Chapter 28

Quantum Mechanics of Atoms

“Your theory is crazy, but it's not crazy enough to be true”

N. Bohr to W. Pauli

Limitations of the Bohr Model

- The model was a great break-through, but there were issues:
  - the nature of angular momentum quantization was not clear, and L being multiples of $h/2\pi$ looked like a coincidence
  - the model did not describe atoms with ≥ 2 electrons
- The theory was not crazy enough to be true
  - more radical departures from classical concepts were needed

Particles as Waves

- Light, which everybody thought was waves, also behaves like particles
- How about particles? Maybe they can also behave like waves?
    - Searching for symmetries in nature is extremely fruitful!

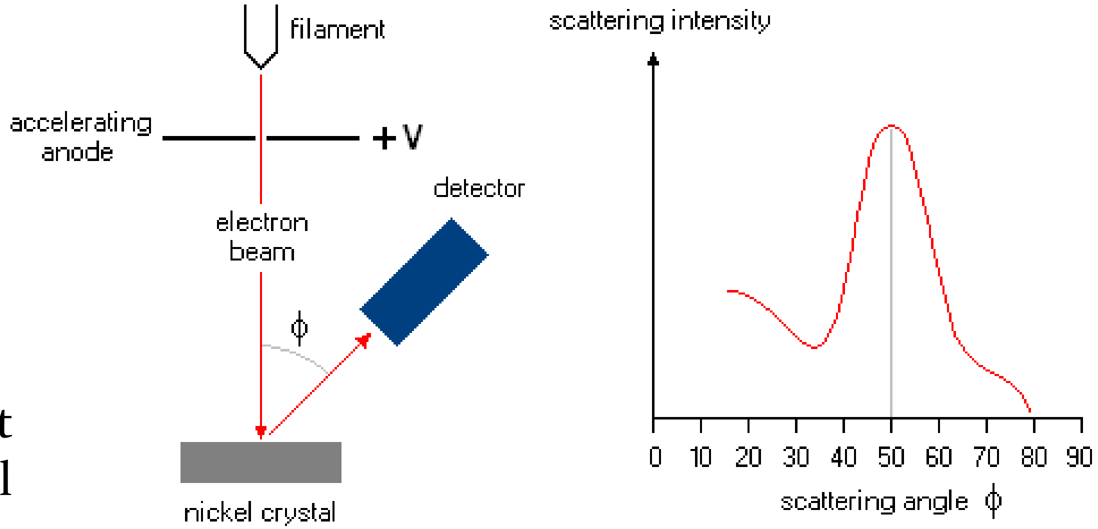
De Broglie: electron can behave like a wave, and its wavelength is $\lambda = h/p$

same as photon

Electron Diffraction

- Davisson & Germer (1927): a beam of electrons is diffracted on a crystal, much like the X-rays
    - they were able to measure the electron wavelength from the diffraction pattern, and knowing the electron speed, confirm that

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



* It was later confirmed for other particles (e.g. α-particles)
* Macroscopic objects do not exhibit wave properties –the *h* value is small

Uncertainty Principle

- If you want to measure the object position, you will need to touch it. Any touch will change its momentum!
- Even if you just look at an object, if you see it, it means that photons stroke the object and got reflected into your eye. The strike changed the object’s momentum!

Uncertainty Principle

- To see an object, we need wavelengths less than its size
  - can't see atoms with eyes! Why?
  - distance ~10^{-10} m, $\lambda=(3-7)\times10^{-7}$ m
- We can only determine distances with accuracy $\Delta x \sim \lambda$
- Suppose we are looking at objects using single photons
  - when the photon strikes an object, it changes its momentum by a value of order of its own momentum:

$$\Delta p \sim p_\gamma = \frac{h}{\lambda} \qquad\qquad \Delta p\,\Delta x \sim h$$

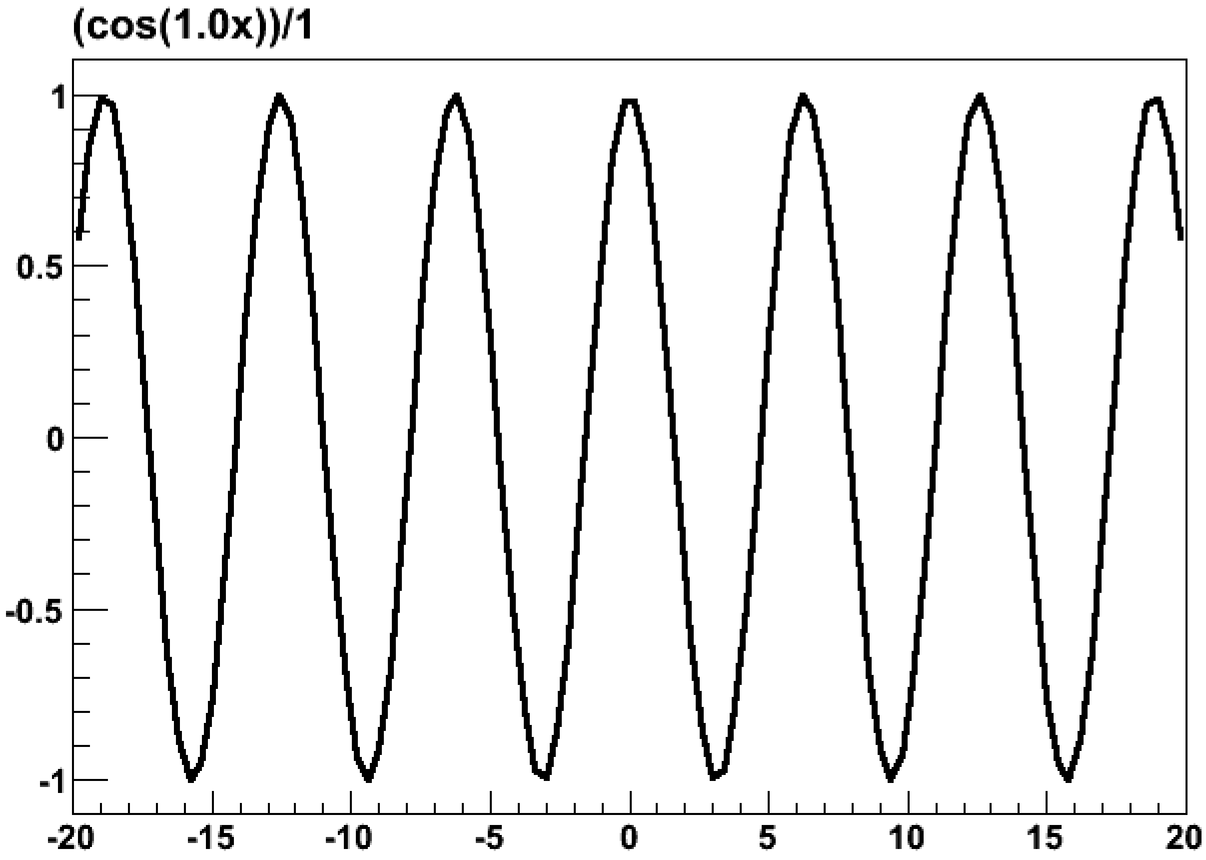
Particles as Waves and Uncertainty Principle

