# Appendix 2

## Quantum Numbers
## (量子数)

# Appendix 2: Quantum Numbers (量子数)

## ➢ Quantum Numbers (量子数)

- ❖ In general, quantum numbers describe values of **conserved quantities** in the dynamics of a quantum system. (广义定义)
- ❖ In particular, quantum numbers can be defined as a set of numerical values that fully specify **the quantum states of electrons in atoms**. (狭义定义)
- ❖ In an atom, the electronic states can be fully determined by **4 quantum numbers**:

  1) the **principal quantum number** $n$; 2) the **azimuthal quantum number** $l$,

  3) the **magnetic quantum number** $m$; 4) the **spin quantum number** $m_s$.

- ❖ The 4 quantum numbers correspond to **a CSCO of the system**, i.e., $\hat{H}$, $\hat{L}^2$, $\hat{L}_z$, and $\hat{s}_z$.

# Appendix 2: Quantum Number (量子数)

## ➢ Principal Quantum Number (主量子数)

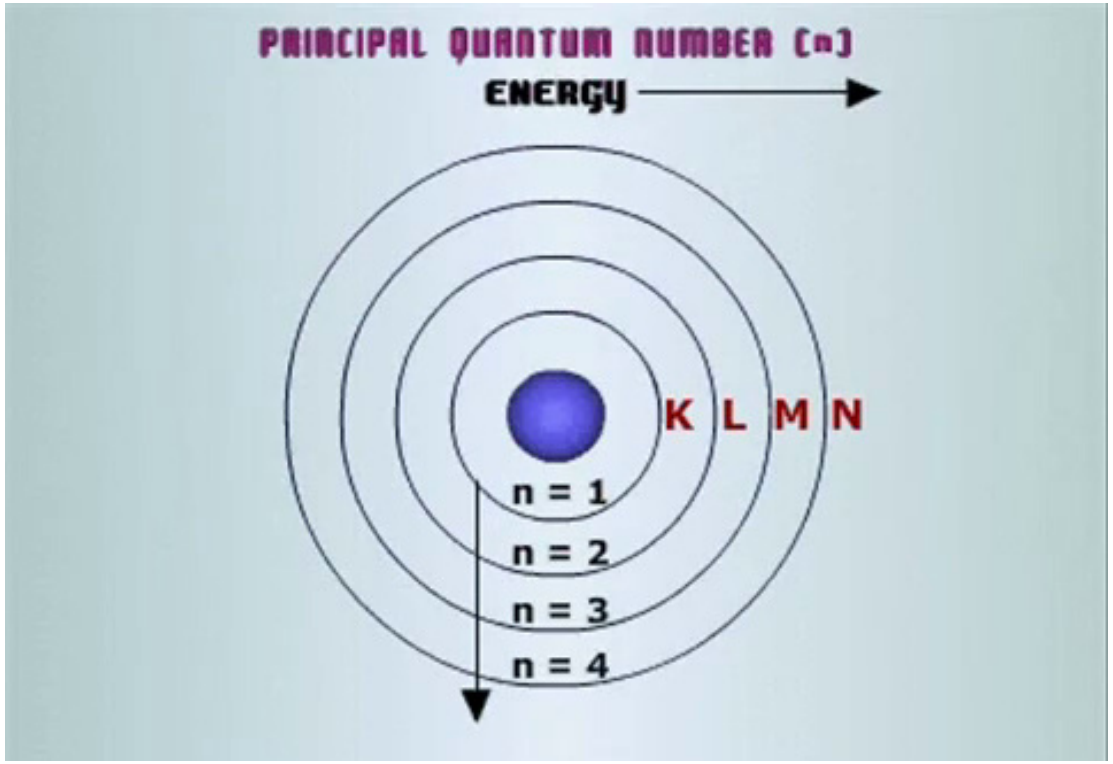
❖ The principal quantum number ($n$) corresponds to the eigenvalues **of total energy** ($\hat{H}$) by considering only the radial coordinates.

In the case of hydrogen atom:

$$E_n = \frac{E_1}{n^2} = \frac{-13.6\ \text{eV}}{n^2}$$

$$n = 1, 2, 3, \cdots$$

$\mathbf{K}, \mathbf{L}, \mathbf{M}, \cdots$ are used to specify the electron shell.



