Quantum Numbers and Atomic Orbitals

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CHEMISTRY 161
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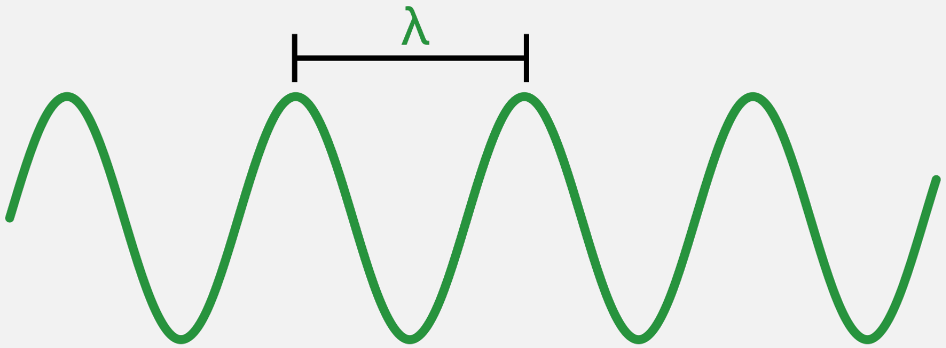
ELECTRONS: Wave-Particle Duality

Q: What is an electron?

Is it a wave that carries energy? ELECTRON AS A WAVE

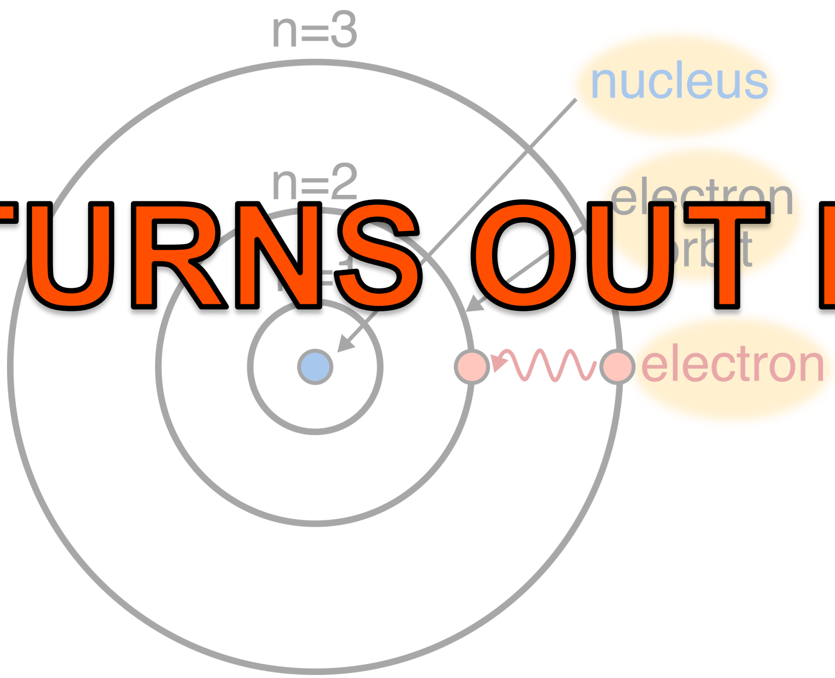


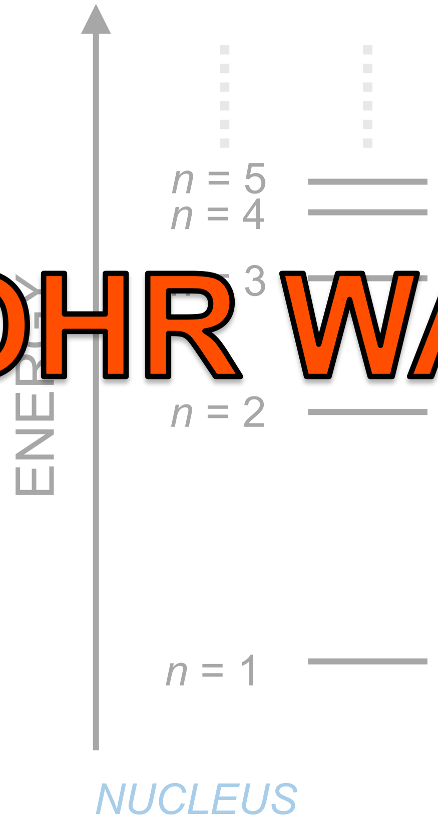
Is it a negatively charged particle? ELECTRON AS A PARTICLE

A: It behaves as both a wave and a particle.

ELECTRONS BEHAVE VERY MUCH LIKE LIGHT!

The Bohr Model: Quantization



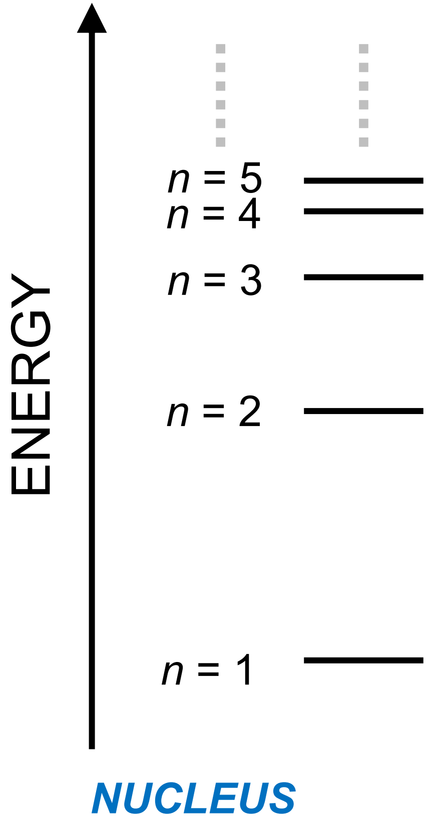


If we imagine the nucleus at the center, then:

- n = 1 has the lowest energy.
- n = 2 has the second lowest energy.
- The energies get higher the farther we get from the nucleus.
- The spacing between states also gets smaller!

TURNS OUT BOHR WAS WRONG!

MODERN ATOMIC THEORY



- Electrons are likely to be found near the nucleus.
  → Energy diagram to the left is not horrible but could be better.
- However, at the same time, electrons can be anywhere really—think back to the wave-like properties of electrons (or light).
- We don't really know how the electron moves (Heisenberg uncertainty principle), but we know where it probably is.
- ORBITAL: The space around the nucleus where the electron's location is most probable, often called the wave function (Ψ^2).

LET’S WORK THROUGH THE QUANTUM NUMBERS

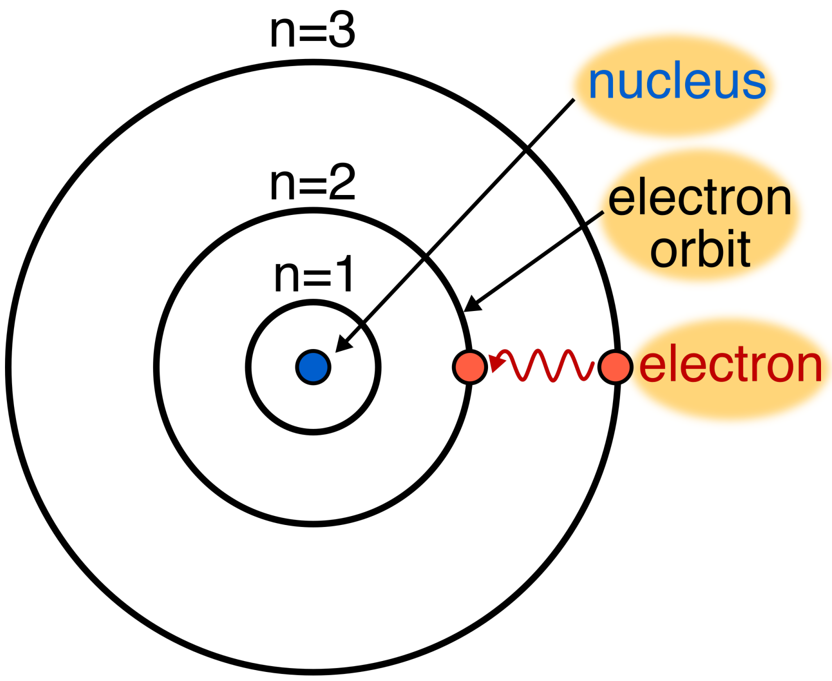
AND ATOMIC ORBITALS NOW.

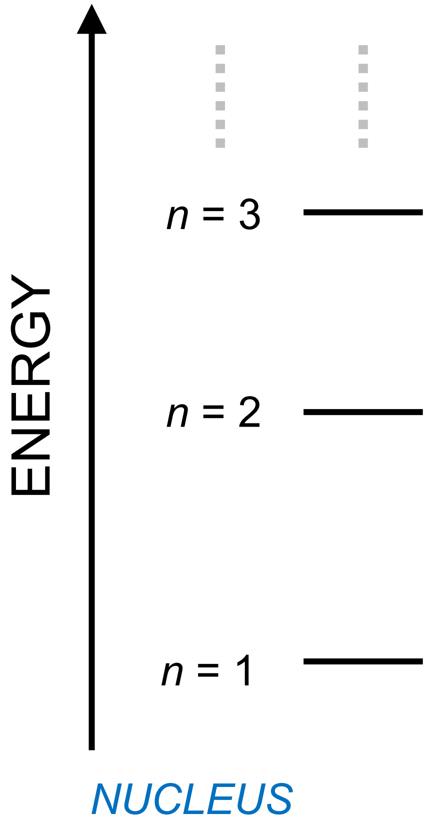
What are quantum numbers anyway though?

Quantum numbers are a unique set of numbers that define an orbital or an electron.

Every orbital and every electron has a unique set of quantum numbers.

n: Principal Quantum Number



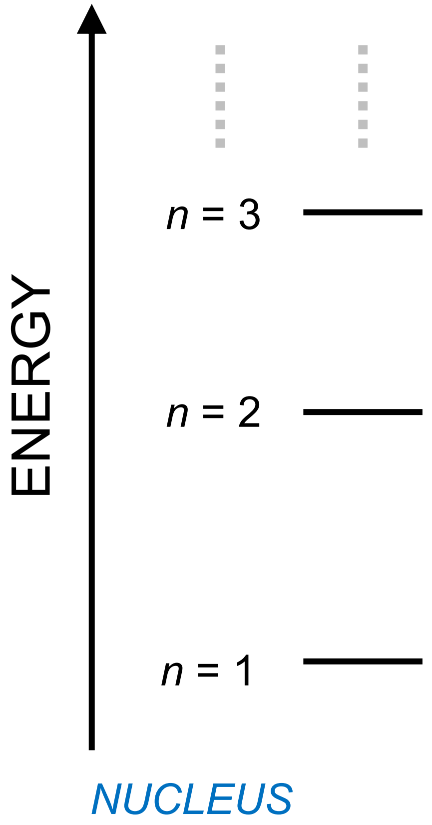


The principal quantum number (*n*) is very much like that of Bohr's notation. It simply tells us the relative size and energy of an orbital.

Generally, the larger the value of *n*, the larger the orbital and the higher its energy.