$$\psi = \sin(kx - \omega t)$$

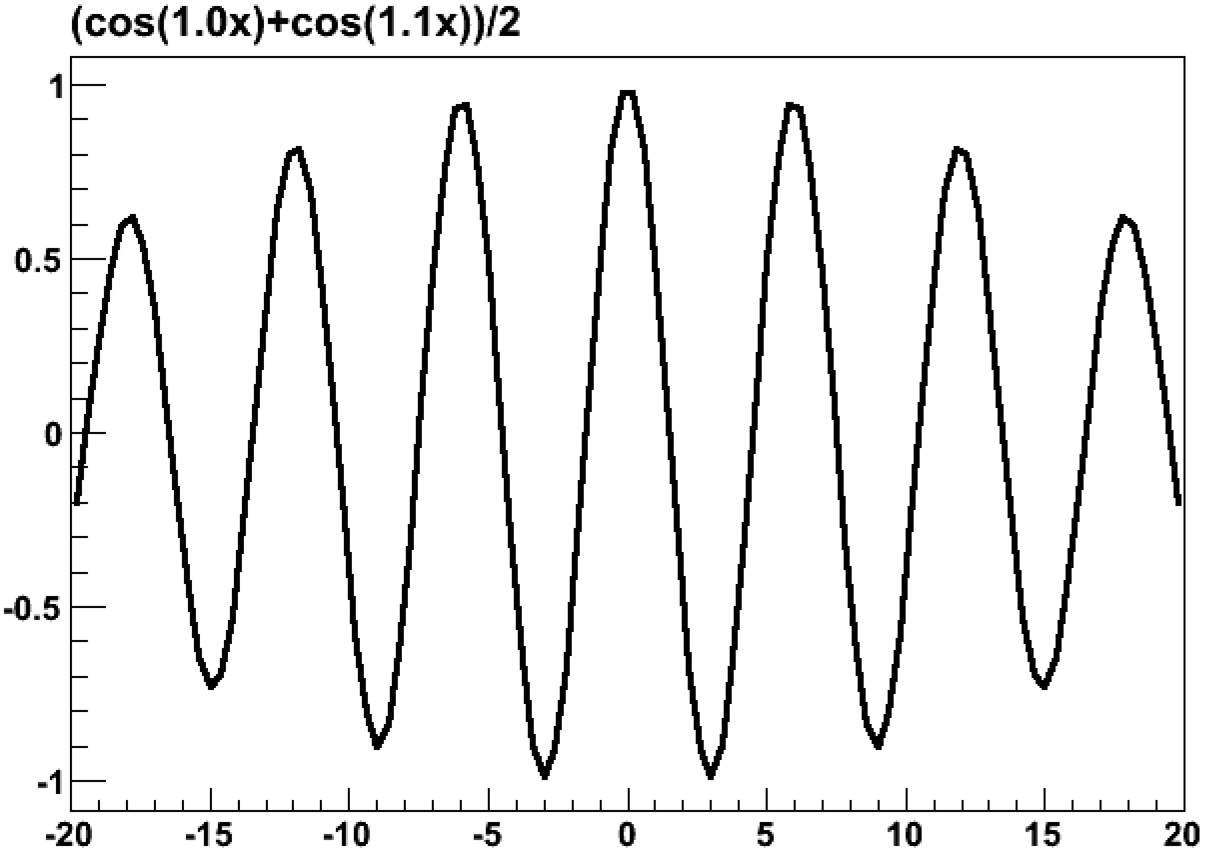
$$k = \frac{2\pi}{\lambda} = \frac{p}{\hbar}$$

- If we know wave number k (and momentum p) precisely, we have no clue where the particle is
- If we don't know the wave number well, the particle looks like a mixture of waves with different k
  - this is what is called a wave packet
- The wider is the k spread, the narrower is the wave packet

