CHAPTER 12

Quantum Physics

> While it is never safe to affirm that the future of Physical Science has no marvels in store even more astonishing than those of the past, it seems probable that most of the grand underlying principles have been firmly established and that future advances are to be sought chiefly in the rigorous application of these principles to all the phenomena which come under our notice.
>
> It is here that the science of measurement shows its importance—where quantitative results are more to be desired than qualitative work. An eminent physicist has remarked that the future truths of Physical Science are to be looked for in the sixth place of decimals.
>
> —Albert Abraham Michelson

How ironic that it was Michelson who said this. He thought of himself as a pillar of classical physics, devoting his life to measuring the speed of light more and more accurately. Yet the Michelson–Morley experiment showed that light behaves in a completely unexpected way. It was a signpost on the way, an indication, as seen from our present vantage point, that our understanding of the natural world would be fundamentally different in the future.

There were others. X-rays were discovered by Röentgen in 1895. Today we know that they are electromagnetic waves emitted by atoms or by accelerated charges. Radioactivity was discovered in 1896 by Becquerel. Radioactive emissions come from the nuclei of atoms, but the existence of nuclei was not even suspected at that time. In 1897 J. J. Thomson found that the constituents of a beam of what we now call electrons always have the same ratio of charge to mass, and hence he is usually credited with the discovery of the electron.

In the first part of the twentieth century there were further discoveries in atomic and nuclear physics, one piled on the other. Some of the experiments seemed to contradict well-established knowledge. This was especially true for the observations that showed light to have the seemingly irreconcilable properties of both waves and particles. Attempts to eliminate the difficulties had only limited success. New insights and understanding came, sometimes slowly, sometimes quickly, but the first quarter of the century is now seen as a time of transition.

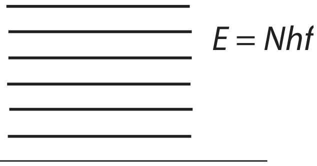
The resolution came in 1925, with the development of quantum mechanics and its synthesis of the wave and particle aspects, not only of light and other electromagnetic radiation, but also of matter and all of its constituents.

12.1 The "old" quantum physics

The year 1900 saw the discovery that would later be seen as leading to the most profound and influential changes in our view of nature. Like the Michelson–Morley experiment it was not just new, but showed that what was thought before was fundamentally flawed. It took years for the implications of the new idea to be understood and to become part of the mainstream of science.

As was true for Michelson, Max Planck saw himself as firmly rooted in the past, and believed that he was just applying Maxwell's work to a different situation. He tried to look at the details of the electromagnetic radiation emitted by hot bodies, such as a red-hot stove, the white-hot wire in a light bulb, or the sun. Experiments had shown that the radiation and its distribution of wavelengths are closely the same at any given temperature, regardless of the nature of the hot material.

He succeeded in developing a formula that describes the way the intensity of the radiation is distributed among the different wavelengths, in other words, the *spectrum* of the radiation. There was, however, a totally unexpected feature. The formula seemed to imply that the particles that make up a hot body, and whose vibrations lead to the emission of the radiation, cannot vibrate with just any frequency, but only with a discrete set of definite, equally spaced frequencies, each of which corresponds to a definite, discrete energy of the vibrating system. There was a lowest frequency, f. All other possible frequencies were multiples of it, Nf. Each was proportional to the corresponding energy of the vibrating body: $E \propto Nf$, where N is a whole number. The proportionality constant is given the symbol h, so that $E = Nhf$. h is a constant of nature and it came to be known as Planck's constant.



The idea that only certain frequencies, and therefore only certain energies are possible is called the *quantization* of energy. It was so at variance with anything that had been previously thought of that no one quite knew whether and how to take it seriously. Einstein, five years later, was the first to take the result to the next logical step. If the emitting material can have only certain definite energies, then in keeping with the law of conservation of energy, the emitted radiation can also not have any arbitrary energy, but must consist of definite amounts (*quanta*) of energy. Einstein introduced the idea of this definite amount, or quantum, of electromagnetic energy, later called a *photon*. Its energy is hf, where this time f is the frequency of the radiation and h is Planck's constant.

The new concept of the photon made it possible to understand the until then mysterious *photoelectric effect*. This is the emission of electrons from a material that is illuminated by electromagnetic radiation, and it had until then been quite incomprehensible. Einstein showed that the energy of each photon of the radiation (hf) is given to the electron as kinetic energy, except for the amount of energy that is necessary to liberate the electron from the material of which it initially forms a part.

Succeeding years brought further seemingly compelling evidence that a beam of light or other electromagnetic radiation consists of photons, particles with energy hf and momentum $\frac{hf}{c}$.

