CH-110 Advanced General Chemistry I

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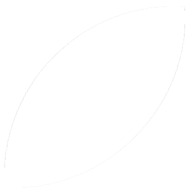
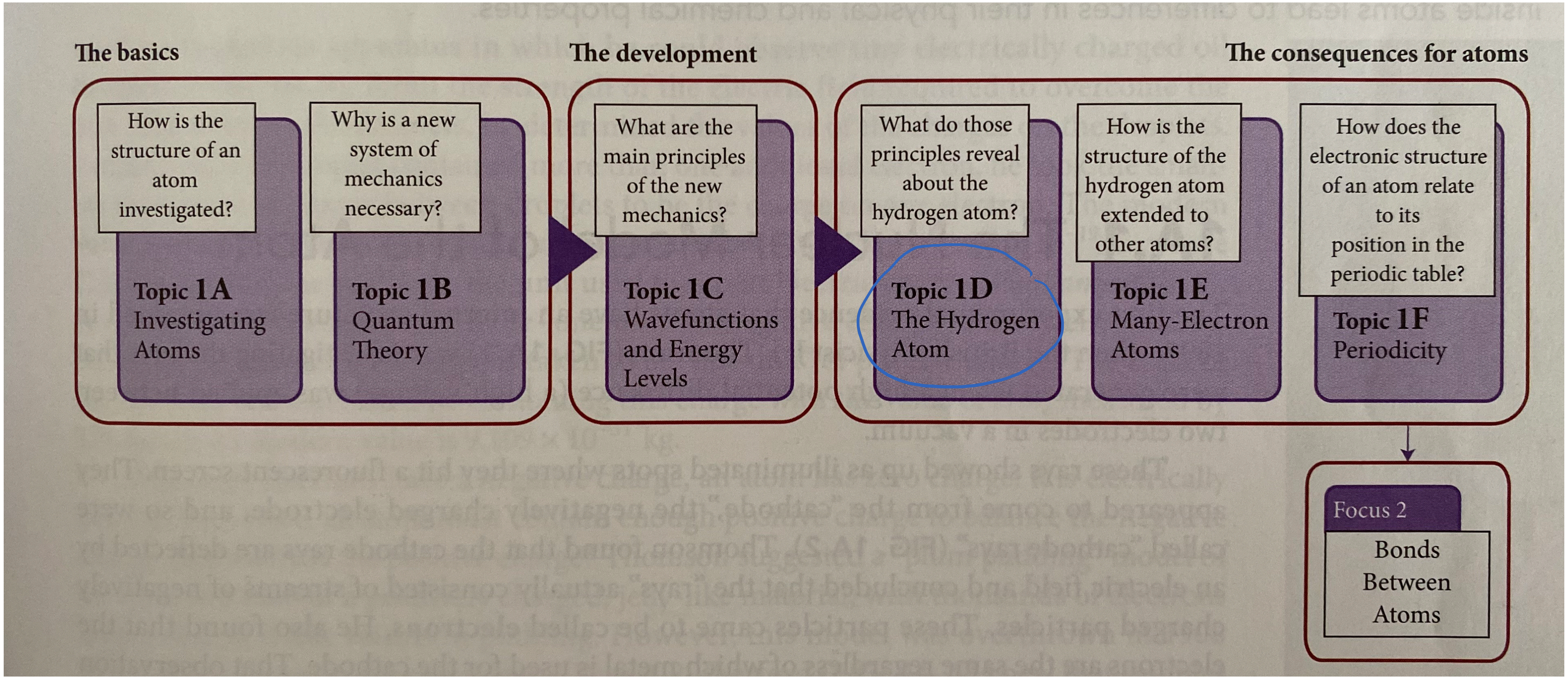
The Hydrogen Atom

Topic 1D



Overview Chapter 1 (Focus 1: Atoms)



The basics

How is the structure of an atom investigated?

Topic 1A
Investigating Atoms

Why is a new system of mechanics necessary?

Topic 1B
Quantum Theory

The development

What are the main principles of the new mechanics?

Topic 1C
Wavefunctions and Energy Levels

The consequences for atoms

What do those principles reveal about the hydrogen atom?

Topic 1D
The Hydrogen Atom

How is the structure of the hydrogen atom extended to other atoms?

Topic 1E
Many-Electron Atoms

How does the electronic structure of an atom relate to its position in the periodic table?

Topic 1F
Periodicity

Focus 2
Bonds Between Atoms

Topic 1D

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

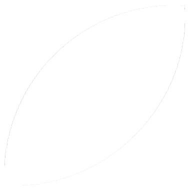
$$\boxed{\nu = R\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right), n_1 = 1,2, \dots, and\ n_2 = n_1 + 1, n_1 + 2, \dots}$$

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

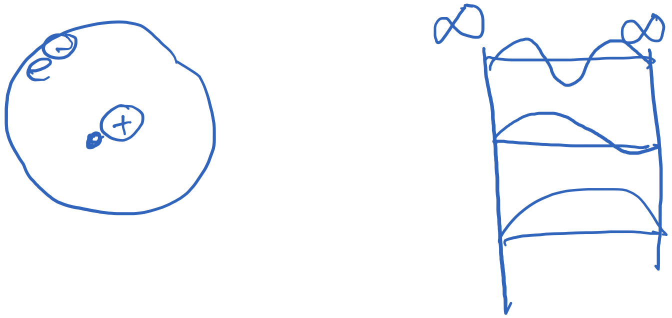
- Why such a **pattern** and why does R have that **value**?
- Example 1C.1 gave clues: lines in spectrum are due to transitions between allowed energy levels of the atom, the difference in energy is carried awway by a photon of energy $h\nu$
- **Aim of this topic**: construct a quantum mechanical model of the hydrogen atom using the fact that an electron has wave-like properties and is described by a wavefunction, and has quantized energy levels.

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. 1D → 3D
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 $+e$:

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

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:

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

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

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

Important formula.
Need to know how to apply.

