3.3 The Quantum Mechanical Model of the Atom

LEARNING TIP

What Is Quantum Mechanics?
Classical mechanics is the branch of physics that studies the motion of macroscopic objects. Quantum mechanics is the study of motion at the atomic level, where the laws of classical mechanics do not apply because particles behave like waves.

Weaknesses in theories and models provide opportunities for science to improve. It is impossible to devise a perfect theory or model the first time around. Instead, science usually involves years and years of revisions and new discoveries. Science is constantly changing by identifying and improving on weaknesses. The success of the Bohr atomic model was important because it showed that electrons exist in discrete energy levels. Also, it explained experimental observations of line spectra in terms of quantum theory. But there were weaknesses in this model that other scientists identified, which paved the way for the complete development of the quantum model of the atom.

By the mid-1920s, it had become apparent that the Bohr model could not explain and make predictions about multi-electron atoms. A new approach was needed. Three physicists were at the forefront of this effort: Erwin Schrödinger, Louis de Broglie, and Werner Heisenberg. The approach they developed to explain properties of matter is called wave mechanics or, more commonly, **quantum mechanics**. CAREER LINK

quantum mechanics the application of quantum theory to explain the properties of matter, particularly electrons in atoms

Schrödinger's Standing Wave

Louis de Broglie, a French physicist, originated the idea that the electron, previously considered just a particle, has wave properties. Pursuing this line of reasoning, Erwin Schrödinger, an Austrian physicist, decided to approach the problem of atomic structure by focusing on the wave properties of the electron. To Schrödinger and de Broglie, an electron bound to a nucleus in an atom resembled a standing wave, so they began research on a description of the atom based on wave behaviour instead of particle behaviour.

The strings on instruments such as guitars and violins are attached at both ends. When you pluck the string, it vibrates and produces a musical tone. The waves produced by the plucking are standing waves. They are called "standing" because they appear to be stationary. The motions of the string are a combination of simple waves of the type shown in **Figure 1**.

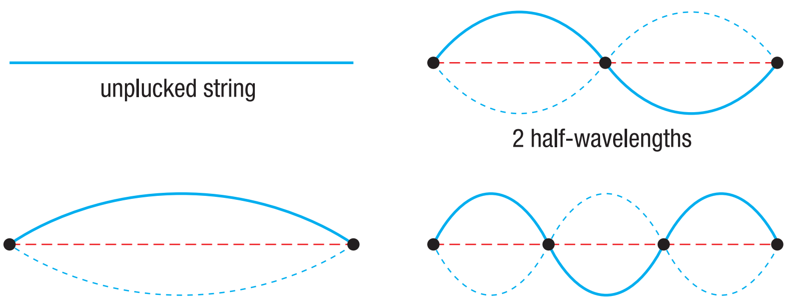

Figure 1 The standing waves caused by the vibration of a guitar string fastened at both ends. Each black dot represents a node (a point of zero displacement), which never moves.

The black dots in Figure 1 represent the nodes, or points, of zero lateral (sideways) displacement for a given wave. Between two nodes, at the point where the amplitude of the wave is at its maximum, is the antinode. Note that there are limitations on the allowed wavelengths of the standing wave. Each end of the string is fixed, so there is always a node at each end. This means that there must be a whole number of half-wavelengths in any of the allowed motions of the string.

Figure 2 shows how standing waves can be produced by a wave generator.

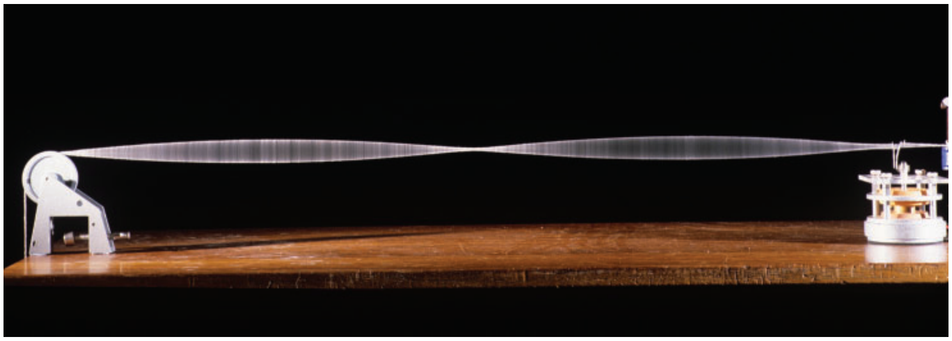

Figure 2 This wave generator is set to produce standing waves that are two half-wavelengths (one wavelength) long.

