## 4 Quantum Numbers

$n$ ~ PRINCIPAL ~ 1, 2, 3, ...

$\ell$ ~ ANGULAR MOMENTUM ~ 0, 1, ..., n-1

$m_\ell$ ~ MAGNETIC ~ $-\ell, \ldots, +\ell$

$m_s$ ~ SPIN ~ $-\frac{1}{2}, +\frac{1}{2}$

$n$ ~ SHELL

$n, \ell$ ~ SUBSHELL

$n, \ell, m_\ell$ ~ ORBITAL

Q. How many e⁻s can occupy a particular subshell?

- PAULI exclusion PRINCIPLE.
  - each e⁻ has its own unique set of 4 QN's.

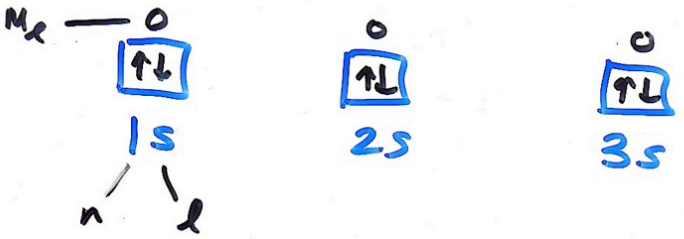
ex: any s-subshell (1s, 2s, 3s, ...)

$\ell = 0$

$\Rightarrow m_\ell = -\ell, \ldots, +\ell = 0$

$n, \ell = 0, m_\ell = 0, \Rightarrow m_s = \pm\frac{1}{2}$

ex: 1s subshell
2s "
3s "
} only hold (2e⁻s.)

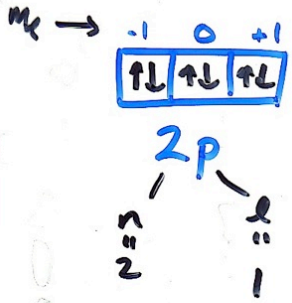


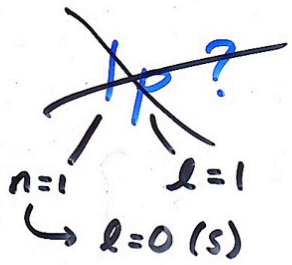
ex: any p-subshell. (2p, 3p, 4p, ...)

$\ell = 1$

$m_\ell = -\ell, \ldots, +\ell$

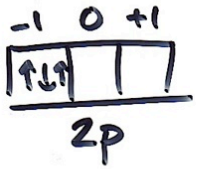
$= -1, 0, +1$




$\Rightarrow m_s = \pm\frac{1}{2}$

$\Rightarrow$ 6 e⁻s in each p-subshell.



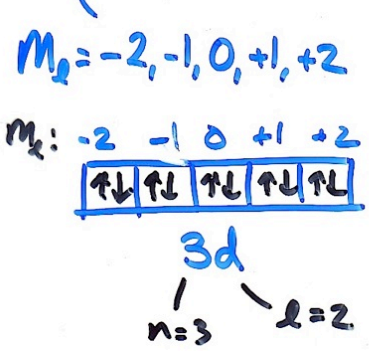

| | n | ℓ | $m_\ell$ | $m_s$ |
|---|---|---|---|---|
| $e^-(1)$ | 2 | 1 | −1 | $+\frac{1}{2}$ |
| $e^-(2)$ | 2 | 1 | −1 | $-\frac{1}{2}$ |
| ~~$e^-(3)$~~ | ~~2~~ | ~~1~~ | ~~−1~~ | ~~$+\frac{1}{2}$~~ |

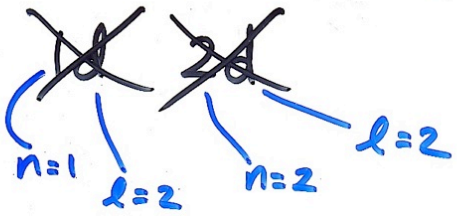
not allowed (PAULI)

d-subshells (3d, 4d, 5d, ...)