Think back to Bohr's picture and why that might be true. As we get farther and farther from the nucleus, the orbital is larger (the electron is found farther from the nucleus) and as a result the energy is higher.

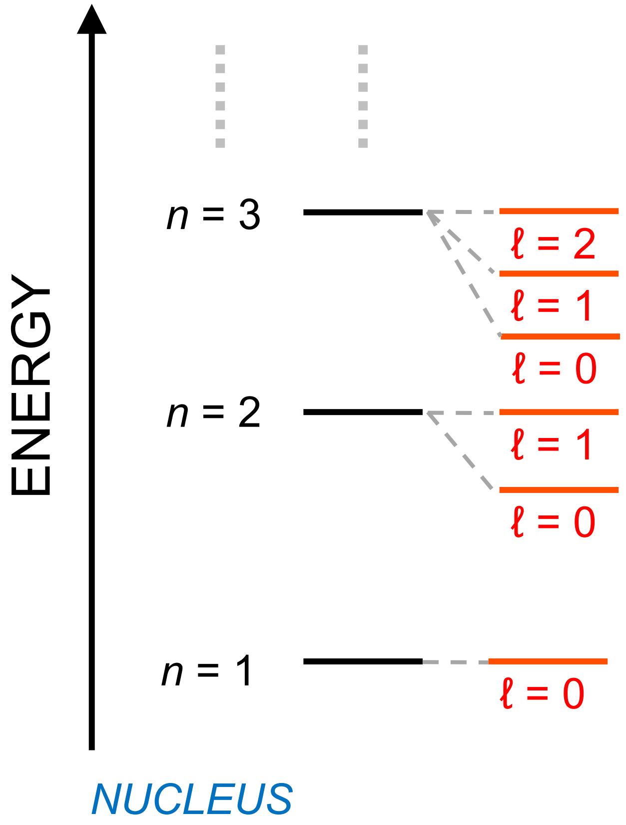
ℓ: Angular Momentum Quantum Number



The angular momentum quantum number (ℓ) defines the shape of our orbital.

The values of ℓ range from 0 to (n – 1).

ℓ: Angular Momentum Quantum Number



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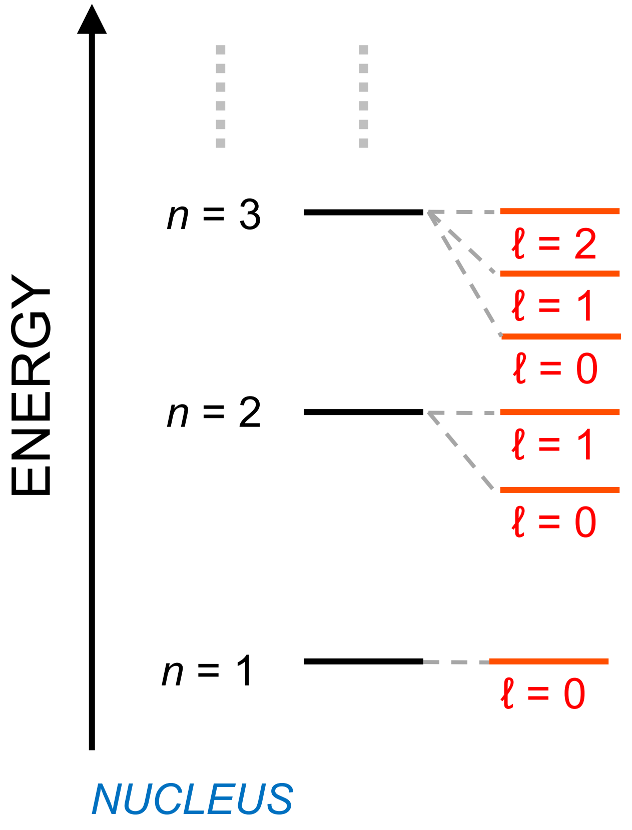


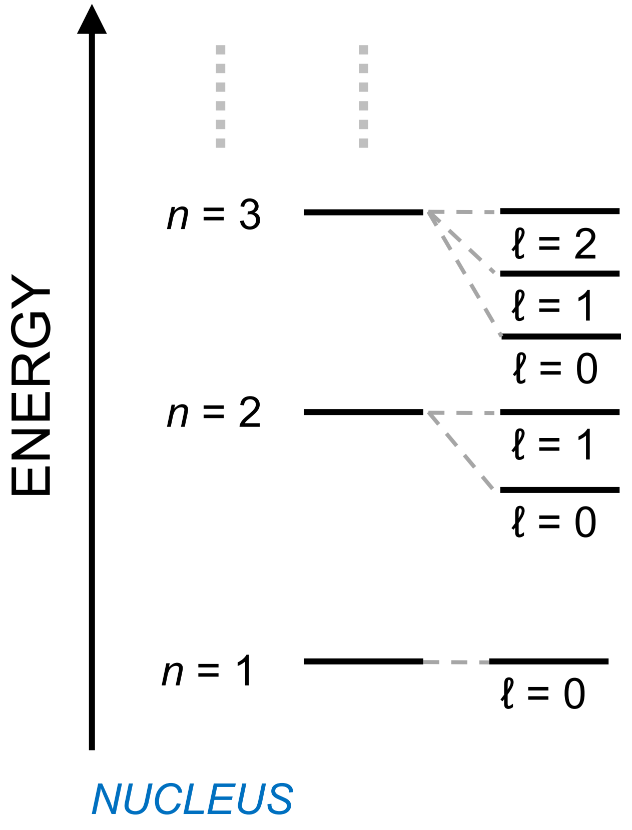
The angular momentum quantum number (ℓ) defines the shape of our orbital.

The values of ℓ range from 0 to (n – 1).
We associate the values of ℓ with letters, such that:

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

We'll go through what this means visually in a bit.

m_ℓ: Magnetic Quantum Number



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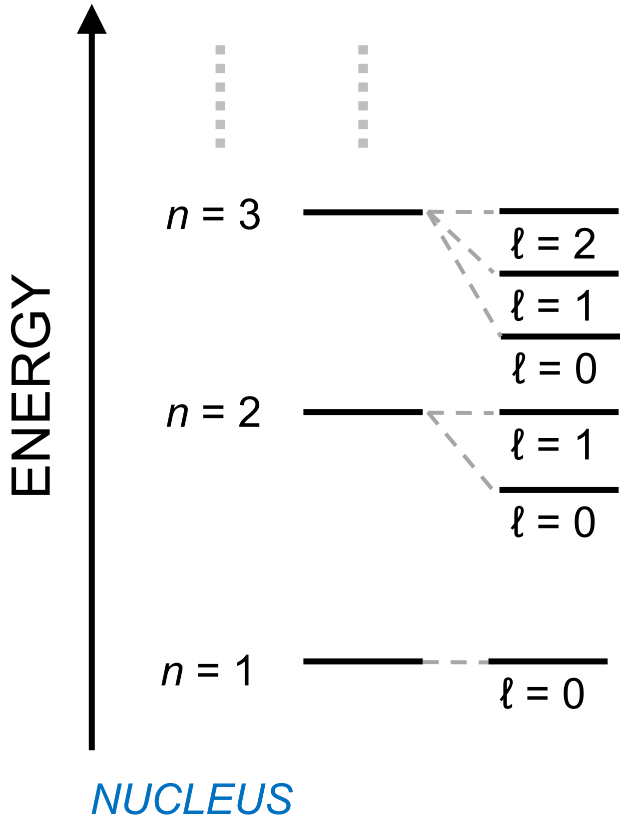
m_ℓ: Magnetic Quantum Number

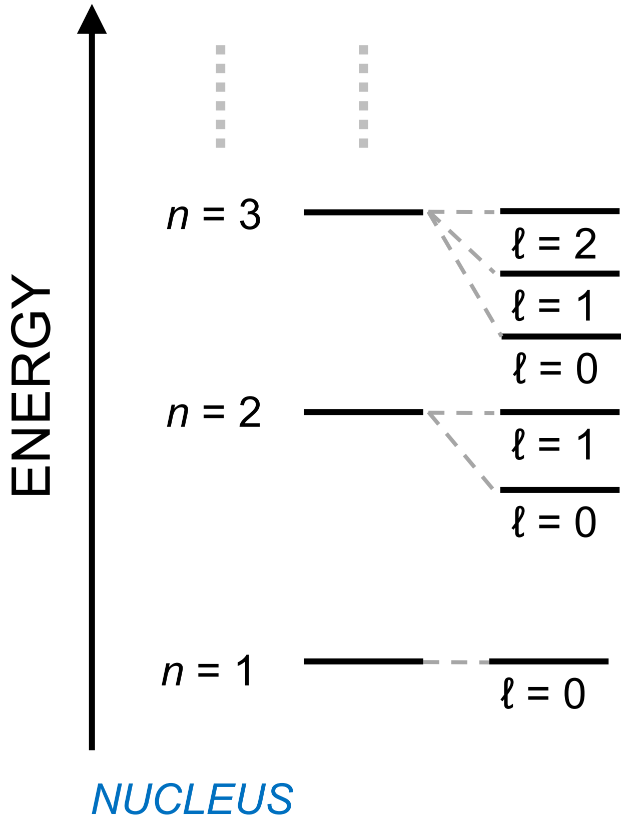


The magnetic quantum number (m_ℓ) defines the orientation of the orbital.

The values of m_ℓ range from $-\ell$ to $+\ell$.

Value of ℓ	**0**	**1**	**2**
Orbital Type	***s***	***p***	***d***
Values of m_ℓ	**0**	**−1, 0, +1**	**−2, −1, 0, +1, +2**

