbau)

Within a sublevel, electrons will have their spin unpaired as much as possible (due to spin-spin interaction contribution to energy)

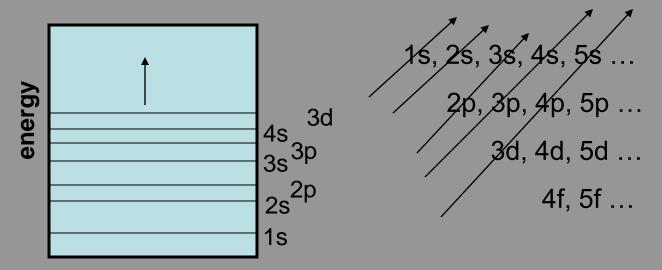
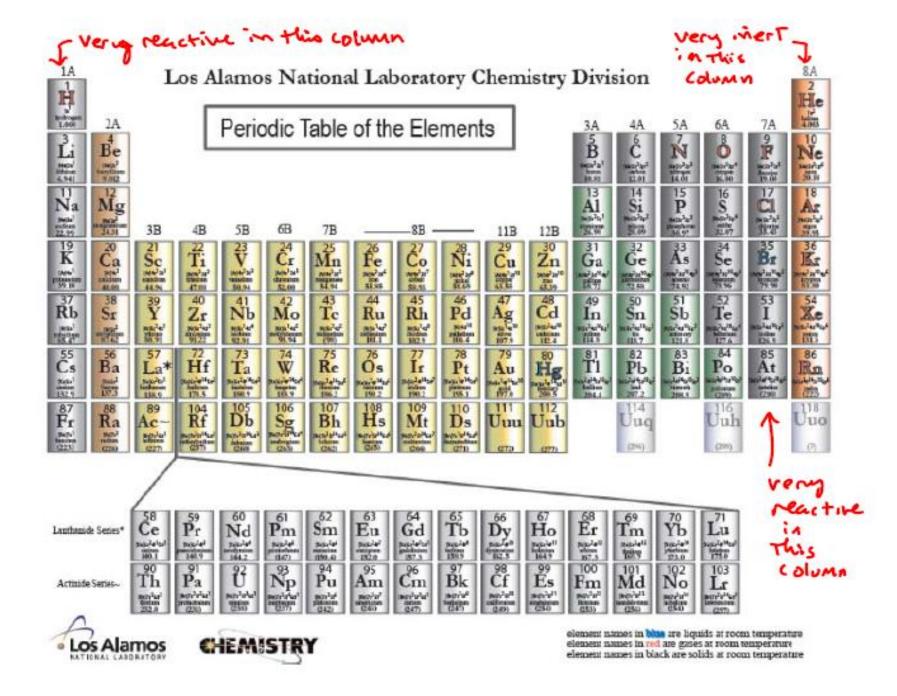


TABLE 39–1 Quantum Numbers for an Electron						
Name	Symbol	Possible Values				
Principal	n	1, 2, 3, …, ∞.				
Orbital	l	For a given $n: \ell$ can be $0, 1, 2, \dots, n - 1$.				
Magnetic	m_{ℓ}	For given n and ℓ : m_{ℓ} can be $\ell, \ell - 1, \dots, 0, \dots, -\ell$.				
Spin	ms	For each set of n, ℓ , and $m_{\ell}: m_s$ can be $+\frac{1}{2}$ or $-\frac{1}{2}$.				

L shall Kchell 1 ----Nelell Energy (n) level 3 2 . 5 sublevel (1) 5 1 1 s P Z=≠e-My==1 My=0 My=1 15' Н ۱ 152 12 2 3 7 5 He 152 25 12 Li 152252 Be 16 1k В 1525220' 12 12 6 CN O 12 14 7 10 14 8 12 11 16 152522p 1 9 F 12 11 14 12 Ne 12 16 12 12 11 10 Na 11 12 14 11 12 11 :



P.A.M. Dirac - on the development of quarture mechanics "The underlying laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are Thus completely known."

