

VI. The Basics of Quantum Mechanics

ψ : The wave function or orbital

- The mathematical description of an electron as a three-dimensional standing wave
- Defined or labeled by three quantum numbers: n , l , and m_l (see below)
- Undergoes constructive interference, destructive interference, and diffraction like any other wave
- The electron's amplitude; cannot be observed directly (also true of any wave)

The 4 Quantum Numbers (QN's), Their Rules, and Their Roles

QN	Name	Allowed Values	What It Determines
n	principal	1, 2, 3, ...	Total number of nodes = $n - 1$ \Rightarrow energy of a 1-electron species \Rightarrow <u>average</u> distance of e- from nucleus
l	angular momentum	0, 1, 2, ..., $n - 1$	Number of angular nodes = l \Rightarrow shape of ψ
Note: $l = 0 \Rightarrow s$ $l = 1 \Rightarrow p$ $l = 2 \Rightarrow d$ $l = 3 \Rightarrow f$ $l = 4 \Rightarrow g$ $l = 5 \Rightarrow h$			
m_l	magnetic	$-l, -l + 1, \dots, 0, \dots, l$ ($2l + 1$ possible values)	Orientation of ψ [with respect to a magnetic field]

Orbital: A wave function with a given value of n , l , and m_l

Subshell: A set of orbitals with the same values of n and l (m_l can take on any allowed value)

Shell: A set of orbitals with the same value of n (l and m_l can take on any allowed values)

m_s	spin	$+\frac{1}{2}, -\frac{1}{2}$	Orientation of an electron's intrinsic angular momentum [with respect to a magnetic field]
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So each orbital can hold two electrons, one of spin $+\frac{1}{2}$, and the other of spin $-\frac{1}{2}$

ψ^2 : The probability density or charge density

- The electron's intensity; can be observed directly (*e.g.* scanning tunneling microscopy)
- $\psi^2 \cdot \text{volume} =$ the probability of finding an electron in that volume

$(4\pi r^2 \Delta r)\psi^2$: The radial distribution function (RDF)

- The probability of finding an electron at a distance r from the nucleus
- $(4\pi r^2 \Delta r)\psi^2$ can never equal one (that is, 100% probability) at any one point in space. That is, we can never completely localize the electron (Heisenberg uncertainty principle).
- $(4\pi r^2 \Delta r)\psi^2$ (and ψ^2 and ψ) does equal zero at a node. We can say where the electron can't be with 100% certainty!