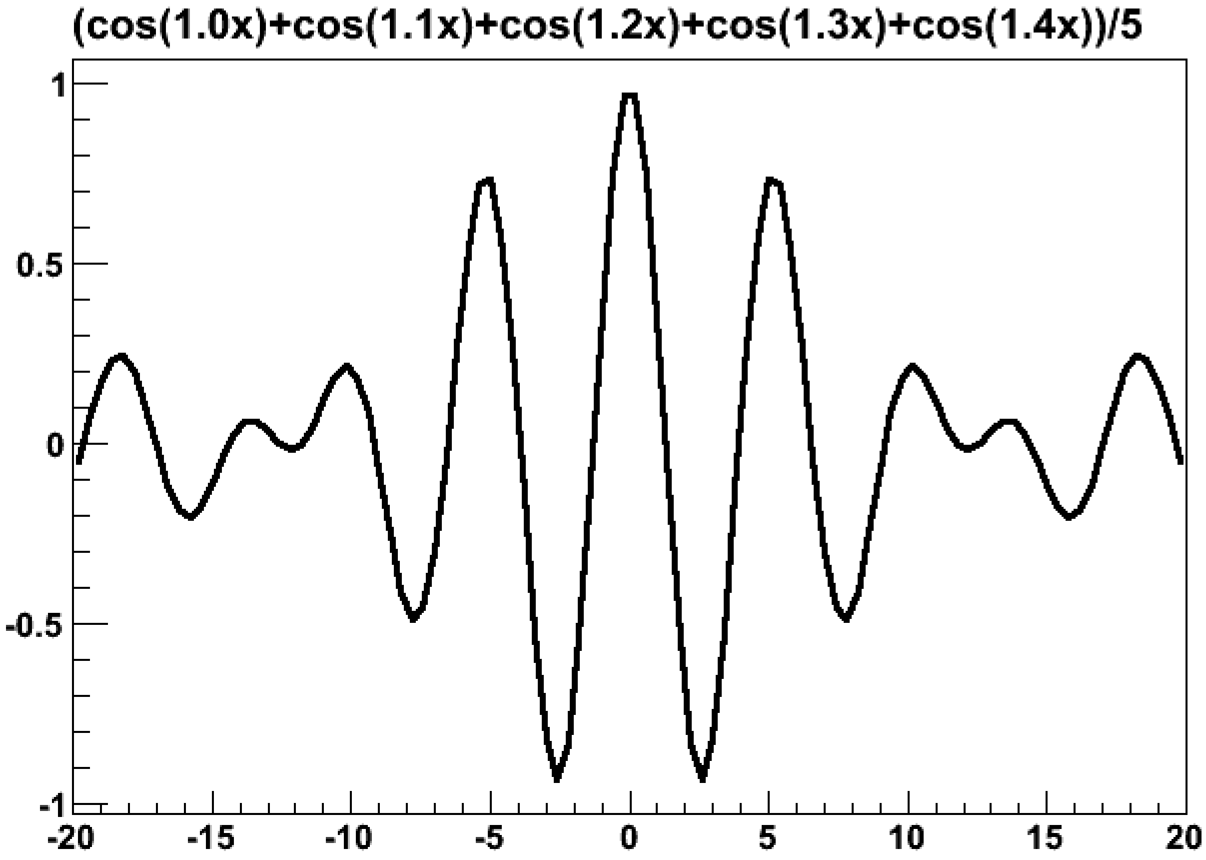
Particles as Waves and Uncertainty Principle



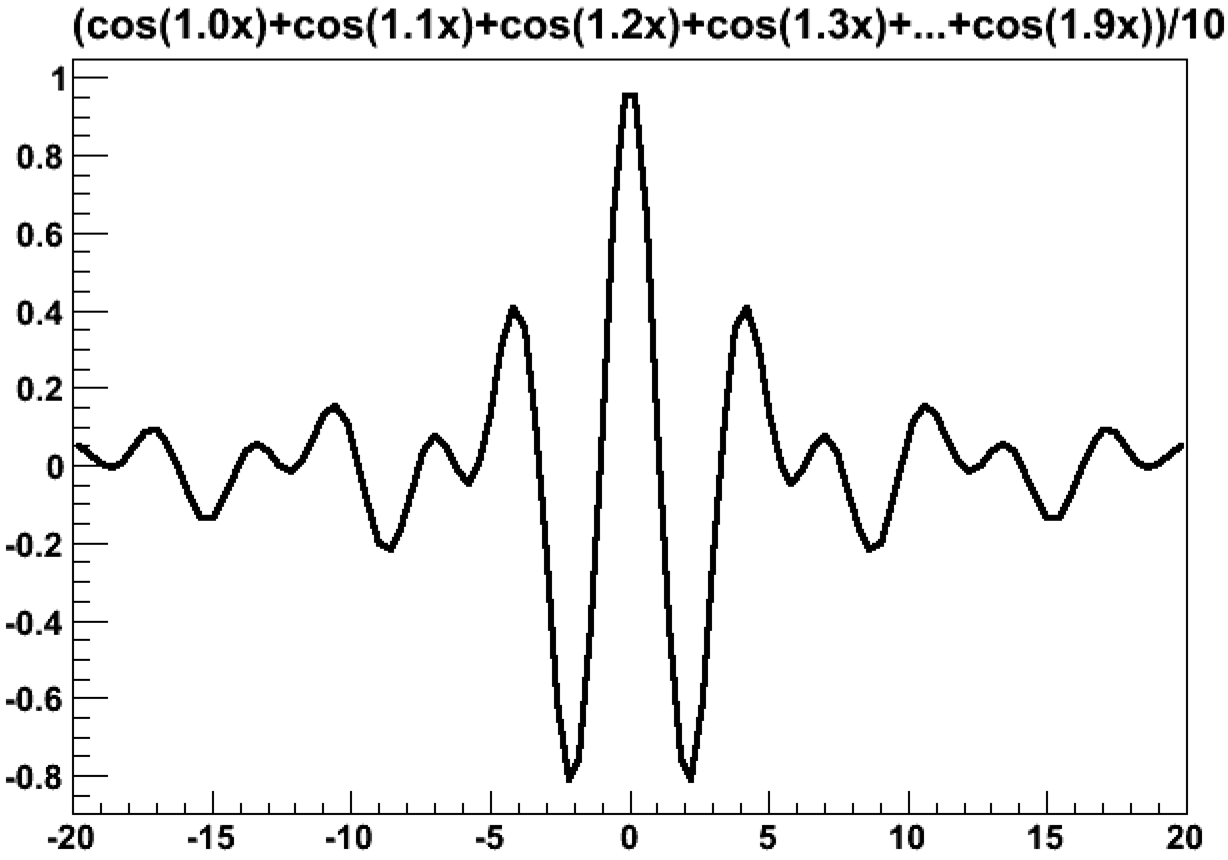
Particles as Waves and Uncertainty Principle



