# Schrödinger Wave Equation for One-Electron Atoms

$$\mathcal{H}\Psi = E\Psi$$

| | | |
|---|---|---|
| $E$ | = | energy of the system (*eigen value*) |
| $\Psi$ | = | wave function solution (*eigen function*) |
| $\mathcal{H}$ | = | Hamiltonian operator, expressing potential and kinetic energy of the system |

Explicit wave equation for hydrogen:

$$\left[-\frac{h^2}{8\pi^2 m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)-\frac{e^2}{r}\right]\Psi = E\Psi$$

Each $\Psi$ solution is a mathematical expression that is a function of three *quantum numbers*: $n$, $l$, and $m_l$.

## Probability of Finding the Electron Somewhere Around the Nucleus

For light, intensity is proportional to amplitude squared:

$$I \% A^2$$

By analogy, the "intensity" of an electron at a point in space (i.e., its *probability*) is proportional to the amplitude of its wave function squared, $\Psi^2$:

$$P \% \Psi^2$$

This is the "Copenhagen Interpretation" of the wave function, due to Max Born and co-workers.

> Einstein to Born:
>
> "Quantum mechanics is certainly imposing. But an inner voice tells me that it is not yet the real thing. The theory says a lot, but does not really bring us any closer to the secret of the 'old one'. I, at any rate, am convinced that He is not playing at dice."
>
> ["The Born-Einstein Letters," translated by Irene Born. New York: Walker and Company, 1971, pp. 90-91.]

## Restrictions on $\Psi$

1. *$\Psi$ has a value for every point in space.* Otherwise the probability would be undefined somewhere.

2. *$\Psi$ can have only one value at any point.* Otherwise the probability would be ambiguous at some points.

3. *$\Psi$ cannot be infinite at any point in space.* Otherwise its position would be fixed, in violation of the Heisenberg Uncertainty Principle.

4. *$\Psi$ can be zero at some points in space (node).* This means the electron is not there.

5. *The sum of $\Psi^2$ over all space is unity.*

   $$\int \Psi^2 \, d\tau = 1$$

   The electron must be somewhere.

# Quantum Numbers

**Principal quantum number, *n***
Determines *energy* by the equation,

$$E = \frac{-2\pi^2 m Z^2 e^4}{n^2 h^2} = \frac{-BZ^2}{n^2}$$

Values: $n$ = 1, 2, 3, ...
Related to concept of *shells*.

**Angular momentum (azimuthal) quantum number, *l***
Determines *shape* of the probability distribution.
Values: $l$ = 0, 1, 2, ..., $n$ - 1
Related to the concept of *subshells*.

| Value of $l$ | 0 | 1 | 2 | 3 | 4 | ... |
|---|---|---|---|---|---|---|
| Subshell Label | *s* | *p* | *d* | *f* | *g* | ... |

**Magnetic quantum number, $m_l$**
Determines *orientation* of the probability distribution.
Values: $m_l = -l, (-l + 1), ..., 0, ..., (l - 1), l$
Related to concept of *orbitals*.

## Orbitals of the First Four Shells

| $n$ | $l$ | Subshell Notation | Allowed $m_l$ values | Orbitals per Subshell |
|---|---|---|---|---|
| 1 | 0 | 1*s* | 0 | 1 |
| 2 | 0 | 2*s* | 0 | 1 |
| | 1 | 2*p* | -1, 0, +1 | 3 |
| 3 | 0 | 3s | 0 | 1 |
| | 1 | 3*p* | -1, 0, +1 | 3 |
| | 2 | 3*d* | -2, -1, 0, +1, +2 | 5 |
| 4 | 0 | 4*s* | 0 | 1 |
| | 1 | 4*p* | -1, 0, +1 | 3 |
| | 2 | 4*d* | -2, -1, 0, +1, +2 | 5 |
| | 3 | 4*f* | -3, -2, -1, 0, +1, +2, +3 | 7 |