Mini **Investigation**

Modelling Standing Electron Waves

Skills: Performing, Observing, Analyzing, Evaluating, Communicating SKILLS HANDBOOK A2.3

Schrödinger's standing waves can be simulated with a mechanical model. A mechanical oscillator causes a loop of wire to vibrate at varying frequencies. Creating vibrations at one point along the wire causes waves throughout the remainder of the wire. This activity is like holding the edge of a stretched Slinky and moving it up and down to produce waves along it. When waves return toward the original direction, they encounter other waves: If they meet constructively, there will be an increase in amplitude. If they meet destructively, there will be a decrease in amplitude. Standing waves result in stationary nodes (no amplitude) and antinodes (at maximum amplitude).

Equipment and Materials: oscillator; stand; loop of wire

When unplugging the oscillator, pull on the plug, not the cord.

Ask your teacher to check the attachment of the wire to the oscillator.

1. Position the oscillator on a laboratory stand. Attach the wire. Position the wire so that its loop is horizontal.
2. Turn the frequency as low as it will go. Plug in the oscillator, then turn it on.
3. Increase the frequency a little. Observe the changes in the waves on the wire.
4. Increase the frequency setting slowly until you can no longer see the nodes and antinodes.
5. Decrease the frequency slowly to the starting point. Observe the simulation in reverse order.
6. Repeat this procedure as necessary.

A. Describe what the nodes and antinodes look like. K/U T/I

B. Do all frequencies result in standing wave patterns? Explain. K/U T/I

C. List the number of nodes and antinodes you were able to observe. K/U T/I

D. How do the waves produced by the oscillator compare with waves in an atom? What are some limitations of the standing wave model of the atom? K/U T/I A

Schrödinger and de Broglie took the idea of standing waves and applied it to the electron in a hydrogen atom. In their model, the electron is a circular standing wave around the nucleus (**Figure 3**). This circular standing wave consists of wavelengths that are multiples of whole numbers ($n = 1, 2, 3, 4, \ldots$). Only certain circular orbits have a circumference into which a whole number of wavelengths can fit.

Any other orbits of the standing electron wave are not allowed because they would cause the standing wave to cancel out or collapse, that is, undergo destructive interference (Figure 3(c)). This model seemed like a possible explanation for the observed quantization of the hydrogen atom: the whole-number multiples of wavelengths correspond to multiples of fixed quanta of energy that the electron can have in the hydrogen atom. However, the new question that this model raised was this: where is the electron located in the hydrogen atom?

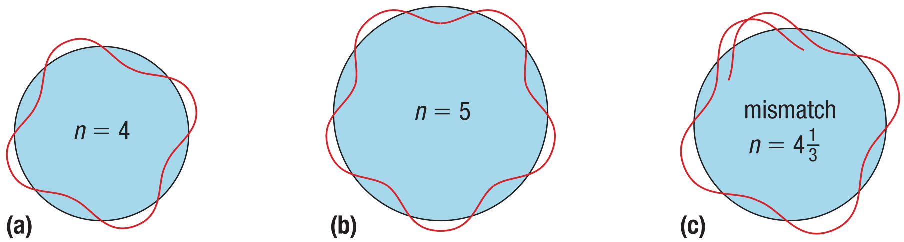

Figure 3 The hydrogen electron visualized as a standing wave around the nucleus. In (a) and (b), the circumference of a particular circular orbit corresponds to a whole number of wavelengths. (c) Otherwise, destructive interference occurs. This model is consistent with the idea that only certain electron energies are allowed, because the atom is quantized. Although this idea encouraged scientists to use a wave theory, it does not mean that the electron travels in circular orbits around the nucleus.