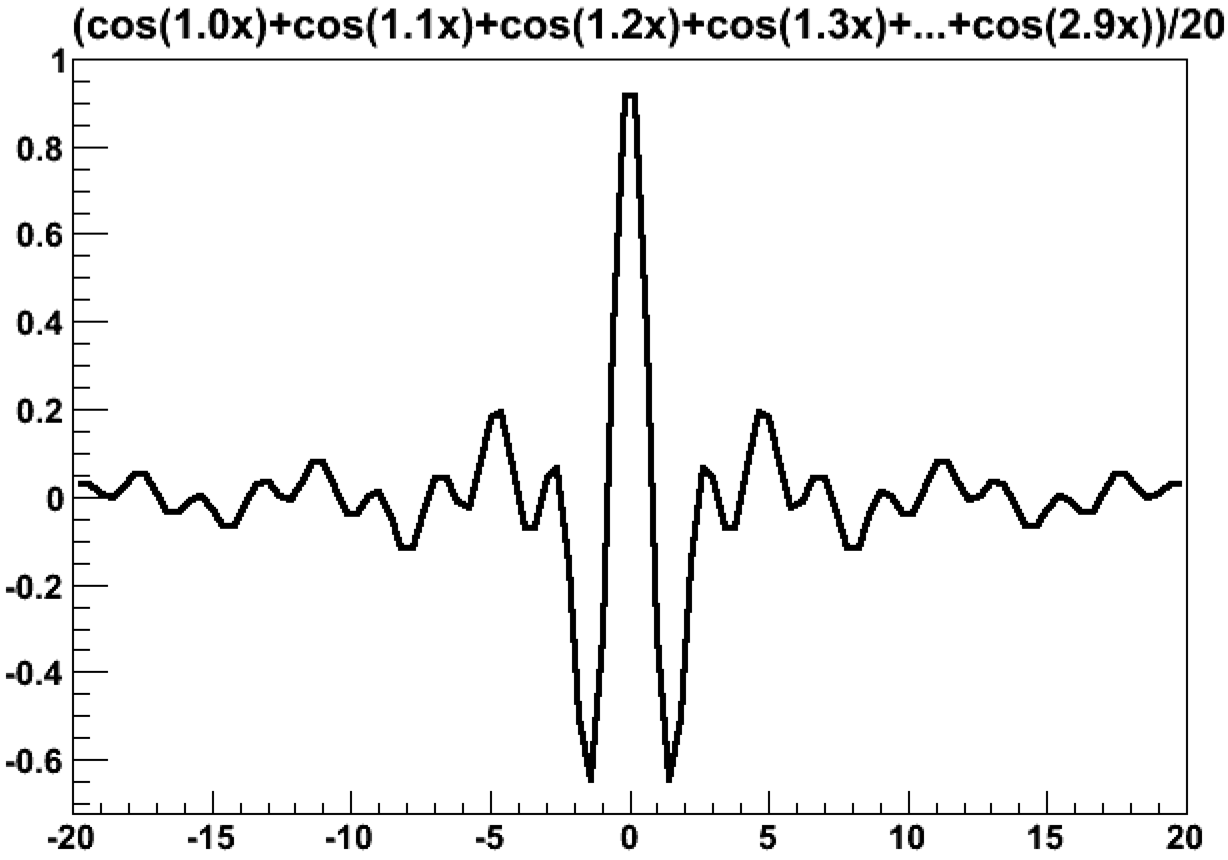
Particles as Waves and Uncertainty Principle



Particles as Waves and Uncertainty Principle



Particles as Waves and Uncertainty Principle



Uncertainty Principle

- If a particle is also a wave, then it doesn't have a definite trajectory. If we know well its direction, then we don't know well its position and vice versa.

Heisenberg uncertainty principle(s):

$$\Delta x \, \Delta p_x \geq \hbar \qquad \Delta t \, \Delta E \geq \hbar$$

Probability vs Determinism

- Classical view: if the initial conditions (positions and velocities) and the forces are known, the motion is determined (always the same).
- Quantum world: particles released in the same way will not all end in the same place!
  - double slit experiment with single photons or electrons
- Probability in QM is not a limitation of our tools – it's inherent.
- Space-time description of atoms and electrons is not possible. They are spread over time/space.

Particles and Waves

- Light is EM waves, what is oscillating is electric and magnetic fields
- When we are talking about other particles, what is oscillating?
  - Probability.