It was clear that the experimental evidence for the existence of photons was revolutionary. It was quite unclear how it could be reconciled with the electromagnetic theory, which was firmly supported by other experiments that demonstrated clearly that light was propagated as waves.

The photoelectric effect

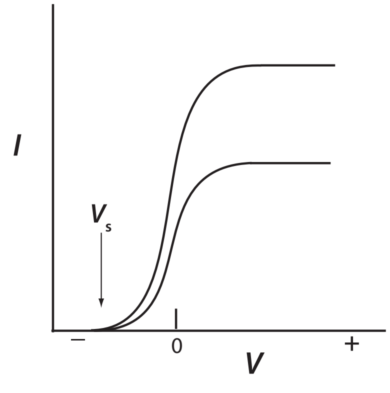
When doors open automatically as we come near, or when an alarm is set off when we cross a certain line, it probably happens because a light beam shining on a *photocell* is interrupted. The light shines on a piece of metal in the photocell and causes electrons to be emitted from the metal. This is called the photoelectric effect, and it has been known since the late nineteenth century.

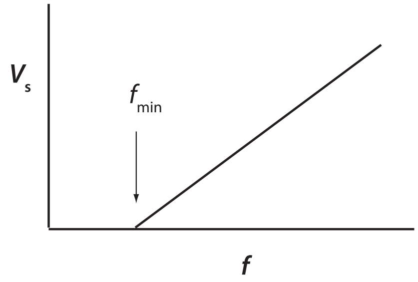
At that time it was confidently expected that like other electric phenomena it would be explained by the electromagnetic theory, which had shown light to be electromagnetic waves. The general features of an explanation seemed clear. An electromagnetic wave has an oscillating electric field. As the wave hits a metal, the electrons in the metal find themselves in this field, and experience an oscillating force. We would expect that if this force is strong enough it can shake some electrons loose, and so explain how the photoelectric effect comes about.

Experiments, however, turned up puzzles and discrepancies. The first is that the effect depends on the color of the light. When the frequency is too small (the wavelength too large), no electrons are liberated, regardless of how much light there is.

The second puzzle concerns the energy of the electrons. It is measured by examining how large a voltage is required to stop the electrons. This is like measuring the kinetic energy of a marble by seeing how high a hill it can climb before it stops. The expectation was that more light would lead to a higher energy of the electrons. The results showed, however, that for a given frequency (i.e., for a particular color) of light, the energy of the electrons does not change, no matter what the intensity of the light is. Only the number of emitted electrons is affected. On the other hand, the energy changes when the frequency of the light is different.

These features can be seen in the two kinds of graphs shown here. Each graph in the figure below shows the current of photoelectrons for light of a given frequency. The upper curve is for a greater light intensity. Here V is the voltage between the metal that emits the photoelectrons and an electrode close to it. When V is negative on this graph, it tends to stop the emitted electrons. Beyond some negative value of V





there is no current. This is the "stopping potential," V_s, and it measures the electron energy. When an electron is stopped in an electric field, its kinetic energy is converted to electric potential energy. The charge of the electron times the stopping potential is equal to this potential energy, and therefore it is also equal to the kinetic energy that the electron has before it is stopped.

We see that the magnitude of the current is greater for the greater light intensity of the upper curve, but the energy of the electrons, as measured by the stopping potential, remains the same.

The second graph shows the stopping potential as a function of the frequency of the light. It is even more unexpected. Below a certain frequency no electrons are emitted, and for higher frequencies the electron energy, as measured by the stopping potential, increases linearly with frequency. With different metals the results are similar, but with different minimum frequencies. The consistent pattern of a "threshold" necessary for electron emission was strange and unexpected.

Eventually the puzzling features were explained by Einstein in 1905, but at a startling expense. The explanation did not use the electromagnetic theory. Instead Einstein used the concept of quantized energy, so reluctantly invented by Planck five years earlier. He said that the emitted light consists of bundles of energy (the photons) that behave like particles and not at all like waves.

Planck had considered only the material that emits the waves. To fit the experiments he had been forced to the conclusion that only certain energies were possible for the material as it emitted the waves. He did not really seem to trust this revolutionary discovery, and it was not carried further in the next few years. Einstein realized that if the emitting material could exist only with certain energies, then the emitted light would also have to exist in bundles of definite energy. When the emitting material goes from one definite energy to another, the light carries away the difference in energy, and must also consist of definite amounts or *quanta* of electromagnetic energy, which were subsequently called "photons."