$\ell = 2$

$m_\ell = -2, -1, 0, +1, +2$




$\ell = 0, \ldots, n-1$

$\Rightarrow$ 10 e⁻s max

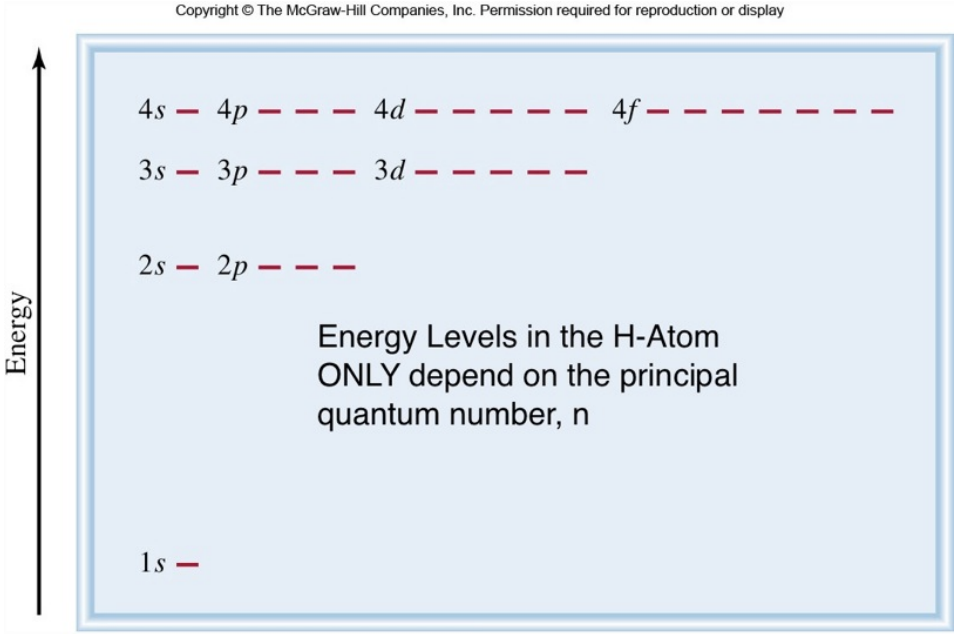
| subshell | s | p | d | f |
|---|---|---|---|---|
| max # e⁻s | 2 | 6 | 10 | 14 |

**Table 7.2 Relation Between Quantum Numbers and Atomic Orbitals**

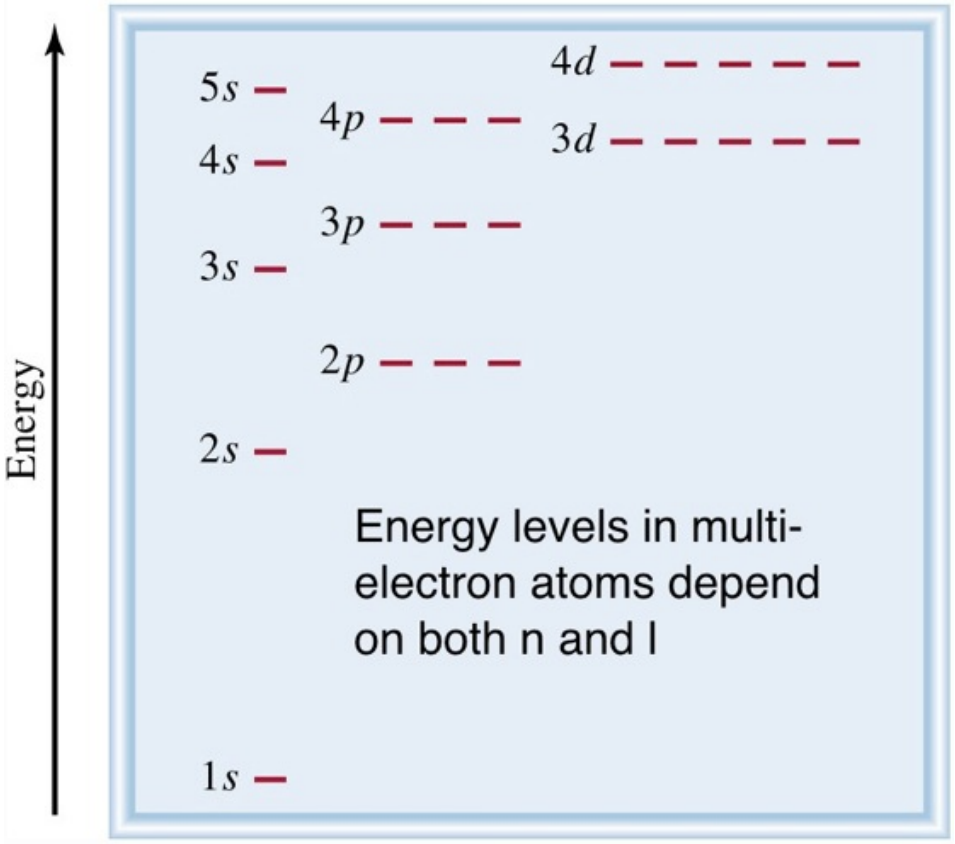
| $n$ | $\ell$ | $m_\ell$ | Number of Orbitals | Atomic Orbital Designations |
|---|---|---|---|---|
| 1 | 0 | 0 | 1 | $1s$ |
| 2 | 0 | 0 | 1 | $2s$ |
| | 1 | −1, 0, 1 | 3 | $2p_x$, $2p_y$, $2p_z$ |
| 3 | 0 | 0 | 1 | $3s$ |
| | 1 | −1, 0, 1 | 3 | $3p_x$, $3p_y$, $3p_z$ |
| | 2 | −2, −1, 0, 1, 2 | 5 | $3d_{xy}$, $3d_{yz}$, $3d_{xz}$, $3d_{x^2-y^2}$, $3d_{z^2}$ |
| ⋮ | ⋮ | ⋮ | ⋮ | ⋮ |