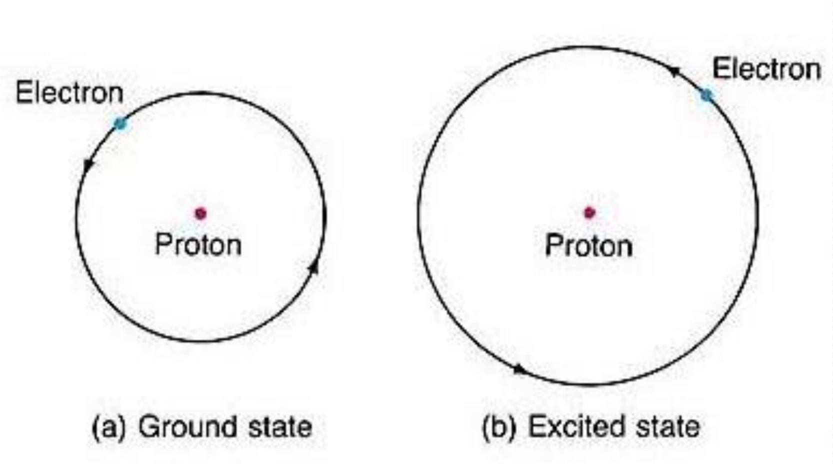
$$\psi(x, y, z, t)$$

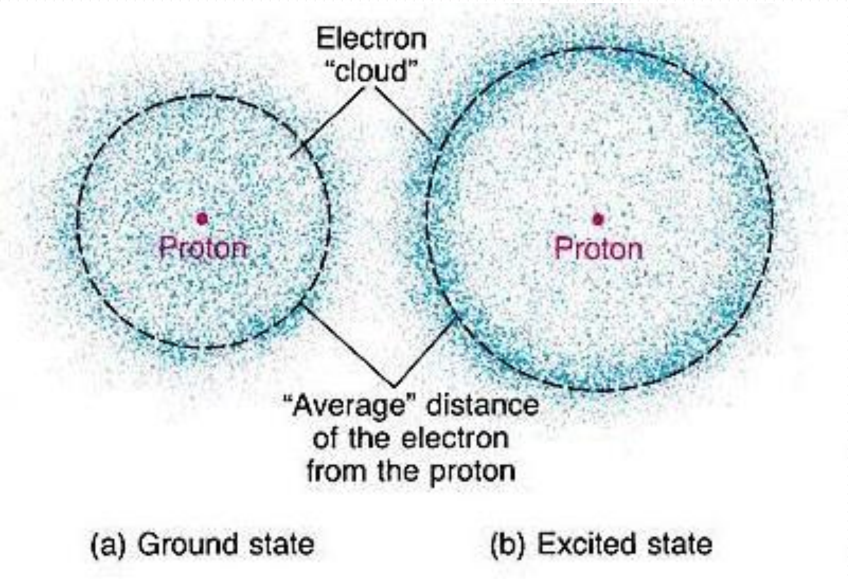
wave function = probability amplitude

$|\psi|^2$ is the probability to find a particle at x, y, z, at time t

Quantum Mechanics and Atoms

- Electrons do not follow orbits – they form “clouds”
- The ground state in hydrogen is spherically symmetric (not a circle!)





Atom: Quantum Numbers

- Principal quantum number *n*: like Bohr said

$$E_n = -\frac{13.6 \text{ eV}}{n^2}$$

- *n* can have any integer value (1, 2, …)

- It determines the total energy of a state in the hydrogen atom

Atom: Quantum Numbers

- Orbital quantum number l: yes, the angular momentum is quantized
- l can be an integer from 0 to (n-1)

larger than $l\hbar$

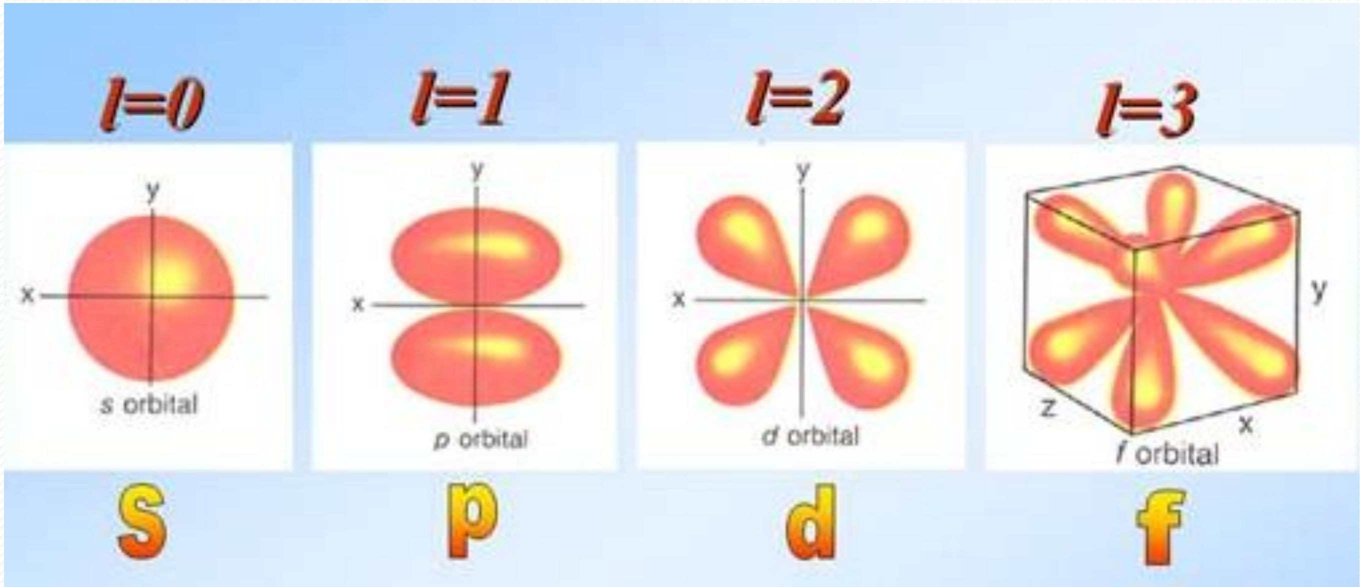
$$L = \sqrt{l(l+1)}\hbar$$

- Magnetic quantum number m_l: determines the momentum direction
- m_l can be an integer between $-l$ and l

