

Week 6 & 7: H Atom & Periodic Table Announcements

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Hydrogen Atom (Solution 3)

- Use the V from Coulombic potential energy of one proton and one electron (H atom) in S .

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\Psi = 0 \quad V(r) = \frac{-Zq^2}{4\pi\epsilon_0 r}$$

- Get a separable wave function in spherical coordinates

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

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Quantum Numbers

- Since the wave function ψ must be well behaved, continuous, etc., there are only certain values of the quantum numbers: n, l, m_l and m_s which can be used
- Principal quantum number:

- Orbital angular momentum number:

- Magnetic quantum number:

- Spin

Radial Wave Function

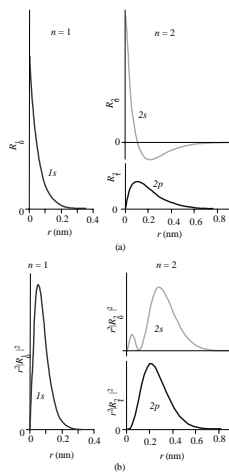


Fig. 3.21: (a) Radial wavefunctions of the electron in a hydrogenic atom for various n and ℓ values. (b) $r^l R_{nl}$, $\ell \geq 0$

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Spherical Harmonic Wave Function

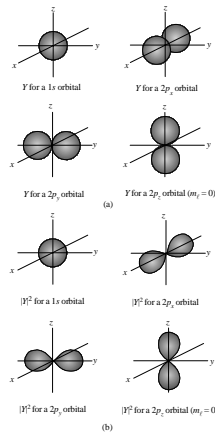


Fig. 3.22: (a) The polar plots of $Y_{n,m}(\theta, \phi)$ for 1s and 2p states. (b) The angular dependence of the probability distribution which is proportional to $|Y_{n,m}(\theta, \phi)|^2$.

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Orbitals

- These are **not orbits but an orbitals!**
- For **s-states**, Ψ function does not depend on r
 - $R(r)$ is spherical symmetric and we think of s states as spherical orbitals, where the electron density is constant everywhere
 - Probability highest in a shell near
 - For example for H atom: $r=a_0=0.0529$ nm
 - » This is the **1st Bohr radius** of the H atom
 - » a_0 is the radius of the ground state
- **P-states** have directionality: these come about in Y (angular) component

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Energy Levels

- The energy of the level is determined by n

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

- Now for H, where $Z=1$, the lowest energy state is 1s, and the energy of that state is called ionization energy:

$$E_I = \frac{mq^4}{8\epsilon_0^2 h^2} = 13.6eV$$

- For other atoms and other energy levels:

$$E_n = -\frac{Z^2 E_I}{n^2}$$

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Energy Levels of H Atom

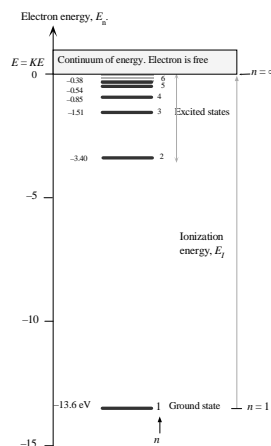


Fig. 3.23: The energy of the electron in the hydrogen atom ($Z = 1$). 30

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Electron in a Box

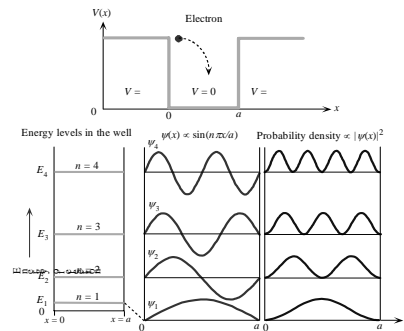


Fig. 3.15: Electron in a one-dimensional infinite PE well. The energy of the electron is quantized. Possible wavefunctions and the probability distributions for the electron are shown.

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Compare Energy States of H with Electron in a Box

- Unlike the electron in a box, the energy states get closer together as n increases, instead of further apart.
- Higher states have smaller (negative) energy values...Why the difference??

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Absorption & Emission Spectra

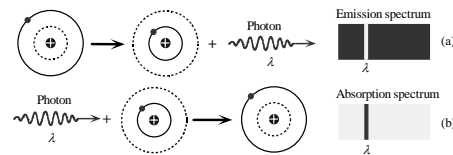


Fig. 3.24: The physical origin of (a) emission and (b) absorption spectra.

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Excitation & Emission

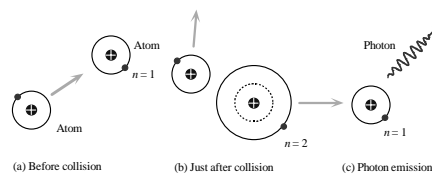


Fig. 3.25: An Atom can become excited by a collision with another atom. When it returns to its ground energy state, it emits a photon.

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Orbital Angular Momentum: l

- l and m_l: Quantize the magnitude of the orbital angular momentum (just like energy is quantized)
- Orbital angular momentum exists due to the fact that the electron is attracted to the nucleus with a certain force

$$L = \hbar[l(l+1)]^{1/2}$$

- l gives the shape of the orbitals

Orbital Angular Momentum

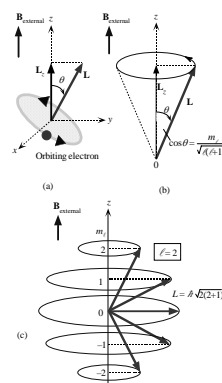


Fig. 3.26(a) The electron has an orbital angular momentum which has a quantized component, L_z , along an external magnetic field, B_{external} . (b) The orbital angular momentum vector L rotates about the z -axis. Its component L_z is quantized and therefore the orientation of L , the angle θ is also quantized. L traces out a cone. (c) According to quantum mechanics, only certain orientations (θ) for L are allowed as determined by l and m_l .

