

Chapter IV

Introduction to Quantum Mechanics – The Schrödinger Equation

I/ The wave properties of the electron

De Broglie's equation says that every moving object has a wavelength.

Louis de Broglie said that a free electron of mass (m) and speed (v) has a wave with a wavelength (λ) given by:

$$\lambda = \frac{h}{mv}$$

h : Planck's constant
 m : the mass

v : the velocity
 λ : the wavelength

The wave behavior of a particle is stronger when its wavelength is larger — that means when the particle's mass or energy is smaller.

A moving electron has both particle and wave nature. However, it is considered sometimes as a wave and sometimes as a particle, depending on the phenomenon studied.

The electron is neither a wave nor a particle; it is a quantum particle.

II/ Standing wave of Louis de Broglie

In Niels Bohr's model, the electron is a particle moving in a circular path called a stationary orbit.

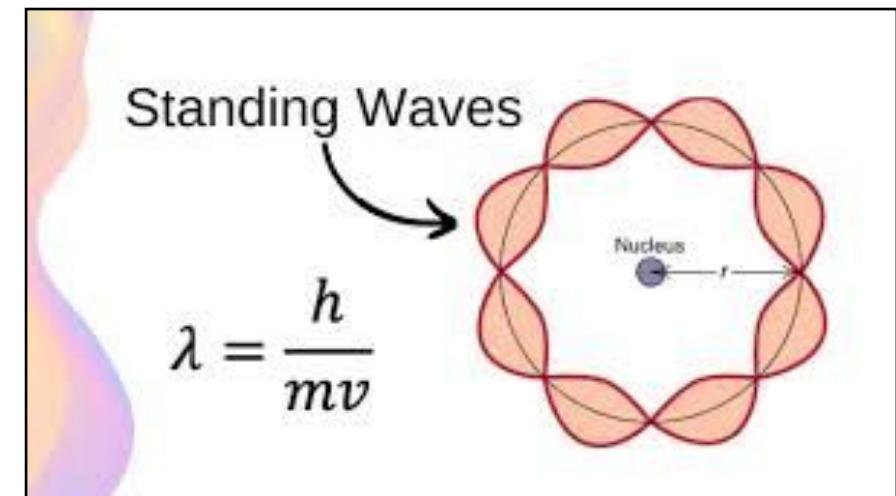
De Broglie gave a simple explanation of this stationary orbit condition.

In De Broglie's model, the electron is described by a standing wave such that:

Therefore:

$$2\pi r = n (h / mv)$$

That is, the total length of the orbit is equal to an integer number of De Broglie wavelengths.



The De Broglie wave closes in on itself after making one complete turn around the nucleus.

III/ The uncertainty principle

Heisenberg showed that if we know the exact position of the electron, we cannot know its speed precisely; and if we know its energy exactly, we cannot know its position for sure.

Heisenberg concluded that it is impossible to know exactly at the same time the position of an electron and its energy if it is described as a wave.

$$\Delta p \Delta x \geq \frac{h}{2\pi}$$

$$P = mv$$

$$m \Delta v \Delta x \geq \frac{h}{2\pi}$$

h: Planck's constant

m: the mass of the particle

p: the momentum

X: the position of the particle

Consequence of Heisenberg's uncertainty principle for the electron:

- ✓ The trajectory cannot be determined using classical mechanics.
- ✓ The particle (corpuscular) nature cannot be used.
- ✓ The wave nature must be used.

Quantum mechanics replaces classical mechanics by defining the electron through its energy and its probability of being at a given point in space.

Schrödinger's equation (1926): a fundamental relation of quantum mechanics, suitable for particles with very small mass.

Solving it makes it possible to find the energy values available to the electron and the mathematical functions that describe its behavior.

I. History of the Atomic Theory-time line

1803	1897	1909	1913	1935	Today	
solid particle	electron	proton	e- orbit nucleus	neutron	Quantum Atom theory	
Dalton	Thomson	Rutherford	Bohr	Chadwick	Schrodinger and others	

IV/ The hydrogen atom according to Schrödinger's model and the wave function

The model of the hydrogen atom developed by Schrödinger is based on representing the electron as a wave, not as a particle.