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

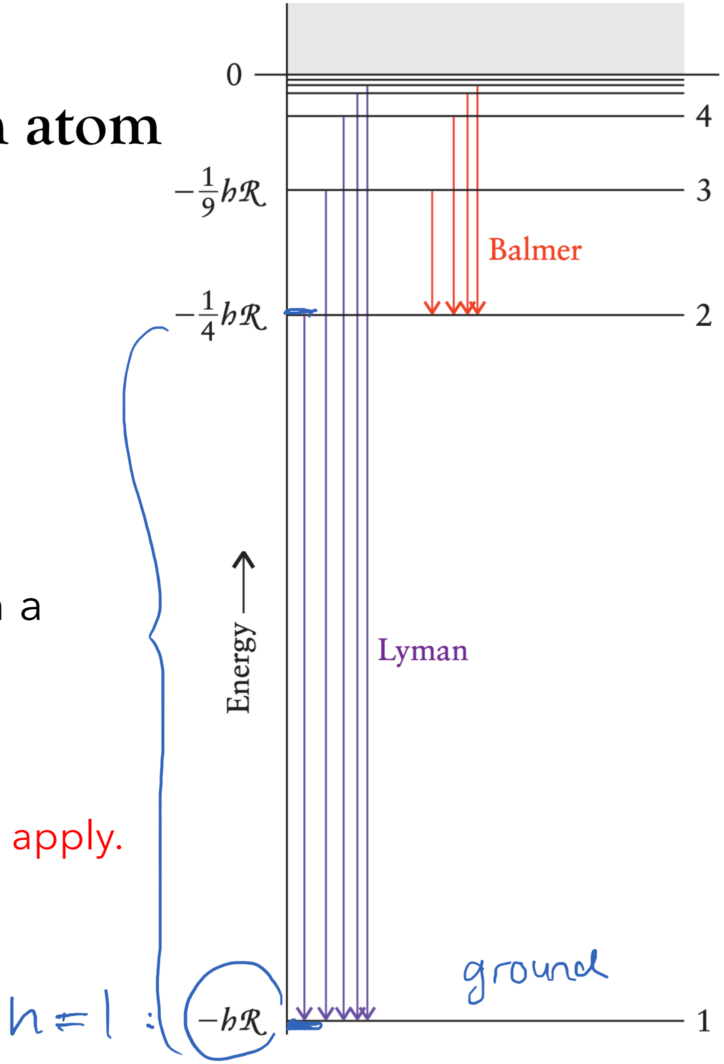


Figure 1D.1

1D.1 Energy levels

What does this equation tell you?

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

Important formula.
Need to know how to apply.

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

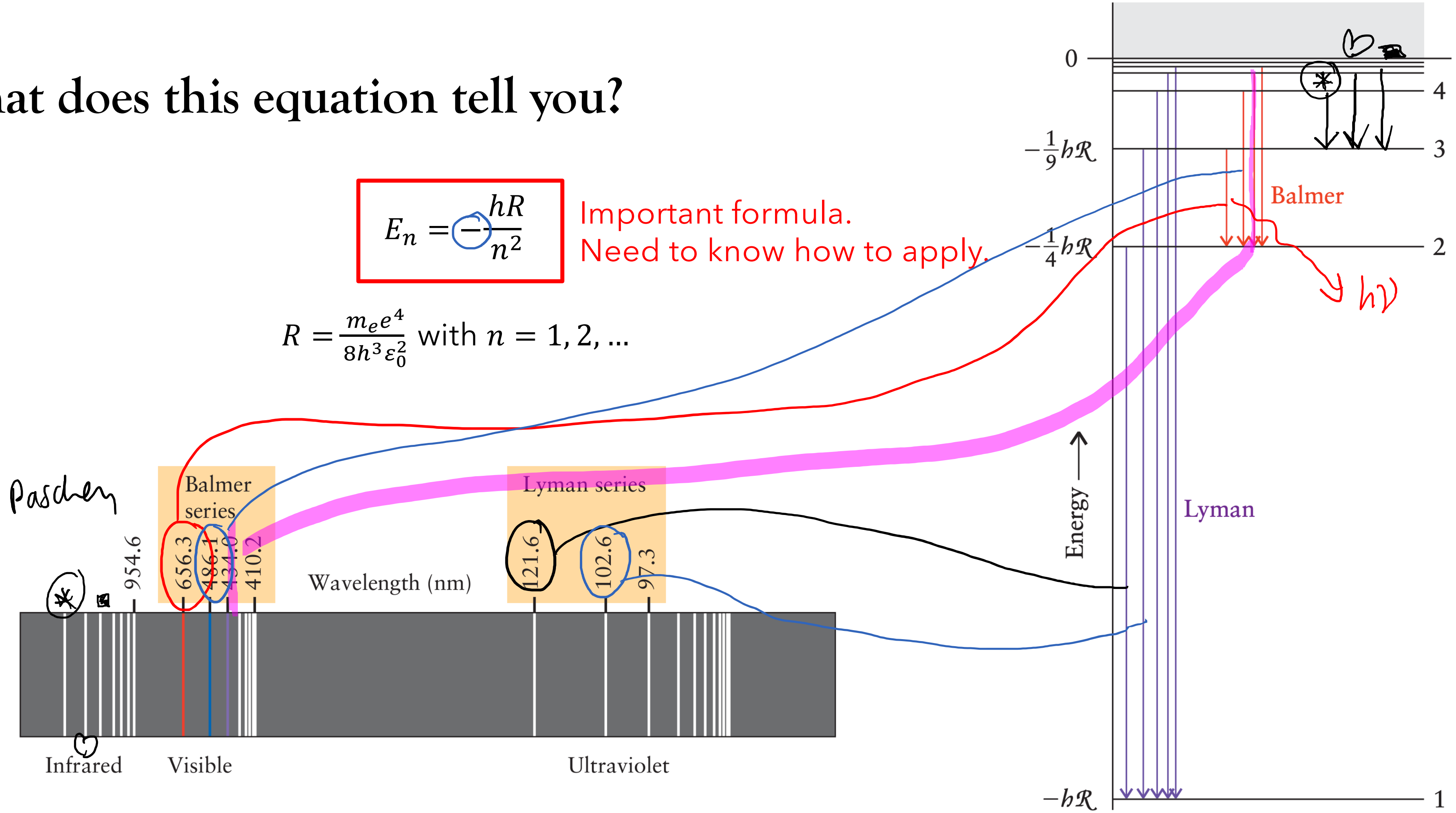


Figure 1D.1

1D.1 Energy levels

What does this equation tell you?

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

Important formula.
Need to know how to apply.

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

- All energies are **negative**: electron has a *less negative* energy far from the nucleus, it takes energy to remove an electron from an atom.
- Energy is quantizied, with **quantum number**, *n*, like for the particle in a box.
- *n* appears in the **denominator**: as *n* increases, the energy becomes less negative and approaches zero, where the electron escapes.