m_ℓ: Magnetic Quantum Number



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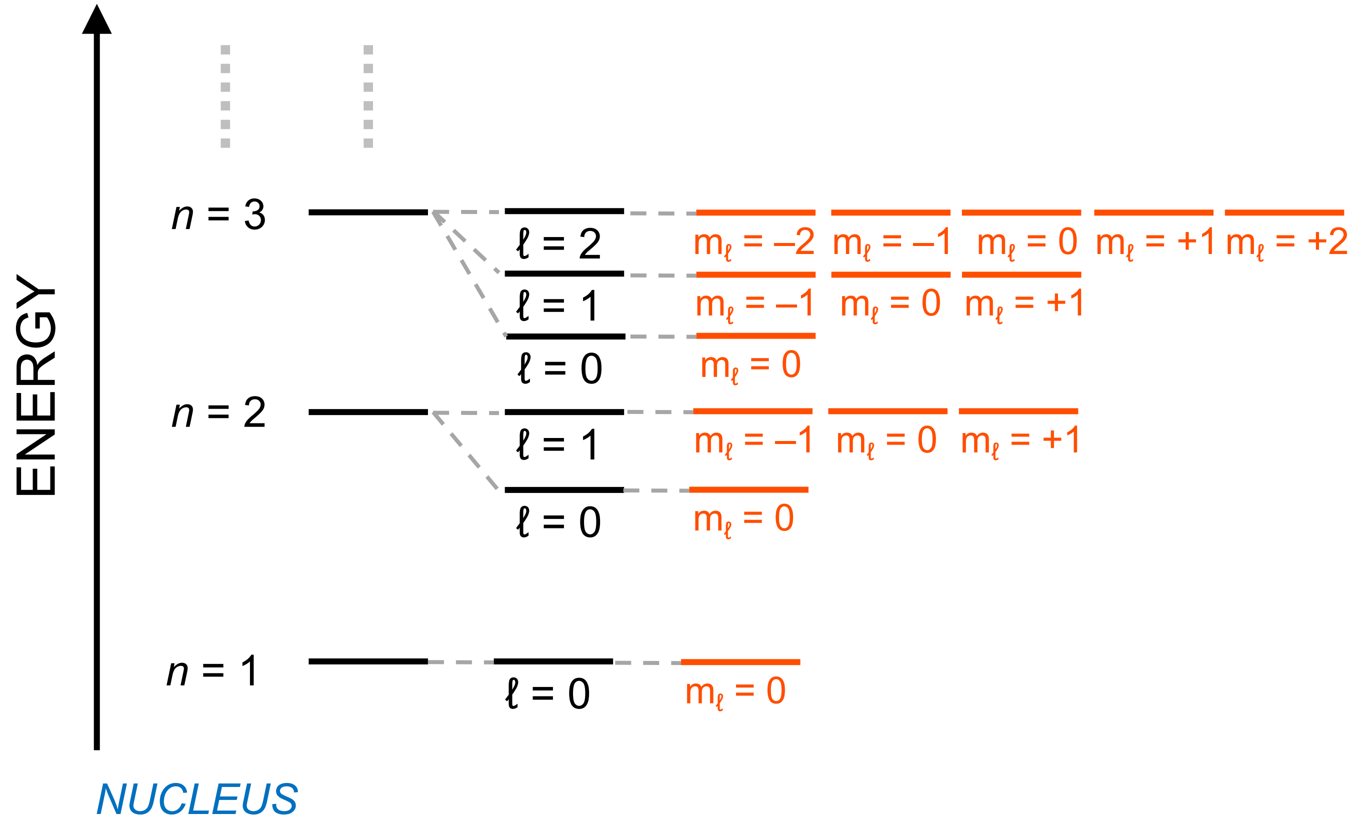
The values of m_ℓ range from $-\ell$ to $+\ell$.
The number of possible m_ℓ tells us how many orbitals exist for a given ℓ.

Value of ℓ	0	1	2
Orbital Type	*s*	*p*	*d*
Values of m_ℓ	0	−1, 0, +1	−2, −1, 0, +1, +2
(# of m_ℓ)	(1)	(3)	(5)

m_ℓ: Magnetic Quantum Number



The magnetic quantum number (m_ℓ) defines the orientation of the orbital.

The values of m_ℓ range from –ℓ to +ℓ.
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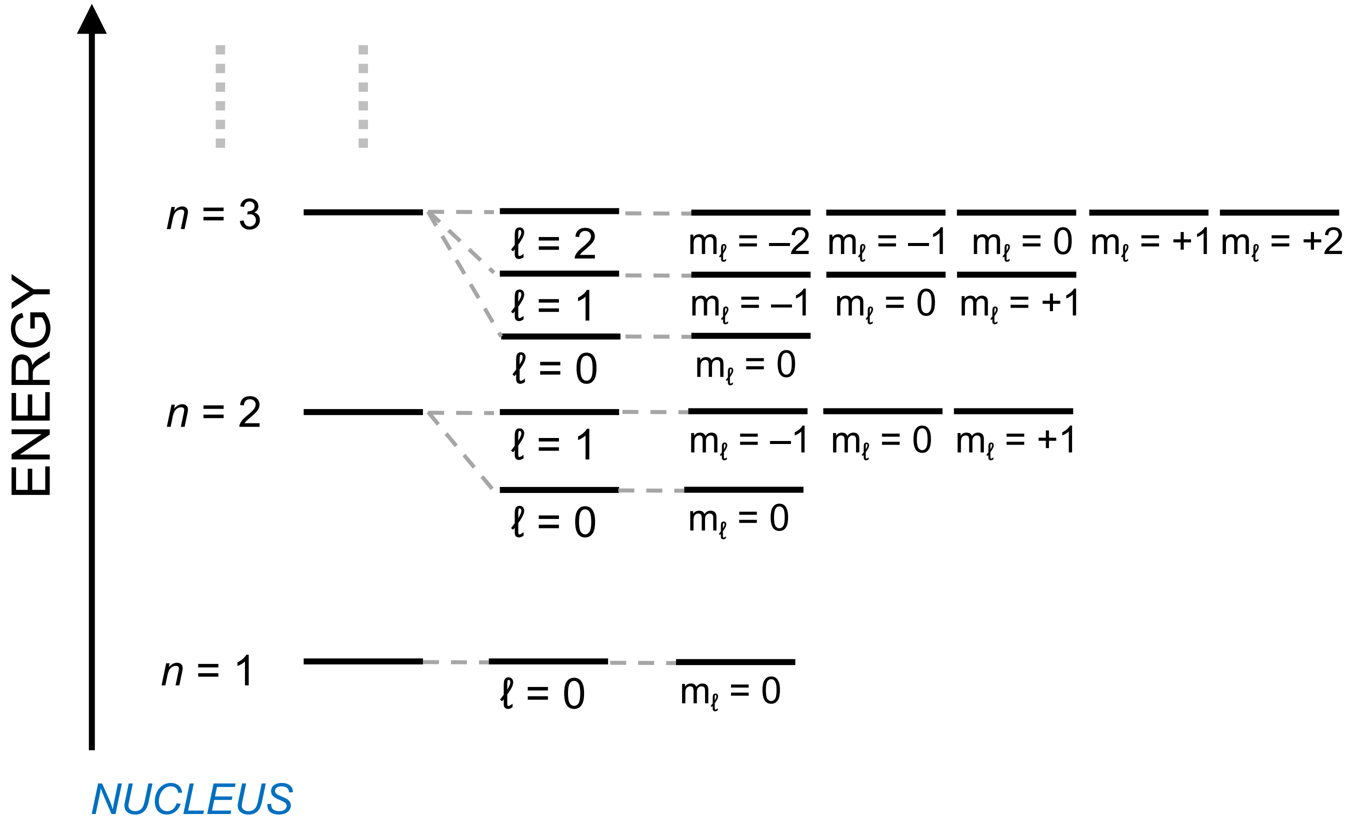
Quantum Numbers ⇔ Atomic Orbitals



PUTTING IT ALL TOGETHER:

- The principal quantum number (n) tells us the relative size and energy of an orbital.

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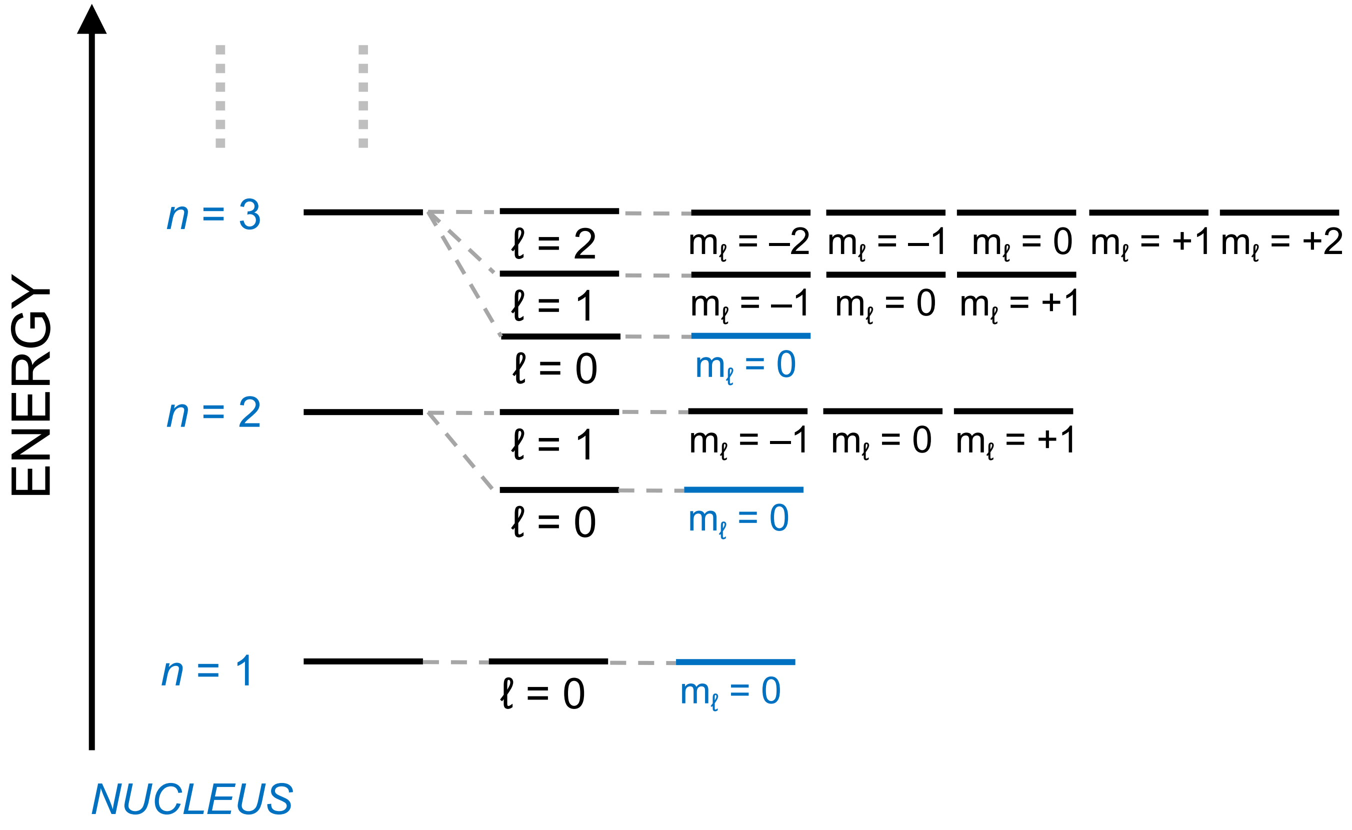

PUTTING IT ALL TOGETHER:

- The principal quantum number (*n*) tells us the relative size and energy of an orbital.
- This is easiest to show with the ℓ = 0 (*s* type) orbitals with different *n* values.

