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)

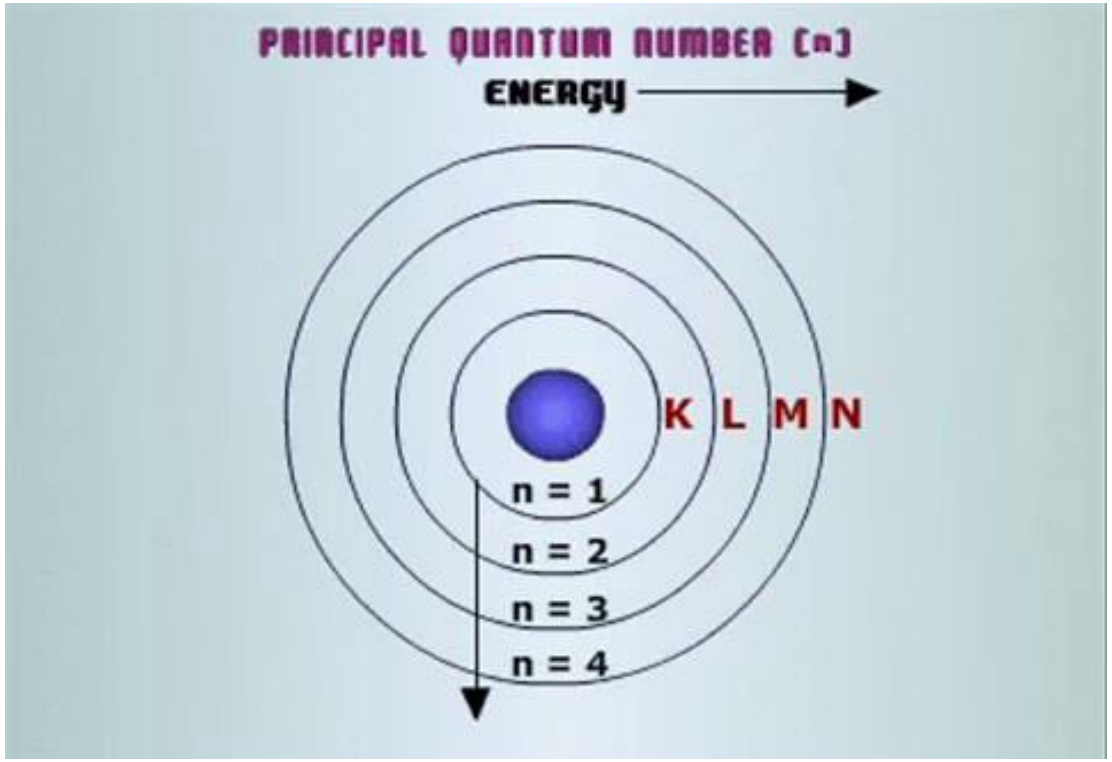
❖ The principal quantum number (n) corresponds to the eigenvalues **of total energy** ($\hat{H}$) by considering only the radial coordinates.

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.



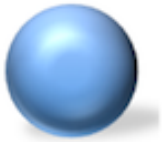
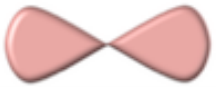
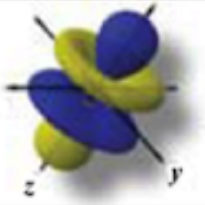
Appendix 2: Quantum Number (量子数)

➢ Azimuthal Quantum Number (角量子数)

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

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

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

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

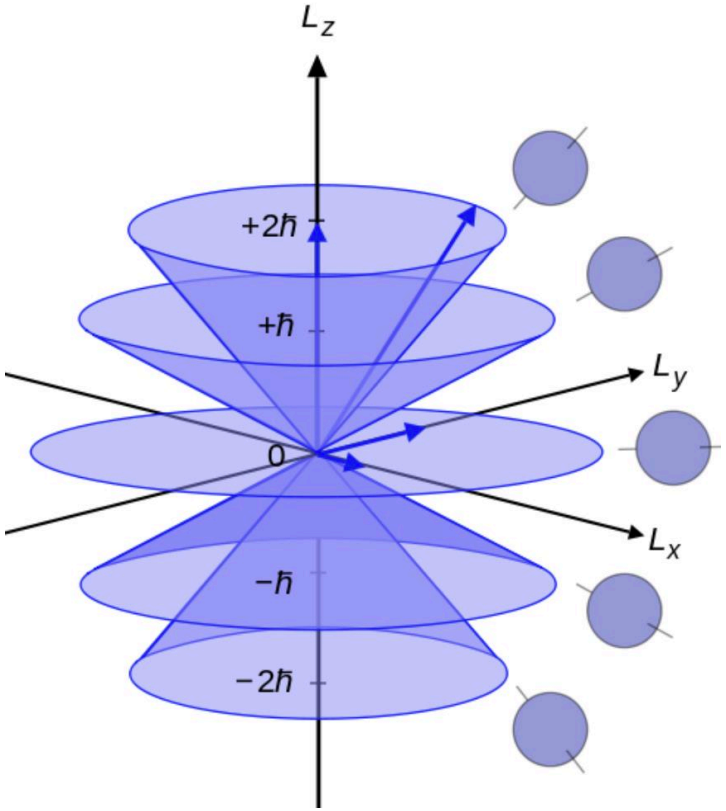
Appendix 2: Quantum Number (量子数)

