"Oh boy . . ."

Sam Beckett (from Quantum Leap)

Unit 8

Building Atoms with Quantum Leaps

Physicists Put Atom in Two Places at Once

This was the headline in the science section of the *New York Times* on May 28, 1996. "Impossible!" you say. "How could they do that?" you wonder. This event is impossible at the macroscopic level at which classical mechanics governs the world. But it is entirely possible according to quantum mechanics, which governs the particulate world of atoms, protons, and electrons. The physicists who caused a single beryllium atom to exist in two states at the same time, separated by a distance of 83 nanometers, made use of a quantum mechanical trait called spin.

Quantum Numbers

The spin attribute is one of the four quantum mechanical characteristics needed to describe an electron completely. Each of these characteristics is described by what is known as a quantum number. If we consider quantum numbers to be the "address" of each electron within an atom, each address has four parts, and no two electrons have the exact same address.

The Bohr model of the hydrogen atom gave us our first understanding that electrons were governed by non-classical mechanics, and this model worked well for explaining the properties of the electron in the hydrogen atom. However, it failed for all other atoms. In 1926, Erwin Schrödinger devised a new model of the atom which is now known as the quantum mechanical model.

The Quantum Mechanical Model of the Atom Schrödinger's atomic model is framed mathematically in terms of what is known as a wave equation. Solutions of wave equations are called wave functions. The solutions to a wave equation define the volume in space where an electron with a particular energy is likely to be found. This volume in space is called an orbital. Each orbital is characterized by three quantum numbers.

The Pauli Exclusion Principle This principle states that no two electrons in an atom can have the same four quantum numbers. If two electrons occupy the same orbital, they must have different spins.

The four quantum numbers are:

1. The principal quantum number, n.

   The allowed values of the principal quantum number are $n = 1, 2, 3, ..., 7$. Electrons with the same value of n are said to have the same principal energy level.

2. The angular momentum quantum number, ℓ.

   Angular momentum quantum numbers depend on principal quantum numbers. For $n = 1$, $\ell = 0$. For $n = 2$, $\ell = 0$ or 1. For $n = 3$, $\ell = 0$, 1, or 2. For $n = 4$, $\ell = 0$, 1, 2, or 3. This pattern can be summarized as $\ell = 0, 1, ..., n - 1$. Notice that all principal energy levels are divided into one or more sublevels.

   Angular momentum quantum numbers are often referred to by using letter designations which correspond with the numerical values. $\ell = 0$ is also called the s sublevel, $\ell = 1$ is p, $\ell = 2$ is d, and $\ell = 3$ is f. Electron energies are described by the principal energy level and the sublevel. Thus an electron with $n = 3$ and $\ell = 1$ is referred to as a 3p electron.

3. The magnetic quantum number, m_ℓ

   Magnetic quantum numbers depend on angular momentum quantum numbers. The pattern is $m_\ell = -\ell ..., 0, ..., +\ell$. Thus for $\ell = 0$, the only allowed value of m_ℓ is 0. When $\ell = 1$, m_ℓ can be –1, 0, or +1. For $\ell = 2$, $m_\ell = -2, -1, 0, +1$, and +2. When this pattern is followed for $\ell = 3$, there are seven possible m_ℓ values (can you write them?).

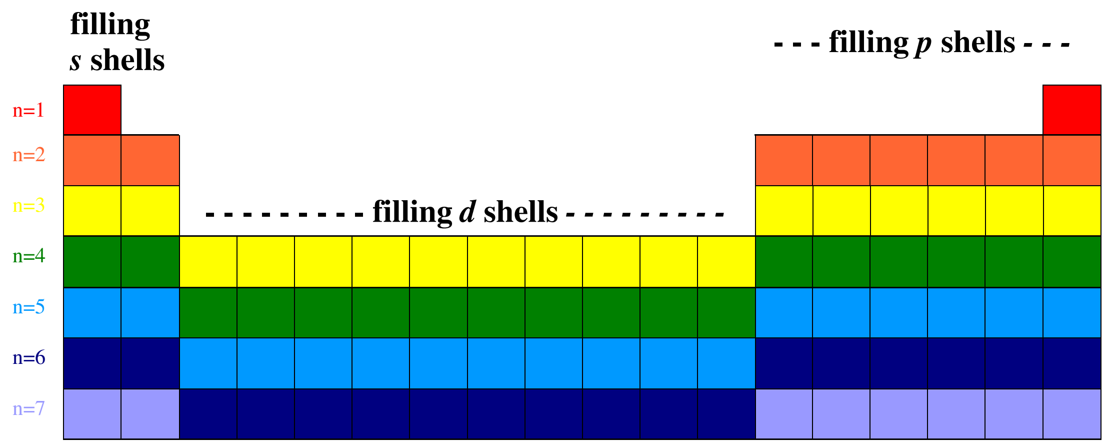
4. The electron spin quantum number, m_s.