nothing known about L_x, L_y

$$L_z = m_l\hbar$$

Electron Cloud Shapes



Spin

- Each spectral line of hydrogen actually consists of two very close lines ("fine structure")
- The splitting is ~$(Z\alpha)^2$, where $\alpha = \dfrac{ke^2}{\hbar c} \approx \dfrac{1}{137}$
  - Hypothesis: this is due to angular momentum associated with spinning of the electron (planetary model)
  - Can't be true (electrons are point-like), however electrons do have some intrinsic property which looks like an angular momentum
- m_s can be +1/2 or −1/2

$$S_z = m_s \hbar$$

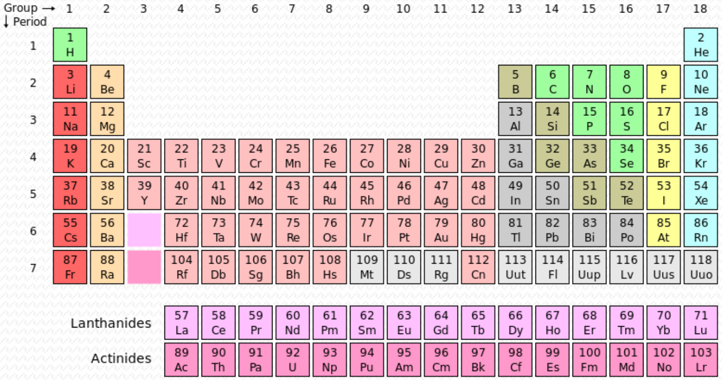
Pauli Exclusion Principle

- No two electrons in an atom can occupy the same quantum state
- Closely related to spin: refer to particles with half-integer spin (electrons, protons), but not to particles with integer spin (photons)

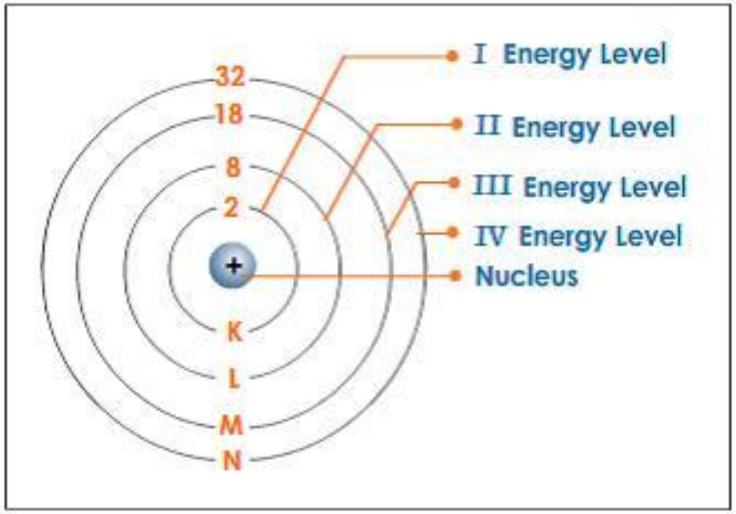
fermions

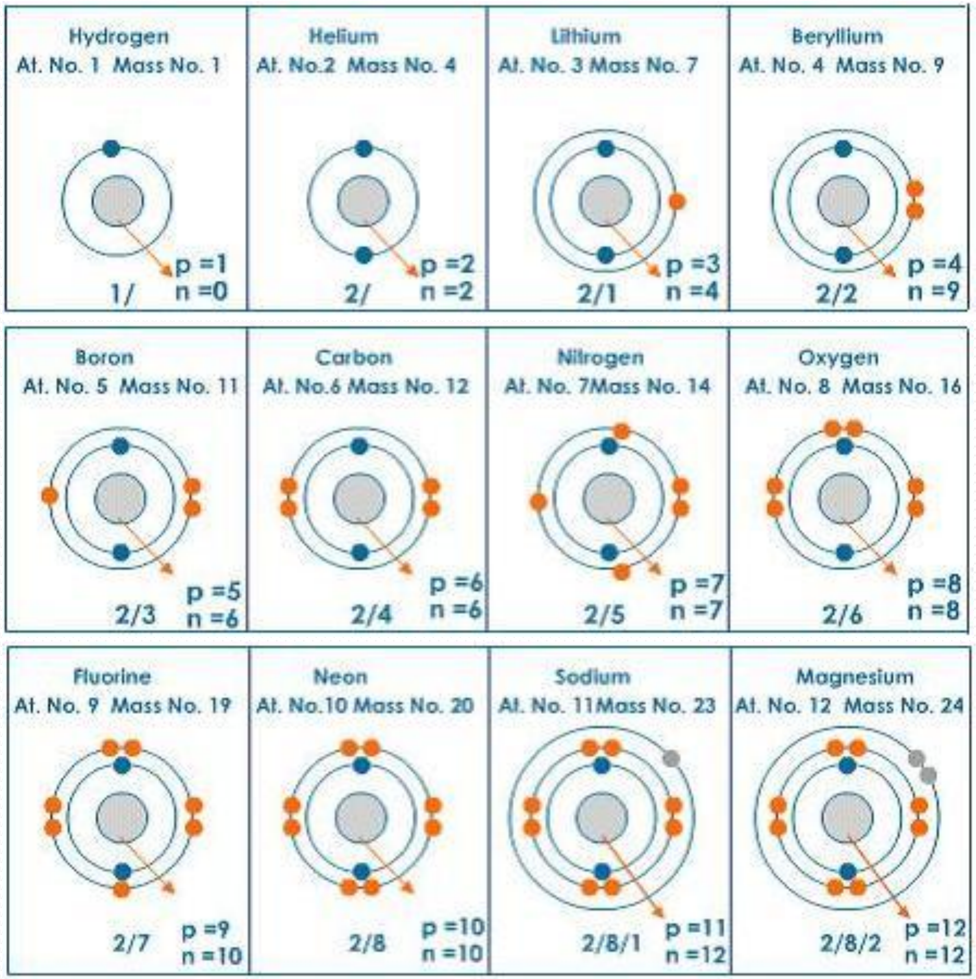
bosons

The Periodic Table of Elements



Group → ↓ Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra		104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Fl	115 Uup	116 Lv	117 Uus	118 Uuo
Lanthanides				57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
Actinides				89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr