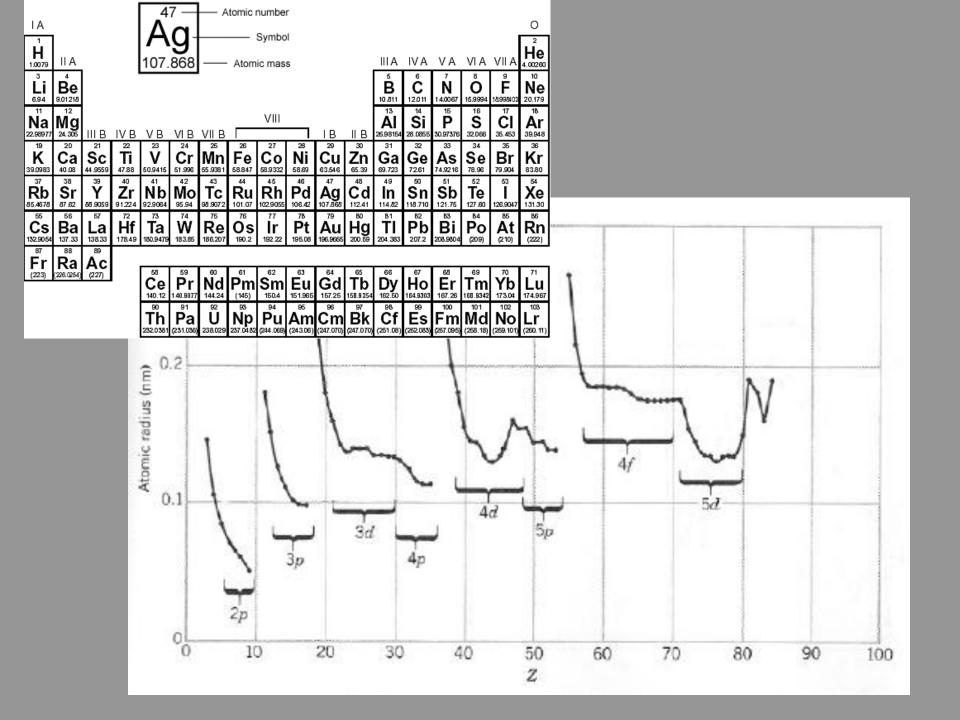


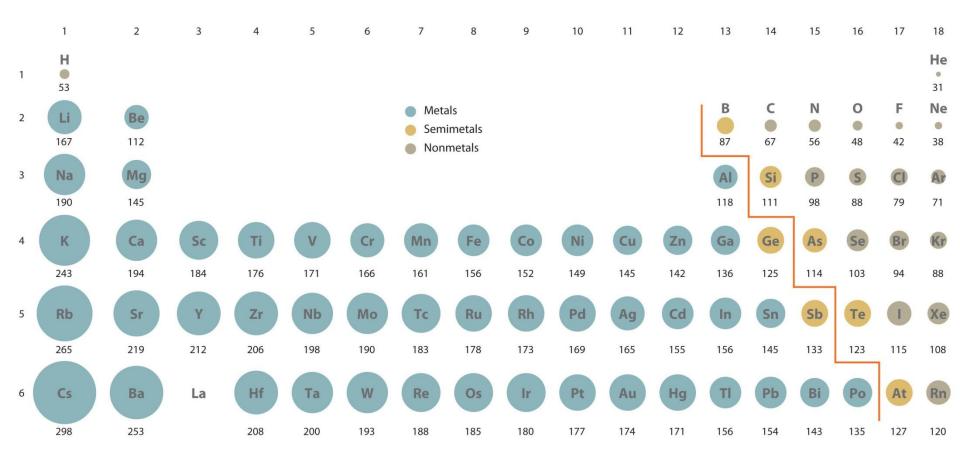
47 — Atomic number	
Ag Symbol	
	V A VI A VII A 4.00260 7 8 9 10
Li Be 6.94 9.01218 B C 10.011 12.011	N O F Ne
11 12 Na Mg 22.56977 24.305 B IV B V B VI B VI B B B 25.95154 25.0555	15 16 17 18 P S CI Ar 30.97376 32.066 35.453 39.948
19 20 21 22 23 24 25 26 27 28 29 30 31 32 K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge 39,0983 40,08 44,9559 47,88 60,9415 51,996 55,9381 68,847 68,9332 58,69 63,546 65,39 69,723 72.61	33 34 35 36
37 38 39 40 41 42 43 44 45 46 47 48 49 60	
55 56 57 72 73 74 75 76 77 7B 79 80 B1 82	83 84 85 86
87 88 89	Bi Po At Rn 200.8004 (209) (210) (222)
Fr Ra Ac (223) (226.0064) (227) Ce Pr Nd Pm Sm Eu Gd ⁶⁴ ⁶⁵ ⁶⁶ ⁶⁷	⁶⁸ T ^m Y ^b L ⁷¹
140.12 140.9077 144.24 (145) 150.4 151.965 157.25 158.9254 152.50 184.8303 90 91 92 93 94 95 96 97 98 99	167.26 168.9342 173.04 174.967 100 101 102 103