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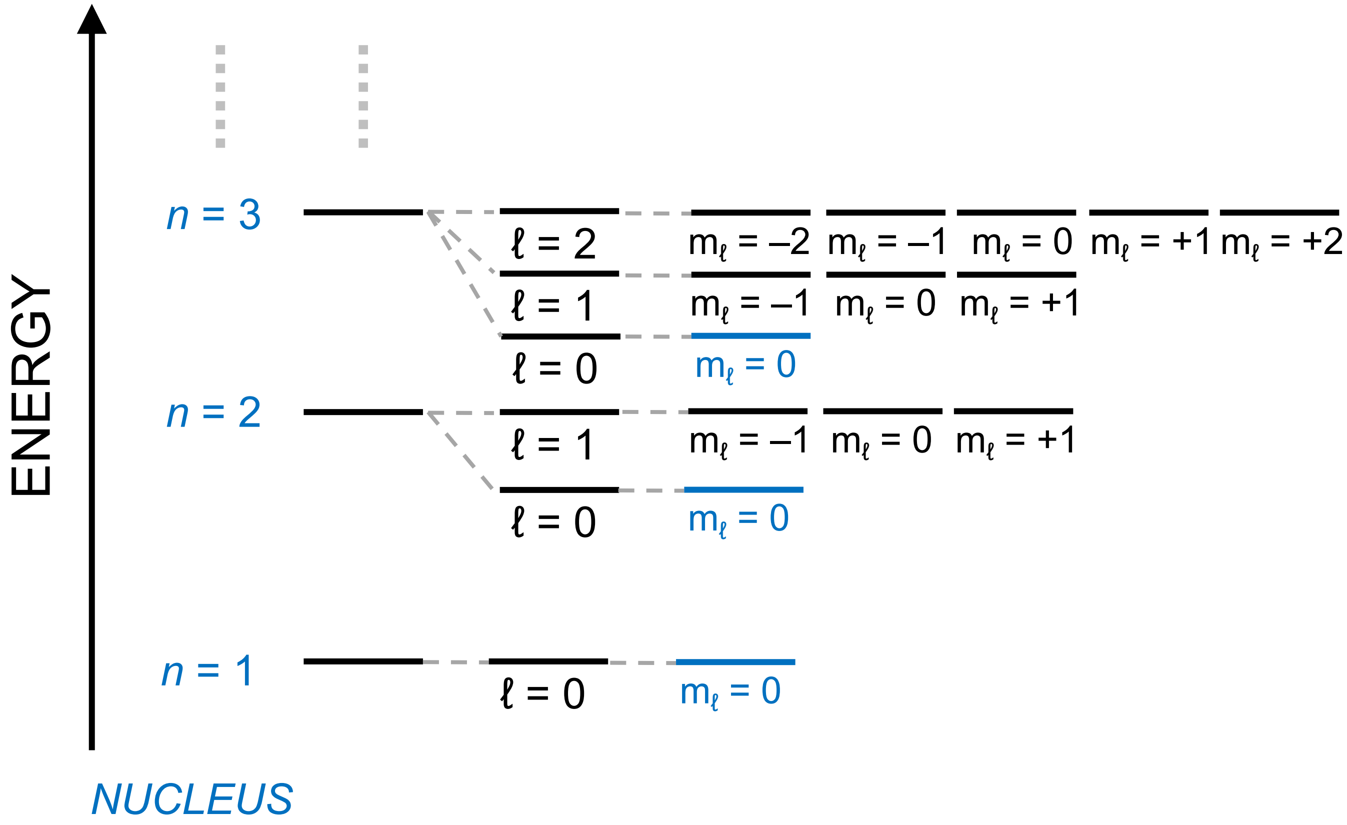
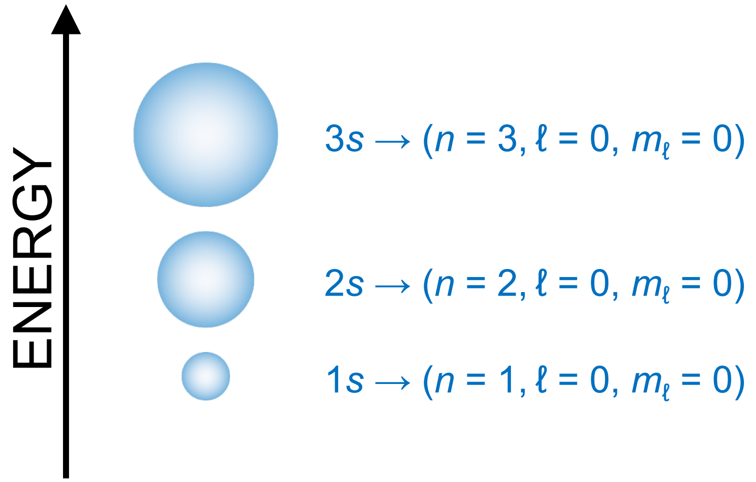


<u>PUTTING IT ALL TOGETHER:</u>

- The principal quantum number (n) tells us the relative size and energy of an orbital.
- This is easiest to show with the ℓ = 0 (s type) orbitals with different n values.
- The farther we get from the nucleus, the larger the orbital shape and the higher the energy:



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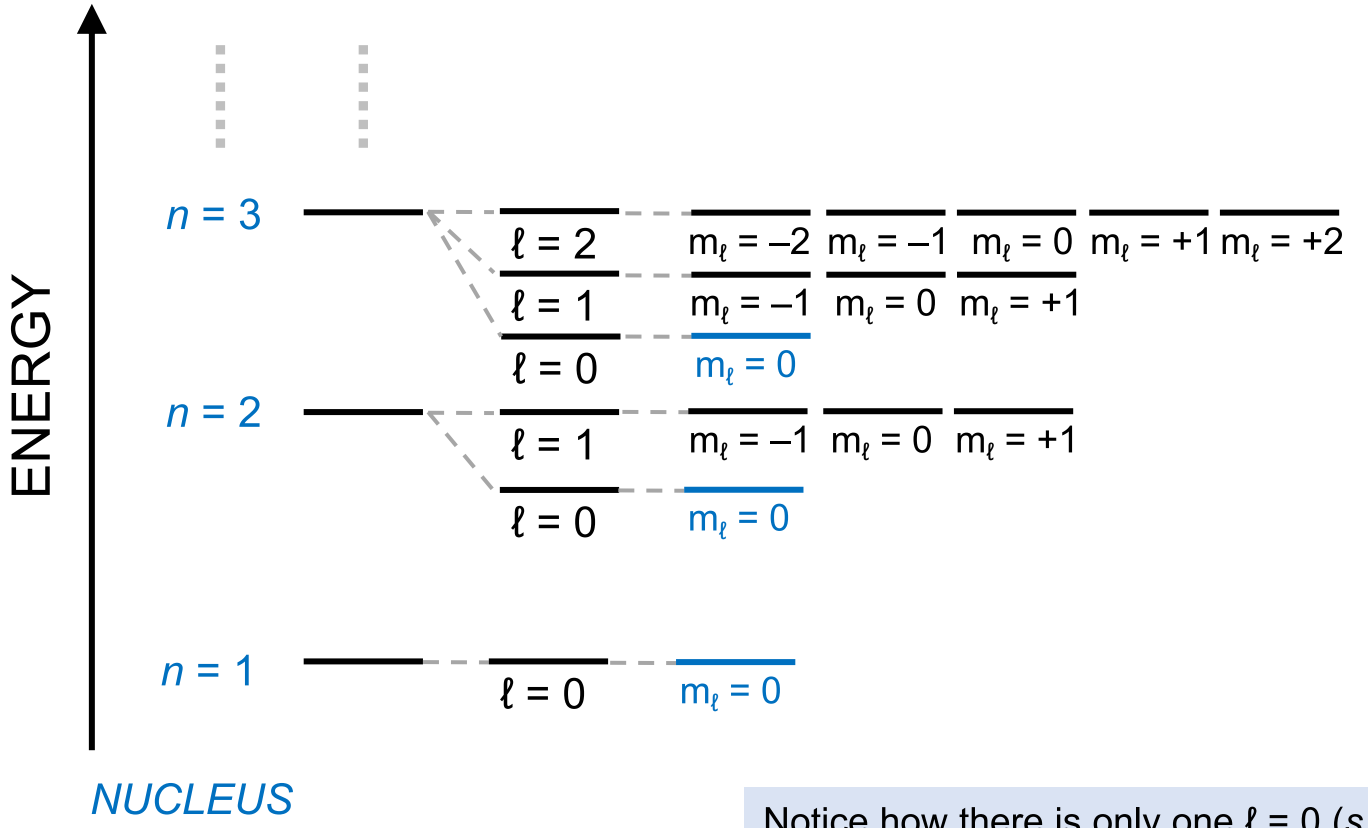

Notice how there is only <u>one</u> ℓ = 0 (s type) orbital per n level because there is only one possible value of $m_\ell = 0$.

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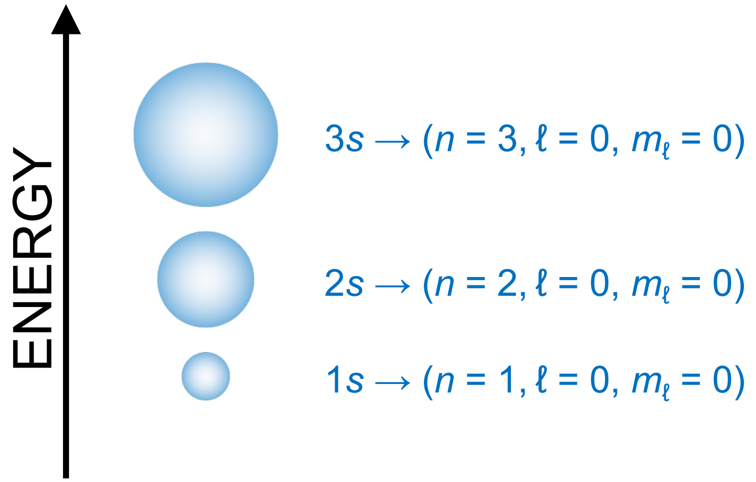

