

## Chapter 1: 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

### $\psi^2$ : The probability density or charge density.

- The electron's intensity; can be observed directly (*e.g.* by the technique of scanning tunneling microscopy)
- $\psi^2 * \text{volume}$  = the probability of finding an electron in that volume
- $\psi^2 * \text{volume}$  can never equal one (that is, 100% probability) at any one point in space. That is, we can never completely localize the electron. (Bohr was wrong!)
- $\psi^2$  (and  $\psi$ ) does equal zero at a node. We can say where the electron can't be.

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

| QN   | Name  | Allowed Values                   | What It Determines   |
|--|---|----------------------------------|--|
| $n$  | principal   | 1, 2, 3, ...                     | Total number of nodes = $n - 1$<br>$\Rightarrow E = -2.179 \times 10^{-18} \text{ J } \frac{Z^2}{n^2}$<br>for a 1-electron atom or ion |
| $l$  | angular momentum<br><br>[ $L^2 = l(l + 1) \hbar^2 / 4\pi^2$ ] | 0, 1, 2, ..., $n - 1$            | Number of angular nodes = $l$<br>$\Rightarrow$ shape of $\psi$<br>$\Rightarrow$ Number of radial nodes = $n - l - 1$                   |
| 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  | $-l, -l + 1, \dots, 0, \dots, l$ | Orientation of $\psi$<br>[with respect to a magnetic field]<br>$\Rightarrow 2l + 1$ possible orientations                              |
| <p><u>Orbital</u>: A wave function with a given value of <math>n</math>, <math>l</math>, and <math>m_l</math></p> <p><u>Subshell</u> or <u>Sublevel</u>: A set of orbitals with the same values of <math>n</math> and <math>l</math> (<math>m_l</math> can be anything)</p> <p><u>Shell</u>: A set of orbitals with the same value of <math>n</math> (<math>l</math> and <math>m_l</math> can be anything)</p> |   |                                  |  |
| $m_s$  | spin  | $+\frac{1}{2}, -\frac{1}{2}$     | Orientation of an electron's<br>intrinsic angular momentum<br>(with respect to a magnetic field)                                       |