The explanation of the photoelectric effect now becomes amazingly simple. Each photon can liberate an electron. It takes a certain amount of energy to do that, different for different materials, depending on how strongly the electrons are attached, or *bound*. The amount of energy to free the electrons—their "binding energy" E_B—is also the minimum energy that a photon must have if an electron is to be emitted. Any extra energy is given to the electron as kinetic energy.

If the photon energy is hf, the kinetic energy of the electron is K, and the smallest energy that it takes to liberate the electron is E_B, then $hf = K + E_B$. This is the result for which Einstein was awarded the Nobel Prize, but not until 17 years later. (For metals the smallest amount of energy that will liberate electrons is called the *work function*).

The equation was immediately successful. It explained the photoelectric effect and established the existence of photons. The question of what happened to the wave theory, which was supported by many experiments, and which had seemed to be firmly established until that time, was left unanswered.

Go to the PhET website and open the simulation *Photoelectric Effect*.

You can vary the material of the target. You can also vary three quantities with sliders: the light intensity, the battery voltage, and the wavelength.

Choose sodium.

(a) Set the intensity at 35% and the wavelength at about 150 nm. Check "current vs battery voltage."

Vary the battery voltage with the slider on the battery on both sides of zero and observe the first graph, current against voltage. Compare the graph to the corresponding graph in the text. Why are the shapes somewhat different there? Observe the electrons in each of the voltage regions. At what battery voltage does the current go to zero? This is the "stopping potential." What is the energy of the photoelectrons?

Increase the intensity to 60%. What are the stopping potential and the photoelectron energy now?

(b) Check the boxes to see the other two graphs. What do you see on the second graph as you change the battery voltage? What do you see on the third graph? Does it correspond to your prediction?

(c) Uncheck the boxes for the second and third graphs so that you see only the first. Set the wavelength at about 300 nm. Again vary the battery voltage. What are the stopping potential and the photoelectron energy? What is the frequency of the light?

What do you expect for the graph of photoelectron energy vs. light frequency? Turn on the third graph vary the wavelength, and see whether your prediction was correct.

(d) Why is it that below a certain frequency there are no photoelectrons? What is that frequency for sodium? What quantity in the Einstein photoelectric equation can you calculate from that frequency? What is it, from your graphs, for sodium?

(e) Put the intensity again at 35% and set V at 0.

Vary the wavelength and observe the third graph, electron energy against frequency.

(f) Choose zinc. Find its work function from the graphs of the simulation.

EXAMPLE 1

In zinc the minimum amount of energy that it takes to remove an electron is 4.3 eV.

(a) What minimum energy and frequency must a photon have to produce a photoelectron?

(b) What is the wavelength of that photon?

(c) A photoelectron is produced by a photon that has an energy twice the minimum. What is the energy of the photoelectron?

Ans.:

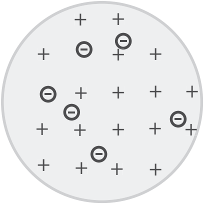
(a) The minimum energy of the photon is 4.3 eV. This energy is equal to hf. Planck's constant, h, is equal to 6.63×10^{-34} Js. Before we can use the relation $E = hf$, we have to convert the value of the energy to SI units: $E = (4.3)(1.6 \times 10^{-19}) = 6.9 \times 10^{-19}$ J. Now we can use $f = \frac{E}{h} = \frac{6.9\times10^{-19}}{6.63\times10^{-34}} = 1.04 \times 10^{15}\,\mathrm{s}^{-1}$ or 1.04×10^{15} Hz.

(b) $\lambda = \frac{c}{f} = \frac{3\times10^{8}}{1.04\times10^{15}} = 2.9 \times 10^{-7}\,\mathrm{m} = 290\,\mathrm{nm}$.

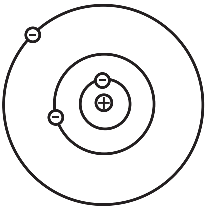
(c) If the photon energy is twice 4.3 eV, the energy above 4.3 eV goes to the photoelectron. Here this energy is 4.3 eV.

Bohr's vision of the atom

The greatest triumph of the early quantum theory came with Bohr's model of the hydrogen atom in 1913. There had been an earlier atomic model by J. J. Thomson that envisioned electrons stuck in a ball of positive charge. This model could not predict any of the observed atomic properties and had to be abandoned.



Thomson



Bohr

Bohr's "planetary" model of electrons in orbit around a nucleus gave a more realistic view of atomic structure. It led to the correct allowed, quantized, energies of the hydrogen atom and to values of the atom's size that are closely related to what we know today. It also has the advantage that it uses only some elementary mechanics and Coulomb's law.