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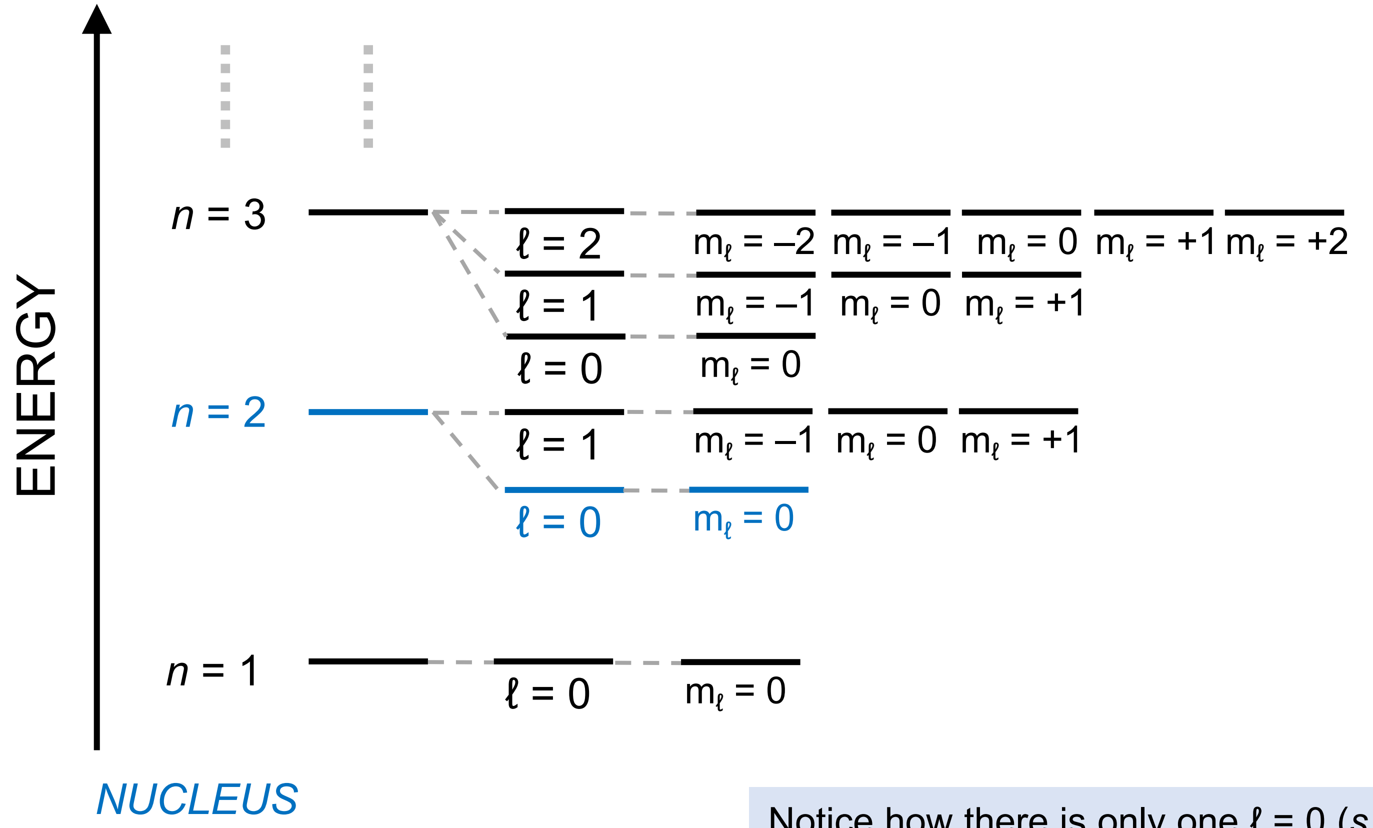
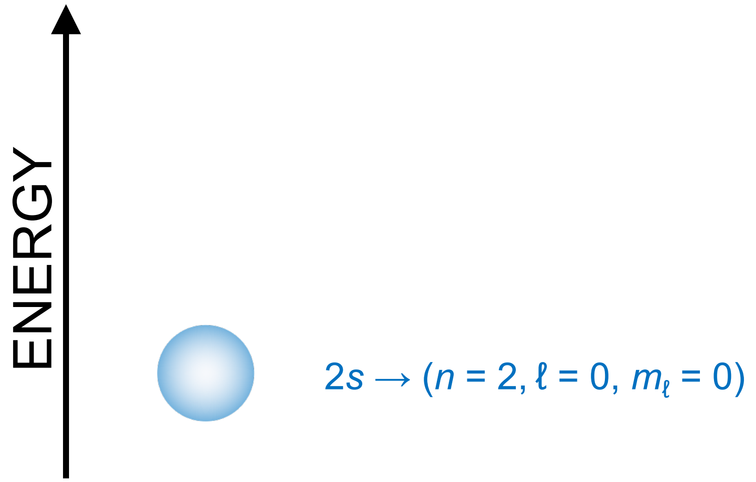


PUTTING IT ALL TOGETHER:

- The angular momentum quantum number (m_ℓ) tells us the shape of the orbital.
- We've already seen what an ℓ = 0 orbital (s type) looks like.

Notice how there is only <u>one</u> ℓ = 0 (s type) orbital per n level because there is only one possible value of $m_\ell = 0$.



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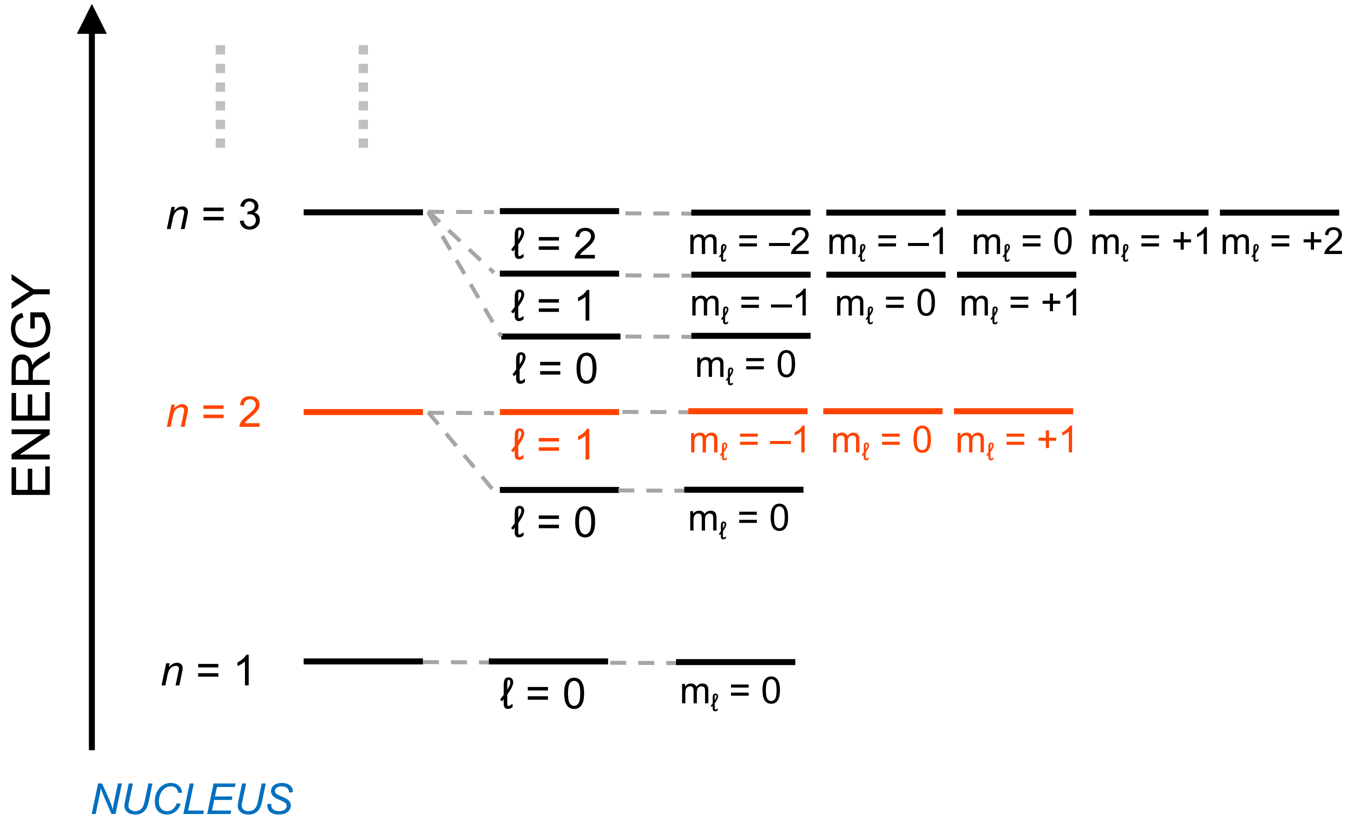

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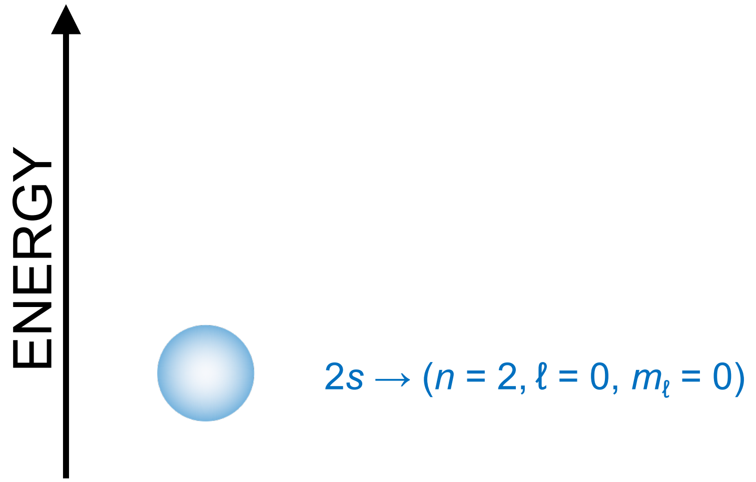
- What about an ℓ = 1 orbital (*p* type)?



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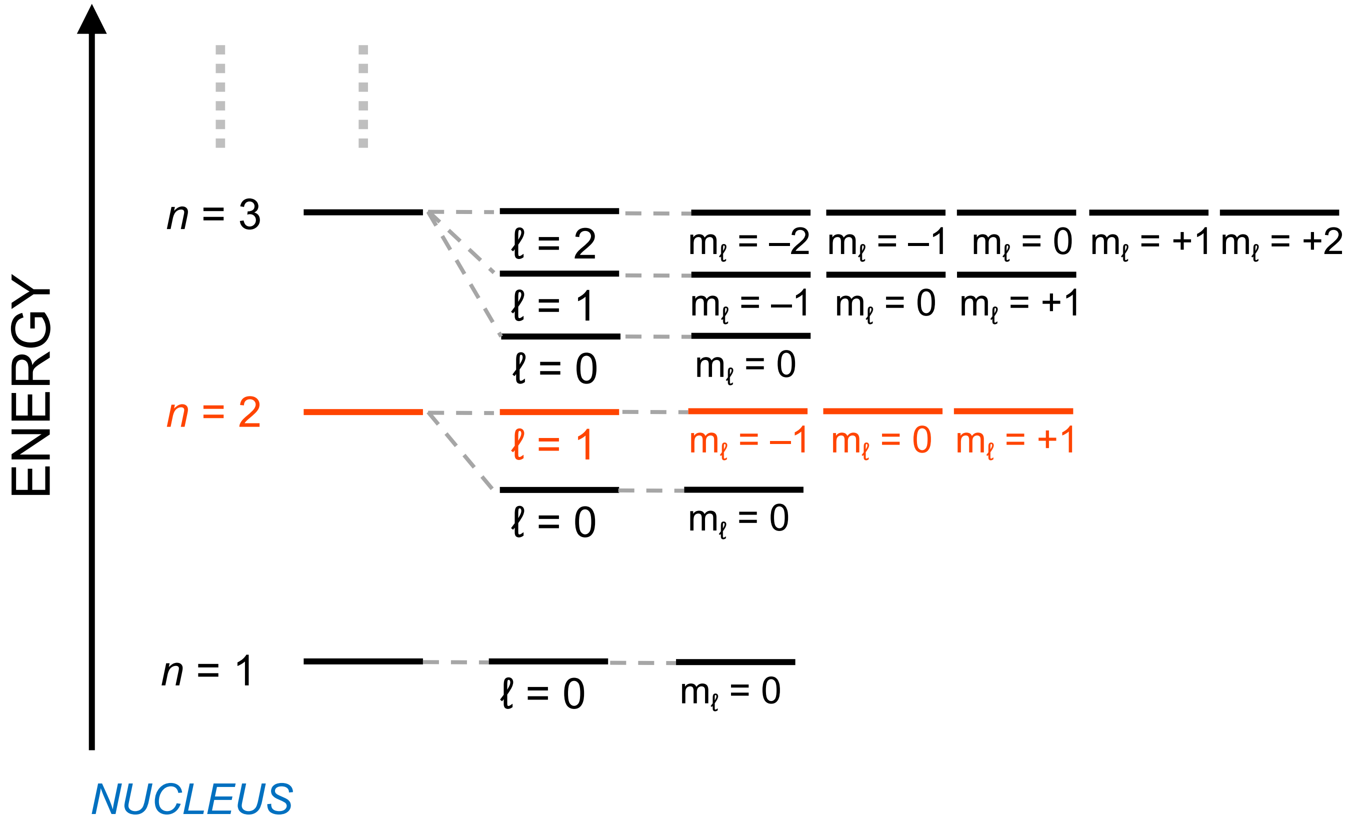