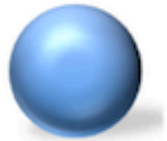
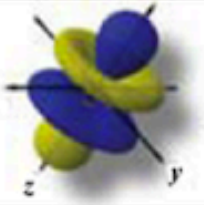
# Appendix 2: Quantum Number (量子数)

## ➢ Azimuthal Quantum Number (角量子数)

❖ The azimuthal (angular) quantum number ($\boldsymbol{l}$) corresponds to the eigenvalues of **angular momentum** ($\widehat{\boldsymbol{L}}^{\boldsymbol{2}}$)

$$\widehat{\boldsymbol{L}}^{\boldsymbol{2}}\boldsymbol{\psi} = \hbar^{\boldsymbol{2}}\boldsymbol{l}(\boldsymbol{l}+\boldsymbol{1})\boldsymbol{\psi},$$

$$\boldsymbol{l} = \boldsymbol{0}, \boldsymbol{1}, \boldsymbol{2}, \cdots \boldsymbol{n}-\boldsymbol{1} \quad (\boldsymbol{n} \text{ total})$$

| Angular Momentum Quantum Number, $\ell$ | Name of Subshell | Shape | |
|---|---|---|---|
| 0 | s | Sphere |  |
| 1 | p | Dumbbell |  |
| 2 | d | Complex/double dumbbell |  |
| 3 | f | More complex/ multiple lobes |  |

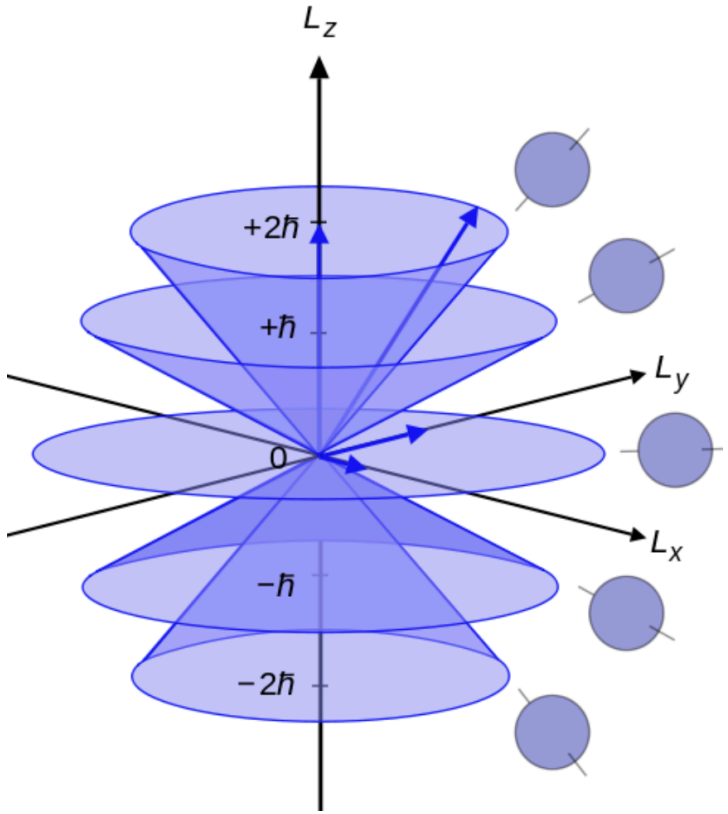
# Appendix 2: Quantum Number (量子数)

## ➢ Magnetic Quantum Number (磁量子数)

❖ The magnetic quantum number ($\boldsymbol{m}$) corresponds to the eigenvalues of the **angular momentum in the $z$ direction** ($\widehat{\boldsymbol{L}}_{\boldsymbol{z}}$)