The Bohr model is easy to visualize and is relatively simple. As a result it has continued to have a life far beyond the time in 1925 when it was replaced by a model based on *quantum mechanics*, the modern theory of matter, which requires more complicated mathematical methods. The picture of electrons moving in circles or ellipses about the nucleus is still widely used to illustrate what atoms are like, in spite of the fact that it is obsolete and even misleading.

It is therefore a legitimate question whether there is any value in going into detail about the

Bohr model. We will do so, briefly, because of its historical importance and because it allows us to introduce some important concepts.

We need not stay with Bohr's original sequence and terminology, and will use modern terms wherever possible. We will emphasize which aspects are still regarded as correct and which have to be discarded.

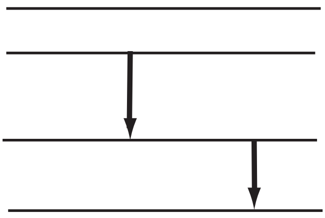
As we show where it falls short, we will be able to introduce some of the features of today's quantum mechanics that are startlingly different, but have proved themselves to be enormously more powerful in their description and analysis of atoms and their combinations.

Here are the basic ingredients of the Bohr model of the atom.

1. *The atom consists of a nucleus and electrons.*

   The existence of the nucleus was known from the work of Rutherford. He bombarded atoms (in a gold foil) with radioactive particles (alpha particles, which he later showed to be helium nuclei). By analyzing the way they bounced off, he showed that almost all of the atom's mass is concentrated in a minute piece in its middle, the nucleus.
2. *The only force acting between the nucleus and the electrons is the electric force, as described by Coulomb's law.*

   The gravitational force is too weak, and the nuclear forces, which were then unknown, act only over much smaller distances. The realization that the electric force is the only force that acts between the nucleus and the electrons (as well as between atoms), and that it has precisely the same form there as in the macroscopic domain, is still fundamental to all our understanding of atomic phenomena.
3. *The atom can exist only in states with certain total energies or "energy levels."*

   This is as in Planck's original hypothesis. The allowed energies can be described in an *energy level diagram*. Each allowed energy is represented by a horizontal line. The lines are spaced along a vertical scale that is proportional to the energy.
4. *The atom can make transitions between energy levels with the emission or absorption of energy.*

   One way it can do this is by the emission or absorption of a photon, a quantum of electromagnetic energy, hf, equal to the energy difference between the levels before and after the emission or absorption, so that energy is conserved. The emitted photon has exactly the energy equal to the energy difference between the initial and final energy levels. Similarly, a photon is absorbed only if its energy is exactly equal to the energy difference between the initial and some final level. If there is no such level the photon is not absorbed, i.e., a collection of such atoms is *transparent* to photons of that frequency and energy.

Each of these statements remains as valid today as it was when Bohr used them in 1913. Bohr, however, imagined definite mechanical orbits for the electrons. Today we know that there are no circular or other geometric orbits, and that we can only determine the probability of finding the electron in a particular region or at some particular distance from the nucleus.

Now we come to the actual calculation of the energy levels for the simplest atom, that of hydrogen. According to Bohr's initial model its single electron moves in a circle around the proton at its center.

Bohr knew that there was a problem with the orbits. An electron moving in a circle is accelerated (with the centripetal acceleration $\frac{v^2}{r}$), and Maxwell's theory shows that an accelerated charge radiates, and so loses energy. This happens, for instance, in modern synchrotrons, where electrons race around a circular track, and which are used as sources of intense electromagnetic radiation. Bohr simply said ("postulated") that this doesn't happen in atoms, and that the energy remains constant as long as an electron moves in one of the orbits allowed to it.

This was his major contribution, together with the prescription for finding the allowed orbits, or, as we would prefer to say today, the allowed energy levels. He did this by making a further postulate, known as the *quantization* *condition*, that said that the angular momentum of the electron (mvr) could only be a multiple of Planck's constant divided by 2π, i.e., $\frac{h}{2\pi}$, today written as $\hbar$ (pronounced "h-bar"). In other words, $mvr = n\hbar$, where the *quantum number*, n, can take on the values 1, 2, 3, and so on, up to infinity.

He tried to justify this choice, but the major justification came from the fact that the quantization condition could be used, together with Coulomb's law, to calculate the allowed energy levels, and that they came out correctly, i.e., in accord with the experimentally observed radiation from hydrogen.

Here is the result: the allowed energies of the hydrogen atom are described by the formula $E_n = \frac{E_1}{n^2}$, where $E_1 = -13.6\,\text{eV}$. The negative sign follows from the choice of the reference level as $E = 0$ when the electron and the nucleus are far apart, i.e., when $\frac{1}{r} = 0$. When the hydrogen atom is in one of the allowed, stable states, energy needs to be given to it to bring it to this reference level. In other words, its energy needs to be raised to bring it to zero. All the allowed energies are therefore negative.

