CH-110 Advanced General Chemistry I

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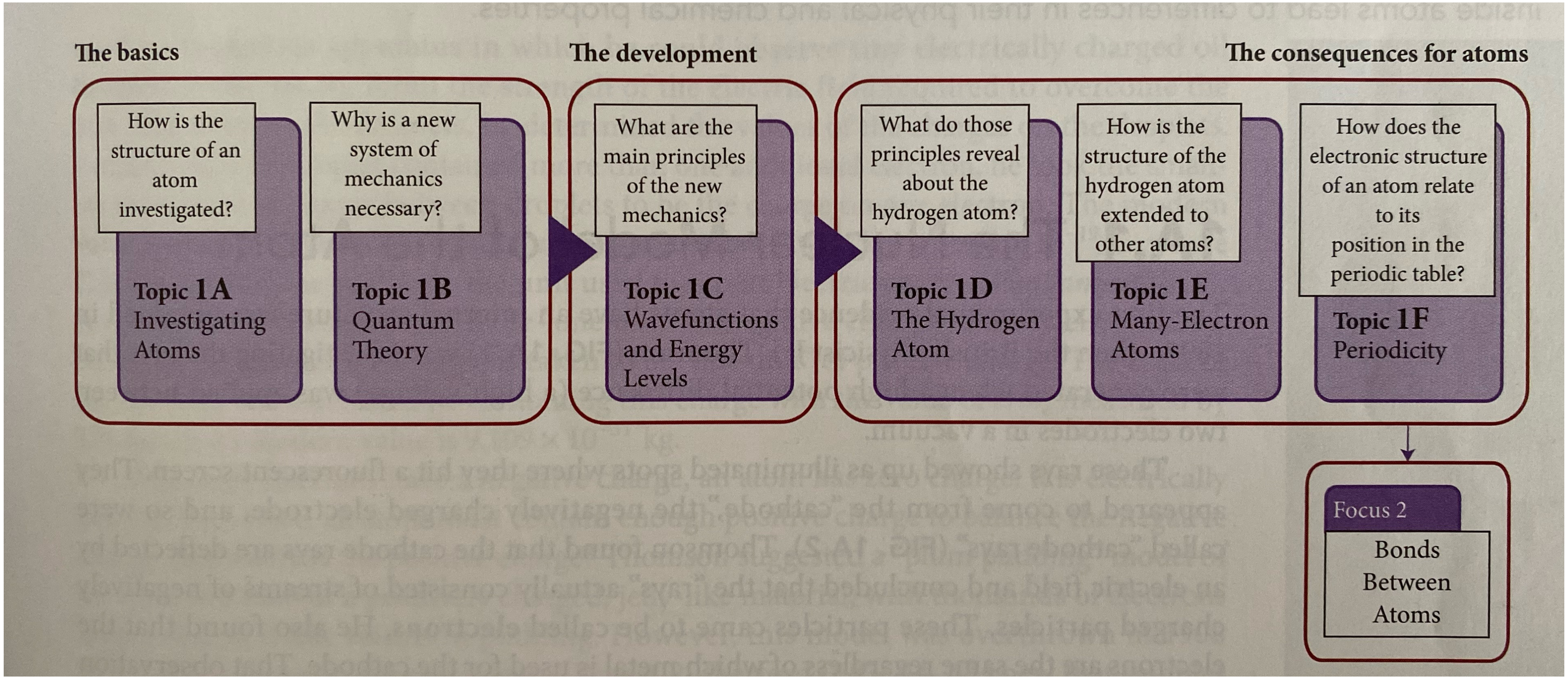
The Hydrogen Atom

Topic 1D

Overview Chapter 1 (Focus 1: Atoms)



Topic 1D.1 Energy levels
Topic 1D.2 Atomic orbitals
Topic 1D.3 Quantum numbers, shells, and subshells
Topic 1D.4 The shapes of orbitals
Topic 1D.5 Electron spin
Topic 1D.6 The electronic structure of hydrogen: a summary

WHY DO YOU NEED TO KNOW THIS MATERIAL?

- The hydrogen atom is the **simplest atom of all** and is used to discuss the **structures of all atoms**.
- It is therefore **central** to many explanations in chemistry.

WHAT DO YOU NEED TO KNOW ALREADY?

- Features of spectrum of atomic hydrogen (Topic 1A)
- Concepts of wavefunction and energy level in quantum mechanics (Topic 1C)

1D The hydrogen atom

Setting the stage

In Topic 1A, we have seen this puzzle

$$\nu = R\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right), n_1 = 1,2, \ldots, and\ n_2 = n_1 + 1, n_1 + 2, \ldots$$

Value of Rydberg constant, $R = 3.29 \text{ x } 10^{15} Hz$

Energy Levels

Topic 1D.1

1D.1 Energy levels

Recap

- **Again:** an **electron** in an atom is like a **particle** in a box in the sense that it is confined within the atom, not by the **walls**, but by the **electrostatic pull of the nucleus**.
- Solving Schrödinger equation for the hydrogen atom will result in existence of **discrete energy levels**.

1D.1 Energy levels

Allowed energy levels for electron in hydrogen atom

To find allowed energy levels of an electron in a hydrogen atom, you need to solve appropriate Schrödinger equation. Consider:

1. Motion in three dimensions.
2. Instead of simple walls, the electron experiences a **Coulomb potential** due to the nucleus. The Coulomb potential energy of an electron of charge $-e$ at a distance r from the nucleus of charge $+e$:

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

ε_0: electric constant

1D.1 Energy levels

Allowed energy levels for electron in hydrogen atom

Schrödinger managed to solve his equation with this potential energy:

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

He found that the allowed energy levels of an electron in a hydrogen atom are:

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

Important formula.
Need to know how to apply.

$$R = \frac{m_e e^4}{8h^3\varepsilon_0^2} \text{ with } n = 1, 2, \ldots$$

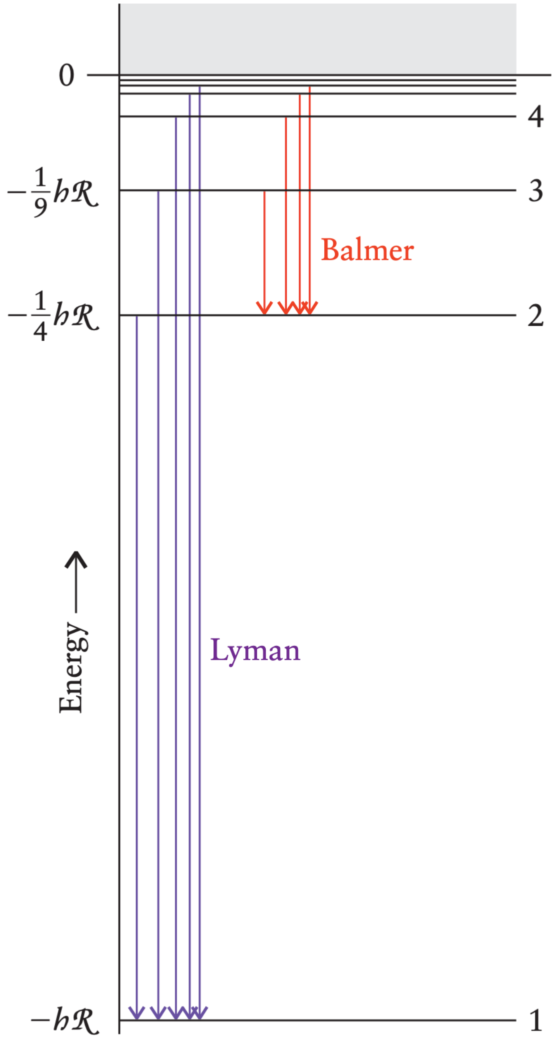


Figure 1D.1

1D.1 Energy levels

What does this equation tell you?

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

Important formula.
Need to know how to apply.

$$R = \frac{m_e e^4}{8h^3\varepsilon_0^2} \text{ with } n = 1, 2, \ldots$$

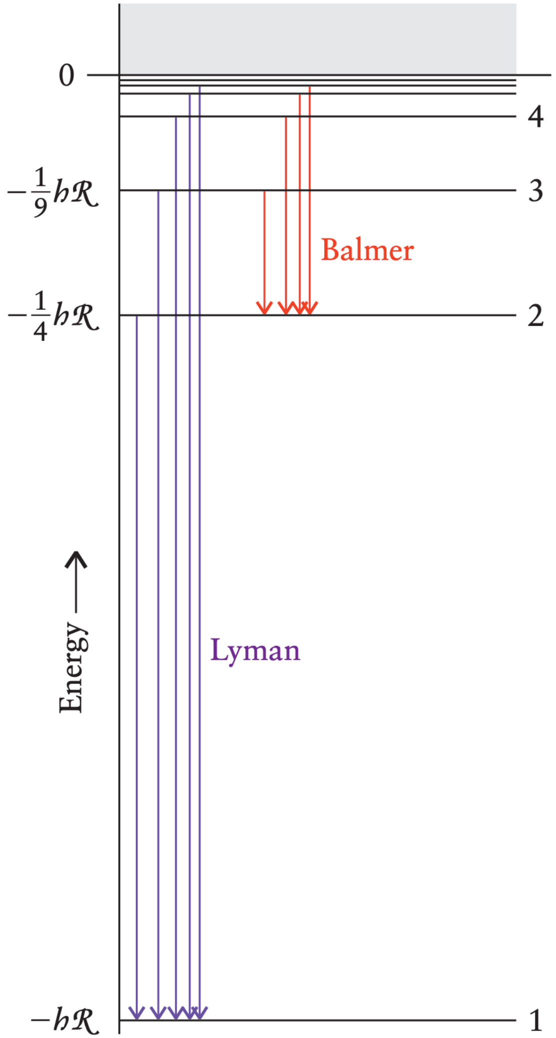


Figure 1D.1

1D.1 Energy levels

Relationship to Bohr frequency condition

1D.1 Energy levels

Finally, it makes sense

You can now see:

- Lyman series, for example, arises from transitions starting at $n_2 = 3, 4, 5 \ldots$ and all ending at $\boldsymbol{n_1 = 2}$
- Balmer series: $n_2 = 2, 3, 4, 5 \ldots$ to $\boldsymbol{n_1 = 1}$

Rydberg constant

$$R = \frac{m_e e^4}{8h^3 \varepsilon_0^2} = \mathbf{3.29 \times 10^{15}}\ \boldsymbol{Hz}$$

- Imagine Schrödinger calculating this constant!