➢ 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** ($\widehat{\boldsymbol{L}}_{\boldsymbol{z}}$)

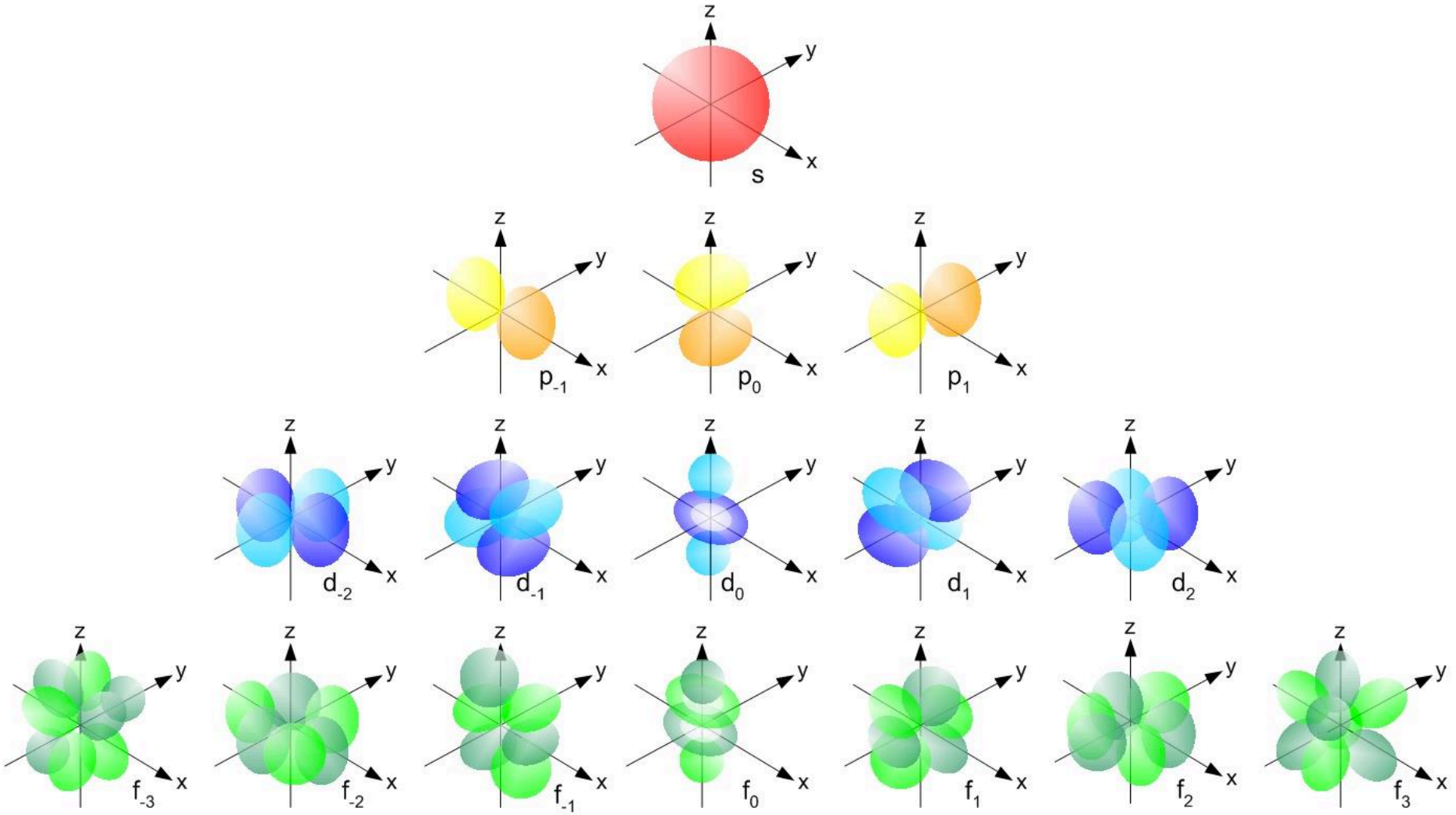
$$\widehat{\boldsymbol{L}}_{\boldsymbol{z}}\boldsymbol{\psi} = \boldsymbol{m}\hbar\boldsymbol{\psi}$$

