

## VI. The Basics of Quantum Mechanics

### $\psi$ : 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 $\psi$
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 $\psi$ [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  $-\frac{1}{2}$

### $\psi^2$ : 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  $\psi^2$  and  $\psi$ ) does equal zero at a node. We can say where the electron can't be with 100% certainty!