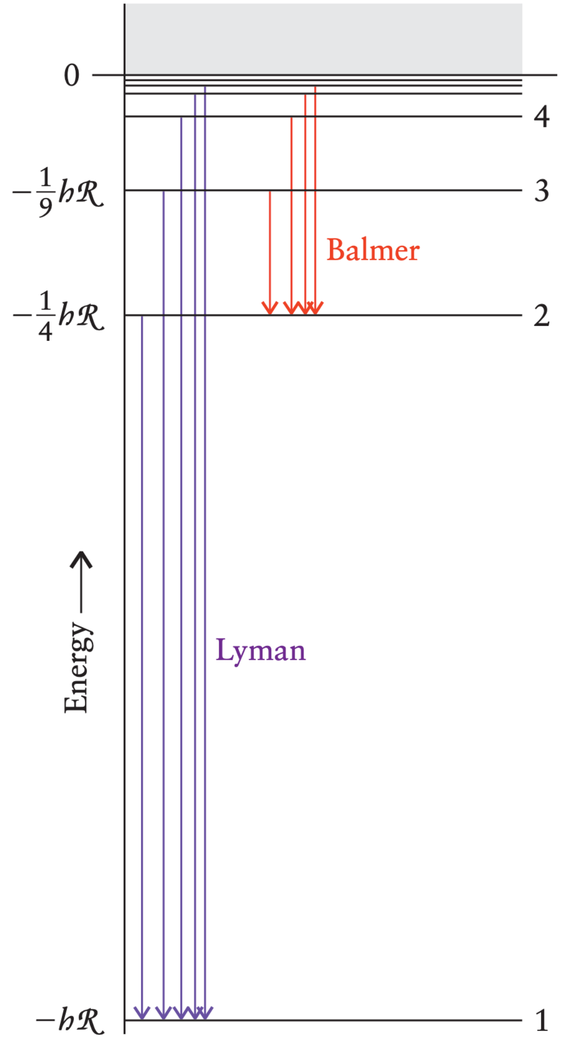


Figure 1D.1

1D.1 Energy levels

Finally, it makes sense

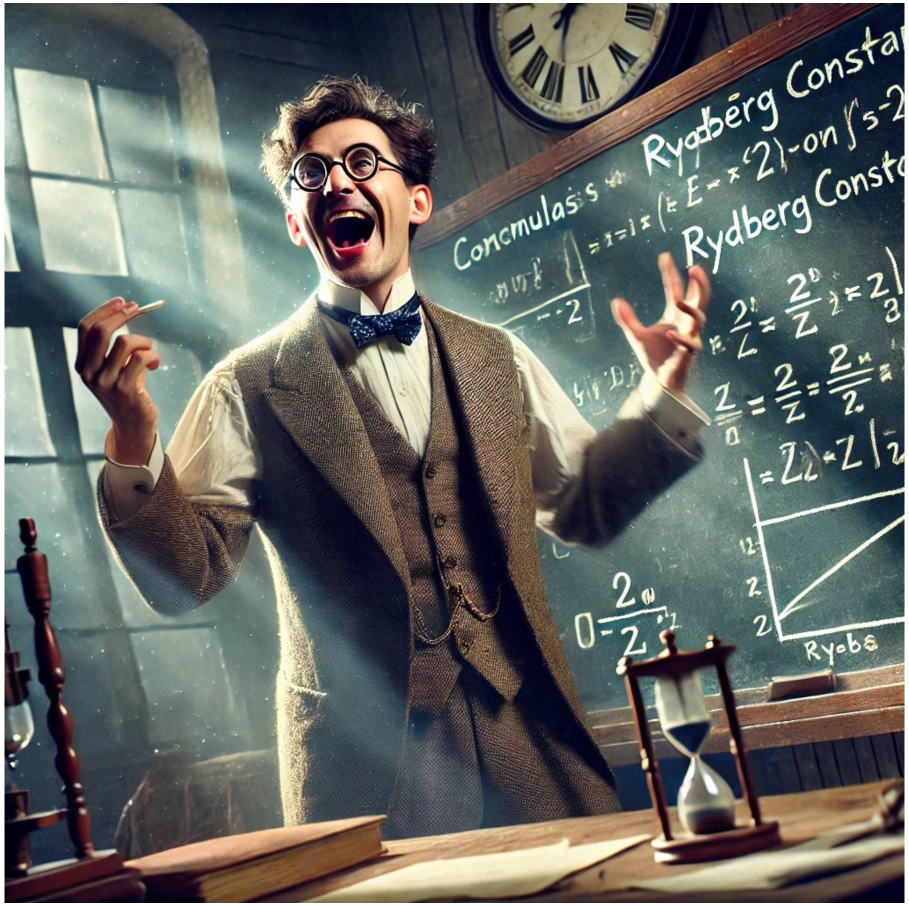


Image source: ChatGPT (2024)
Schrödinger's Eureka Moment.

1D.1 Energy levels

Generalization to other one-electron ions possible

Schrödinger was able to generalize this equation

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

$$R = \frac{m_e e^4}{8h^3\varepsilon_0^2} \text{ with } n = 1, 2, \ldots$$

to other one-electron ions such as He^+ and even C^{5+}.

For a nucleus with atomic number Z and charge Ze, the energy levels are:

$$E_n = -\frac{Z^2 hR}{n^2} \; with \; n = 1, 2, \ldots$$

Important formula.
Need to know how to apply.

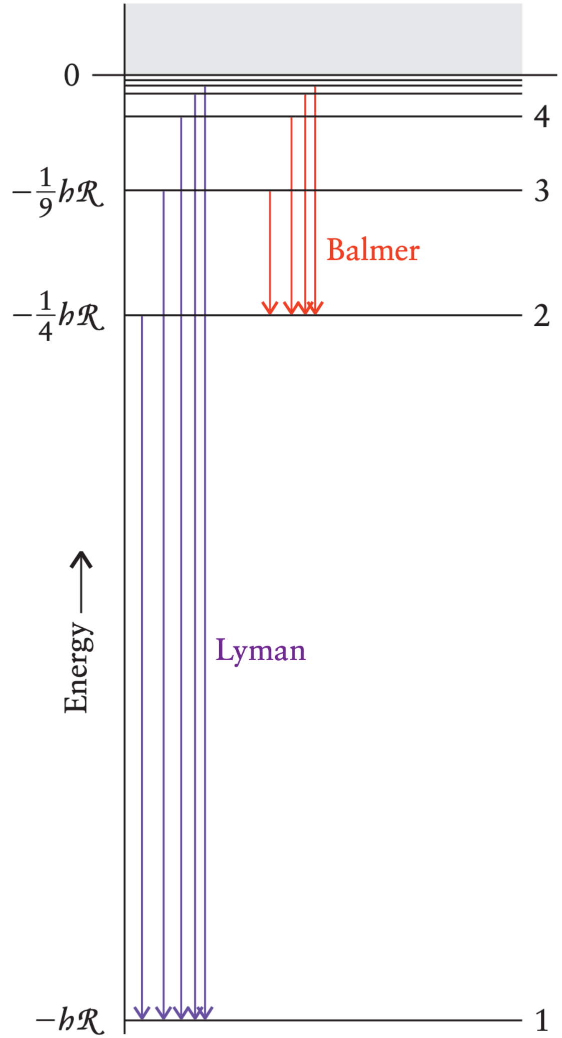
Note:

Larger nuclear charge $Z \rightarrow$ lower (more negative) electron energy → electron more tightly bound.
Equation valid for one-electron ions; many-electron atoms → see Topic 1E.

1D.1 Energy levels

Key terms to remember

- $n = 1$: → ground state with energy $E = -hR$
- Excitation: electron absorbs photon → moves to higher n
- Ionization: $n \rightarrow \infty$; electron removed
- Ionization energy of H (from ground state) = hR $= 2.18 \times 10^{-17} J = 13.6\ eV$
- Extra energy beyond this appears as kinetic energy of the free electron



1D.1 Energy levels

Summary

The energy levels of a hydrogen atom are defined by the principal quantum number, $n = 1, 2, \ldots$, and form a converging ladder, as shown in Figure 1D.1. Spectroscopic lines arise from transitions between the levels.

Atomic Orbitals

Topic 1D.2

1D.2 Atomic orbitals

Wavefunction and atomic orbitals

The wavefunction of an electron in an atom is called an atomic orbital.

$|\psi|^2$: probability density of finding electron in space

For H atom: electron cloud around nucleus; denser regions = higher probability

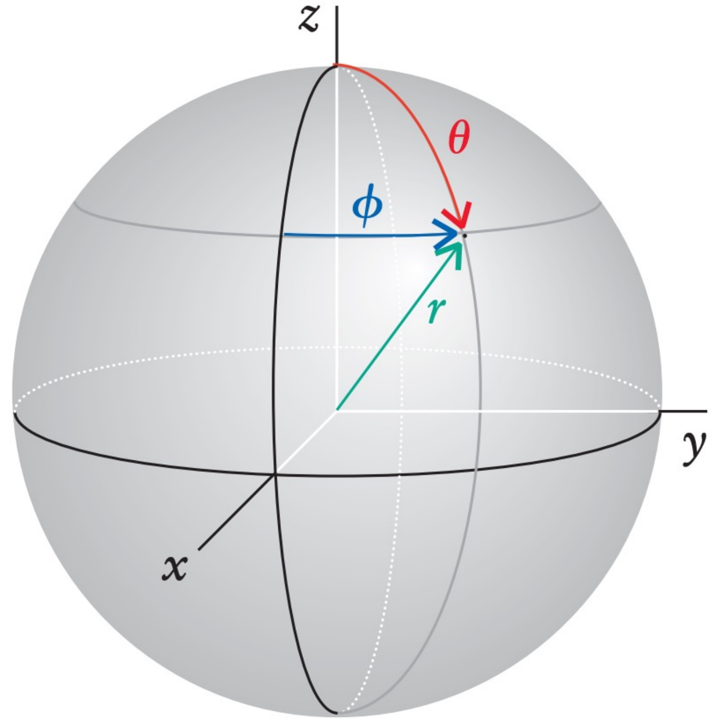
Image source: ChatGPT (2025)
Glossy Hydrogen Balloon Orbitals.