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



Appendix 2: Quantum Number (量子数)

- **Magnetic Quantum Number (磁量子数)**

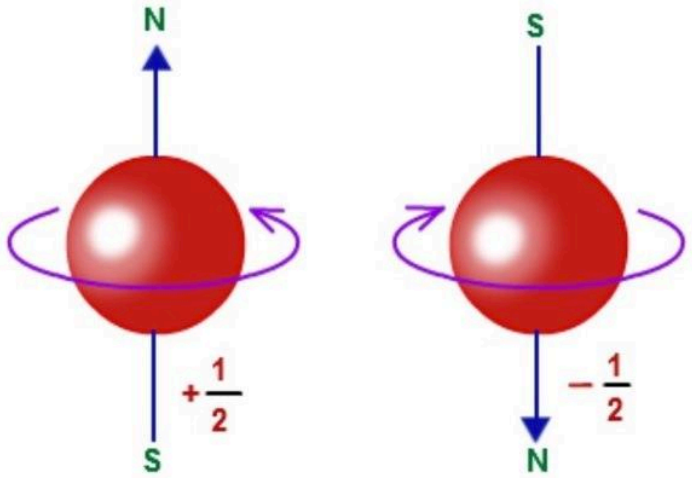


Appendix 2: Quantum Number (量子数)

➢ 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** ($\hat{s}_z$)

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



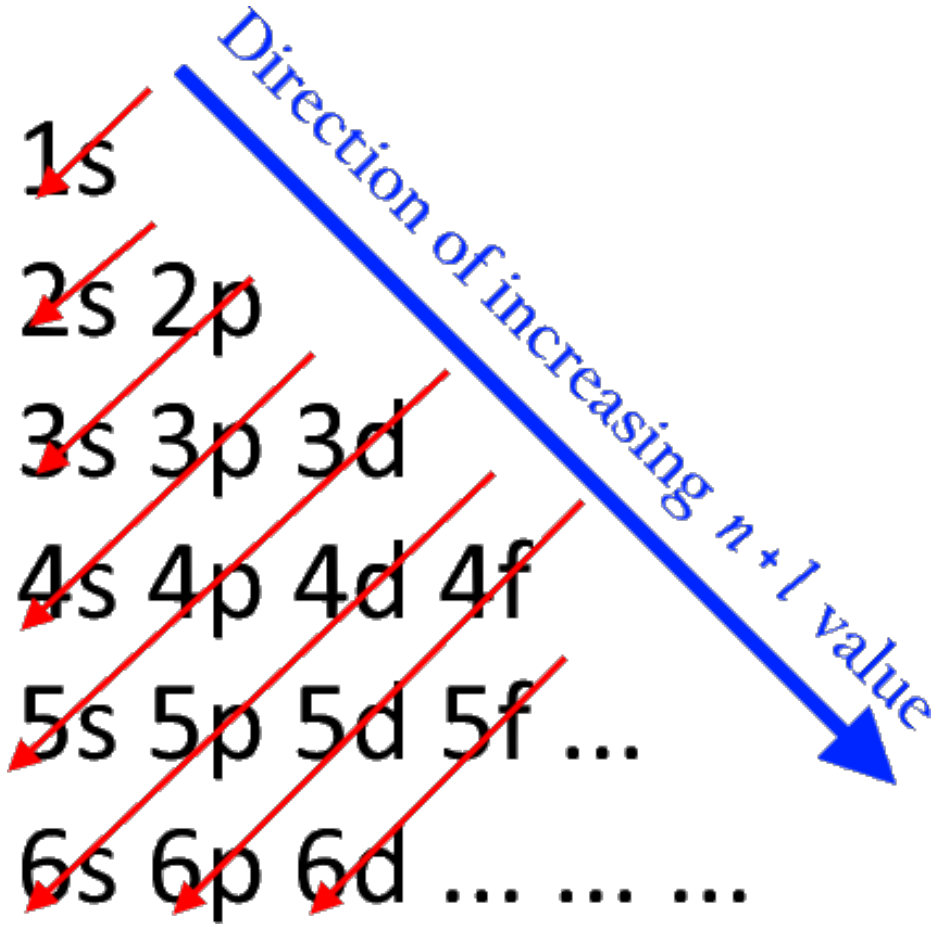
Appendix 2: Quantum Number (量子数)

➢ 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			

Appendix 2: Quantum Number (量子数)

- **Electron Configuration (电子排布)**



Aufbau Principle