Orbitals and Probability Distributions

orbital the region around the nucleus where an electron has a high probability of being found

Heisenberg's uncertainty principle the idea that it is impossible to know the exact position and speed of an electron at a given time

Schrödinger's work on quantum mechanics led to his development of a mathematical equation, called the Schrödinger wave equation, that could be used to calculate electron energy levels. If an electron has a definable energy, then it can be localized in an **orbital**, which is the region around the nucleus where there is a high probability of finding an electron. But how can you locate something as small as an electron?

Werner Heisenberg, who studied with Bohr, came up with a statistical approach for locating electrons. To measure the location and speed of an object, you must be able to observe it. Life-sized objects are easy to locate because you can see them. You can determine both the speed and the location of a moving car using a radar gun and a GPS unit. For atomic-sized particles and smaller, any attempt to probe them changes their position, direction of travel, or both. This idea formed the basis of Heisenberg's uncertainty principle. Heisenberg demonstrated using mathematics that there are limits to knowing both where a subatomic particle is and its speed at a given time. According to **Heisenberg's uncertainty principle**, it is therefore impossible to simultaneously know the exact position and speed of an electron. The best we can do is to describe the probability of finding an electron in a specific location.

An electron orbital is analogous to students at school moving from classroom to classroom during a scheduled break. The students are like electrons, the school is like the atom, and the classrooms are like orbitals. Someone who does not know a student's exact schedule may be able to determine the probability of that student being in a particular classroom at a particular time, but it is not certain. Another analogy with more appropriate relative sizes is a bee in a closed stadium. You know that the bee is inside the stadium, and you can reason that it will most likely be near its nest. However, you cannot pinpoint its exact location.

A **wave function** is a mathematical description of an orbital in an atom where an electron of a certain energy is likely to be found. Note that an orbital is not a Bohr orbit—the electron is not moving around the nucleus in a circle. How, then, is the electron moving? The answer is surprising: we do not know. The wave function gives no information about the detailed pathway of the electron. This idea is somewhat disturbing. When we solve problems involving the motions of objects in the macroscopic world, we are able to predict their pathways. For example, when 2 billiard balls with known velocities collide, we can predict their motions after the collision. However, we cannot predict the electron's motion. It is a mystery what electrons do in the atom. Quantum mechanics does not describe how an electron moves or even if it moves. It only tells us the statistical probability of finding the electron in a given location in an atom. The area or region where we are likely to find an electron is an orbital.

wave function the mathematical probability of finding an electron in a certain region of space

Using wave functions, physicists have created a three-dimensional **electron probability density**, which is a plot that indicates regions around the nucleus with the greatest probability of finding an electron. The electron probability density plot for a hydrogen electron in the ground state (lowest energy state) is spherical and is called the 1*s* orbital (**Figure 4(a)**). The greatest probability of finding the electron occurs at a distance r_{max} from the nucleus (**Figure 4(b)**). This distance is the same as the distance Bohr calculated for the radius of the first circular orbit of hydrogen's electron.

electron probability density the probability of finding an electron at a given location, derived from wave equations and used to determine the shapes of orbitals; also called electron probability distribution

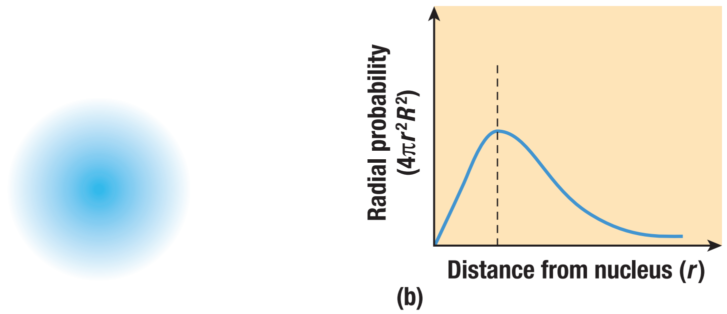

Figure 4 (a) The probability distribution for the hydrogen 1*s* orbital in three-dimensional space. (b) The radial probability distribution is a plot of the total probability of finding the electron as a function of distance from the nucleus.

