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 = $n - 1$ ⇒ energy of a 1-electron species ⇒ average distance of e- from nucleus
l	angular momentum	0, 1, 2, …, n - 1	Number of angular nodes = l ⇒ 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	$-l, -l + 1, \ldots, 0, \ldots, l$ ($2l + 1$ 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	+½, -½	Orientation of an electron's intrinsic angular momentum [with respect to a magnetic field]

So each orbital can hold two electrons, one of spin +½, and the other of spin -½

ψ^2: The probability density or charge density

- The electron's intensity; can be observed directly (*e.g.* scanning tunneling microscopy)
- ψ^2 * volume = the probability of finding an electron in that volume

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

- 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% certainity!