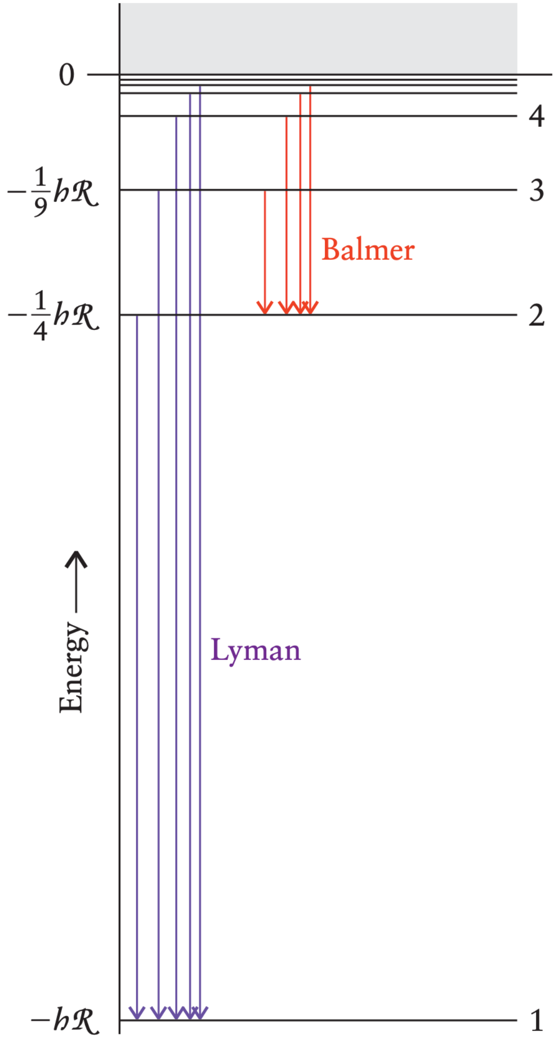


Figure 1D.1

1D.1 Energy levels

Relationship to Bohr frequency condition

Bohr frequency condition:

$$h\nu = \Delta E$$

Insert into previous equation. In the case of the hydrogen atom, if the electron falls from a level with quantum number n_2 to one with quantum number n_1, then:

$$h\nu = \Delta E = \left(-\frac{hR}{n_2^2}\right) - \left(\frac{hR}{n_1^2}\right) = hR\left\{\frac{1}{n_1^2} - \frac{1}{n_2^2}\right\} \; with \; n_1 = 1,2,\ldots, n_2 = n_1 + 1, n_1 + 2, \ldots$$

Compare to previous Rydberg equation:

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

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

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

- Imagine Schrödinger calculating this constant!

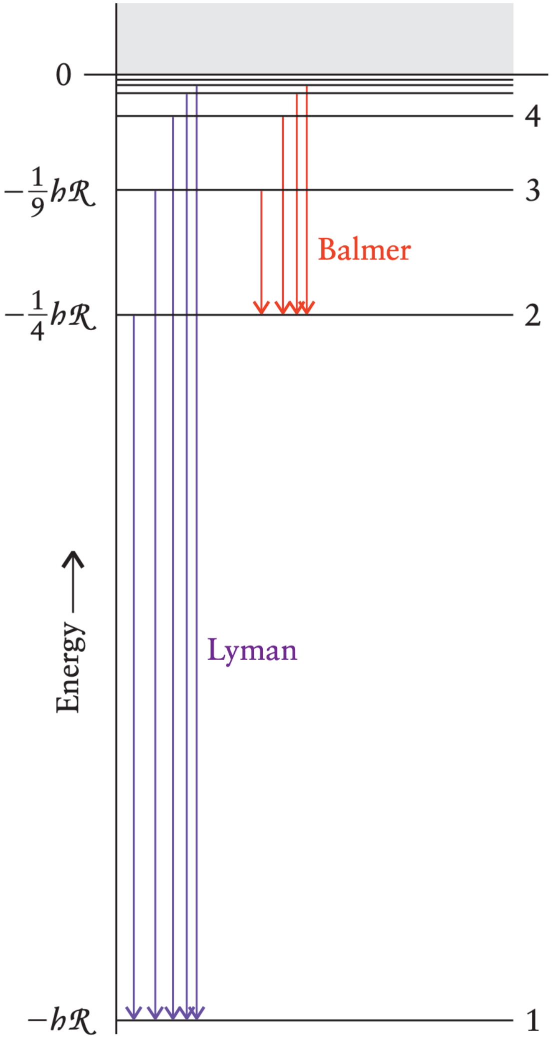


Figure 1D.1

1D.1 Energy levels

Finally, it makes sense

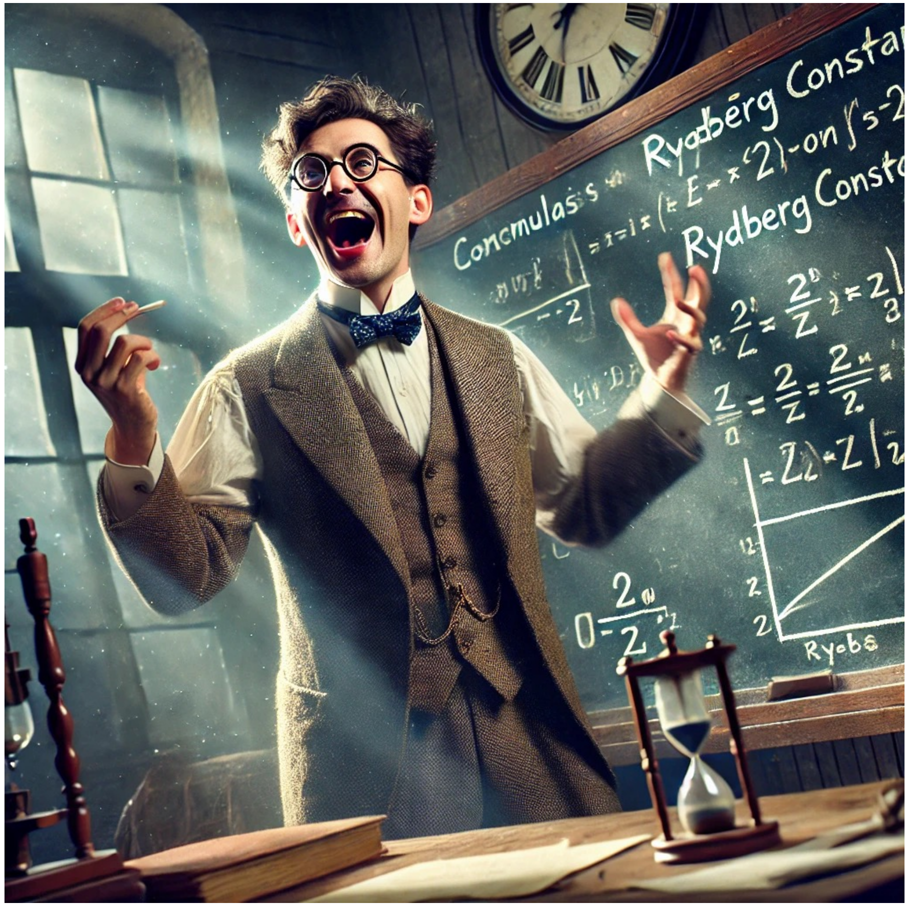


Image source: ChatGPT (2024)
Schrödinger's Eureka Moment.