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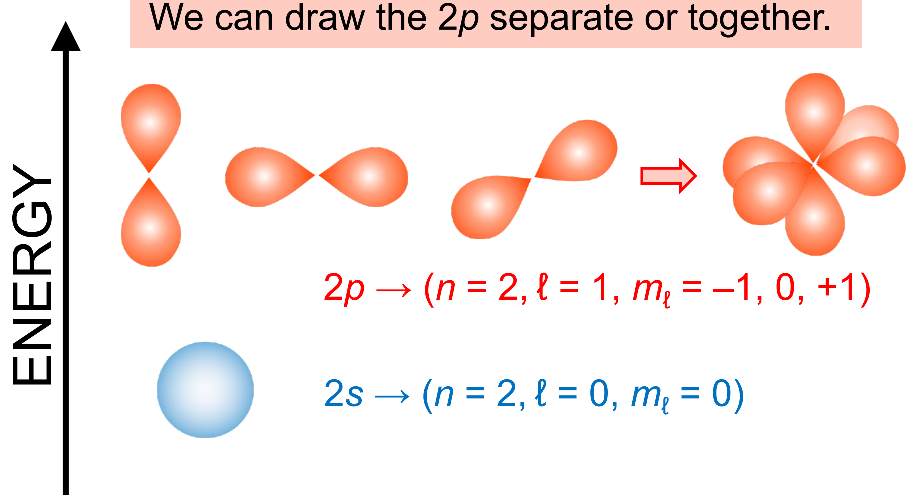
We can draw the 2*p* separate or together.



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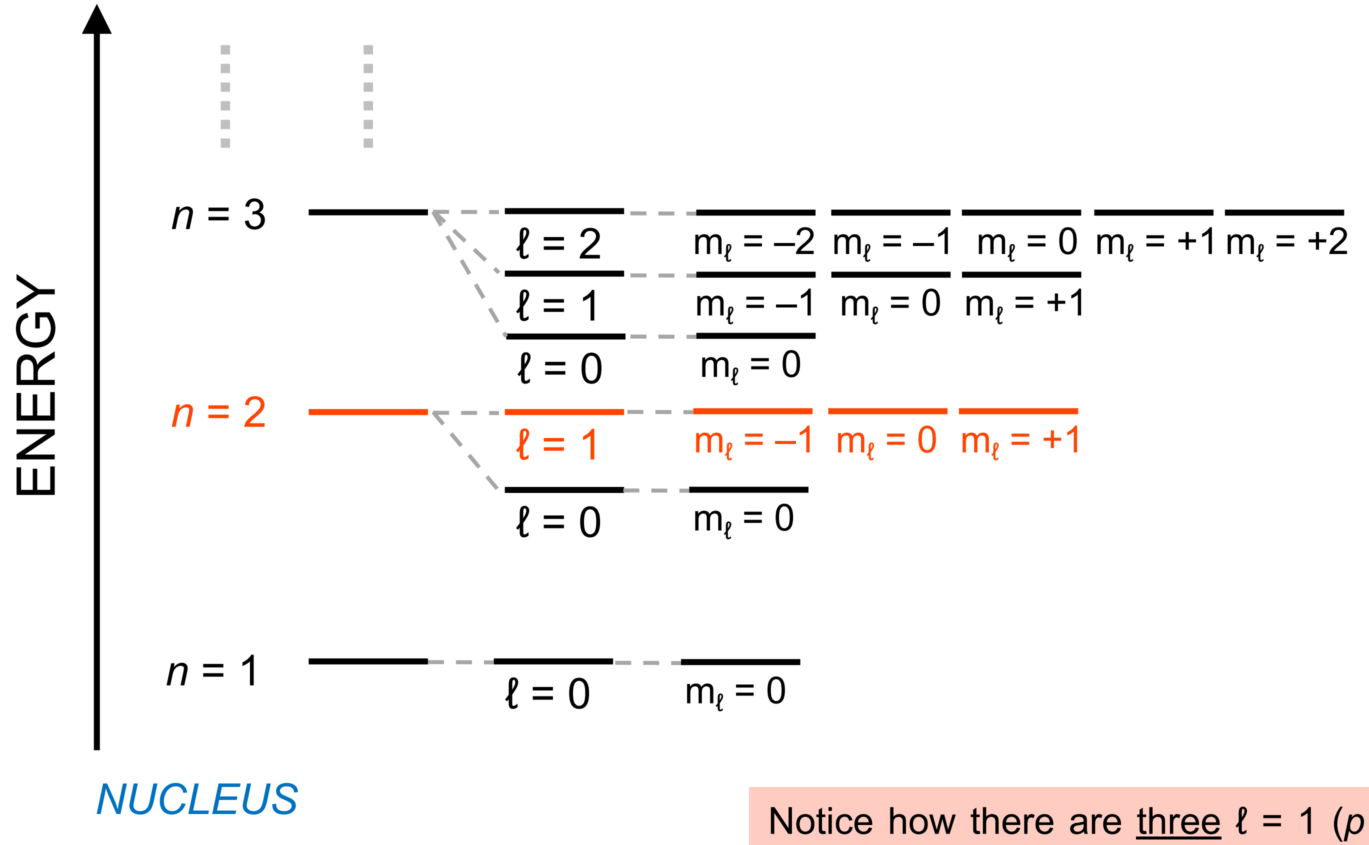

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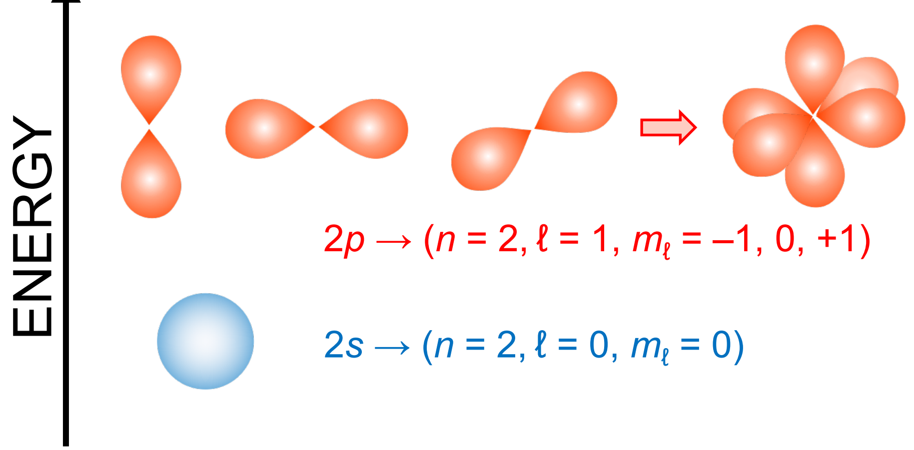
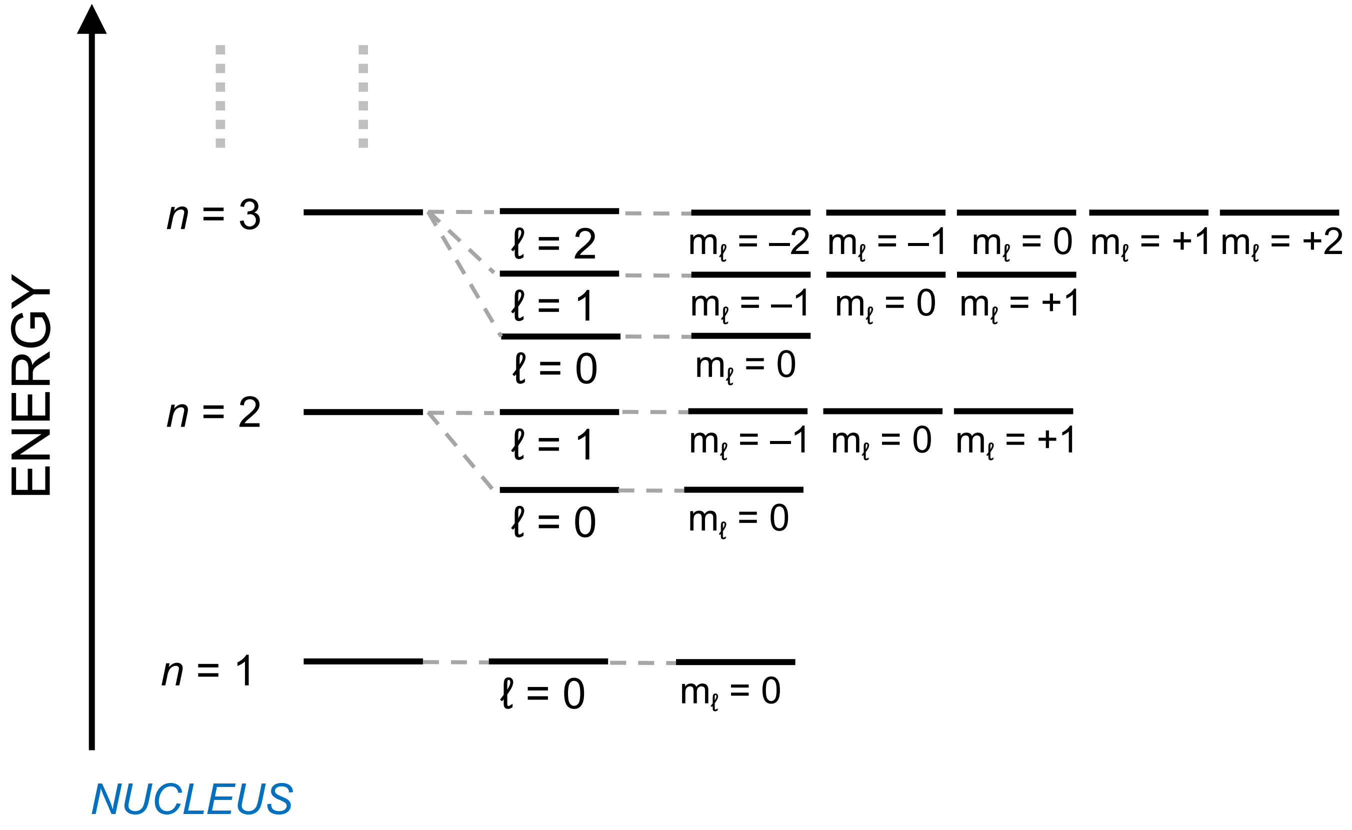