Th Pa U Np Pu Am Cm Bk Cf Es 232.0381 (231.036) 233.029 237.04.82 (244.069) (243.06) (247.070) (247.070) (251.06) (252.065)	Fm Md No Lr (257.096) (258.18) (259.101) (260.11)
	Kelen Lislall Mislall 4F St
	Energy (n) 1 2 Bell Mislull 47 57
	$\frac{(n)}{1e^{n}} = 2 \qquad 3 \qquad (1)$
	$E_{1} = E_{1} = E_{1$
	$\frac{c_{my}}{1e^{1}} \begin{pmatrix} n \\ i \\$
	$\begin{array}{c} & \text{Energy} & (n) \\ & \text{lewel} & (n) \\ & \text{sublewel} & (l) \\ z \\ z \\ & z \\ & He \\ \end{array} \begin{array}{c} (n) \\ & z \\ & s \\ $
	$\begin{array}{c} & & \\$
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	$\begin{array}{c} \underset{l \in w_{1}}{\underset{l \in w_{1}}{(m)}}{\underset{l \in w_{1}}{(m)}} \\ \underset{l \in w_{1}}{\underset{l \in w_{1}}{(m)}}{\underset{l \in w_{1}}{(m)}} \\ \underset{l \in w_{1}}{\underset{l \in w_{1}}{(m)}} \\ \underset{l \in w_{1}}{(m)} \\ \underset{l \in w_{1}$