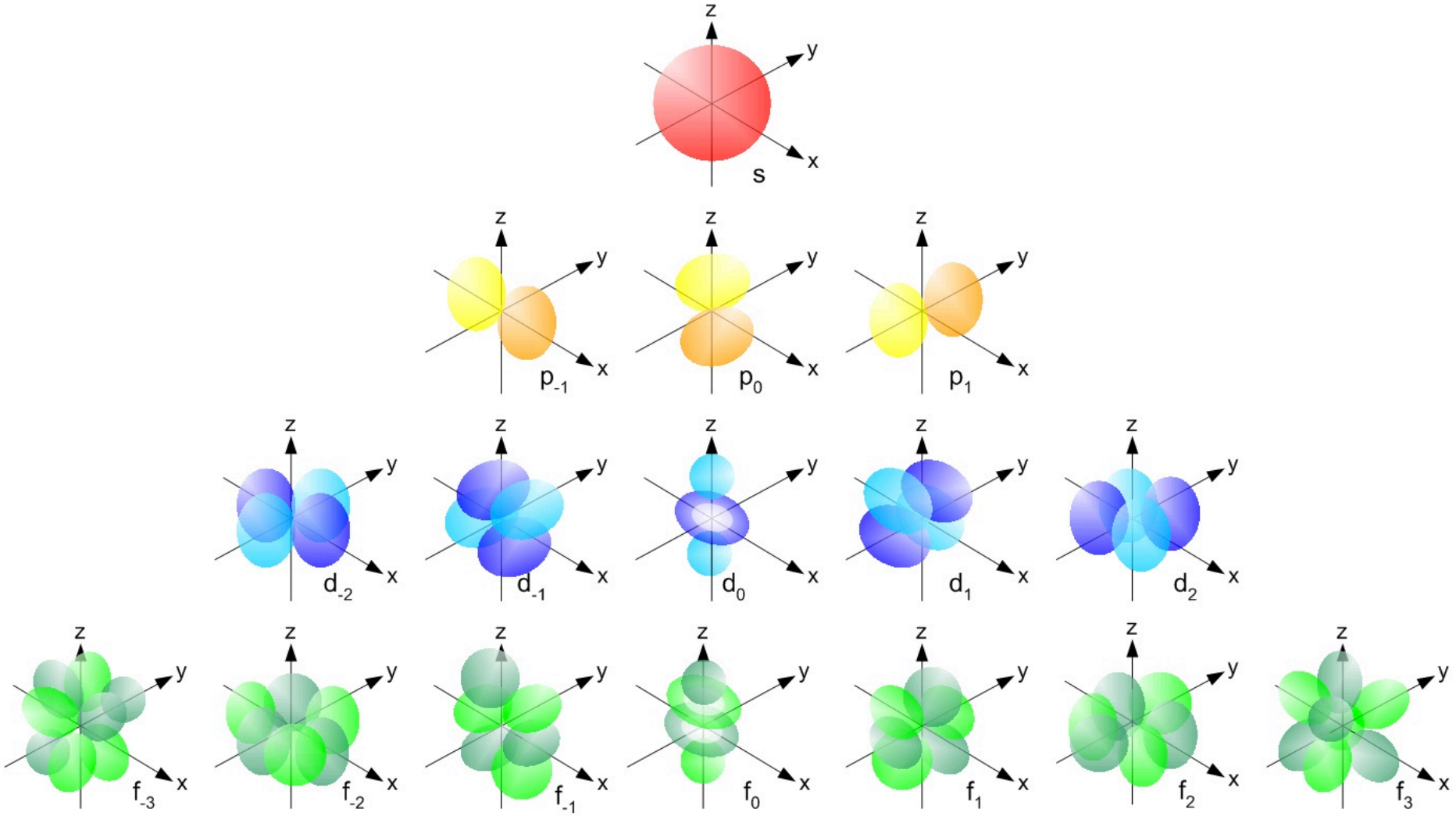
$$\widehat{\boldsymbol{L}}_{\boldsymbol{z}}\boldsymbol{\psi} = \boldsymbol{m}\hbar\boldsymbol{\psi}$$

$$\boldsymbol{m} = -\boldsymbol{l}, \cdots, \boldsymbol{0}, \cdots, \boldsymbol{l} \quad (2\boldsymbol{l} + \boldsymbol{1} \text{ total})$$



# Appendix 2: Quantum Number (量子数)

- **Magnetic Quantum Number (磁量子数)**

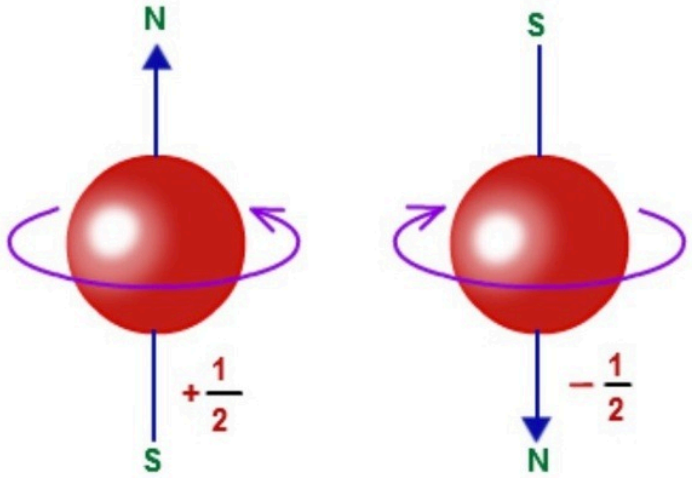


# Appendix 2: Quantum Number (量子数)

## ➢ Spin Quantum Number (自旋量子数)

❖ The spin quantum number ($\boldsymbol{m_s}$) corresponds to the eigenvalues of the **spin momentum in the $z$ direction** ($\hat{s}_z$)

$$\hat{s}_z\psi = m_s\hbar\psi, \qquad m_s = -s, \cdots, s \ \ (2s+1 \text{ total})$$