1D.2 Atomic orbitals

Spherical polar coordinates

The atom is a sphere (3D):

- *r* is the **radius**, the distance from the nucleus
- θ (theta) is the **colatitude**, the angle from the positive *z*-axis (the «north pole»), the geographical «latitude» (north or south)
- ϕ (phi) is the **azimuth**, the angle about the *z*-axis, the geographical «longitude» (east or west)

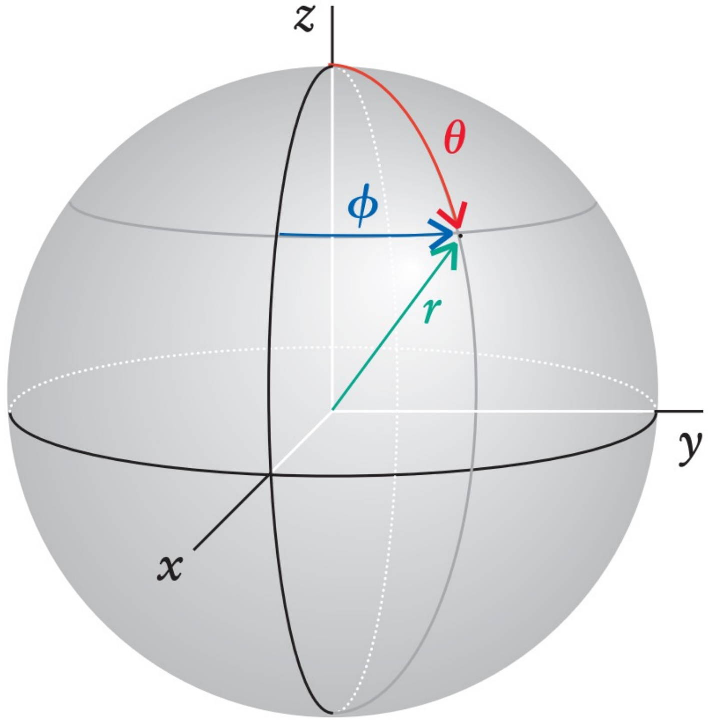


1D.2 Atomic orbitals

Spherical polar coordinates

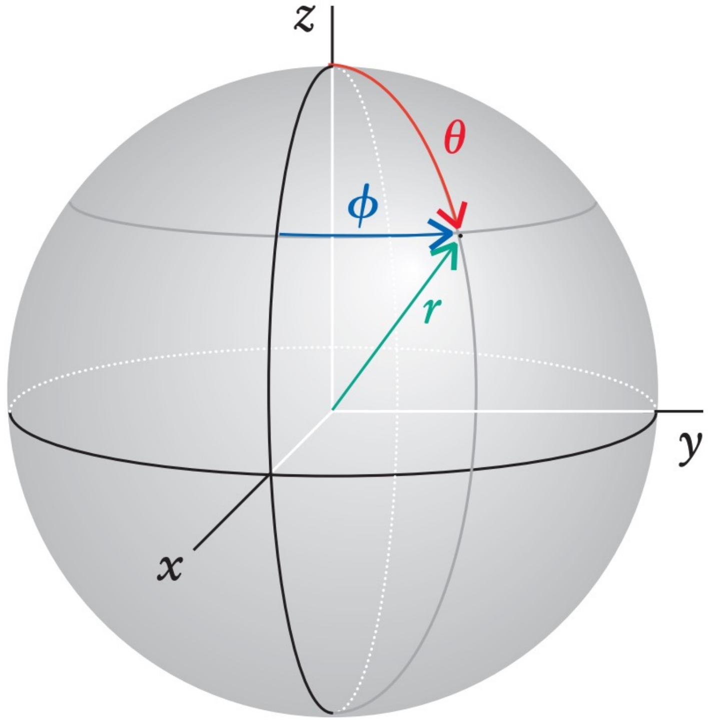
The below applet allows you to see how the location of a point changes as you vary r, θ, and φ

https://mathinsight.org/spherical_coordinates



1D.2 Atomic orbitals

Wavefunction and atomic orbitals



Hydrogen ground state orbital ($n = 1$)

- Wavefunction:

$$\Psi(r, \theta, \phi) = \left(\frac{1}{\pi a_0^3}\right)^{\frac{1}{2}} e^{-\frac{r}{a_0}}$$

- a_0: Bohr radius (52.9 pm)
- **Spherically symmetric**: independent of θ and ϕ, same value in all directions
- **Exponential decay:** Probability density is highest close to the nucleus (at r = 0, $e^0 = 1$)
- Unlike particle in a box: no physical, confining walls for electron in atom, but **the pull of nucleus** weakens with distance.

1D.2 Atomic orbitals

TABLE 1.2 Hydrogenlike Wavefunctions* (Atomic Orbitals), $\psi = RY$

(a) Radial wavefunctions

n	l	$R_{nl}(r)$
1	0	$2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$
2	0	$\frac{1}{2\sqrt{2}}\left(\frac{Z}{a_0}\right)^{3/2}\left(2-\frac{Zr}{a_0}\right)e^{-Zr/2a_0}$
	1	$\frac{1}{2\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2}\left(\frac{Zr}{a_0}\right)e^{-Zr/2a_0}$
3	0	$\frac{2}{9\sqrt{3}}\left(\frac{Z}{a_0}\right)^{3/2}\left(3-\frac{2Zr}{a_0}+\frac{2Z^2r^2}{9a_0^2}\right)e^{-Zr/3a_0}$
	1	$\frac{2}{9\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2}\left(2-\frac{Zr}{3a_0}\right)e^{-Zr/3a_0}$
	2	$\frac{4}{81\sqrt{30}}\left(\frac{Z}{a_0}\right)^{3/2}\left(\frac{Zr}{a_0}\right)^2 e^{-Zr/3a_0}$

(b) Angular wavefunctions

l	"m_l"†	$Y_{l,m_l}(\theta,\phi)$
0	0	$\left(\frac{1}{4\pi}\right)^{1/2}$
1	x	$\left(\frac{3}{4\pi}\right)^{1/2}\sin\theta\cos\phi$
	y	$\left(\frac{3}{4\pi}\right)^{1/2}\sin\theta\sin\phi$
	z	$\left(\frac{3}{4\pi}\right)^{1/2}\cos\theta$
2	xy	$\left(\frac{15}{16\pi}\right)^{1/2}\sin^2\theta\sin 2\phi$
	yz	$\left(\frac{15}{4\pi}\right)^{1/2}\cos\theta\sin\theta\sin\phi$
	zx	$\left(\frac{15}{4\pi}\right)^{1/2}\cos\theta\sin\theta\cos\phi$
	x^2-y^2	$\left(\frac{15}{16\pi}\right)^{1/2}\sin^2\theta\cos 2\phi$
	z^2	$\left(\frac{5}{16\pi}\right)^{1/2}(3\cos^2\theta-1)$

*Note: In each case, $a_0 = 4\pi\varepsilon_0\hbar^2/m_e e^2$, or close to 52.9 pm; for hydrogen itself, $Z = 1$.

†In all cases except $m_l = 0$, the orbitals are sums and differences of orbitals with specific values of m_l.

1D.2 Atomic orbitals

Example from Table 1.2

- For example, a $2p_x$-orbital (n = 2, l = 1, «m_l» = x) of hydrogen (Z = 1) is

$$\Psi(\mathrm{r},\theta,\phi) = R_{2,1}(r)\times Y_{1,x}(\theta,\phi) = \frac{1}{2\sqrt{6}}\left(\frac{1}{\mathrm{a}_0}\right)^{\frac{3}{2}}\frac{r}{a_0}\,e^{-\frac{r}{2a_0}}\times\left(\frac{3}{4\pi}\right)^{\frac{1}{2}}\sin(\theta)\cos(\phi)$$

1D.2 Atomic orbitals

Summary

The distribution of an electron in an atom is described by a wavefunction known as an atomic orbital.

Quantum Numbers, Shells, and Subshells

Topic 1D.3

1D.3 Quantum numbers, shells, and subshells

Three quantum numbers for the hydrogen atom

When the Schrödinger equation is solved for the hydrogen atom, **three quantum numbers** are needed to specify each wavefunction:

1D.3 Quantum numbers, shells, and subshells

1. Principal quantum number n

Principal quantum number n is related to the **size** and **energy** of the orbital, all orbitals with the same principal quantum number have the same energy, belong to the same **shell** of the atom.

1D.3 Quantum numbers, shells, and subshells

2. Orbital angular quantum number l

Quantum number l is related to its **shape**

It can take on the following values:

$$l = 0, 1, 2, \ldots, \boldsymbol{n-1}$$

Orbitals with principal number n are divided into **subshells $\boldsymbol{l}$**:

For $n = 1$: there is only one subshell $l = 0$

For $n = 2$: there are two subshells $l = 0, 1$

For $n = 3$: there are three subshells $l = 0, 1, 2$

1D.3 Quantum numbers, shells, and subshells

s-, p-, and d-orbitals

$l = 0$: s-orbital (origin: s-orbital spectroscopic lines described as "sharp")

$l = 1$: p-orbital (origin: "principal")

$l = 2$: d-orbital (origin: "diffuse")

Value of *l*	0	1	2	3
Orbital type	s	p	d	f

Higher values of l are possible (g-, h-, … orbitals) are possible, but not often needed in practice.

1D.3 Quantum numbers, shells, and subshells

2. Orbital angular quantum number *l*

The orbital angular quantum number (ℓ) can be used to calculate the magnitude of the orbital angular momentum (L) of an electron:

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

- s (ℓ=0): $L = 0$ (not circulating around nucleus, and evenly distributed around it)
- p (ℓ=1): $L = \sqrt{2}\hbar$
- d (ℓ=2): $L = \sqrt{6}\hbar$
- f (ℓ=3): $L = \sqrt{12}\hbar$

L is measure of the rate (in classical terms) at which the electron circulates around the nucleus

1D.4 The shapes of orbitals

Analogy: angular momentum to swinging ball on string.