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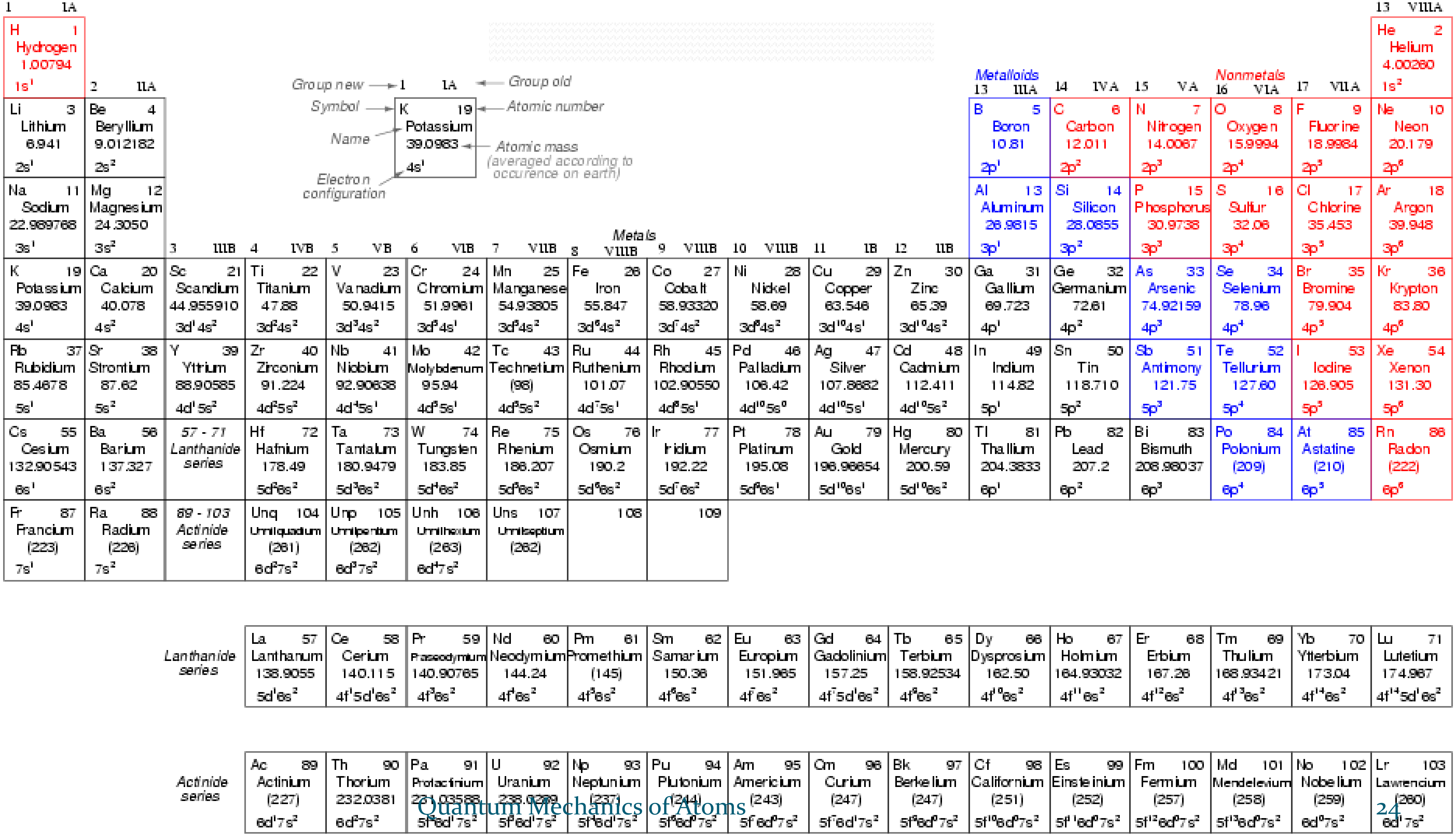

Group new → 1 IA ← Group old

Symbol → K 19 ← Atomic number

Name → Potassium

39.0983 ← Atomic mass (averaged according to occurence on earth)