# Electron Configurations / Orbital Diagrams

- tell us how e⁻s are arranged in the atom.
- Place e⁻s in Lower energy orbitals before higher energy orbitals.
- Building-up principle.
  - AUF BAU principle





**Hydrogen** $Z=1$ $1p^+, 1e^-$ (atom)

$1e^-$ occupies $1s$ orbital

$e^-$ configuration: $1s^1$

orbital diagram 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**Helium** $Z=2$, $2p^+$, $2e^-$

$2e^-$s occupy $1s$ orbital

$e^-$ conf: $1s^2$

orbital diag: 


**Lithium** $Z=3$, $3e^-$

$2e^-$s occupy $1s$ orbital

$1e^-$ " $2s$ "

$e^-$ conf: $1s^2 2s^1$

orb. diag. 


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**Be** $Z=4$

$4e^-$s: $2e^- \rightsquigarrow 1s$

$2e^- \rightsquigarrow 2s$

$1s^2 2s^2$ 


$e^-$ config orb. diag.

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**B** $Z=5$

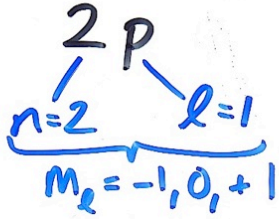
$5e^-$s: $2e^- \longrightarrow 1s$

$2e^- \longrightarrow 2s$

$1e^- \longrightarrow 2p$

$1s^2 2s^2 2p^1$ 


$e^-$ config orbital diagram



C, Z=6  6e⁻

$1s^2 2s^2 2p^2$

e⁻ config

(A) 1s 2s 2p ✗

(B) 1s 2s 2p ✓

(C) 1s 2s 2p ✗

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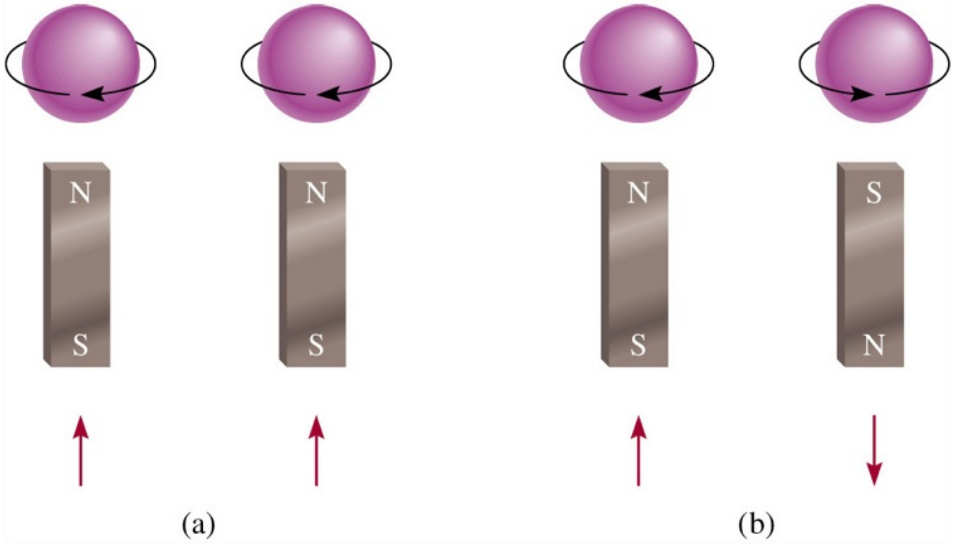
2 types of materials