Imagine a ball attached to a string, representing an electron in a p-orbital. When you swing this ball around in a circle, it has a certain angular momentum. The faster you swing it, the farther it moves away from the center. If you try to bring the ball closer to the center, it becomes difficult; the tension in the string and the motion cause the ball to naturally stay at a distance from the center, similar to how a p-orbital behaves with a non-zero angular momentum.

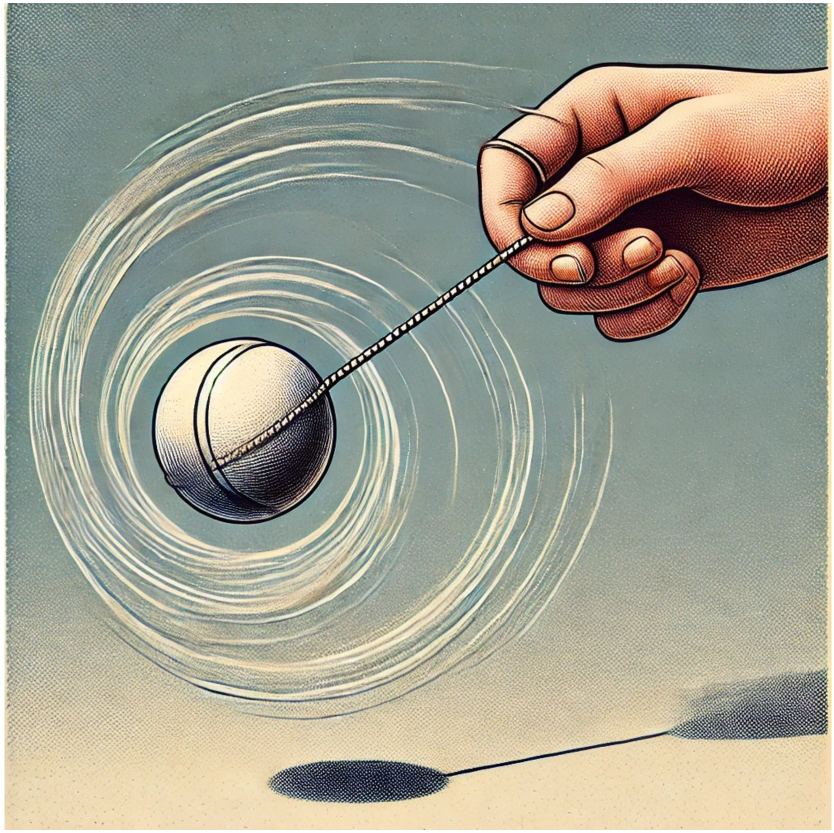


Image source: ChatGPT (2024). *Angular Momentum of Ball on a String.*

1D.3 Quantum numbers, shells, and subshells

3. Magnetic quantum number m_l

Distinguishes the **individual orbitals within a subshell**

Can take positive and negative integer values:

$$m_l = l, l-1, \dots, -l$$

E.g.

- p-orbital with $l = 1$ and $m_l = +1, 0, -1$
- d-orbital with $l = 2$ and $m_l = +2, +1, 0, -1, -2$

1D.3 Quantum numbers, shells, and subshells

3. Magnetic quantum number m_l

- Specifies **orientation of orbital motion of electron**
- $m_\ell = +1$: motion one way; $m_\ell = -1$: opposite way
- $m_\ell = 0$: no circulation around that axis (symmetrically distributed)

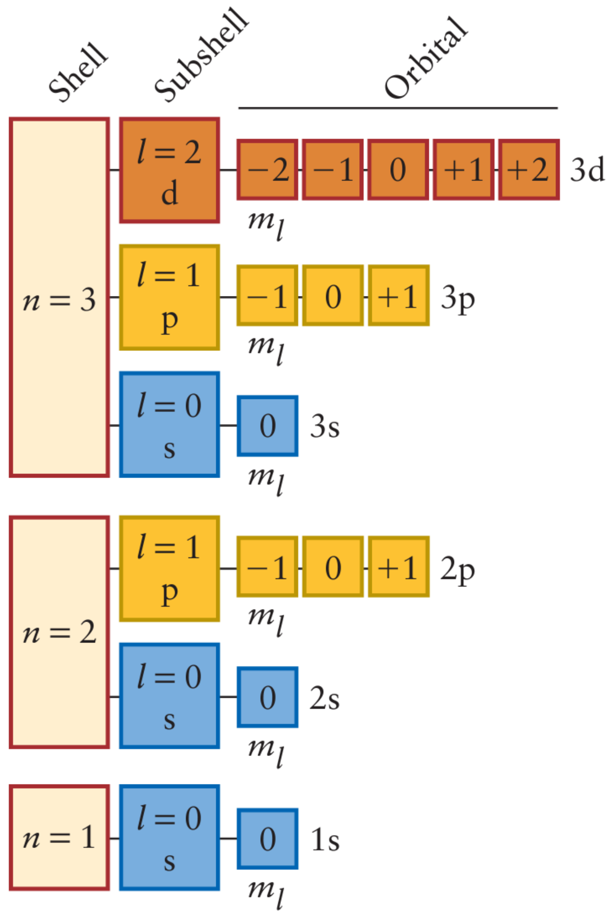


Figure 1D.3

1D.3 Quantum numbers, shells, and subshells

Summary

Atomic orbitals are designated by the quantum numbers n, l, and m_l and fall into shells and subshells.

TABLE 1.3 Quantum Numbers for Electrons in Atoms

	Name	Symbol	Values	Specifies	Indicates
	principal	n	$1, 2, \ldots$	shell	size
	orbital angular momentum*	l	$0, 1, \ldots, n-1$	subshell: $l = 0, 1, 2, 3, 4, \ldots$ s, p, d, f, g, ...	shape
	magnetic	m_l	$l, l-1, \ldots, -l$	orbitals of subshell	orientation
Chapter 1D.5:	spin magnetic	m_s	$+\frac{1}{2}, -\frac{1}{2}$	spin state	spin direction

*Also called the azimuthal quantum number.

The Shapes of Orbitals

Topic 1D.4

1D.4 The shapes of orbitals

s-orbitals

- Each orbital is defined by three quantum numbers n, ℓ, m_ℓ (the electron's "address").
- Example: hydrogen ground state → $n = 1, \ell = 0, m_\ell = 0$ → the **1s orbital**.
- Each shell has one s-orbital, named ns (1s, 2s, 3s …).

1D.4 The shapes of orbitals

s-orbitals are spherically symmetrical

- **Spherically symmetric**: independent of θ and ϕ, same value in all directions
- **1s orbital:** Probability density at $(\mathrm{r}, \theta, \phi) = |\, \psi_{1s} \,|^2$:

$$\Psi^2(\mathrm{r}, \theta, \phi) = \frac{1}{\pi a_0^3}\, e^{-\frac{2r}{a_0}}$$

- The 1s probability cloud extends infinitely, but beyond **~250 pm** the chance of finding the electron is negligible → the atom is effectively very small.

1D.4 The shapes of orbitals

s-orbitals are spherically symmetrical

High electron density at the nucleus: in an s-orbital, probability at the nucleus is nonzero.

Reason: with $\ell = 0$, there is no angular momentum barrier that keeps the electron away from the nucleus.

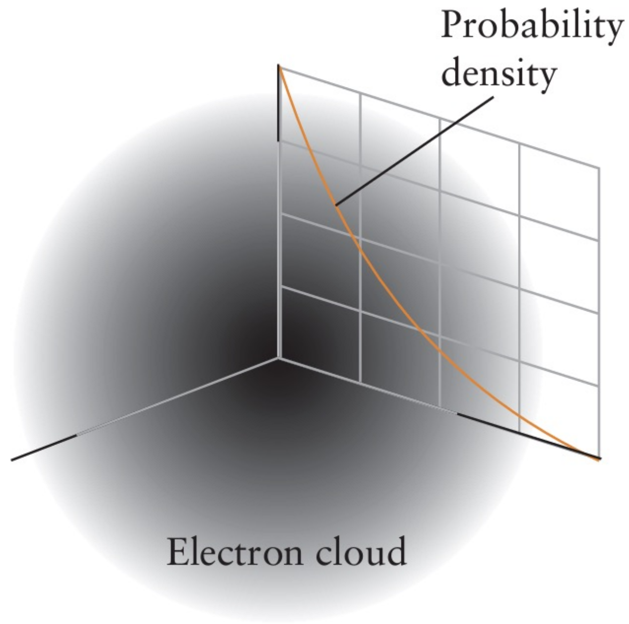


Figure 1D.4

1D.4 The shapes of orbitals

Example 1D.1: Calculating the probability of finding an electron at a certain location

Suppose an electron is in a 1s-orbital of a hydrogen atom.

What is the **probability** of finding the electron in a small region a **distance a_0** from the nucleus **relative** to the probability of finding it in the small region located right **at the nucleus**?

Anticipate: the probability density decreases exponentially with distance from the nucleus.

Plan: compare the probability densitites at the two locations: ratio of the squares of the wavefunctions at the two locations.