1D.1 Energy levels

Generalization to other one-electron ions possible

Schrödinger was able to generalize this equation

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

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

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:

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

Important formula.
Need to know how to apply.

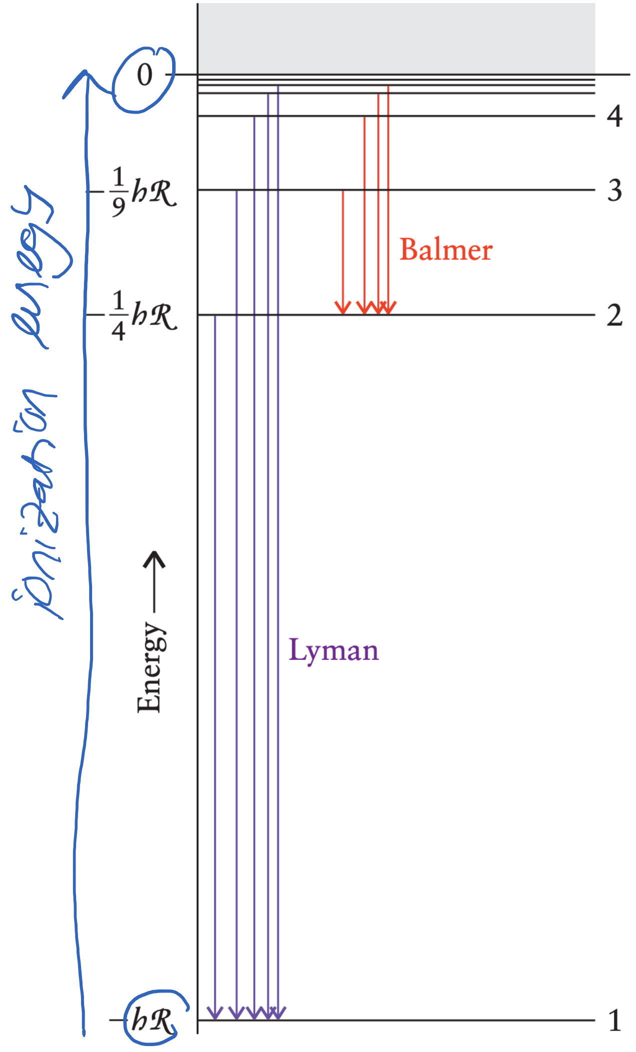
Note:

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



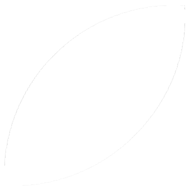
1D.1 Energy levels

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

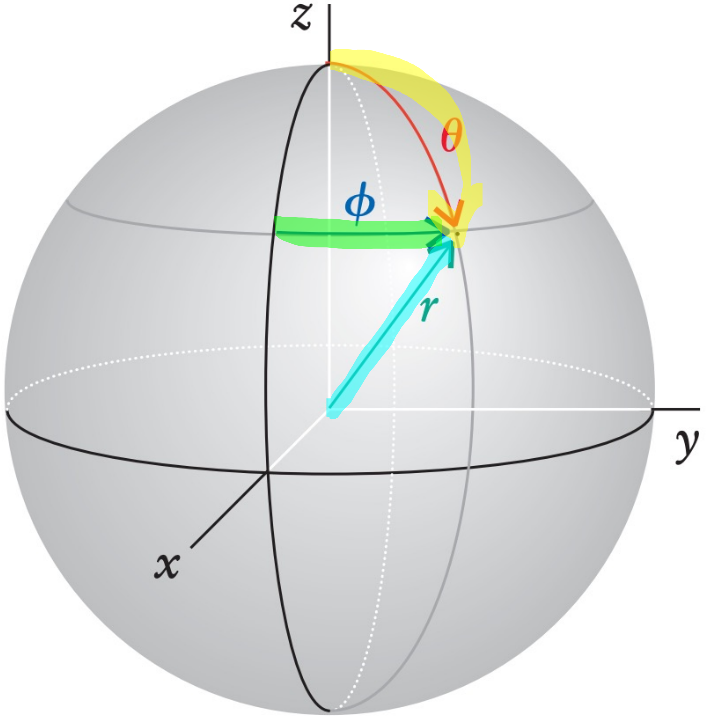
Image source: ChatGPT (2025)
Glossy Hydrogen Balloon Orbitals.

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)