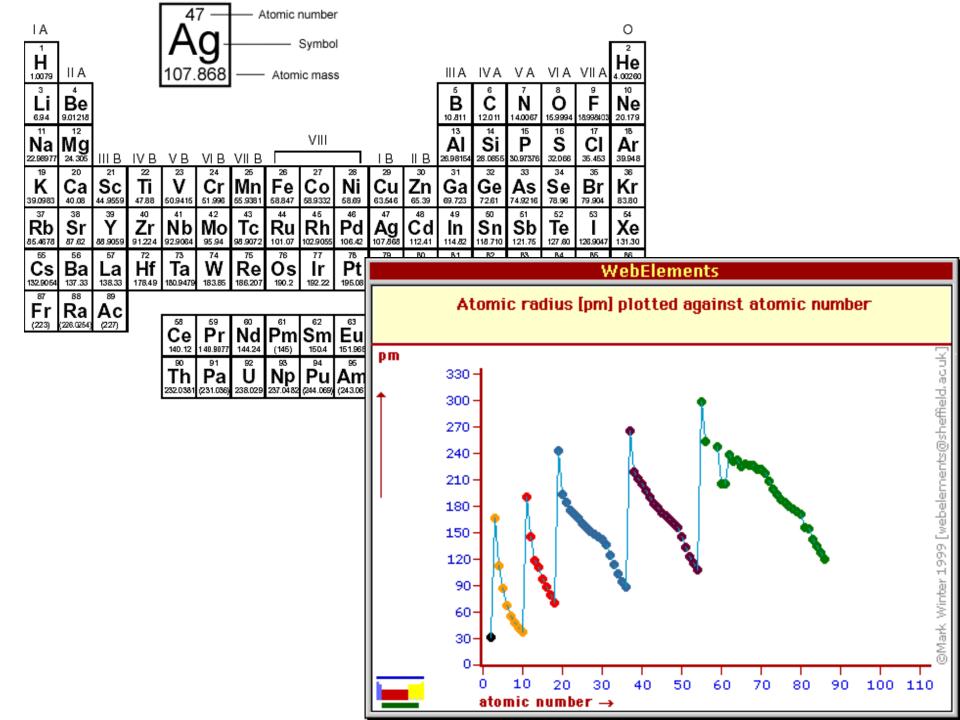
Check out

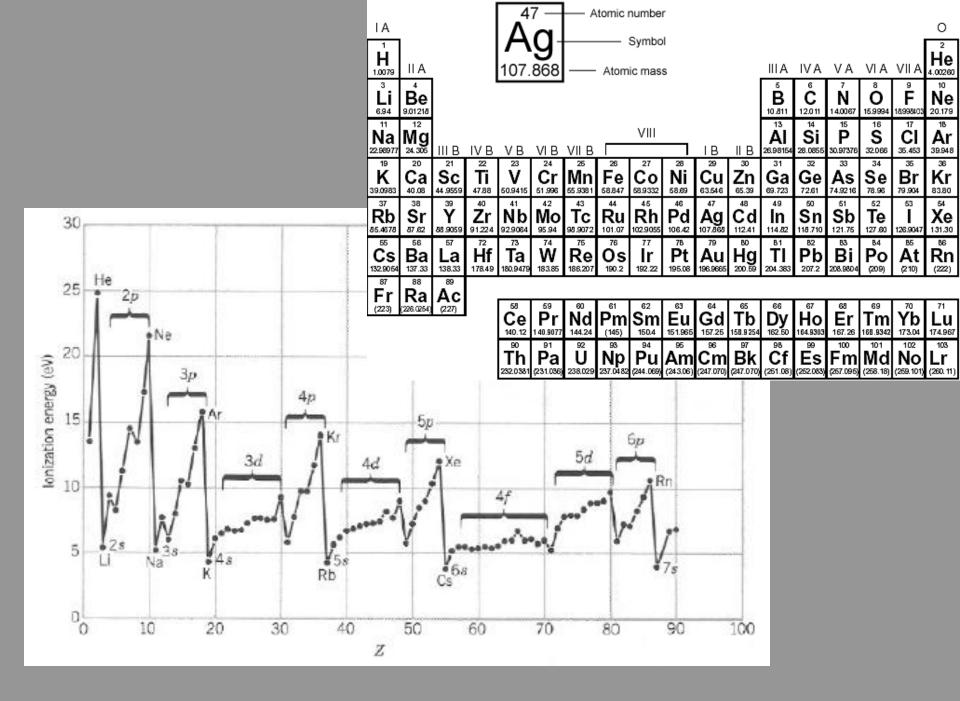
http:www.chemicool.com

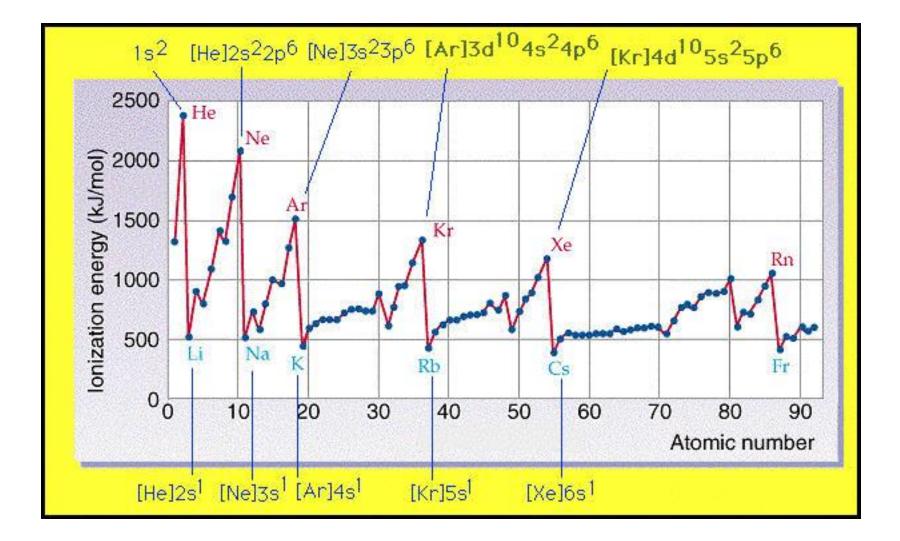
Interactive periodic chart











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H				/ \	9			0,00									Н́е
1.0079	IIA		107.868 — Atomic mass									IIIA		VA		VIIA	4.00260
³ Li	₿e									Å	ċ	Ň	ů	Å	Ňе		
	9.01218											10.811	12.011	14.0067	15.9994	18,998103	20.179
Na	Mg	VIII								Â	Ši	P	S 16	ČI	År		
22.96977	24,306	III B	IV B	VВ	VIВ	VII B				IВ	IIВ	26.98154	28.0855			35.453	39.948
19	20	21	22	23	24	25 N A	26	27	28	29	30	31	32	33	34	35	38
K 39.0983	Ca 40.08	Sc 44.9559	Ti 47.88	V 50.9416	61.996	65.8381	Fe 58.847	Co 68.9332	Ni 68.69	Cu 63.646	Zn 65.39	Ga 69.723	Ge 72.61	AS 74.9216	Se 78.96	Br 79.904	Kr 83.80