Each value of the *quantum number*, n, corresponds to one of the allowed values of the energy. For $n = 2$, the energy is $+\frac{13.6}{4}$ eV, or -3.4 eV, and so on. The radius of the atom is $n^2 r_1$, where r_1, the radius of the atom when it is in its lowest (ground-state) energy level, is 0.53×10^{-10} m or 0.053 nm. (A unit that is often used for atomic distances is the *Angstrom*, equal to 10^{-10} m, so that the ground–state radius of the hydrogen atom according to Bohr is 0.53 Å.)

As n increases, and the energy gets closer to zero, the radius becomes larger. When n goes to infinity, r also goes to infinity, and the electron and the proton are completely separated.

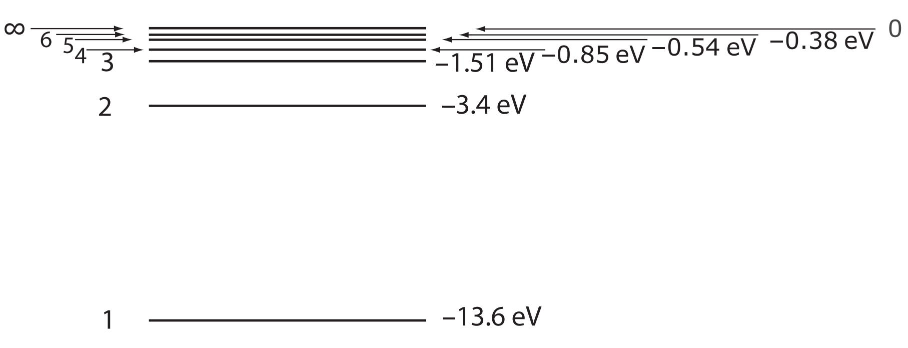
Bohr's assumption of circular electron orbits was wrong. His method of calculating the energies was wrong. The values of angular momenta of his quantization condition turned out to be wrong. But the notion of energy levels is correct, and he got the right values for them for the hydrogen atom. His model also led to values for the radii of the orbits, and so to the atomic size. The picture of atoms with exact radii later had to be abandoned and replaced by the statements of quantum mechanics, which allow us to say only what the probability is of finding the electron at a given distance from the nucleus. The probabilities turned out to have maxima at or close to the Bohr orbits, so that the model was basically successful in describing the atomic size.

The successes were so impressive that it was difficult to doubt that Bohr had shown the correct path. Over the next decade attempts were made by Bohr and others to extend the model to atoms with more than one electron and to describe other atomic properties. Success seemed tantalizingly close, but more and more assumptions had to be made, and it proved more and more difficult to find agreement between theory and observation. It was eventually realized that radically new ideas were required, and they came, starting in 1924, in a torrent of activity and creativity, and with astonishing success.

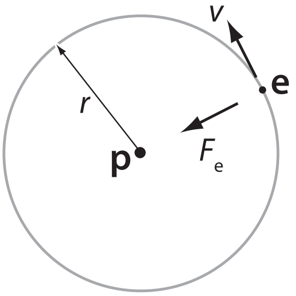
Bohr's calculation

Here is the Bohr model calculation for the energy levels and the radii of the hydrogen atom.

Bohr's electron moves in a circle, so that there must be a force on it toward the center (a centripetal force) equal to $\frac{mv^2}{r}$. In this case the force is the electric force of attraction to the



proton, $\frac{ke^2}{r^2}$, where e is the magnitude of the charge on the electron or the proton.



The first equation is therefore

$$F = \frac{ke^2}{r^2} = \frac{mv^2}{r}$$

which we can rewrite as $v^2 = \frac{ke^2}{mr}$.

The second equation is the quantization condition, which says that the angular momentum of the atom is a multiple of $\hbar$:

$$mvr = n\hbar$$

so that $v = \frac{n\hbar}{mr}$.

We can square it and set the two relations for v^2 equal to each other, to get

$$\frac{ke^2}{mr} = \frac{n^2\hbar^2}{m^2r^2}$$

which we can solve for r, to get

$$r = n^2 \frac{\hbar^2}{kme^2}$$

For $n = 1$, the radius is $r_1 = \frac{(1.055\times10^{-34})^2}{(9\times10^9)(0.91\times10^{-30})(1.6\times10^{-19})^2}$, which is 0.53×10^{-10} m or 0.53 Å.