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Magnetic Quantum Number: m_l

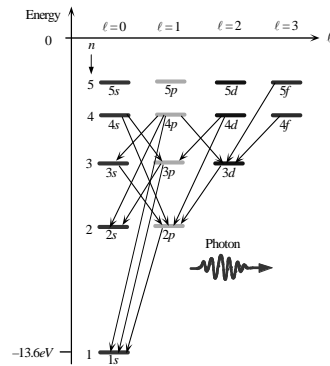
- In the presence of an external magnetic field: the orbital angular momentum becomes quantized according to m_l

$$L_z = m_l \hbar$$

Absorption/ Emission

- When an atom absorbs energy, an electron can be excited up a level
- When an electron drops down a level, energy can be emitted
- Electrons & photons must obey conservation of momentum
- If a photon is given off or absorbed, the momentum of the electron must change

Selection Rules: rules that govern allowable electron transitions



- n must change
- $\Delta l = \pm 1$
- $\Delta m_l = 0, \pm 1$

Fig. 3.27: An illustration of the allowed photon emission processes. Photon emission involves $\Delta l = \pm 1$.

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Spin: m_s

- Each state has two electrons
- Each electron has a "spin" $\pm 1/2$
 - "spin" is not really accurate
 - a better way to picture that our electrons have two states is to keep in mind that moving charge has a magnetic field associated with it and picture the 2 spin options as equivalent to N & S of a magnet

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Spin

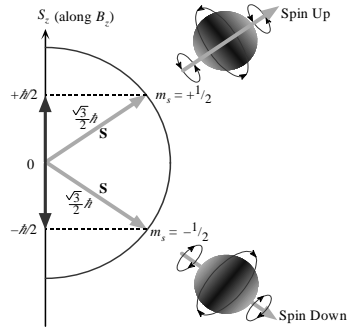


Fig. 3.28: Spin angular momentum exhibits space quantization. Its magnitude along z is quantized so that the angle of S to the z -axis is also quantized.

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Calculations with Quantum Numbers

$$L = \hbar[l(l+1)]^{1/2}$$

$$L_z = m_l \hbar$$

$$S = \hbar[s(s+1)]^{1/2}$$

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

$$S_z = m_s \hbar$$



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Multi-electron Atoms

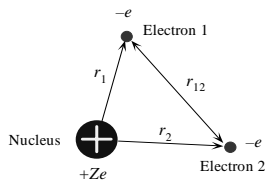


Fig. 3.32: A helium-like atom. The nucleus has a charge of $+Ze$, where for He $Z = 2$. If one electron is removed, we have the He^+ ion which is equivalent to the hydrogenic atom with $Z = 2$.

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Multi-electron Atoms

- In atoms with more than one electron, there is an "effective nuclear charge": SCREENING
 - Outer electrons are far from the ion core
 - Inner electron charges can screen the positive nuclear charge
- He atoms has 2 electrons
 - $V(r)$ now depends also on inter-electron distance
 - Where r_{12} is the distance between the 2 electrons
 - First is Coulombic attraction, the second is repulsion
- This causes the SWE to have a different set of wave functions as solutions
 - Since the "l" quantum numbers determine the orientation of the electron orbitals, the energy now depends not just on n but also on l
 - $E_{n,l}$ increases with both n and l

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Energy Levels in Multi-electron Atoms

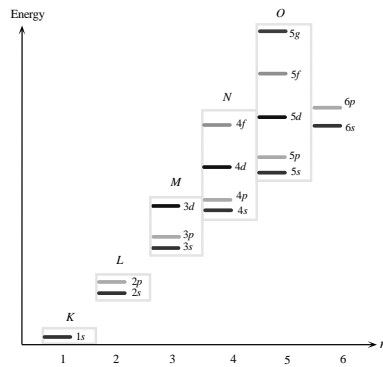


Fig. 3.33: Energy of various one-electron states. The energy depends on both n and l 40

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Aufbau Chart

1s			
2s	2p		
3s	3p	3d	
4s	4p	4d	4f
5s	5p	5d	5f
6s	6p	6d	6f

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Use Chart for Filling Orbitals

- **Example Fe (26)**
- PEP does not tell us how electrons distribute themselves among the energy levels when there is degeneracy.
- Suppose we have 6 electrons
 - 2 x 1s states. 2 x 2s states.
 - How do the other 2 occupy the 2p states, since there is room for 6 electrons?
 - They could pair their spins and occupy only one m_l state
 - or align their spins and occupy different m_l states.

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Hund's Rule:

- Observations show: electrons in same n, l subshell prefer to have spins parallel
- This is because by aligning spins, they occupy different orbitals
- If they were crammed into the same orbital with different spin states, there would be a large Coulombic repulsion because they occupy the same region of space.
- Try C(6), N(7), O(8), F(9), Ne(10)

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Filling Orbitals

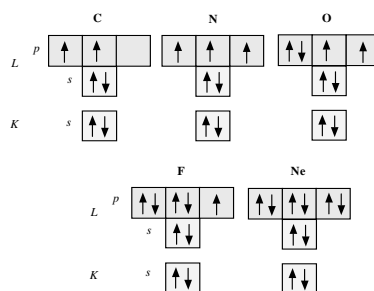


Fig. 3.36: Electronic configurations for C, N, O, F and Ne atoms. Notice that Hund's rule forces electrons to align their spins in C, N and O. The Ne atom has all the *K* and *L* orbitals full.

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