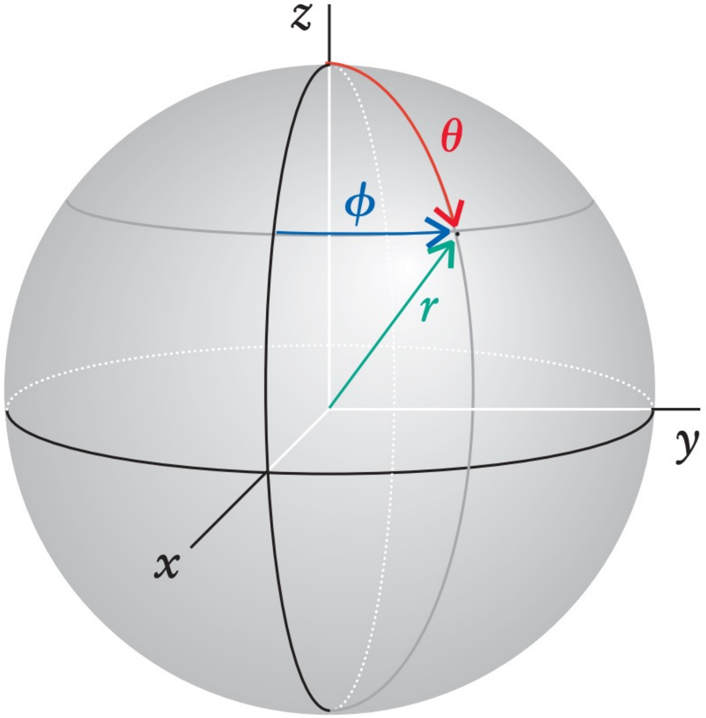


1D.2 Atomic orbitals

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

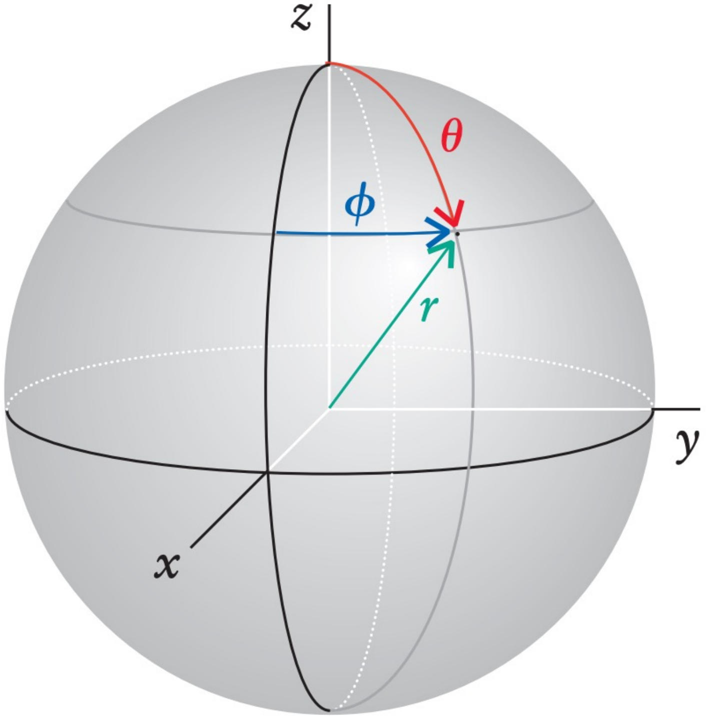
Each wavefunction depends on three coordinates:

$$\Psi(\mathrm{r},\theta,\phi) = \mathrm{R}(\mathrm{r}) \times Y(\theta,\phi)$$

→ Product of a radial $\mathrm{R}(\mathrm{r})$ and angular part $Y(\theta,\phi)$.

$R(r)$**: radial wavefunction**, expresses how the wavefunction varies with distance from the nucleus.

$Y(\theta,\phi)$: **angular wavefunction**, expresses how the wavefunction varies as the angles θ and ϕ change.



1D.2 Atomic orbitals

Hydrogen ground state orbital $\boxed{(\boldsymbol{n} = \mathbf{1})}$

- Wavefunction:

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

- 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	$\boxed{2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}}$
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	$\left(\frac{5}{16\pi}\right)^{1/2}(3\cos^2\theta-1)$

→ double-check

See next two slides!

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[*] 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

Addition: From radial and angular parts to the full ground-state orbital

What we're doing here: we take the radial part $R_{nl}(r)$ and the angular part $Y_{l,m_l}(\theta,\phi)$ from the table, and multiply them to obtain the full wavefunction $\psi(r,\theta,\phi)$. For the ground state of hydrogen ($n=1, l=0, m_l=0$) this looks like:

$$\psi(r,\theta,\phi)=2\left(\frac{1}{a_0}\right)^{\frac{3}{2}}e^{-\frac{r}{a_0}}\times\left(\frac{1}{4\pi}\right)^{\frac{1}{2}}$$

Step 1: Put constants together:

$$\psi(r,\theta,\phi)=\left[2\left(\frac{1}{a_0}\right)^{\frac{3}{2}}\times\left(\frac{1}{\sqrt{4\pi}}\right)\right]e^{-\frac{r}{a_0}}$$

Step 2: Simplify the factor with 2 and $\sqrt{4\pi}$:

$$\frac{2}{\sqrt{4\pi}}=\frac{2}{2\sqrt{\pi}}=\frac{1}{\sqrt{\pi}}$$

1D.2 Atomic orbitals

Addition: From radial and angular parts to the full ground-state orbital

Step 3: Collect powers of a_0

$$\left(\frac{1}{a_0}\right)^{\frac{3}{2}} = \frac{1}{a^{\frac{3}{2}}}$$

So the prefactor becomes:

$$\frac{1}{\sqrt{\pi}} \times \left(\frac{1}{a^{\frac{3}{2}}}\right) = \frac{1}{\sqrt{\pi a_0^3}}$$

Step 4: Write the final result

$$\psi(r, \theta, \phi) = \frac{1}{\sqrt{\pi a_0^3}}\, e^{-\frac{r}{a_0}}$$

Evaluate: This equation matches the one on slide 27. OK.

1D.2 Atomic orbitals

Example from Table 1.2

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

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

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:

1. Principal quantum number n is related to the **size** and **energy** of the orbital
2. Quantum number l is related to its **shape**
3. Quantum number m_l is related to its **orientation in space**

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.

main shell

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:

$$\boxed{l = 0, 1, 2, \dots, \boldsymbol{n} - \mathbf{1}} \leftarrow$$

Orbitals with principal number n are divided into **subshells l**:

For $\underline{n =} 1$: there is only one subshell $\underline{l = 0}$

For $n = 2$: there are two subshells $\underline{l = 0, 1}$

For $n = 3$: there are three subshells $\underline{l = 0, 1, 2}$

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:

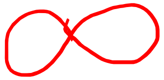
$$\boxed{L = \sqrt{\ell(\ell+1)}\,\hbar}$$

- 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

p_x :



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.