The other radii are $r_n = n^2 r_1$, four times as large for $n = 2$, nine times as large for $n = 3$, and so on for other values of n.

Now we can find the energies. Instead of calculating the kinetic energy and the potential energy separately, we see that the Coulomb's law relation can also be written $\frac{ke^2}{r} = mv^2$, where the left side is the negative of the potential energy and the right side is twice the kinetic energy, $2K$. We will follow the established practice and call the potential energy U in the rest of this chapter so that $-U = 2K$. The total energy is $E = U + K$ or $U - \frac{U}{2}$, so that $E = \frac{U}{2}$ or $\frac{-ke^2}{2r}$.

With our earlier value for r this is equal to

$$E = -\frac{ke^2}{2}\frac{kme^2}{n^2\hbar^2}$$

or

$$-\frac{1}{n^2}\frac{k^2me^4}{2\hbar^2}$$

For $n = 1$ this is $-\frac{(9\times10^9)^2(0.91\times10^{-30})(1.6\times10^{-19})^4}{(2)(1.055\times10^{-34})}$ J or -13.6 eV. The other energies can be written as $E_n = (\frac{1}{n^2})E_1$, so that they are $-\frac{13.6\,\text{eV}}{4}$ for $n = 2$, $-\frac{13.6\,\text{eV}}{9}$ for $n = 3$, and so on, up to $E = 0$ as n approaches infinity.

The lowest state ($n = 1$) is the *ground state*. The others are the *excited states*. The atom will, unless something prevents it from doing so, go to the lowest state that is available to it. As it goes to a lower state it gives up the difference in the energy. One way to do this is to emit a photon. Let's look at a transition from the state $n = 3$ to the state $n = 2$. The energies of the excited states are $\frac{E_1}{4} = -3.4$ eV for $n = 2$ and $\frac{E_1}{9} = -1.51$ eV for $n = 3$. The photon energy is $\frac{E_1}{9} - \frac{E_1}{4}$ or $-1.51\,\text{eV} - (-3.4\,\text{eV})$, which is about 1.9 eV. We can also calculate the corresponding frequency and wavelength from the fact that the photon energy is hf and the wavelength is $\frac{c}{f}$. (Just remember that you have to pay attention to the system of units: in the SI system you first have to change from eV to joules, and the wavelength then comes out in meters. The frequency is in hertz [Hz], where 1 Hz is one vibration per second.)

As n increases, and the energy gets closer to zero, the radius (n^2r_1) gets larger. When n and r go to infinity, the electron and the proton are completely separated, and both the kinetic energy and the potential energy go to zero.

Our choice for the reference level leads to the fact that when the electron is closer to the nucleus, so that its potential energy is smaller than at the reference level, both the potential energy and the total energy are then negative.

To take the atom from its ground state to the state where the electron and proton are infinitely far from each other, we have to give it 13.6 eV. This, the energy to destroy the atom, is also called its *binding energy*.

To remove the electron is called to *ionize* the atom. The hydrogen atom's *ionization energy* is therefore also 13.6 eV.

EXAMPLE 2

(a) What is the total energy and what are the potential and kinetic energies of a hydrogen atom in the state with $n = 4$?

(b) What are the energy, frequency, and wavelength of the light emitted by a hydrogen atom in the transition from the state with $n = 4$ to the state with $n = 2$?

Ans.:

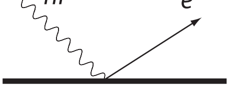
(a) For $n = 4$ the energy is $-\frac{E_1}{4^2} = -0.85$ eV. The potential energy is twice as large and the kinetic energy is 0.85 eV.

(b) The energy is $\Delta E = E_4 - E_2 = -0.85 - (-3.40) = 2.55$ eV.

The frequency is $\frac{\Delta E}{h}$. In SI units the energy is $(2.55)(1.6 \times 10^{-19}\,\text{J}) = 4.08 \times 10^{-19}$ J, and $f = \frac{\Delta E}{h} = \frac{4.08\times10^{-19}}{6.63\times10^{-34}} = 6.15 \times 10^{14}$ Hz. The wavelength is $\frac{c}{f} = \frac{3\times10^8}{6.15\times10^{14}} = 4.88 \times 10^{-7}$ m = 488 nm(= 4880 Å).