Figure 5 illustrates different electron orbitals, or clouds. The electron can jump to any of these orbitals if it absorbs sufficient quanta of energy. Furthermore, these orbitals overlap, rather than being distinct levels as in the Bohr model. You will learn more about electron orbitals in the next sections. WEB LINK

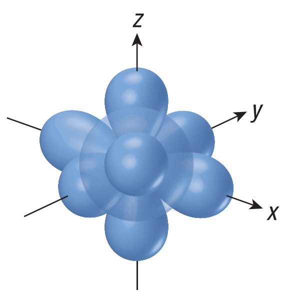

Figure 5 The electron probability density of various orbitals

LEARNING **TIP**

Orbitals versus Orbits

The table below outlines the main differences between orbitals and orbits.

Orbitals	Orbits
2 electrons	$2n^2$ electrons
three dimensions	two dimensions
distance from nucleus varies	distance from nucleus is fixed
no set path	path is elliptical or circular

The two main ideas of the **quantum mechanical model** of the atom are that electrons can be in different orbitals by absorbing or emitting quanta of energy, and that the location of electrons is given by a probability distribution. The quantum mechanical model is a radical departure from earlier atomic models because it is based on uncertainty—the uncertainty of an electron's location within the atom. According to this model, the structure of a tiny atom is much more complex than anyone would have thought possible, as you will see in the next section.

quantum mechanical model a model for the atom based on quantum theory and the calculation of probabilities for the location of electrons

3.3 Review

Summary

- Louis de Broglie originated the idea that the electron has both particle and wave properties.
- The quantum (wave) mechanical model describes an electron as a standing wave.
- The electron can occupy a series of orbitals. Each orbital has a prescribed possible energy value and spatial distribution.
- The exact position of the electron and how it is moving can never both be known. This is consistent with Heisenberg's uncertainty principle, which states that it is impossible to know both the position and the speed of a particle simultaneously.
- Orbitals are described as probability distributions and depicted as electron density plots.
- In the ground state, the single electron in a hydrogen atom resides in a low-energy orbital.
- The two main ideas of the quantum mechanical model of the atom are that electrons can move between orbitals by absorbing or emitting quanta of energy, and that the location of electrons is given by a probability distribution.

Questions

1. Define the following terms and provide an expanded description: K/U
   (a) orbital
   (b) electron probability density
   (c) quantum mechanics
   (d) wave function
   (e) quantum mechanical model
   (f) Heisenberg's uncertainty principle
2. (a) Draw a concept map illustrating the important aspects of the quantum mechanical model of the atom. Include a brief description of each point. Include the terms "wave function," "orbital," "probability density," and "uncertainty principle."
   (b) Expand on your concept map from (a) by including the contributions by Planck, Bohr, de Broglie, Schrödinger, and Heisenberg. K/U C
3. Explain how an electron orbital is not the same as an orbit. K/U
4. What information about the electron cannot be determined from quantum mechanics? K/U A
5. Explain the value of scientists working together and sharing information. How do you think this networking has contributed to current knowledge and understanding of major scientific principles? K/U T/I A
6. Heisenberg, de Broglie, and Schrödinger were all theoretical physicists. Explain why their work is studied in such detail in a chemistry course. K/U T/I A
7. Science is divided into the arbitrary groups of biology, chemistry, and physics. K/U T/I A
   (a) Why do you think science has been so divided?
   (b) This section highlights one area where physics and chemistry overlap. Identify three more areas where the different groups overlap.
   (c) Do you think it makes sense to divide up science into these groups? Explain your reasoning.
8. When most people visualize an atom, they use the Bohr–Rutherford model. K/U T/I A
   (a) Why do you think this is?
   (b) Do you think it is important for most people to understand exactly how the atom functions? Explain your reasoning.
9. Dr. Richard Bader and his research group at McMaster University, Hamilton, are well known for their work on the structure of chemical entities. Research Bader, and determine the nature of his group's work. Prepare a brief, general description of how it relates to quantum mechanics. K/U T/I A
10. Research Schrödinger's wave equation, and identify the different mathematical symbols in it. K/U T/I
11. Research the thought experiment called Schrödinger's cat. What does this thought experiment tell us about the quantum mechanical model of the atom? K/U T/I A

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