37	38	39 V	40	41	42	43	44	45	46	47	48	49	⁶⁰	61	62	63	64
Rb 85.4678	Sr 87.62	Y 88.9059	2r 91,224	Nb 92,9084	Mo 95,94	TC 98,9072	Ru	Rh 102,9055	Pd	Ag 107.868	Cd	114,82	Sn	Sb 121.75	Te 127.60	126,9047	Xe
55	56	67	72	73	74	75	76	77	7B	79	BO	B1	82	83	B4	85	86
CS 132,9054	Ba 137.33	La 138.33	Hf 178.49	Ta 180.9479	W 183.85	Re 186.207	0s	lr 192.22	Pt 195.08	AU 196.9665	Hg 200.59	TI 204.383	Pb 207.2	Bi 208.9804	Po	At (210)	Rn
87	88	89	110.49	100.9419	10.00	100.201	190.2	182.22	190.00	190.9000	200.69	204.303	201.2	206,9604	(209)	(210)	(222)
Fr	Ra	Ac															
(223)	(226.0254)	(227)		се	Pr	Ñd	Pm	Sm	Éи	Ğd	тв	Ďу	Но	Ĕ٢	Г'n	Yb	Lu
					1 40.9077	144.24	(145)	150.4	151.965		158.9254		164.9303		168.8342		174.967
				тh	Pa	92	Ñp	94 Du	Åm	ຕື້	۳Bk	٣f	[®] Es	100 Em	Md	No ¹⁰²	103 1 m
				Th 232.0381		238.029				Cm (247.070)							Lr (260.11)

