Schrödinger Wave Equation
for One-Electron Atoms

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

E = energy of the system (*eigen value*)
Ψ = 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 Ψ 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:

$$I \propto A^2$$

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, Ψ^2:

$$P \propto \Psi^2$$

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 Ψ

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

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

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

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

5. *The sum of Ψ^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