Introduction

We've discussed how Bohr's model predicted the behavior of the hydrogen atom. To describe the other atoms (and get to our goal of actually predicting the behavior of atoms in chemical reactions), we need a more advanced structure than the one Bohr provided. The modern way to discuss the structure of the atom relies on **quantum mechanics**, a way to describe the motion of small particles. An in-depth study of quantum mechanics would require advanced math knowledge, but the findings and underlying concepts we can discuss with simple math and explanation.

A new picture of matter ... waves?

Einstein showed that **light** has properties of both waves and particles. A more radical notion was proposed by de Broglie, who said that **all matter** had properties of both waves and particles. He gave a simple equation that lets you calculate the **wavelength** (λ) of any particle:

$$\lambda = \frac{h}{m \times v}$$

... where

- λ = the wavelength (in m)
- h = Planck's constant = 6.63×10^{-34} J-s
- v = the velocity of the particle (in m/s)

A few things about this equation:

- The mass of the particle is in the denominator. The larger the particle, the shorter the wavelength.
- The speed of the particle is also in the denominator. The faster the particle moves, the shorter the wavelength.

Why aren't the wave properties of things the size of, say, ping pong balls observable? Why don't they sit on a table and oscillate (like you'd expect from a wave)? The equation above holds the answer. As the mass of the object increases, its wavelength decreases. The wavelengths of macroscopic objects aren't large enough to observe. In other words, the ping pong ball **does** have a wavelength, but it's too small to observe.

But how do we know that de Broglie's equation is right? We **can** observe the wave properties of very small particles - namely **electrons**. We've used this to our advantage in the **electron microscope**, which uses electrons for imaging much like an optical telescope uses light waves. Since electrons have a much smaller wavelength than light waves do, we can see objects in much greater detail with an electron microscope than we can with an optical microscope!

So how does this relate to a picture of the atom? This observation is the basis for quantum mechanics. In quantum mechanics, small particles are described using their **wave properties**, and it is for this reason that quantum mechanics is also called **wave mechanics**.

Uncertainty and quantum mechanics

To wrap our brains around quantum mechanics, we first have to discuss what quantum mechanics can tell us and what it can't. In classical physics (**Newtonian mechanics**), we calculate an object's trajectory. For example, you might calculate the position and speed of a ball you've dropped out of a third-story window at different points in time. In quantum mechanics, though, we speak only of the **probability** that a particle might be in a given space at a certain time. We don't speak of the path a particle takes - we just tell whether it's probable the particle is in a given space.

Heisenberg, in fact, said that it was **impossible** to know with absolute certainty both the position and momentum of a particle. This was called the uncertainty principle, and essentially said that the uncertainty in the position and trajectory of a particle the size of an electron was too large to figure our exactly what the position and momentum of an electron inside an atom was. When you talk about objects the size of a ping pong ball, the uncertainty is still there, but since the ball is large and massive compared to an electron, the uncertainty is small compared to the size of the ball and can be ignored..

In quantum mechanics, then, we talk about **wave functions**, which are mathematical expressions of the **probability** of finding an electron in a given space. The wave functions describe the space an electron is likely to be in. Luckily, we don't have to discuss the actual equations, since the important (to us) features of quantum mechanics can be discussed without them.

Quantum numbers: the "phone number" of the electron

So how do we use the wave functions to give us useful information without talking about the actual equations themselves? We can envision the shape of the space mapped out by the wave function - much the same way you can think about a sphere without actually writing the equation for one.

But how do we specify the wave function? We do this with **quantum numbers** - in effect, the "phone number' of an electron in an atom. With the quantum numbers we can describe each electron in an atom. Each electron has **four** quantum numbers, and no two electrons in the same atom have the same four quantum number - much like no two households in the same area have the same phone number.

We'll now discuss the four quantum numbers and what they tell you about an electron.

1: The principal quantum number (n)

The principal quantum number **n** tells you a few things:

- The **shell** an electron is in. Shells correspond to Bohr's **energy levels**.
- The **energy** of an electron. Generally, the higher the n, the higher the energy.
- The **distance** of the electron from the nucleus. The larger the n, the larger the amount of space available to the electron.

The principal quantum number (like all quantum numbers) can only have certain values. These are:

- **n** can be any positive integer. For example, **n** could equal 1, 2 ,3, 4, ...