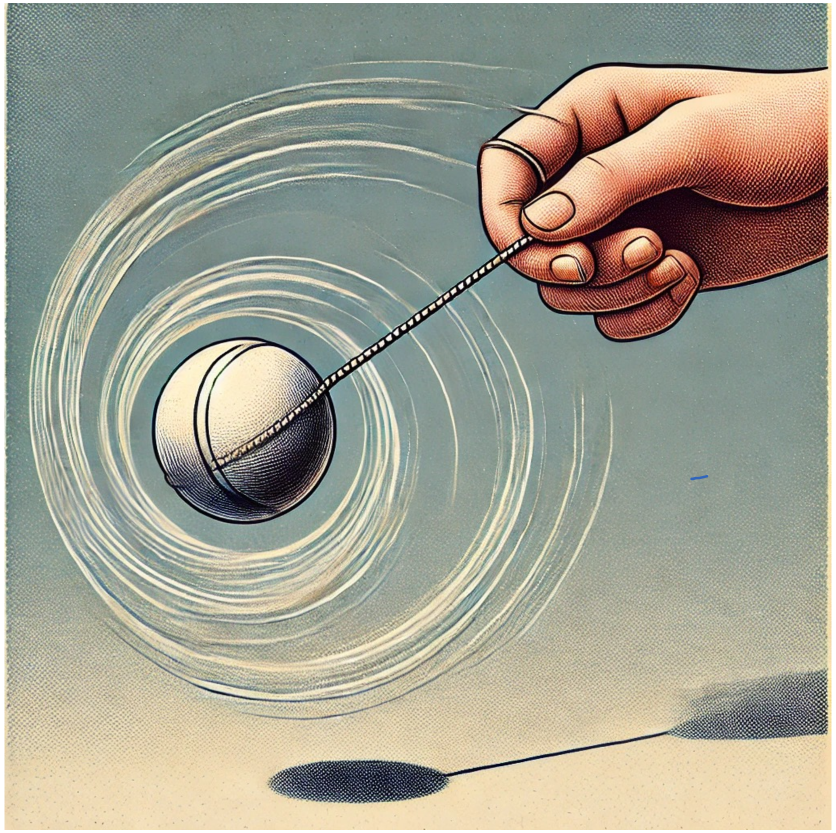


Image source: ChatGPT (2024).
Angular Momentum of Ball on a String.

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 $m_l = +2, +1, 0, -1, -2$

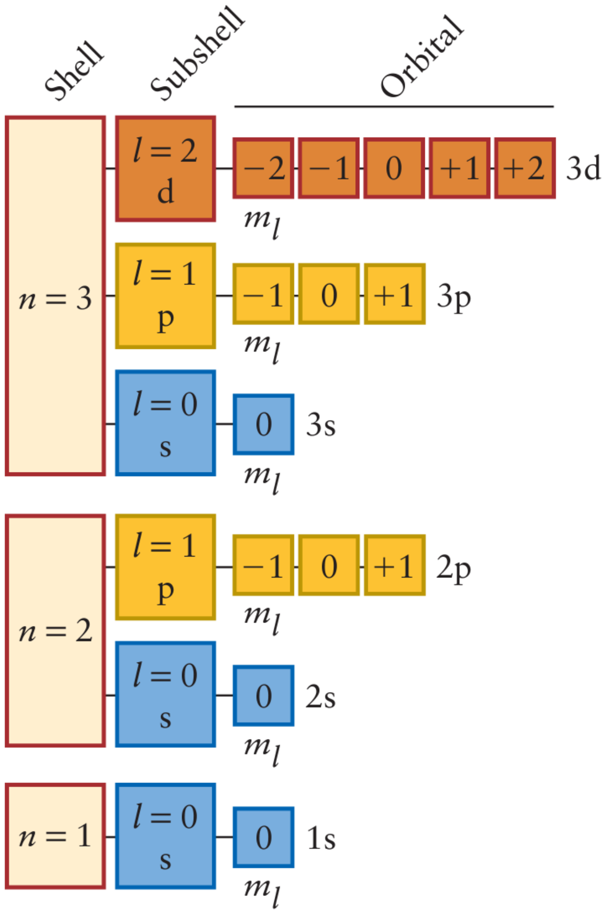


Figure 1D.3

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)

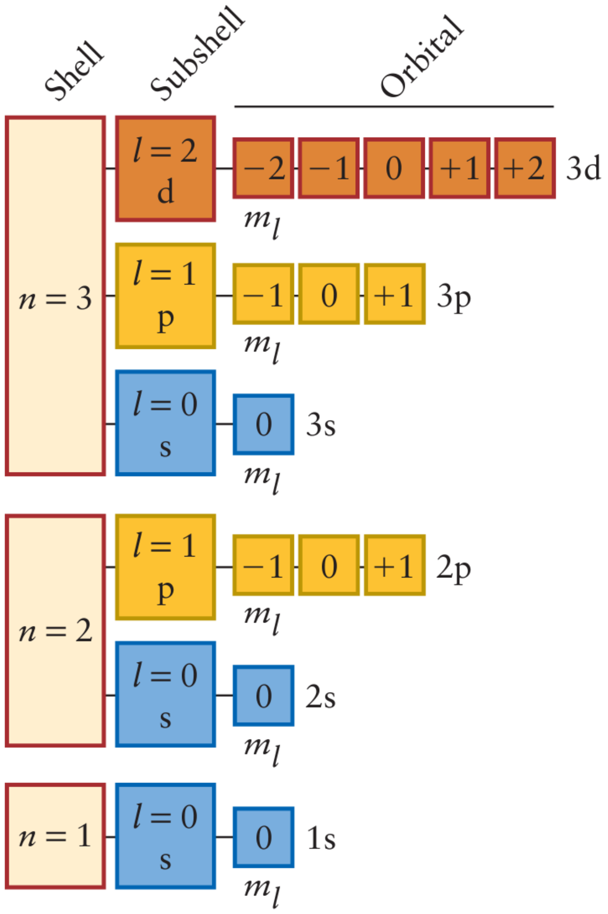


Figure 1D.3

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.