Electron configuration → $4s^1$

1 IA	2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	Metals 8 VIIIB	9 VIIIB	10 VIIIB	11 IB	12 IIB	Metalloids 13 IIIA	14 IVA	15 VA	Nonmetals 16 VIA	17 VIIA	13 VIIIA
H 1 Hydrogen 1.00794 $1s^1$																	He 2 Helium 4.00260 $1s^2$
Li 3 Lithium 6.941 $2s^1$	Be 4 Beryllium 9.012182 $2s^2$											B 5 Boron 10.81 $2p^1$	C 6 Carbon 12.011 $2p^2$	N 7 Nitrogen 14.0067 $2p^3$	O 8 Oxygen 15.9994 $2p^4$	F 9 Fluorine 18.9984 $2p^5$	Ne 10 Neon 20.179 $2p^6$
Na 11 Sodium 22.989768 $3s^1$	Mg 12 Magnesium 24.3050 $3s^2$											Al 13 Aluminum 26.9815 $3p^1$	Si 14 Silicon 28.0855 $3p^2$	P 15 Phosphorus 30.9738 $3p^3$	S 16 Sulfur 32.06 $3p^4$	Cl 17 Chlorine 35.453 $3p^5$	Ar 18 Argon 39.948 $3p^6$
K 19 Potassium 39.0983 $4s^1$	Ca 20 Calcium 40.078 $4s^2$	Sc 21 Scandium 44.955910 $3d^1 4s^2$	Ti 22 Titanium 47.88 $3d^2 4s^2$	V 23 Vanadium 50.9415 $3d^3 4s^2$	Cr 24 Chromium 51.9961 $3d^5 4s^1$	Mn 25 Manganese 54.93805 $3d^5 4s^2$	Fe 26 Iron 55.847 $3d^6 4s^2$	Co 27 Cobalt 58.93320 $3d^7 4s^2$	Ni 28 Nickel 58.69 $3d^8 4s^2$	Cu 29 Copper 63.546 $3d^{10} 4s^1$	Zn 30 Zinc 65.39 $3d^{10} 4s^2$	Ga 31 Gallium 69.723 $4p^1$	Ge 32 Germanium 72.61 $4p^2$	As 33 Arsenic 74.92159 $4p^3$	Se 34 Selenium 78.96 $4p^4$	Br 35 Bromine 79.904 $4p^5$	Kr 36 Krypton 83.80 $4p^6$
Rb 37 Rubidium 85.4678 $5s^1$	Sr 38 Strontium 87.62 $5s^2$	Y 39 Yttrium 88.90585 $4d^1 5s^2$	Zr 40 Zirconium 91.224 $4d^2 5s^2$	Nb 41 Niobium 92.90638 $4d^4 5s^1$	Mo 42 Molybdenum 95.94 $4d^5 5s^1$	Tc 43 Technetium (98) $4d^5 5s^2$	Ru 44 Ruthenium 101.07 $4d^7 5s^1$	Rh 45 Rhodium 102.90550 $4d^8 5s^1$	Pd 46 Palladium 106.42 $4d^{10} 5s^0$	Ag 47 Silver 107.8682 $4d^{10} 5s^1$	Cd 48 Cadmium 112.411 $4d^{10} 5s^2$	In 49 Indium 114.82 $5p^1$	Sn 50 Tin 118.710 $5p^2$	Sb 51 Antimony 121.75 $5p^3$	Te 52 Tellurium 127.60 $5p^4$	I 53 Iodine 126.905 $5p^5$	Xe 54 Xenon 131.30 $5p^6$
Cs 55 Cesium 132.90543 $6s^1$	Ba 56 Barium 137.327 $6s^2$	57 - 71 Lanthanide series	Hf 72 Hafnium 178.49 $5d^2 6s^2$	Ta 73 Tantalum 180.9479 $5d^3 6s^2$	W 74 Tungsten 183.85 $5d^4 6s^2$	Re 75 Rhenium 186.207 $5d^5 6s^2$	Os 76 Osmium 190.2 $5d^6 6s^2$	Ir 77 Iridium 192.22 $5d^7 6s^2$	Pt 78 Platinum 195.08 $5d^9 6s^1$	Au 79 Gold 196.96654 $5d^{10} 6s^1$	Hg 80 Mercury 200.59 $5d^{10} 6s^2$	Tl 81 Thallium 204.3833 $6p^1$	Pb 82 Lead 207.2 $6p^2$	Bi 83 Bismuth 208.98037 $6p^3$	Po 84 Polonium (209) $6p^4$	At 85 Astatine (210) $6p^5$	Rn 86 Radon (222) $6p^6$
Fr 87 Francium (223) $7s^1$	Ra 88 Radium (226) $7s^2$	89 - 103 Actinide series	Unq 104 Unnilquadium (261) $6d^2 7s^2$	Unp 105 Unnilpentium (262) $6d^3 7s^2$	Unh 106 Unnilhexium (263) $6d^4 7s^2$	Uns 107 Unnilseptium (262)	108	109									

Lanthanide series	La 57 Lanthanum 138.9055 $5d^1 6s^2$	Ce 58 Cerium 140.115 $4f^1 5d^1 6s^2$	Pr 59 Praseodymium 140.90765 $4f^3 6s^2$	Nd 60 Neodymium 144.24 $4f^4 6s^2$	Pm 61 Promethium (145) $4f^5 6s^2$	Sm 62 Samarium 150.36 $4f^6 6s^2$	Eu 63 Europium 151.965 $4f^7 6s^2$	Gd 64 Gadolinium 157.25 $4f^7 5d^1 6s^2$	Tb 65 Terbium 158.92534 $4f^9 6s^2$	Dy 66 Dysprosium 162.50 $4f^{10} 6s^2$	Ho 67 Holmium 164.93032 $4f^{11} 6s^2$	Er 68 Erbium 167.26 $4f^{12} 6s^2$	Tm 69 Thulium 168.93421 $4f^{13} 6s^2$	Yb 70 Ytterbium 173.04 $4f^{14} 6s^2$	Lu 71 Lutetium 174.967 $4f^{14} 5d^1 6s^2$
Actinide series	Ac 89 Actinium (227) $6d^1 7s^2$	Th 90 Thorium 232.0381 $6d^2 7s^2$	Pa 91 Protactinium 231.03588 $5f^2 6d^1 7s^2$	U 92 Uranium 238.0289 $5f^3 6d^1 7s^2$	Np 93 Neptunium (237) $5f^4 6d^1 7s^2$	Pu 94 Plutonium (244) $5f^6 6d^0 7s^2$	Am 95 Americium (243) $5f^7 6d^0 7s^2$	Cm 96 Curium (247) $5f^7 6d^1 7s^2$	Bk 97 Berkelium (247) $5f^9 6d^0 7s^2$	Cf 98 Californium (251) $5f^{10} 6d^0 7s^2$	Es 99 Einsteinium (252) $5f^{11} 6d^0 7s^2$	Fm 100 Fermium (257) $5f^{12} 6d^0 7s^2$	Md 101 Mendelevium (258) $5f^{13} 6d^0 7s^2$	No 102 Nobelium (259) $6d^0 7s^2$	Lr 103 Lawrencium (260) $6d^1 7s^2$