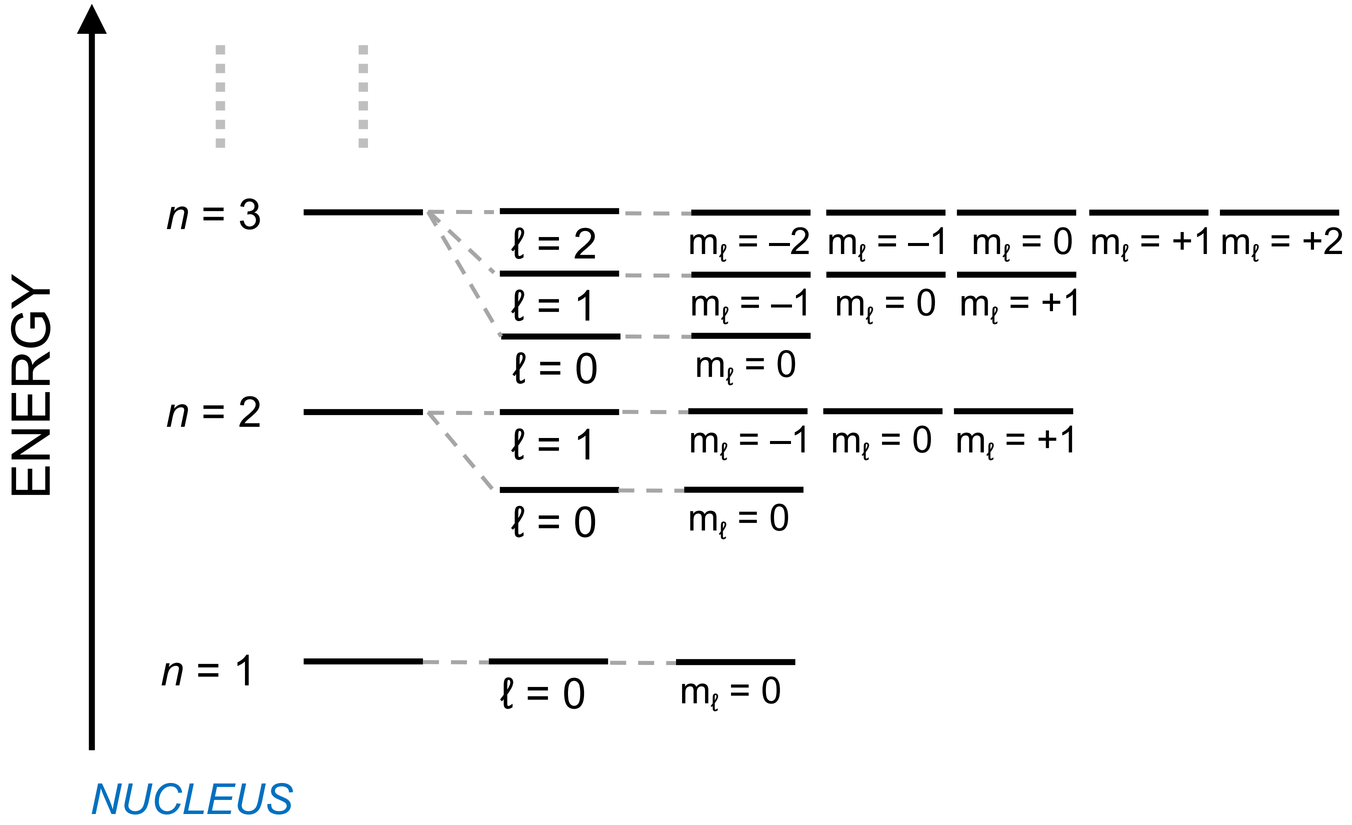
Notice how there are <u>three</u> ℓ = 1 (*p* type) orbitals per *n* level because there are three possible values of m_ℓ = (–1, 0, +1).

m_s: Spin Magnetic Quantum Number



The spin magnetic quantum number (m_s) defines the orientation of the electron.

m_s: Spin Magnetic Quantum Number



The spin magnetic quantum number (m_s) defines the orientation of the electron.

The values of m_s are either –½ or +½.

Value of ℓ	**0**	**1**	**2**
Orbital Type	***s***	***p***	***d***
Values of m_ℓ	**0**	**–1, 0, +1**	**–2, –1, 0, +1, +2**
(# of m_ℓ)	**(1)**	**(3)**	**(5)**
Values of m_s	**–½, +½**	**–½, +½**	**–½, +½**

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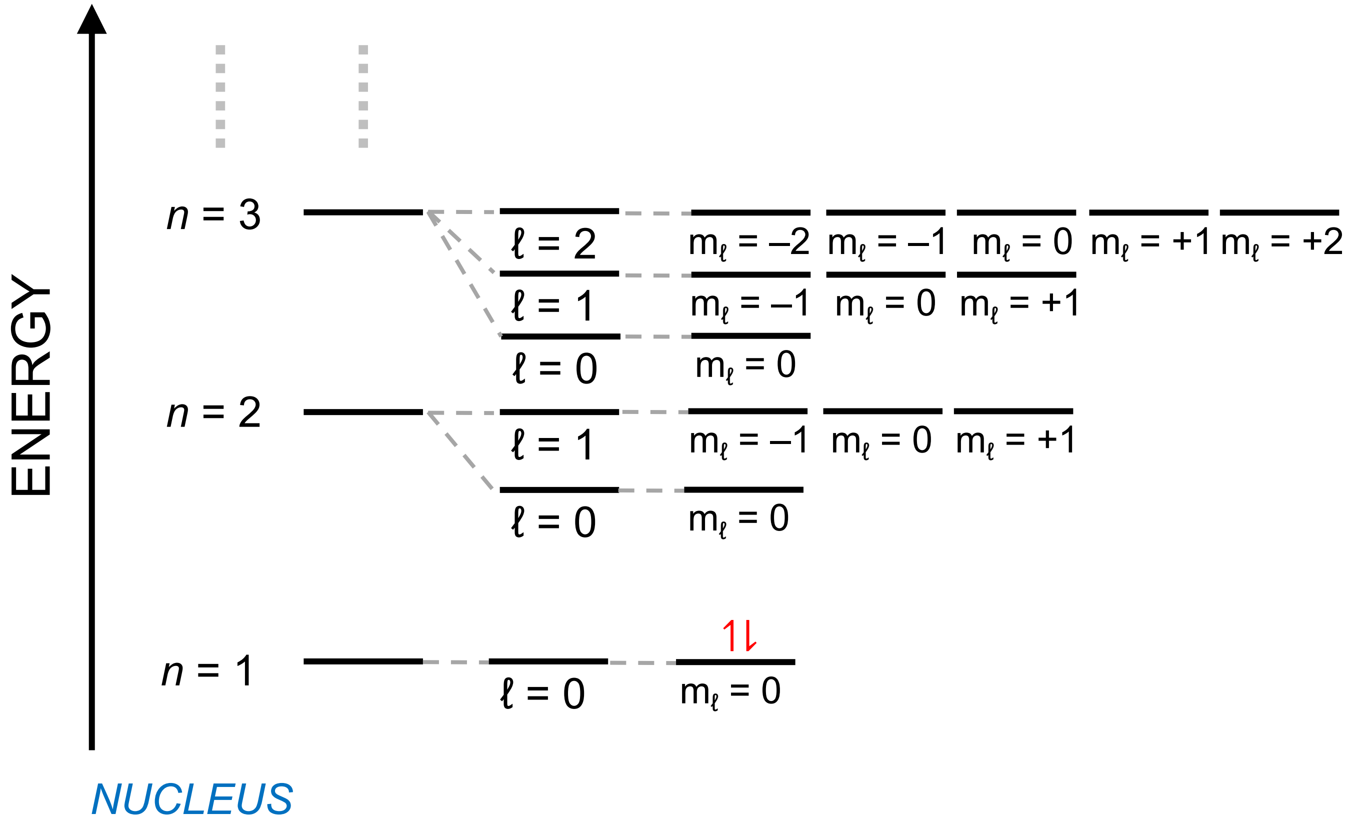


The spin magnetic quantum number (m_s) defines the orientation of the electron.

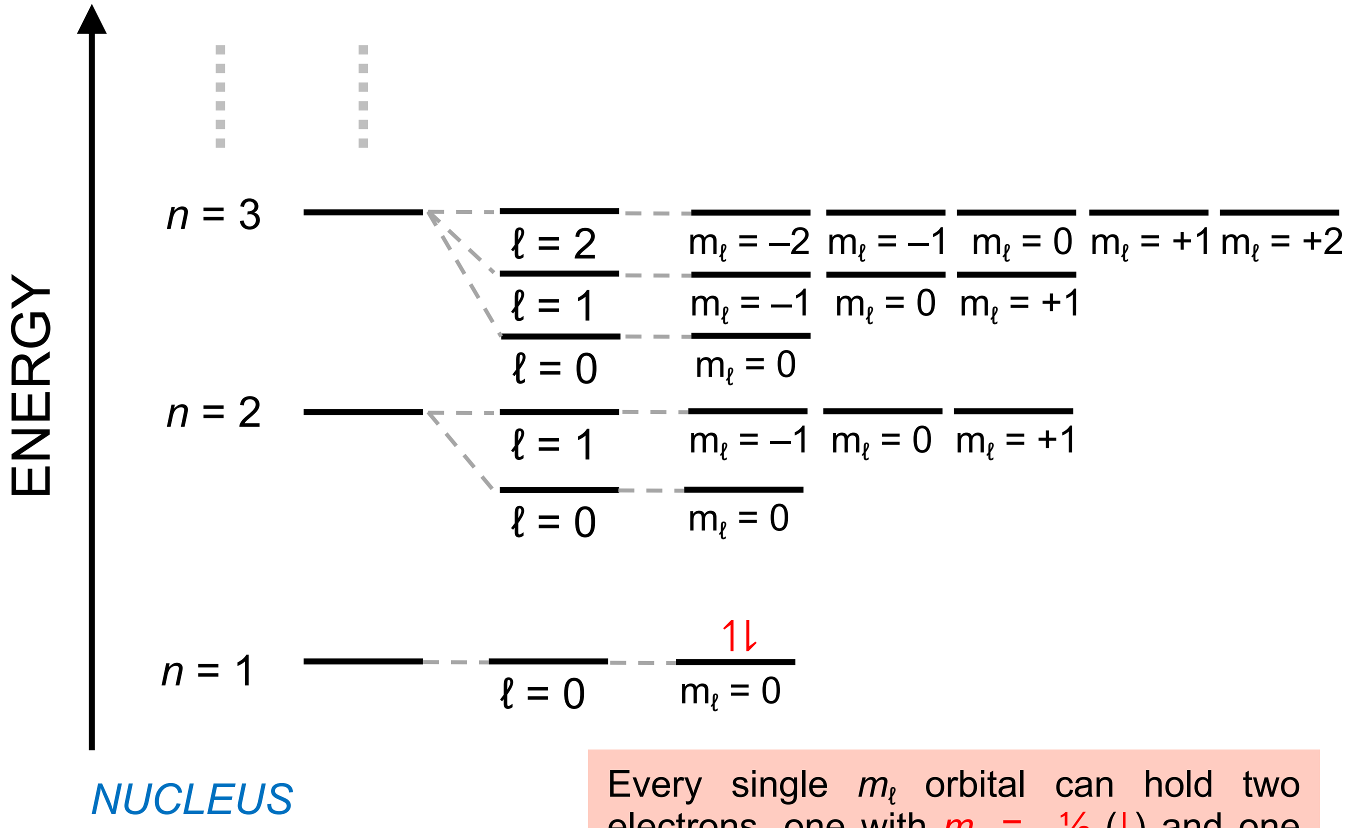
The values of m_s are either –½ or +½.
The value of m_s tells us the "spin" of the electron, which is either "up" or "down".*

↿ ⇂

Value of ℓ	0	1	2
Orbital Type	*s*	*p*	*d*
Values of m_ℓ	0	–1, 0, +1	–2, –1, 0, +1, +2
(# of m_ℓ)	(1)	(3)	(5)
Values of m_s	–½, +½	–½, +½	–½, +½

** Spin doesn't mean the electron is physically spinning in space, so "up" and "down" don't have any physical meaning. We just need to designate two different orientations and "up" and "down" are easiest.*

m_s: Spin Magnetic Quantum Number



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Value of ℓ	0	1	2
Orbital Type	***s***	***p***	***d***
Values of m_ℓ	**0**	**–1, 0, +1**	**–2, –1, 0, +1, +2**
(# of m_ℓ)	**(1)**	**(3)**	**(5)**
Values of m_s	**–½, +½**	**–½, +½**	**–½, +½**

Every single m_ℓ orbital can hold two electrons, one with $m_s = -½$ (⇂) and one with $m_s = +½$ (↿).