For 1s: $\psi(r, \theta, \phi)$ becomes $\psi(r)$

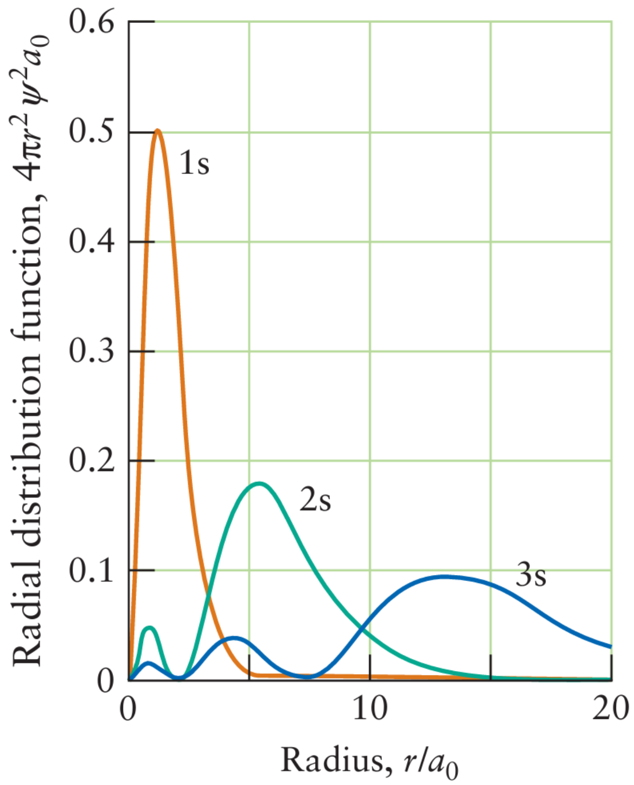
1D.4 The shapes of orbitals

Example 1D.1: Calculating the probability of finding an electron at a certain location

1D.4 The shapes of orbitals

Why we need the radial distribution function

Figure 1D.5

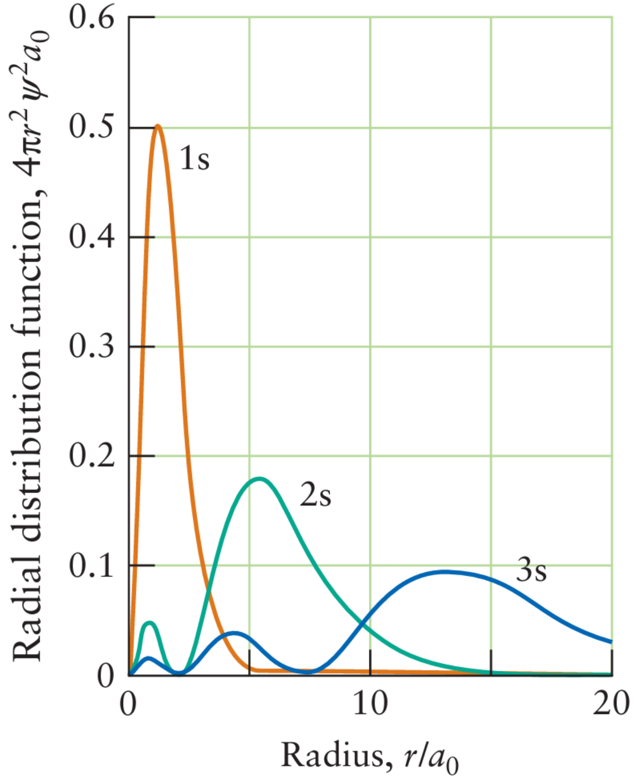


1D.4 The shapes of orbitals

The probability density vs. radial distribution function

- The wavefunction itself tells you, through $\psi^2(r, \theta, \phi)\delta V$, the probability of finding the electron in the **small volume δV at a particular location** specified by r, θ, and ϕ.
- The radial distribution function tells you, through $P(r)\delta\mathrm{r}$, the probability of finding the electron anywhere in the **spherical shell** between r and $\mathrm{r} + \delta\mathrm{r}$

Figure 1D.5



1D.4 The shapes of orbitals

The radial distribution function

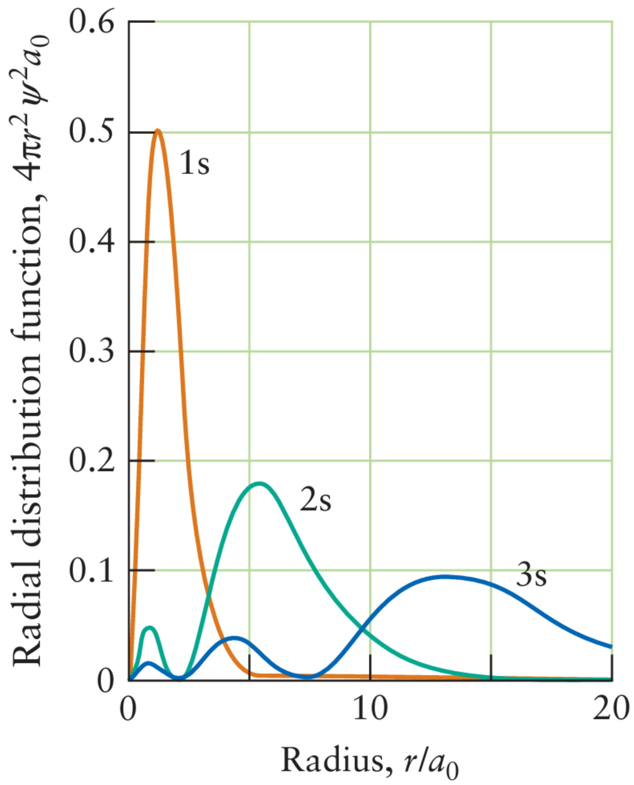
Radial distribution at the nucleus

- $P(r) = 4\pi r^2|\psi(r)|^2$ is **zero at** $r = 0$ for all orbitals (shell volume = 0).
- For **s-orbitals**, $|\psi(0)|^2$ is nonzero, but multiplying by r^2 makes $P(0) = 0$.

Shape of $P(r)$ for 1s

- As r inceases:
  - *$4\pi r^2$grows (bigger shell)*
  - *$|\psi(r)|^2$ decays*
- Product → rises from 0, peaks, then falls to 0.
- Maximum at **Bohr radius** a_0= most probable distance of electron in 1s orbital.

Figure 1D.5



1D.4 The shapes of orbitals

Boundary surface representation

- Encloses most of the electron cloud
- Easier to draw, but atoms really have fuzzy edges
- Still useful: shows where the electron is most likely found.

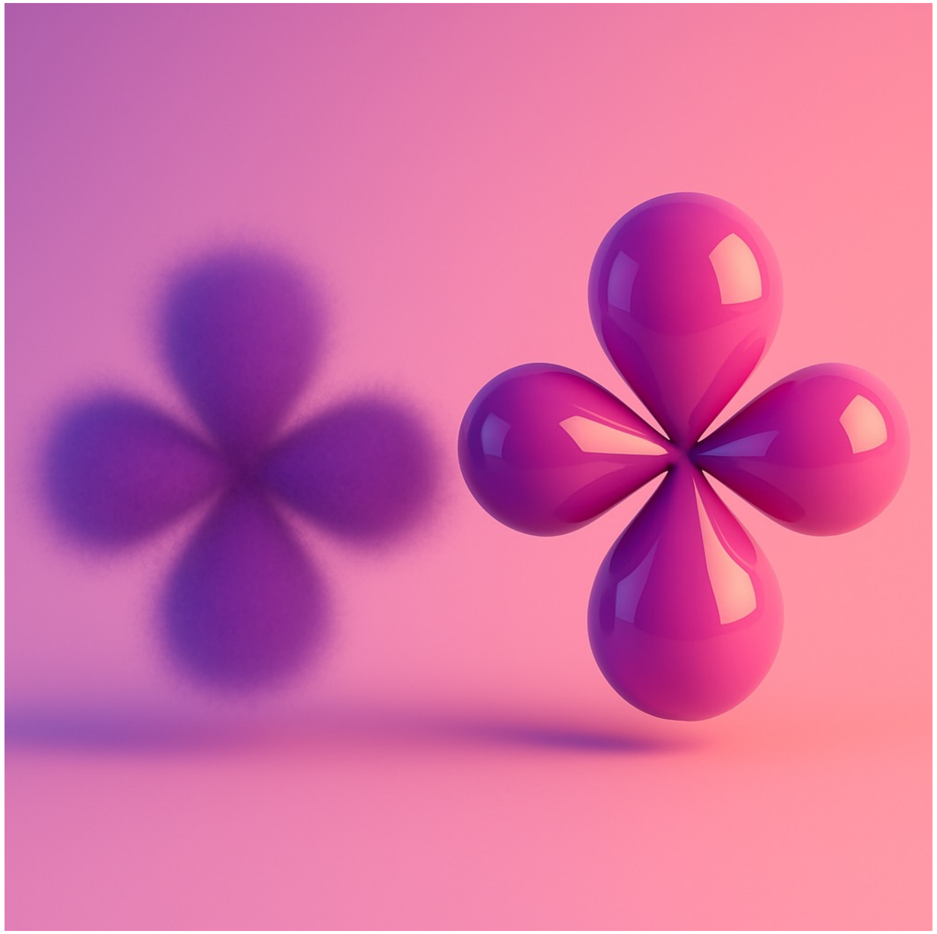


Image source: ChatGPT (2025).
Fuzzy Real vs. Boundary Surface.

1D.4 The shapes of orbitals

Boundary surface of the 1s-orbital

- Keep in mind:
  The probability density inside the boundary surface is not uniform.
- An s-orbital has a spherical boundary surface because the electron cloud is spherical.