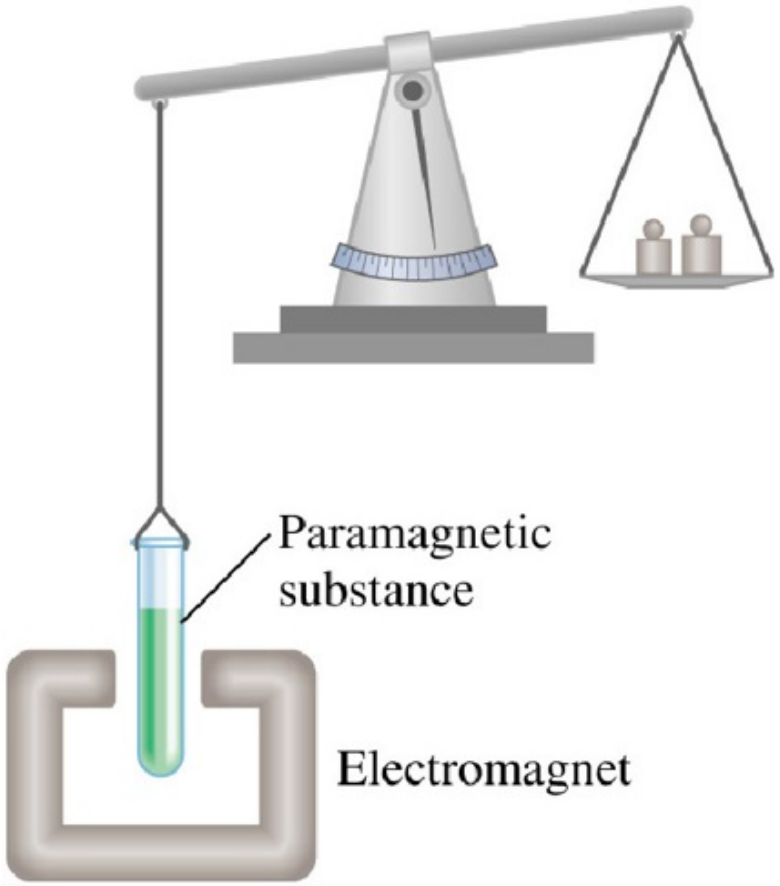
**Paramagnetic**
- attracted into magnetic fields
- caused by unpaired e's
- ↑ ↑

**Diamagnetic**
- repelled away from magnetic fields
- caused by paired e's
- ↑↓

Carbon atoms (in flames) are attracted into a magnetic field ⇒ PARAMAGNETIC!








## Hund's Rule

e⁻s prefer to be unpaired in the same subshell, before pairing up.

ex: Nitrogen, Z=7

$1s^2 2s^2 2p^3$ e⁻ config


orbital diagram

⇒ N atoms are PARAMAGNETIC

ex: O, Z=8

$1s^2 2s^2 2p^4$


ex: F, Z=9

$1s^2 2s^2 2p^5$


ex: Ne, Z=10

$1s^2 2s^2 2p^6$


DIAMAG.

Na  Z = 11

$1s^2 2s^2 2p^6 3s^1$ = [Ne] $3s^1$

$1s^2 2s^2 2p^6$: arranged just like Neon (noble gas) → stable → 'all' subshells are FULL

[Ne]: Noble Gas Core!