   The values of m_s are +½ and –½ . Electrons can be thought of as spinning on an axis, where one m_s value corresponds to a clockwise rotation and the other value corresponds to a counterclockwise rotation.

The Periodic Table

The periodic table serves as a guide to both order of increasing electron energies and the order in which electrons fill orbitals. Electrons occupy the lowest energy orbitals available, and as the numbers of electrons in an atom increases, the outermost electrons occupy higher and higher energy levels. The periodic table on the next page illustrates the correspondence of electron energy levels and position on the periodic table.

Note:



For *s* and *p* orbitals, the period number corresponds with the principal energy level. For *d* orbitals, the fourth period corresponds to $n = 3$, the fifth period to $n = 4$, and so on. The lanthanides and actinides (not shown) result from the filling of the 4*f* and 5*f* orbitals, respectively.

Self Test

1. Complete the chart below by entering all possible values for the quantum numbers. The first line is completed as an example.

n	ℓ	m_ℓ	m_s
1	0	0	+½ , –½
2			
3			
4			

2. The ground-state electron configuration for the single electron in the hydrogen atom is $1s^1$. What are the values of the m_ℓ and m_s quantum numbers for this electron? Explain.

3. The quantum numbers for one of the two electrons of helium are $n = 1$, $\ell = 0$, $m_\ell = 0$, and $m_s = -½$. What are the quantum numbers for the other electron? Write the electron configuration for helium.

4. What are the maximum number of electrons in an atom that can have when $n = 1$ and when $n = 2$? Explain.

Workshop: Building Atoms with Quantum Leaps

1. Count off the numbers from 1 to 36, rotating among the members of your group.

   a) Write the full ground-state electron configuration for each of your elements.

   b) Explain the relationship between the electron configuration and the corresponding principal and angular momentum quantum numbers for each element.

2. Begin by assigning one of each of the following elements to each group member: carbon, nitrogen, fluorine, neon, sodium, aluminum, phosphorus, chlorine, iron (there should be more elements in this list than group members; you may omit an element or two, as necessary). Each person should complete the following five steps for their element:

Step 1: Write the electron configuration of the element. This can be copied from Question 1.

Step 2: Prepare a chart similar to the one shown in the example below, giving the values of each of the four quantum numbers for each electron in the atom.

Step 3: Fill in all of the items in the chart.

Step 4: Create an energy level diagram for your element. Use a line to represent an orbital, and use up and down arrows to represent electrons in each orbital.

Step 5: Fill in the energy level diagram.

We will complete the five steps for boron as an example.

Step 1: Electron configuration

B: $1s^2 2s^2 2p^1$

Steps 2 and 3: Chart of quantum numbers

n	ℓ	m_ℓ	m_s
1	0	0	–½
2	0	0	+½
2	0	0	–½
2	1	–1	+½

Steps 4 and 5: Energy level diagram

$2p$ __↑__   ____   ____
$2s$ __↑↓__
$1s$ __↑↓__

3. Answer each of the following:

a) How many $3p$ electrons does a chlorine atom have?

b) Give the complete set of quantum numbers for all of the chlorine 3*p* electrons.

c) How many *d* electrons does an iron atom have?

d) How many unpaired electrons are in a chlorine atom, an iron atom, and a nitrogen atom?

The group round-robin method works well for this question.

4. Many substances exhibit no magnetic properties except in the presence of a magnetic field. Substances with all paired electrons are weakly repelled by a magnetic field. These substances are called *diamagnetic*. Other substances are attracted to a magnetic field and are called *paramagnetic*. This property is the result of unpaired electrons.

Which of the following do you expect to be paramagnetic? Explain how you reach your conclusions.

a) K

b) Ba^{2+}

c) Fe^{2+}

d) Fe^{3+}

e) F

f) F^{-}

g) Ni^{2+}

5. For each of the following pairs, determine the atom with (i) the largest radius, (ii) the greatest ionization energy, and (iii) the smallest electron affinity. Explain your reasoning in each case.

   a) F or K

b) O or Si

c) Li or Cs

d) F or As

6. Define each of the terms from Question 5: atomic radius, ionization energy, and electron affinity. Consider the following when constructing your definitions:

   a) How can the radius of an atom be experimentally determined?

   b) What is meant by the terms first, second, and third ionization energy?

   c) What is the sign of electron affinity if it is defined as the quantity of energy released? What if it is defined as the energy change? Which definition are you using in your class?

7. Most general chemistry textbooks have a plot of first ionization energy versus atomic number. Find this figure in your textbook. What are the periodic trends in first ionization energy? Specifically, address the following:

a) What is the trend within a group? Why?

b) What is the trend within a period? Why?

c) How do main group elements compare with transition elements?

d) Why are there irregularities in the trends?

8. What is the periodic trend for metallic character? How is this property defined? What is a metal? What is a nonmetal? What are the macroscopic characteristics that distinguish metals from nonmetals? What are the particulate-level characteristics that lead to these two classes? What is a metalloid?