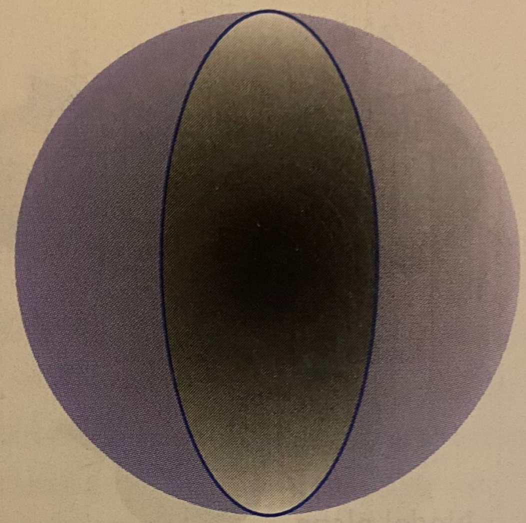


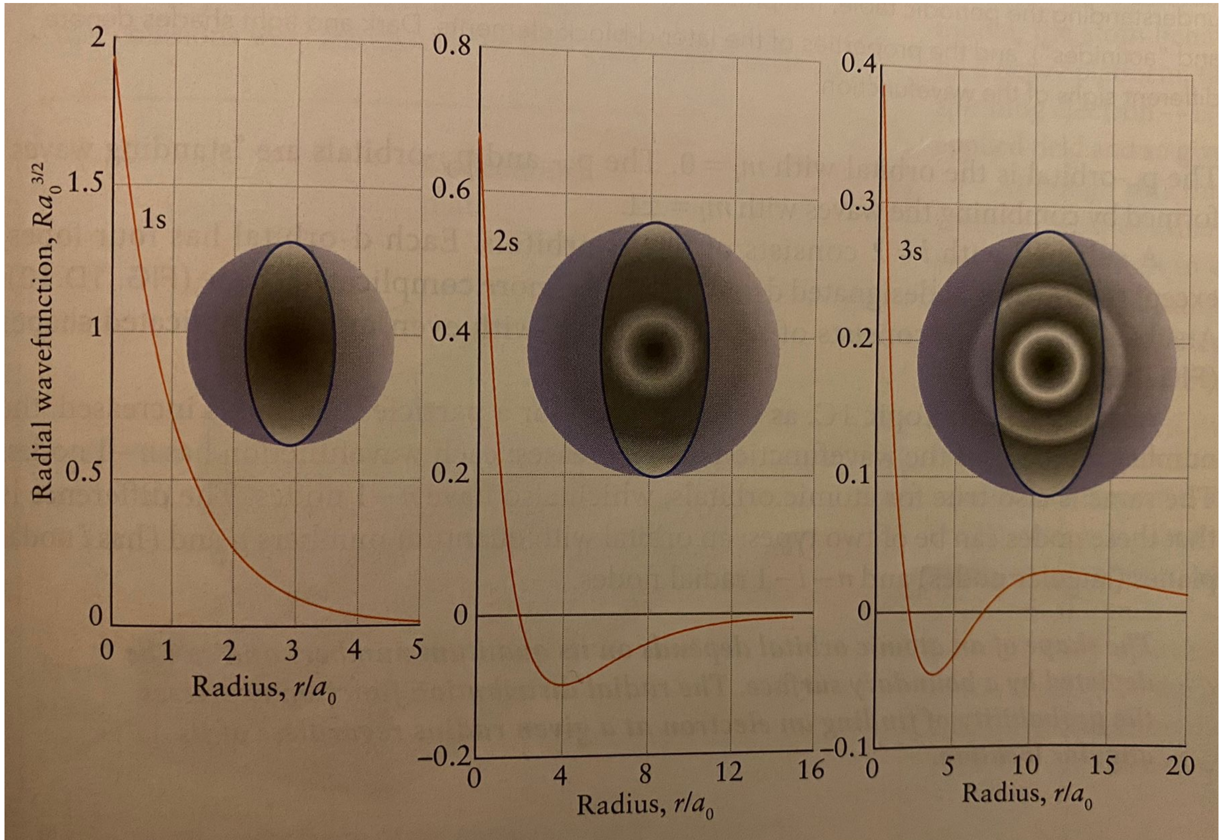
FIGURE 1D.6 The 1s-orbital. The simplest way of drawing an atomic orbital is as a boundary surface (the outer blue sphere), a surface within which there is a high probability (typically 90%) of finding the electron. We use blue to denote s-orbitals, but that color is only an aid to their identification.

1D.3 Quantum numbers, shells, and subshells

Boundary surfaces of higher-order s-orbitals

- The s-orbitals of higher energy have spherical boundary surfaces of greater diameter, **the average distance of the electron** from the nucleus also increases.
- They also have a more complicated radial variation, with **radial nodes**, radii at which the wavefunction passes through zero.

Figure 1D.7



1D.3 Quantum numbers, shells, and subshells

Boundary surfaces of higher-order s-orbitals

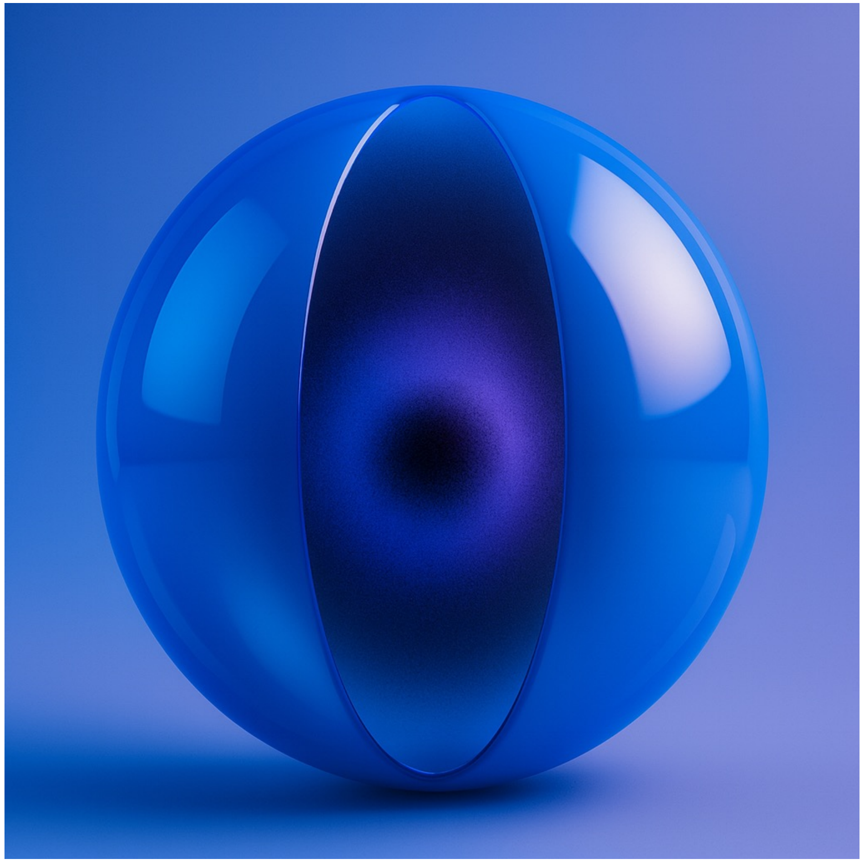


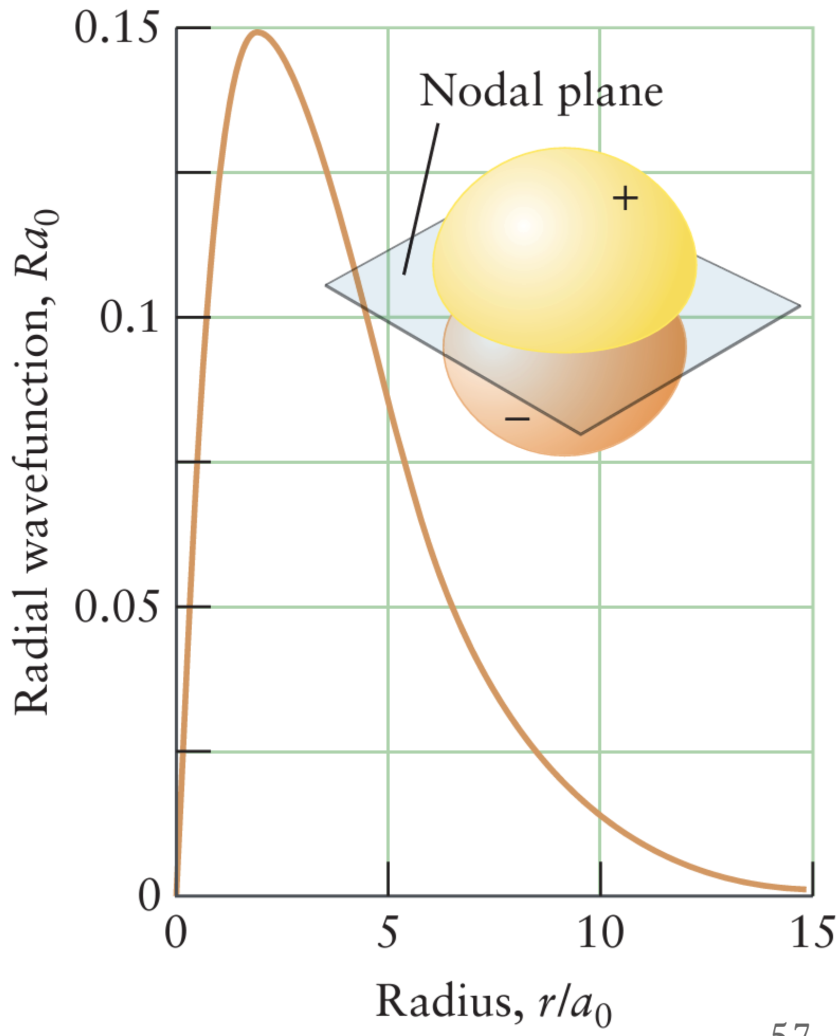
Image source: ChatGPT (2025).
A Glimpse inside a 2s Orbital.

1D.4 The shapes of orbitals

Boundary surfaces of p-orbitals

- Two lobes with signs + and - to signify that wavefunction has two different signs in these two regions
- E.g. $2p_z$ orbital is proportional to $\cos(\theta)$: as θ changes from 0 to π, $\cos(\theta)$ changes from $+1$ through 0 to -1.