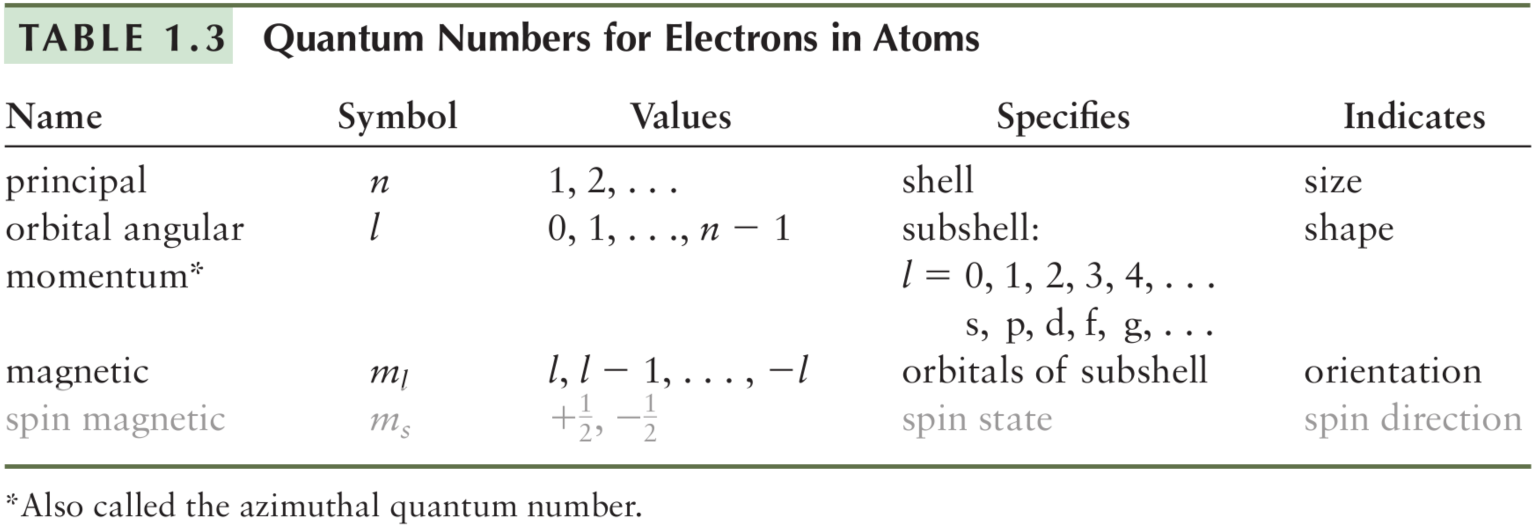


TABLE 1.3 Quantum Numbers for Electrons in Atoms

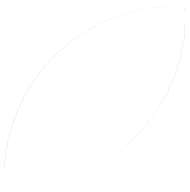
Name	Symbol	Values	Specifies	Indicates
principal	n	1, 2, . . .	shell	size
orbital angular momentum*	l	0, 1, . . ., $n - 1$	subshell: l = 0, 1, 2, 3, 4, . . . s, p, d, f, g, . . .	shape
magnetic	m_l	$l, l - 1, \ldots, -l$	orbitals of subshell	orientation
spin magnetic	m_s	$+\frac{1}{2}, -\frac{1}{2}$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

*Also called the azimuthal quantum number.

Chapter 1D.5:

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 → $\underline{n = 1}, \underline{\ell = 0}, \underline{m_\ell = 0}$ → the **1s orbital**.
- Each shell has one s-orbital, named ns (1s, 2s, 3s …).

2s : $n=2$, $\ell=0$, $m_\ell=0$

$\vdots$

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.

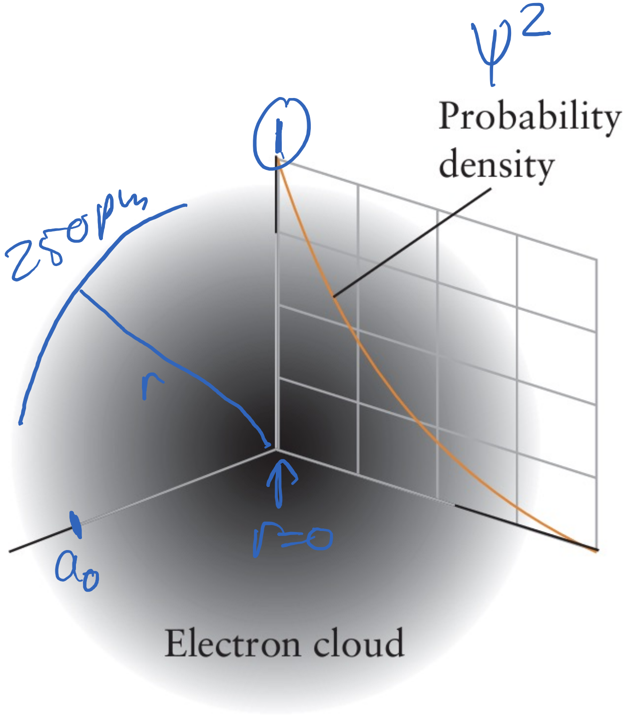


Figure 1D.4

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 $\boldsymbol{a_0}$** 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.

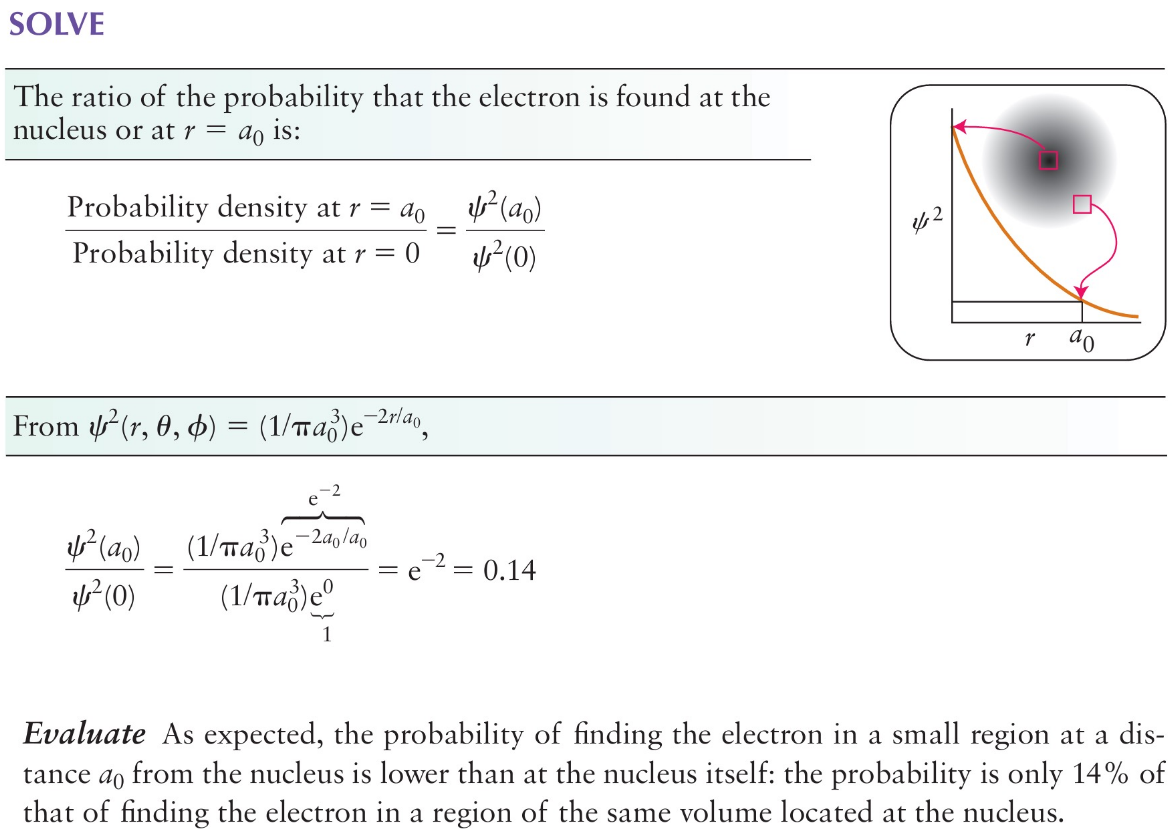
Plan: compare the probability densitites at the two locations: ratio of the squares of the wavefunctions at the two locations. $r=0$, $r=a_0$