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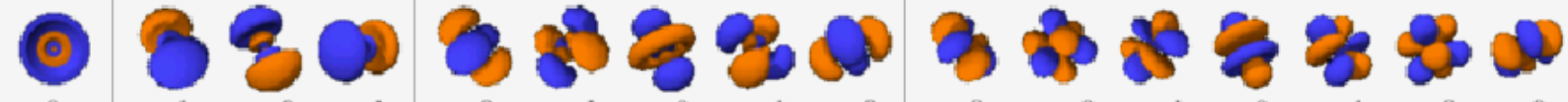
## ➢ Atomic Orbitals (原子轨道)

| | *s* (l=0) | *p* (l=1) | *d* (l=2) | *f* (l=3) |
|---|---|---|---|---|
| n=1 |  m=0 | | | |
| n=2 |  m=0 m=−1 m=0 m=1 | | | |
| n=3 |  m=0 m=−1 m=0 m=1 m=−2 m=−1 m=0 m=1 m=2 | | | |
| n=4 |  m=0 m=−1 m=0 m=1 m=−2 m=−1 m=0 m=1 m=2 m=−3 m=−2 m=−1 m=0 m=1 m=2 m=3 | | | |
| n=5 |  m=0 m=−1 m=0 m=1 m=−2 m=−1 m=0 m=1 m=2 | | | |
| n=6 |  m=0 m=−1 m=0 m=1 | | | |
| n=7 |  m=0 | | | |

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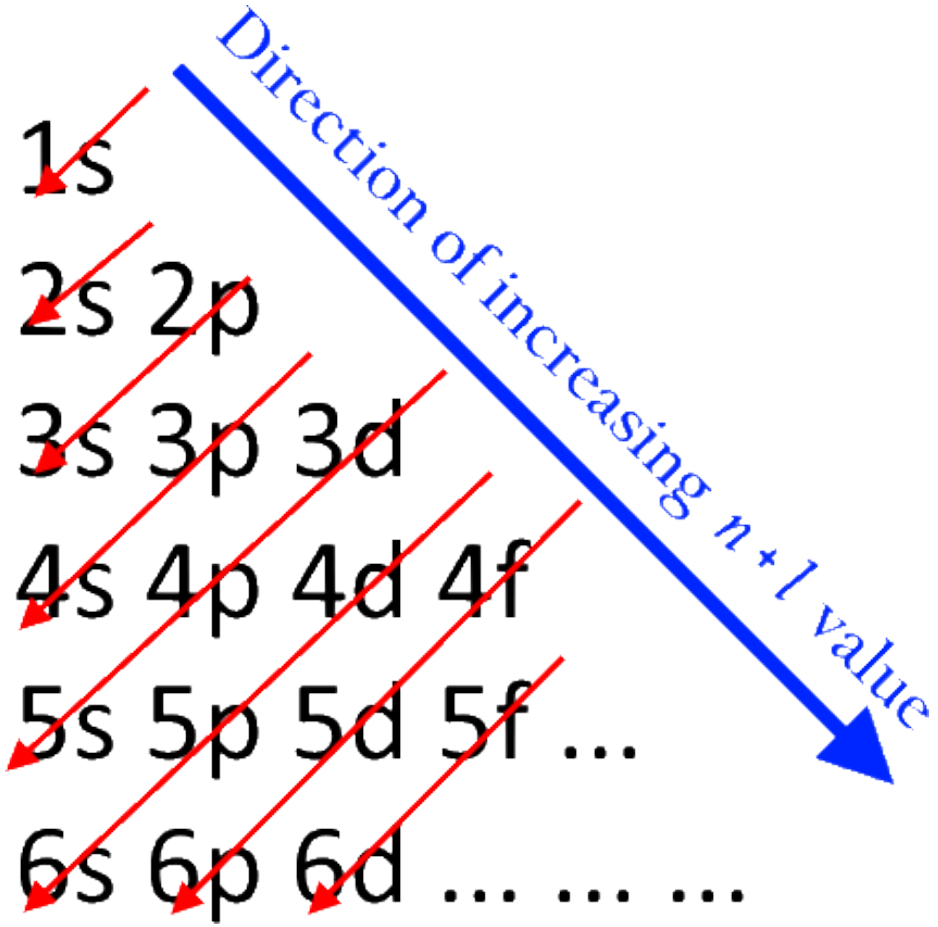
- **Electron Configuration (电子排布)**




**Aufbau Principle**