Figure 1D.8

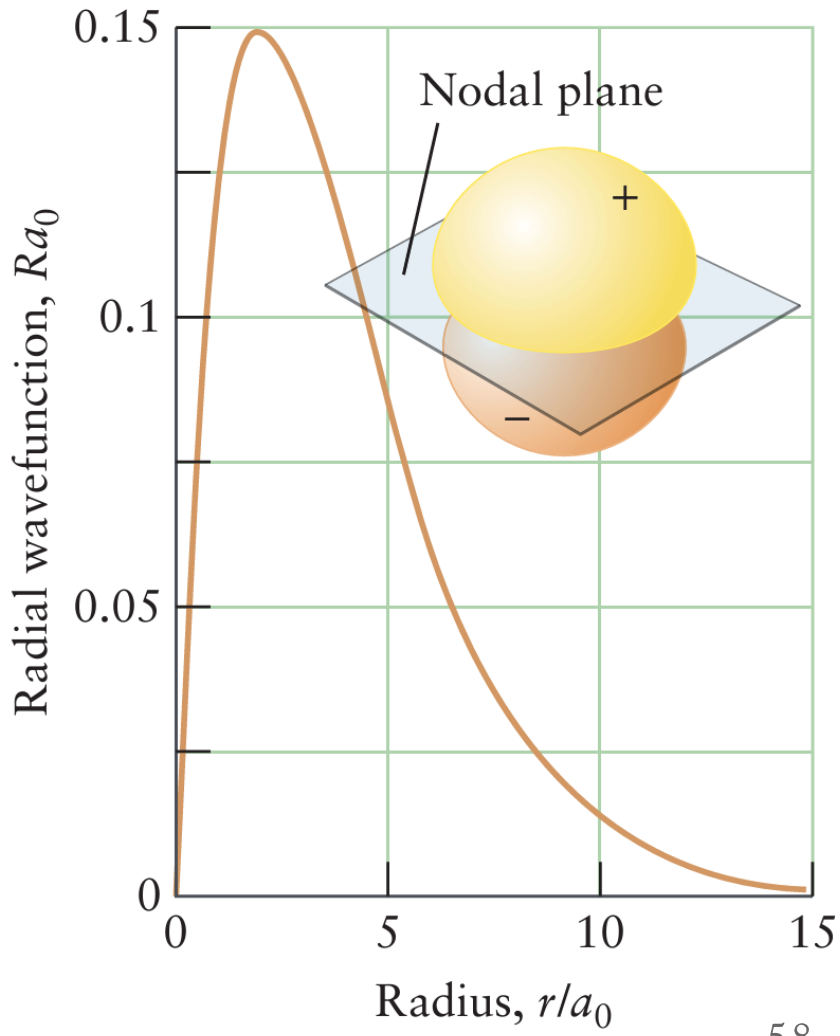


1D.4 The shapes of orbitals

Nodal planes

- The two lobes of a p-orbital are separated by a **nodal plane**, cuts through the nucleus, $\psi = 0$. The wavefunction changes sign **on passing through this plane**.
- Also called **angular nodes** because they occur when the angular wavefunction passes through zero.
- A p-electron will **never be found at the nucleus** because the wavefunction is zero there.
- Electrons in p-orbitals have nonzero angular momentum, which flings them away from the nucleus.

Figure 1D.8

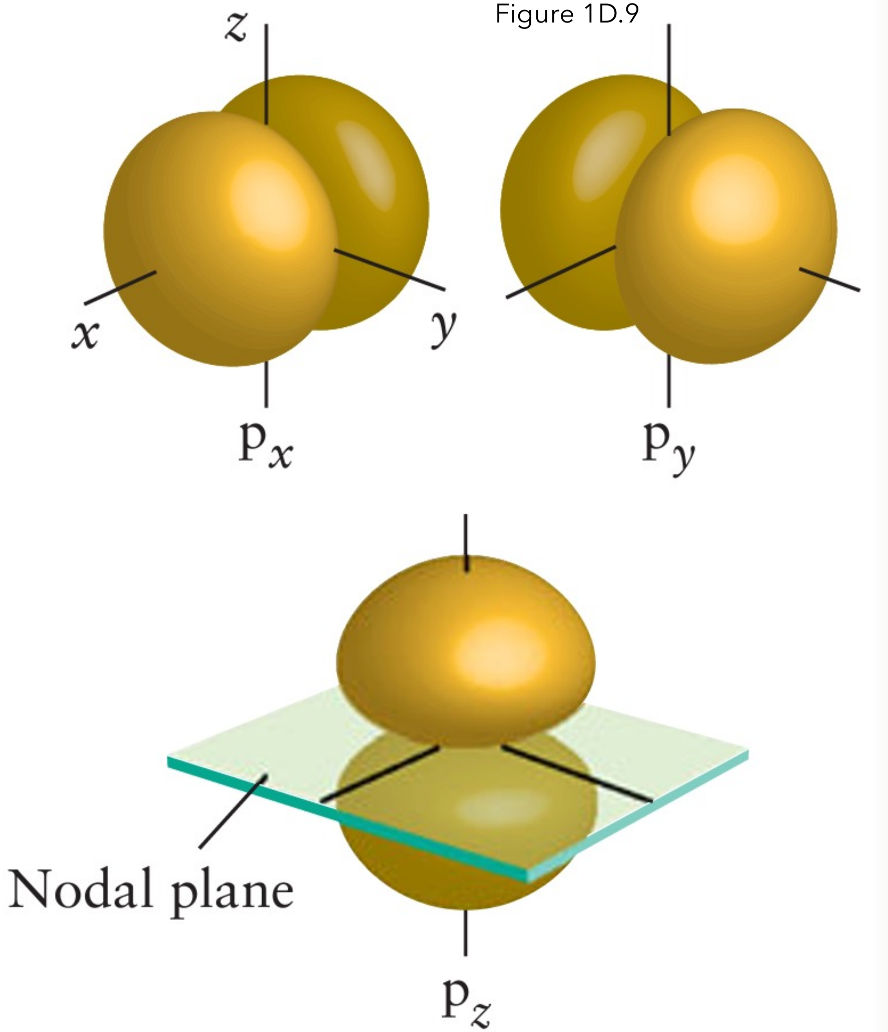


1D.4 The shapes of orbitals

p-orbitals

- Three p-orbitals in each subshell of an atom
- Quantum numbers $m_l = +1, 0, -1$
- Chemists refer to them according to the axes along which the lobes lie: p_x-, p_y-, p_z-orbitals
- p_z-orbital has $m_l = 0$
- p_x-, p_y-orbitals have $m_l = \pm 1$

Figure 1D.9



1D.4 The shapes of orbitals

d-orbitals

- Subshell l = 2 consists of **five d-orbitals**
- Each d-orbital has four lobes, except d_{z^2}

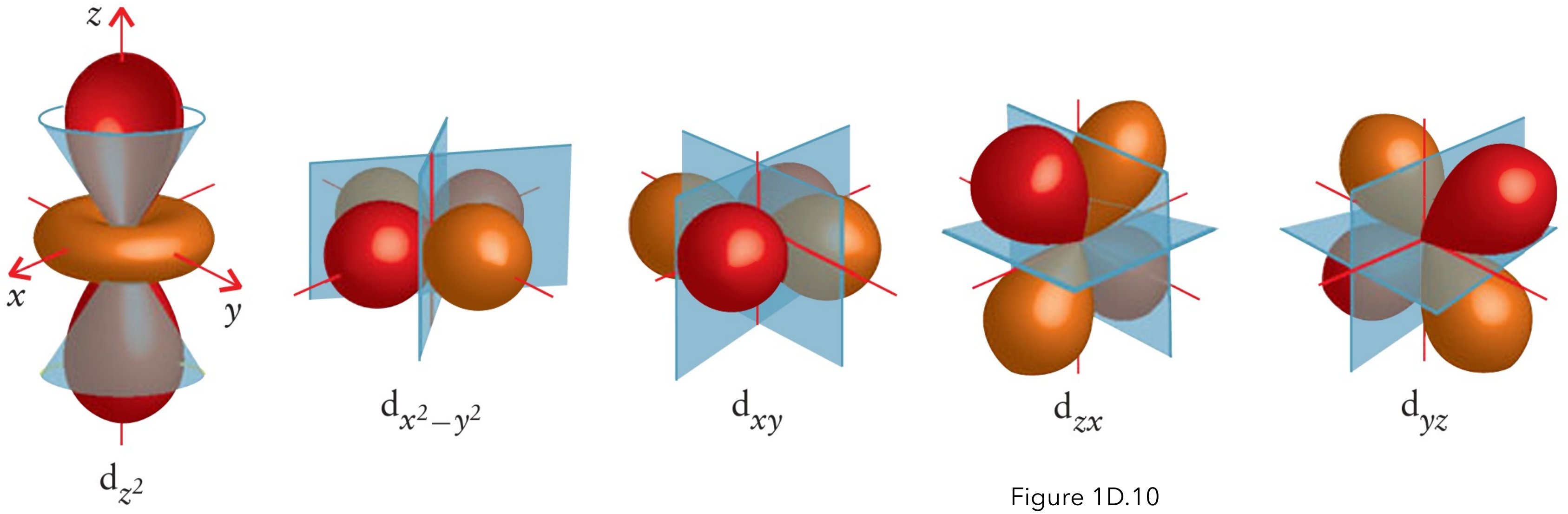


Figure 1D.10

1D.4 The shapes of orbitals

f-orbitals

- Subshell $l = 3$ consists of **seven f-orbitals**.
- Very **complex** appearance.
- Detailed form will not be discussed again in this course.
- Their existence is important for **understanding the periodic table**, the presence of the lanthanoids and actinoids and the properties of the later d-block elements.