Suddenly, photons everywhere

The Bohr model's success confirmed the existence of the photons that Einstein had introduced when he explained the photoelectric effect. We have already discussed the photoelectric effect: the photon hits a material and gives all of its energy to an electron. Part of the energy is used to liberate the electron, i.e., to overcome its binding energy. Whatever is left over is given to the electron as kinetic energy.



$$hf = K + E_B$$

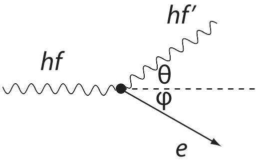
where the left side is the photon energy and the right side is the kinetic energy, K, of the electron plus its binding energy. (The binding energy, E_B, is the energy needed to separate the electron from the material of which it is originally a part.) This is Einstein's photoelectric equation. In the initial experiments the electrons were ejected from metals in which the binding energy of the electrons that are released is typically of the order of a few eV.

The Compton effect

A second interaction between a photon and an electron is the Compton effect. This time the photon gives only part of its energy to an electron and gives the rest to a new photon. The energies are related by

$$hf = hf' + K_e$$

where hf is the energy of the original photon, f' is the frequency of the new photon, which is also called the recoil photon, and K_e is the electron's kinetic energy.



This experiment was done with x-rays with frequencies two or three orders of magnitude greater than those of visible light. The photon energies are therefore also greater (of the order of keV), and the electron's binding energy is so small by comparison that it is usually neglected. The Compton effect can therefore be analyzed as a collision between a photon and an electron in which both energy and momentum are conserved.

The result is a relation between the wavelength, λ, of the original photon and the wavelength, λ′, of the new photon. Their difference is

$$\lambda' - \lambda = \Delta\lambda = \frac{h}{m_e c}(1 - \cos\theta)$$

This result, the *Compton effect equation*, is startling and incomprehensible to anyone who expects the radiation to follow Maxwell's electromagnetic theory. The photon collides with an electron and its energy changes. Its frequency and wavelength change. It is as if a beam of blue light were suddenly to turn red. Once again we are confronted with the particle properties of photons.

EXAMPLE 3

In the Compton effect the most probable angle for the recoil photon is 180°. What is the energy of the Compton electron for this angle when the energy of the original photon is equal to $E_0 = m_e c^2 = 0.51\,\text{MeV}$, the rest energy of an electron?

Ans.:

For $\theta = 180°$, $\cos\theta = -1$, and $(1 - \cos\theta) = 2$.

$\lambda = \frac{c}{f} = \frac{hc}{hf} = \frac{hc}{E}$.

The Compton equation for this angle can now be written as

$\frac{hc}{E'} - \frac{hc}{E} = \frac{2h}{m_e c}$ or $\frac{1}{E'} - \frac{1}{E} = \frac{2}{E_0}$.

We can solve for E' by writing $\frac{1}{E'} = \frac{1}{E} + \frac{2}{E_0} = \frac{2E+E_0}{EE_0}$ so that

$E' = \frac{EE_0}{2E+E_0}$.

For $E = E_0$, E' is equal to $\frac{E_0^2}{3E_0} = \frac{1}{3}E_0$.

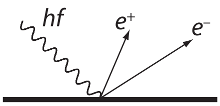
The energy of the electron is $E - E'$, which is $\frac{2E_0}{3}$.

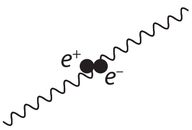
For all other angles the electron energy is less. It ranges from zero to $\frac{2}{3}E_0$.

For higher photon energies the ratio of the electron energy to the photon energy (which here is $\frac{2}{3}$) is closer to one.

Pair production and annihilation

If a photon has still larger energy, of the order of MeV, it can create an electron–positron pair. (The positron is like an electron, but positively charged.) This time the particles are not just knocked out of a material or given some momentum in a collision. They are not there at all to start with, and are created in the process that is called *pair production*. The creation uses up an energy equal to the rest energy of the two particles, which is 1.02 MeV, which is therefore the minimum energy that a photon must have if this process is to occur. If the photon has additional energy it is given to the two particles as kinetic energy.





The photoelectric effect, the Compton effect, and pair production are three processes that are initiated by photons. There are also processes that go in the other direction, initiated by electrons and resulting in photons. One is *pair annihilation*. If an electron and a positron find themselves near each other, they will *annihilate*, i.e., they will both disappear, and give their energy to two photons.

This usually happens when a positron (for example, after being emitted by a radioactive substance) slows down and comes approximately to rest near an electron. The momentum of the two particles at rest is zero, and that is why a single photon cannot be created. It takes two photons, moving off in opposite directions, to satisfy the law of conservation of momentum.

EXAMPLE 4

Most detectors and counters of high-energy photons do not detect or count the photons directly. Instead they count the electrons emitted through one of the *photon-electron interactions*.

A photon has an energy of 2 MeV. What are the three processes by which this photon can lose energy with the emission of one or more electrons? What is the range of energies of the resulting electrons in each case?