The mathematical solution of Schrödinger's equation gives results called wave functions, represented by the symbol Ψ (psi)

From these wave functions, we must remember:

- ✓ Each wave function corresponds to an energy.
- ✓ The square of the wave function (Ψ^2) is related to the probability of finding the electron (electron density).

IV.1/ Energy or eigenvalues

$$E_n = \frac{-13.6}{n^2} \text{ (eV)}$$

- ✓ It is the same result as that obtained with Bohr's model.
- ✓ The energy is quantized.
- ✓ The energy depends on the principal quantum number n.

IV.2/The probability of finding an electron in a volume V

The probability of finding the electron in a volume V is:

$$\int dP = \int_V \Psi^2 dV$$

The electron is not exactly localized around the nucleus. We can only know the probability of its presence within a given volume V.

V/ The quantum numbers

- ✓ The quantum numbers are whole numbers, and their values are not chosen at random.
- ✓ The quantum numbers come from the mathematical solution of Schrödinger's equation applied to an electron considered as having a wave-like nature.

The principal quantum number, $n = 1, 2, 3, \dots$ can take any whole number value from 1 to infinity.

Its value is the main factor that determines the electron's energy.
The size of the orbital increases with n .

The secondary quantum number, $l = 0, 1, 2, \dots, n - 1$ ($l \leq n - 1$)

Electrons in the same shell can be grouped into subshells, which are defined by the secondary quantum number (l).

The magnetic quantum number, $m = 0, -1, +1, -2, +2, \dots, -l, +l$ ($-l \leq m \leq +l$) shows how the orbitals in the same subshell are oriented in space.
They have the same energy but point in different directions.

The quantum number s (or spin quantum number) describes the spin of the electron
Its direction of rotation around its own axis.
It can have only two possible values: $+\frac{1}{2}$ or $-\frac{1}{2}$.

The information given by the quantum numbers

- ✓ The three quantum numbers identify an electron, just like an address.
- ✓ The table below shows the allowed combinations for the three quantum numbers.
- ✓ n = number of subshells in a shell.
- ✓ $2l + 1$ = number of orbitals in a subshell.
- ✓ n^2 = number of orbitals in a shell.

<i>n</i>	<i>l</i>	<i>ml</i>	<i>m_s</i>	Number of orbitals	Orbital Name	Number of electrons	Total Electrons
1 (K shell)	0	0	$\frac{1}{2}$ $-\frac{1}{2}$	1	<i>1s</i>	2	2
2 (L Shell)	0	0	$\frac{1}{2}$ $-\frac{1}{2}$	1	<i>2s</i>	2	8
	1	-1, 0, +1	$\frac{1}{2}$ $-\frac{1}{2}$	3	<i>2p</i>	6	
3 (M-shell)	0	0	$\frac{1}{2}$ $-\frac{1}{2}$	1	<i>3s</i>	2	18
	1	-1, 0, +1	$\frac{1}{2}$ $-\frac{1}{2}$	3	<i>3p</i>	6	
	2	-2, -1, 0, +1, +2	$\frac{1}{2}$ $-\frac{1}{2}$	5	<i>3d</i>	10	
4 (L-shell)	0	0	$\frac{1}{2}$ $-\frac{1}{2}$	1	<i>4s</i>	2	32
	1	-1, 0, +1	$\frac{1}{2}$ $-\frac{1}{2}$	3	<i>4p</i>	6	
	2	-2, -1, 0, +1, +2	$\frac{1}{2}$ $-\frac{1}{2}$	5	<i>4d</i>	10	
	3	-3, -2, -1, 0, +1, +2, +3	$\frac{1}{2}$ $-\frac{1}{2}$	7	<i>4f</i>	14	

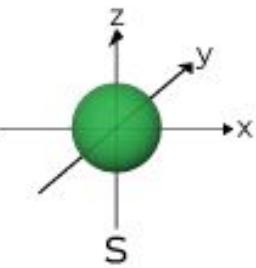
Quantum Number Chart

VI/ The shape of atomic orbitals

When we draw atomic orbitals, we should remember that:

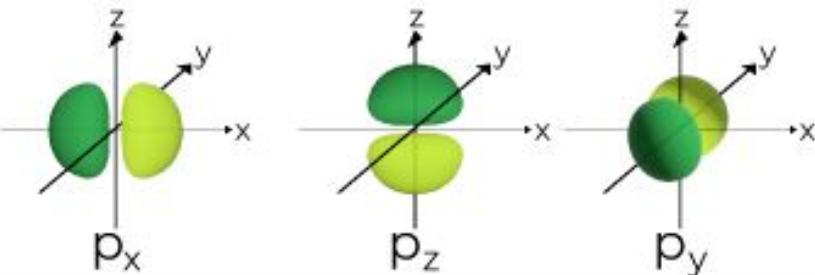
- ✓ There is about 90% chance to find the electron inside the orbital, this number is chosen by convention.
- ✓ The line or surface around the orbital is not a real wall; there is still about 10% chance to find the electron outside it.
- ✓ The electron cloud shows where the electron is most likely to be around the nucleus.
- ✓ The electron is not equally likely to be found everywhere inside the orbital.

S orbital



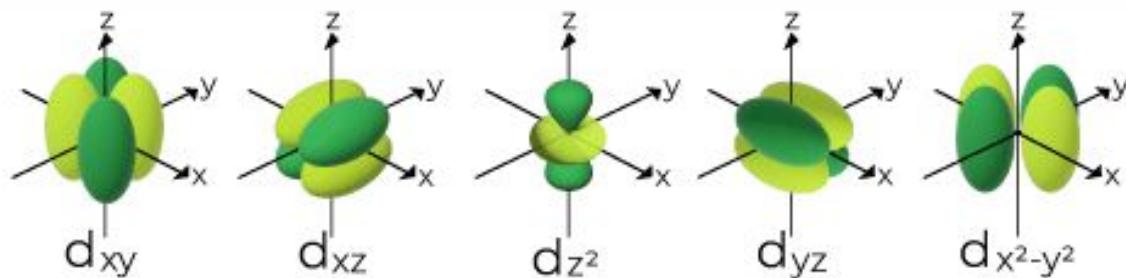
$n = 1, 2, 3, \dots 7$
 $l = 0$
 $m = 0$

p orbital



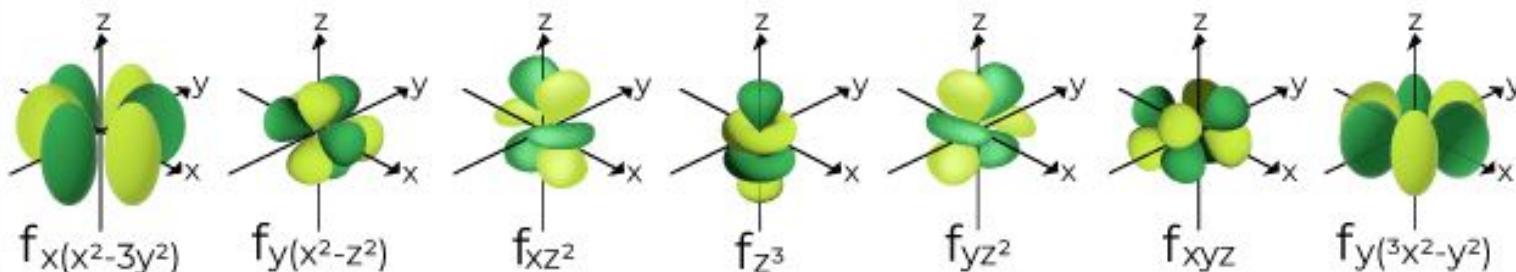
$n = 2, 3, \dots 6$
 $l = 1$
 $m = 0, \pm 1$

d orbital



$n = 3, 4, \text{and } 5$
 $l = 2$
 $m = 0, \pm 1, \pm 2$

f orbital



$n = 4$
 $l = 3$
 $m = 0, \pm 1, \pm 2, \pm 3$