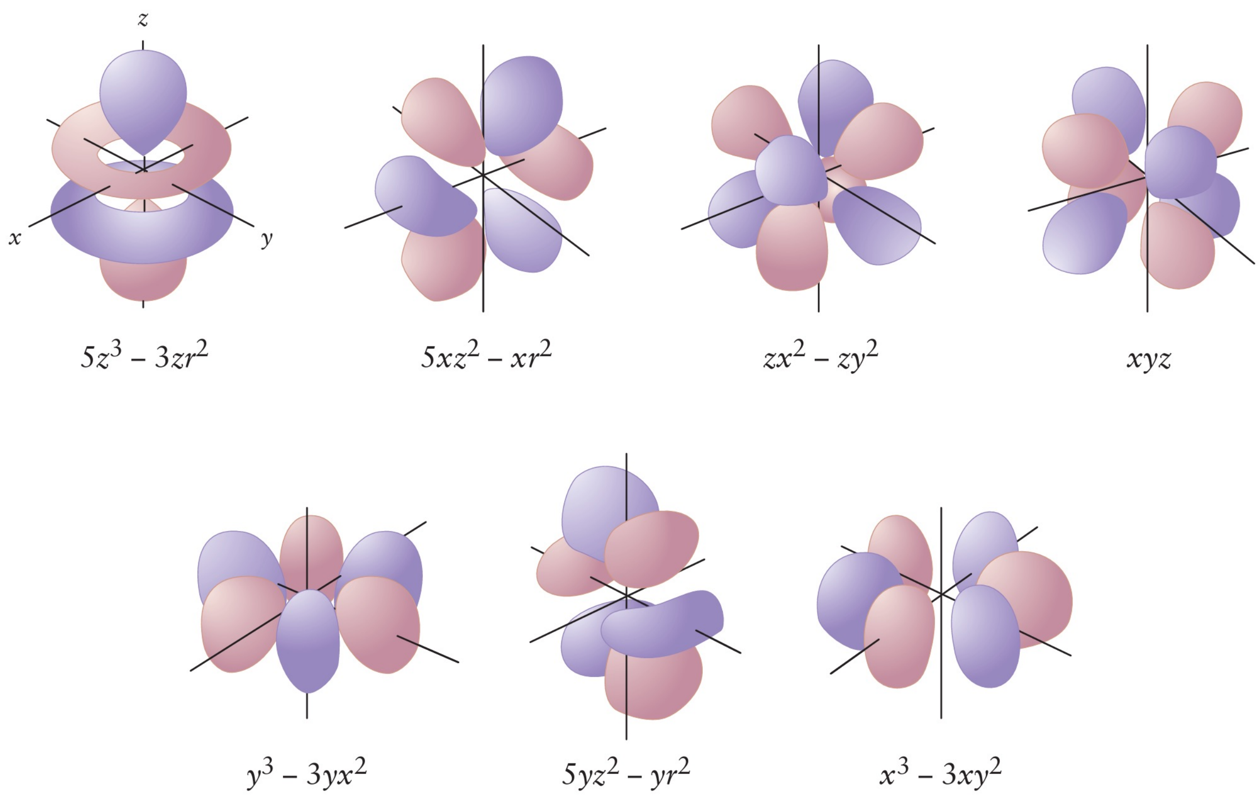


Figure 1D.11

1D.4 The shapes of orbitals

Summary

The shape of an atomic orbital depends on its quantum numbers and can be depicted by a boundary surface. The radial distribution function expresses the probability of finding an electron at a given radius regardless of its angular momentum.

Electron Spin

Topic 1D.5

1D.5 Electron spin

Spin ↑ and ↓

Think of an electron as being able to spin counterclockwise (the ↑ state) and clockwise (the ↓ state) at exactly the same rate.

These two spins are distinguished by a **fourth quantum number**, the spin magnetic quantum number, m_s.

This quantum number can have only one of two values: $+\frac{1}{2}$ (↑) and $-\frac{1}{2}$ (↓).

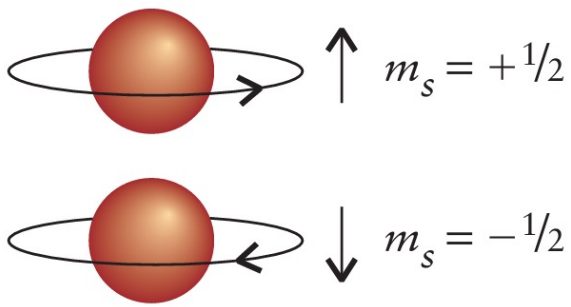


Figure 1D.12

1D.5 Electron spin

Summary

An electron has the property of spin;

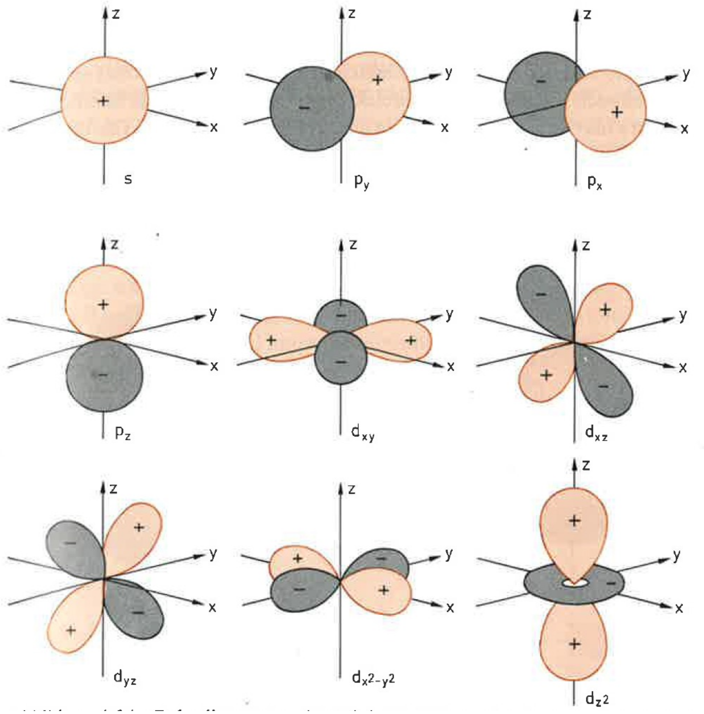
the spin is described by the quantum number $m_s = \pm\frac{1}{2}$.

The Electronic Structure of Hydrogen: A Summary

Topic 1D.6

1D.6 The electronic structure of hydrogen: a summary

Blackboard summary



1D.6 The electronic structure of hydrogen: a summary

1) In the ground state of hydrogen:

$$n = 1, l = 0, m_l = 0, m_s = \pm\frac{1}{2}$$

Both values of m_s are possible, spin orientation does not affect energy.

This is an s-electron with specified spin.

2) When an atom acquires enough energy (by absorbing a photon) for its electron to reach n=2:

It can occupy any of the four orbitals in that shell: one 2s and three 2p orbitals (in hydrogen, they all have the same energy): 2s- or 2p-electron.

Average distance of electron from nucleus increases with increasing *n*: atom is «swelling up» as it is excited energetically.

1D.6 The electronic structure of hydrogen: a summary

3) Atom acquires even more energy:

Electron can move to n = 3 shell

Atom is now even larger

Nine orbitals available (3s, 3p, 3d)

4) More energy still:

Electron can move to n = 4 shell with 16 available orbitals

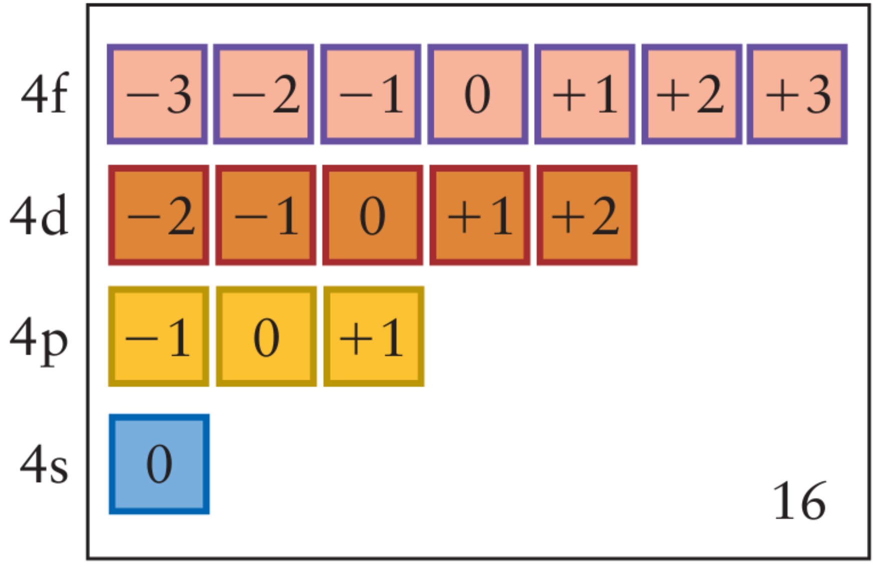


Figure 1D.13

1D.6 The electronic structure of hydrogen: a summary

TABLE 1.3 Quantum Numbers for Electrons in Atoms

Name	Symbol	Values	Specifies	Indicates
principal	n	1, 2, . . .	shell	size
orbital angular momentum*	l	0, 1, . . ., $n - 1$	subshell: l = 0, 1, 2, 3, 4, . . . s, p, d, f, g, . . .	shape
magnetic	m_l	$l, l - 1, \ldots, -l$	orbitals of subshell	orientation
spin magnetic	m_s	$+\frac{1}{2}, -\frac{1}{2}$	spin state	spin direction

*Also called the azimuthal quantum number.

1D.6 The electronic structure of hydrogen: a summary

Summary

The state of an electron in a hydrogen atom is defined by the four quantum numbers n, l, m_l and m_s; as the value of n increases, the size of the atom increases.

The skills you have mastered are the ability to

- Assess the relative probability of finding an electron at a given distance from the nucleus of an atom.
- Name and explain the relation of each of the four quantum numbers to the properties and relative energies of atomic orbitals.
- Describe the properties of electron spin.
- Describe the state of a hydrogen atom in ist ground and excited states.

Summary: You have learned that an electron in a hydrogen atom is described by wavefunctions called atomic orbitals and that each orbital is specified by three quantum numers: n, l, and m_l. You now know that the shape and energy of a given orbital is found by solving the Schrödinger equation for an electron attracted to a nucleus. You also now know that transitions between the allowed energy levels account for the observed patterns of spectroscopic lines. You have also encountered the property of "electron spin" and know that electron spin may have either of two orientations.

	Particle in a box	Hydrogen atom
Dimension of space	1D	3D
Walls	Physical walls	No physical walls, and electrons are confined by pull of the nucleus
Quantization	Energy quantized	
Potential energy	Potential energy inside the box is zero	Potential energy governed by Coulomb potential
Wave function shape	Sinusoidal functions (sine or cosine)	Wave functions (called **orbitals**) are more complex, often **spherical** or **lobed** in shape (spherical harmonics), with both radial and angular components.
Quantum numbers	One quantum number, *n*, which represents the energy level and is related to the number of nodes in the wave function.	Three quantum numbers: ***n***: principal quantum number (energy level), ***l***: angular momentum quantum number (shape of the orbital), $\boldsymbol{m_l}$: magnetic quantum number (orientation of the orbital).
Degeneracy	No degeneracy: each energy level corresponds to one unique state.	Degeneracy in energy levels: for a given principal quantum number *n*, multiple different orbitals (characterized by *l* and m_l) have the same energy.
Boundary conditions	The wave function must go to **zero at the walls** of the box.	The wave function must go to zero at infinity, far from the nucleus.
Physical interpretation	The particle is **free** inside the box but cannot escape due to infinite potential at the walls.	The electron is **bound** to the nucleus due to the attractive Coulomb force, which confines the electron.