<u>2: The angular momentum quantum number (*l*)</u>

The angular momentum quantum number ***l*** describes:

- The **subshell** an electron is in (e.g. the **2s** subshell or the **3p** subshell).
- The **shape** of an **atomic orbital**. **Atomic orbitals** are another name for **wave functions** - the space the electron is likely to be in.
- The **energy**, but to a lesser extent than **n** does. Orbitals with higher values of **l** tend to have higher energies.

The angular momentum quantum number can have only certain values. The possible values for the angular momentum quantum number depend on the value of the principal quantum number, **n**.

- ***l*** may have any integer value from 0 to **n**-1

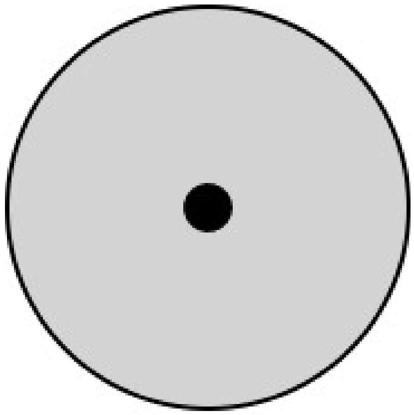
For example, an electron that has **n** = 1 may have ***l*** = 0, but an electron with **n** = 2 may have ***l*** = 0 **or** 1. (It can't have both at the same time, of course!)

It's common practice to talk about the values of ***l*** using letters instead of the integers. Here's a table of the common letters.

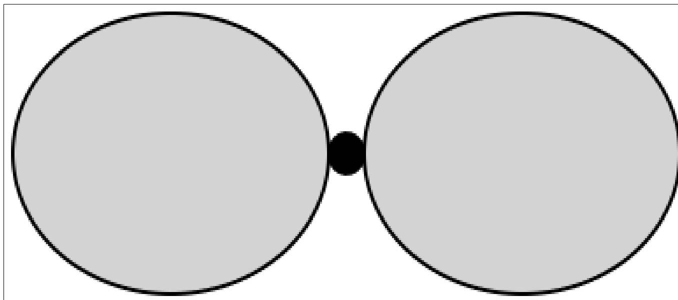
l =	0	1	2	3	4
Letter →	s	p	d	f	g

For example, you would describe an electron with **n** = 1 and ***l*** = 0 as a "1s" electron, while you would call an electron with **n** = 2 and ***l*** = 1 a "2p" electron.

To help us visualize what ***l*** means, let's look at the shapes of a few atomic orbitals graphically. The gray area in each diagram represents the space an electron is likely to be in, while the black dot represents the nucleus (drawn proportionally larger than in a real atom).

	• The "s" orbital is spherical. • As **n** increases, the size of the orbital increases.
Illustration 1 - An "s" orbital in 2D	

The "s" orbital is the simplest shape - it's the sort of arrangement Bohr might have envisioned when he made **his** model of the atom.

	• The "p" orbital is dumbbell-shaped, with two **lobes** pointing in opposite directions. • Electrons may occupy any position in either **lobe** - they're not restricted to one or the other. • The "p" electrons have more energy than the "s" electrons in the same **shell** (same value of **n**)
Illustration 2 - A "p" orbital in 2D	

As you'll find out in the next course, the shape of the "p" orbital is very important in chemical bonding.