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

Student question: *How would I find the probability at a distance x that isn't a multiple of a_0?*
Anwer: *You don't need this yet, but in general you just plug x into $\psi^2(r)$; for a full probability in a region, you'd integrate $|\psi(r)|^2 \cdot 4\pi r^2 dr$ over that range.*

1D.4 The shapes of orbitals

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



SOLVE

The ratio of the probability that the electron is found at the nucleus or at $r = a_0$ is:

$$\frac{\text{Probability density at } r = a_0}{\text{Probability density at } r = 0} = \frac{\psi^2(a_0)}{\psi^2(0)}$$

From $\psi^2(r, \theta, \phi) = (1/\pi a_0^3)e^{-2r/a_0}$,

$$\frac{\psi^2(a_0)}{\psi^2(0)} = \frac{(1/\pi a_0^3)\overbrace{e^{-2a_0/a_0}}^{e^{-2}}}{(1/\pi a_0^3)\underbrace{e^0}_{1}} = e^{-2} = 0.14$$

Evaluate As expected, the probability of finding the electron in a small region at a distance a_0 from the nucleus is lower than at the nucleus itself: the probability is only 14% of that of finding the electron in a region of the same volume located at the nucleus.

At $r = 2a_0$:

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

Ratio becomes:

$e^{-4} = 0.018$

At $r = 3a_0$:

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

Ratio becomes:

$e^{-6} = 0.0025$

1D.4 The shapes of orbitals

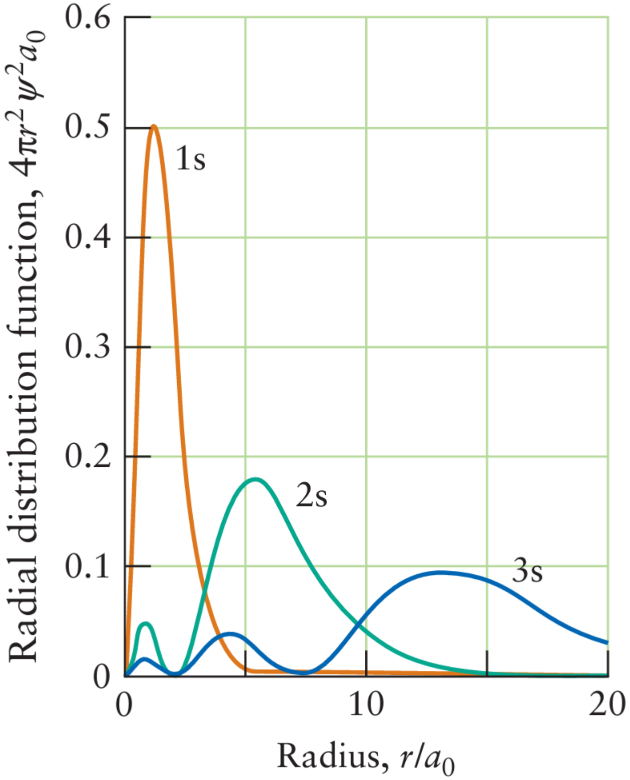
Why we need the radial distribution function

- $|\psi|^2$: probability density at a point (r, θ, ϕ).
- To know probability **at distance r in all directions**, use the **radial distribution function (s-orbitals)**:

$$P(r) = 4\pi r^2 |\psi|^2$$

- **Interpretation**: probability of finding electron in thin shell between r and $r + \delta r$.
- **Analogy**: Earth's population density—zero inside Earth's radius, rises at surface, falls off above it.

Figure 1D.5

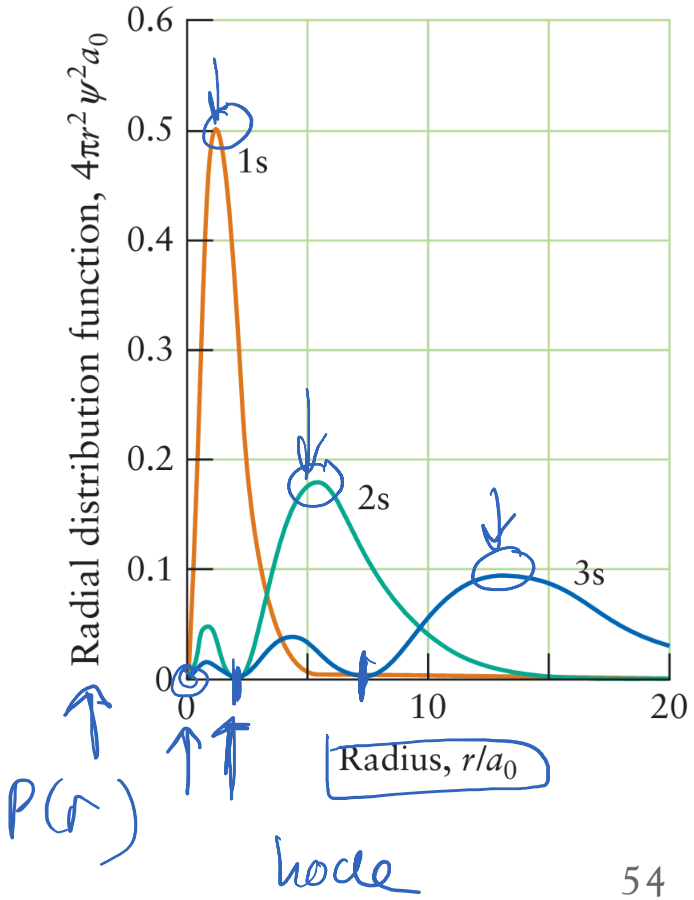


1D.4 The shapes of orbitals

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 $\boxed{P(r)\delta r}$, the probability of finding the electron anywhere in the **spherical shell** between r and r + δr

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