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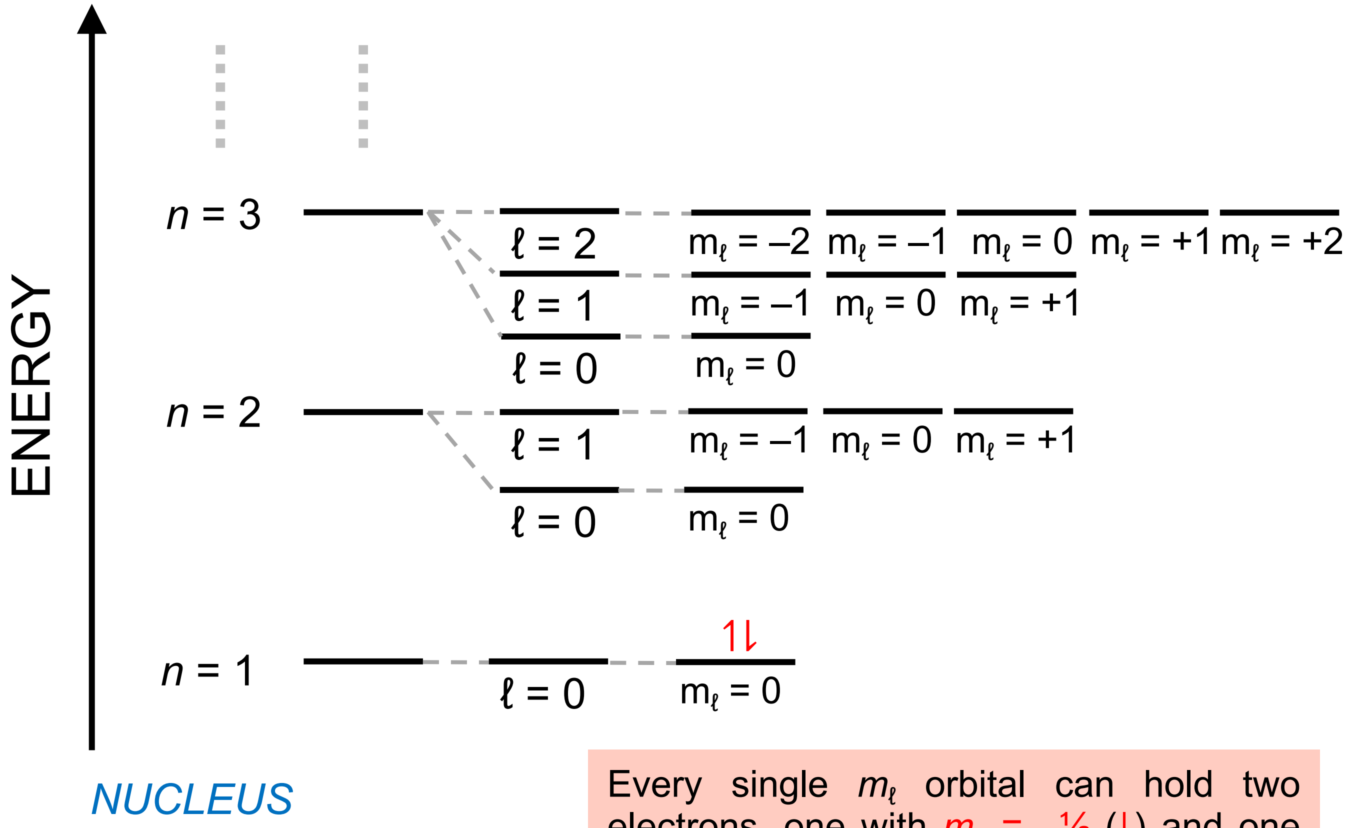

Every single m_ℓ orbital can hold two electrons, one with m_s = –½ (↓) and one with m_s = +½ (↑).

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The values of m_s are either –½ or +½. The value of m_s tells us the "spin" of the electron, which is either "up" or "down".*

↑ ↓

Value of ℓ	0	1	2
Orbital Type	*s*	*p*	*d*
Values of m_ℓ	0	–1, 0, +1	–2, –1, 0, +1, +2
(# of m_ℓ)	(1)	(3)	(5)
Values of m_s	–½, +½	–½, +½	–½, +½
[# of electrons]	[2]	[6]	[10]

** Spin doesn't mean the electron is physically spinning in space, so "up" and "down" don't have any physical meaning. We just need to designate two different orientations and "up" and "down" are easiest.*

What set of orbitals correspond to each of the following sets of quantum numbers? How many electrons can each hold?

n	ℓ	Orbitals	Total number of electrons
2	1		
5	3		
3	2		
4	0		

What set of orbitals correspond to each of the following sets of quantum numbers? How many electrons can each hold?

n	ℓ	Orbitals	Total number of electrons
2	1	2*p*	
5	3	5*f*	
3	2	3*d*	
4	0	4*s*	

What set of orbitals correspond to each of the following sets of quantum numbers? How many electrons can each hold?

n	*ℓ*	Orbitals	Total number of electrons
2	1	2*p*	There are 3 *p*-type orbitals, each with 2 electrons, so 2*p* can hold 6 electrons.
5	3	5*f*	There are 7 *f*-type orbitals, each with 2 electrons, so 5*f* can hold 14 electrons.
3	2	3*d*	There are 3 *d*-type orbitals, each with 2 electrons, so 3*d* can hold 10 electrons.
4	0	4*s*	There is 1 *s*-type orbitals, with 2 electrons, so 4*s* can hold 2 electrons.

Which of the following sets of quantum numbers are allowed?

n	ℓ	m_ℓ	m_s	Allowed or not?
3	2	0	–½	
5	4	4	+½	
3	0	1	+½	
4	4	1	–½	

Which of the following sets of quantum numbers are allowed?

n	ℓ	m_ℓ	m_s	Allowed or not?
3	2	0	–½	For $n = 3$: $\ell = 2 \rightarrow m_\ell = \{-2, -1, 0, +1, +2\}$ $\ell = 1 \rightarrow m_\ell = \{-1, 0, +1\}$ $\ell = 0 \rightarrow m_\ell = 0$
5	4	4	+½	For $n = 5$: $\ell = 4 \rightarrow m_\ell = \{-4, -3, -2, -1, 0, +1, +2, +3, +4\}$ $\ell = 3 \rightarrow m_\ell = \{-3, -2, -1, 0, +1, +2, +3\}$ $\ell = 2 \rightarrow m_\ell = \{-2, -1, 0, +1, +2\}$ $\ell = 1 \rightarrow m_\ell = \{-1, 0, +1\}$ $\ell = 0 \rightarrow m_\ell = 0$
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4	4	1	–½	For $n = 4$: $\ell = 3 \rightarrow m_\ell = \{-3, -2, -1, 0, +1, +2, +3\}$ $\ell = 2 \rightarrow m_\ell = \{-2, -1, 0, +1, +2\}$ $\ell = 1 \rightarrow m_\ell = \{-1, 0, +1\}$ $\ell = 0 \rightarrow m_\ell = 0$

Which of the following sets of quantum numbers are allowed?

n	ℓ	m_ℓ	m_s	Allowed or not?
3	2	0	$-\frac{1}{2}$	For $n = 3$: $\ell = 2 \rightarrow m_\ell = \{-2, -1, 0, +1, +2\}$ $\ell = 1 \rightarrow m_\ell = \{-1, 0, +1\}$ $\ell = 0 \rightarrow m_\ell = 0$ ALLOWED
5	4	4	$+\frac{1}{2}$	For $n = 5$: $\ell = 4 \rightarrow m_\ell = \{-4, -3, -2, -1, 0, +1, +2, +3, +4\}$ $\ell = 3 \rightarrow m_\ell = \{-3, -2, -1, 0, +1, +2, +3\}$ $\ell = 2 \rightarrow m_\ell = \{-2, -1, 0, +1, +2\}$ $\ell = 1 \rightarrow m_\ell = \{-1, 0, +1\}$ $\ell = 0 \rightarrow m_\ell = 0$ ALLOWED
3	0	1	$+\frac{1}{2}$	For $n = 3$: $\ell = 2 \rightarrow m_\ell = \{-2, -1, 0, +1, +2\}$ $\ell = 1 \rightarrow m_\ell = \{-1, 0, +1\}$ $\ell = 0 \rightarrow m_\ell = 0$
4	4	1	$-\frac{1}{2}$	For $n = 4$: $\ell = 3 \rightarrow m_\ell = \{-3, -2, -1, 0, +1, +2, +3\}$ $\ell = 2 \rightarrow m_\ell = \{-2, -1, 0, +1, +2\}$ $\ell = 1 \rightarrow m_\ell = \{-1, 0, +1\}$ $\ell = 0 \rightarrow m_\ell = 0$

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5	4	4	+½	For $n = 5$: $\ell = 4 \rightarrow m_\ell = \{-4, -3, -2, -1, 0, +1, +2, +3, +4\}$ $\ell = 3 \rightarrow m_\ell = \{-3, -2, -1, 0, +1, +2, +3\}$ $\ell = 2 \rightarrow m_\ell = \{-2, -1, 0, +1, +2\}$ $\ell = 1 \rightarrow m_\ell = \{-1, 0, +1\}$ $\ell = 0 \rightarrow m_\ell = 0$ ALLOWED
3	0	1	+½	For $n = 3$: $\ell = 2 \rightarrow m_\ell = \{-2, -1, 0, +1, +2\}$ $\ell = 1 \rightarrow m_\ell = \{-1, 0, +1\}$ $\ell = 0 \rightarrow m_\ell = 0$ NOT ALLOWED because $m_\ell \neq 1$ for $n = 3$ and $\ell = 0$.
4	4	1	–½	For $n = 4$: $\ell = 3 \rightarrow m_\ell = \{-3, -2, -1, 0, +1, +2, +3\}$ $\ell = 2 \rightarrow m_\ell = \{-2, -1, 0, +1, +2\}$ $\ell = 1 \rightarrow m_\ell = \{-1, 0, +1\}$ $\ell = 0 \rightarrow m_\ell = 0$ NOT ALLOWED because $\ell \neq 4$ for $n = 4$.