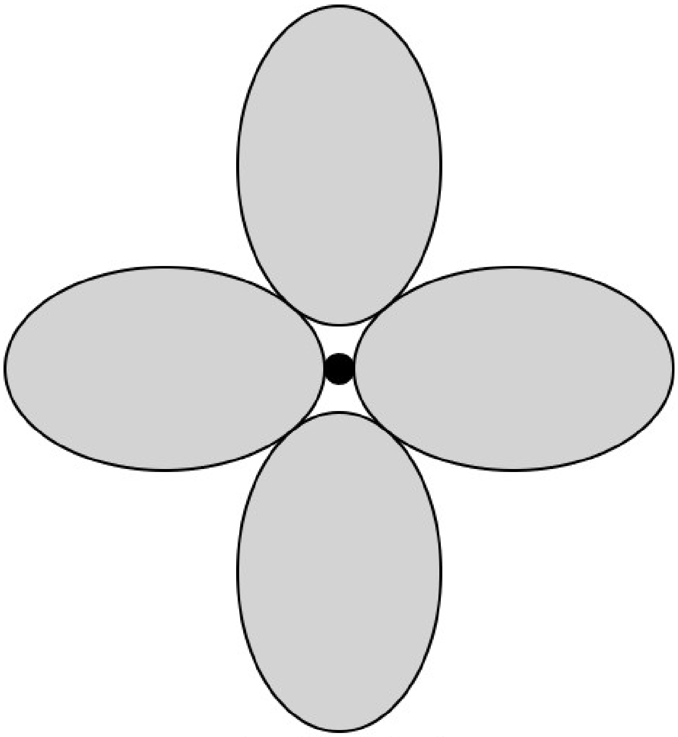


Illustration 3 - A "d" orbital in 2D

- The "d" orbitals have a considerably more complicated shape than "s" or "p" orbitals.
- Most of the "d" orbitals have this flower petal shape, but not **all**!
- Electrons are not restricted to any one **lobe** of this orbital - they may be in any of the four lobes.
- The "d" electrons have more energy than the "s" **or** "p" electrons in the same **shell**.

Some elements (like phosphorus) use their "d" orbitals to form more bonds than you'd normally expect.

3: The magnetic quantum number (m_l)

The magnetic quantum number **m_l** describes the **orientation** of the orbital. Like the other quantum numbers, it can only have certain values.

- **m_l** can be any integer from -***l*** to ***l***

So, for an "s" orbital (***l*** = 0), **m_l** must be 0. This should make sense to you, because no matter how you orient a **sphere** it still looks the same. For a "p" orbital (***l*** = 1), possible values of **m_l** are -1, 0, and 1. This should also make sense, as you can arrange a dumbbell three ways about the axes - along the x axis, along the y axis, and along the z axis.

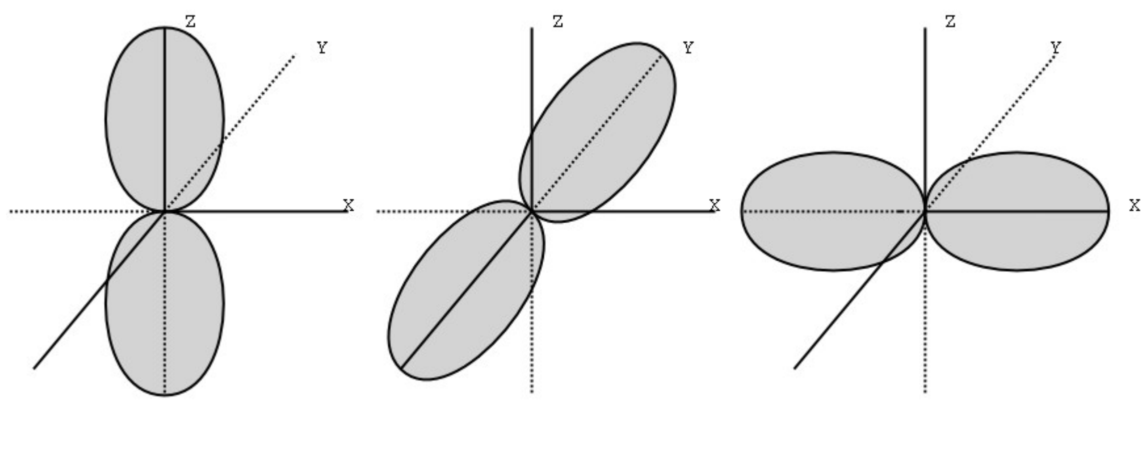


Illustration 4 - The three orientations of "p" orbitals

The "d" orbitals (***l*** = 2) can be oriented about the axes in **five** ways - $\mathbf{m}_l$ can be -2, -1, 0 , 1, or 2, but that gets difficult to draw!

The first three quantum numbers (**n**, ***l***, and $\mathbf{m}_l$) define the **atomic orbital** the electron is in. The last tells us how many electrons can be in the orbital.

4: The spin quantum number (m_s)

The spin quantum number $\mathbf{m}_s$ represents the spin of the electron. You can think of electrons as spinning either clockwise or counterclockwise.

The spin quantum number can have only two values.

- $\mathbf{m}_s$ may be either +½ or -½.

In essence, what this tells us is that each orbital (for example, the 1s orbital, or the 2p orbital that points along the x axis) can hold only two electrons. This will be important when we discuss electron configuration.

Summary

We've learned that matter (and particularly, electrons) behaves as waves and can be described by mathematical equations called **wave functions**. We've also discussed how we can describe the electrons in an atom using the **quantum numbers**, and what each of the quantum numbers represents. Soon, we will use the quantum numbers to determine the **electron configuration** of atoms.