Ans.:

The three processes are the photoelectric effect, the Compton effect, and pair production. In the photoelectric effect the photon loses all of its energy. A few eV are used to liberate the electron, but most of the 2 MeV go to the photon.

In the Compton effect part of the energy goes to the electron and part goes to the recoil photon. The Compton-effect equation shows that the largest difference between the initial photon and the recoil photon occurs when the angle between them is 180°. This, then, is the angle between them for which the electron energy is largest. The previous example showed that the energy of the recoil photon for this angle is $E' = \frac{EE_0}{2E+E_0}$. The corresponding electron energy is $E_e = E - E' = E - E' = E - \frac{EE_0}{2E+E_0} = \frac{E(2E+E_0)-EE_0}{2E+E_0} = E\frac{2E}{2E+E_0}$.

For a 2-MeV photon this is $\frac{4}{4.51}E = 1.77\,\text{MeV}$. The electron can have any energy from zero up to this maximum.

In pair production 1.02 MeV ($= 2E_0$) is used to create the pair. The rest, 0.98 MeV, is shared as kinetic energy between the electron and the positron.

EXAMPLE 5

A positron and an electron are at rest next to each other. What happens?

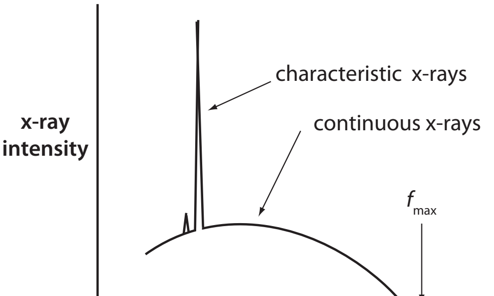
Ans.:

The positron and the electron disappear. They *annihilate*. In their place two photons appear, going in opposite directions, each with the energy $E_0 = 0.51\,\text{MeV}$.

X-rays

The final process that we will consider is x-ray production. Actually there are two processes. They occur together when a beam of electrons hits a target material. (In commercial x-ray tubes it is usually a metal high up in the periodic table of elements, because the emission of x-rays is then more likely.)

When the electrons hit the target, they are stopped. This means that they undergo an acceleration, and we already mentioned in connection with the Bohr model that accelerated electrons are expected to radiate. In x-ray production this actually happens. The result is easily understood in terms of photons. The electrons can give the photons various amounts of energy, but the maximum energy that a photon can get is equal to the energy of an electron in the beam. The emitted photons have a maximum energy and frequency and a corresponding minimum wavelength. All lower energies are possible, and the process is therefore called *continuous x-ray production*.



The second process that occurs simultaneously is the result of the fact that the electrons can raise the atoms of the target material to higher energy levels or knock electrons out completely. The target atoms will come back to the ground state with the emission of photons. The photons have the energies characteristic of the energy-level structure of the target atoms and are therefore called *characteristic x-rays*. Because the target is a heavy metal, the x-ray energies are in the range of 1000 eV (keV) rather than the eV of the hydrogen atom.

EXAMPLE 6

The electrons in an x-ray tube are accelerated by a potential difference of 12 kV in an electron gun. What are the minimum and maximum energies, frequencies, and wavelengths of the x-rays that are produced?

Ans.:

The maximum x-ray energy is 12 keV and the minimum is zero. The minimum frequency is zero and the maximum wavelength is infinite. The maximum frequency is $\frac{E}{h} = \frac{(12000)(1.6\times10^{-19})}{6.63\times10^{-34}} = 2.9\times10^{18}\,\text{Hz}$. The corresponding wavelength is $\frac{c}{f} = \frac{3\times10^{8}}{2.9\times10^{18}} = 1.03\times10^{-10}\,\text{m} = 0.103\,\text{nm}$.

12.2 The new synthesis

Photons and electromagnetic waves

There was an overwhelming amount of evidence that showed that light and other kinds of electromagnetic radiation consist of photons, each with a definite amount of energy and a definite amount of momentum, both proportional to the frequency.

But what does it mean to have a photon with a certain frequency? Frequency and wavelength are the attributes of waves, not of particles. What happened to the electromagnetic waves that had so successfully explained the phenomena of light earlier? There seemed to be no way that a particle theory could explain interference and polarization.

What a dilemma! More and more phenomena were discovered that could be explained only by assuming that light consists of photons. At the same time the phenomena of interference and polarization seemed to make it clear that light is a wave phenomenon. Two theories seemed to be necessary to describe light, and the two were quite incompatible.

So which is it? Does light consist of particles or waves? Is it just one of the two, or both, or neither one? The question is at the heart of the difference between classical physics, i.e., Newtonian mechanics and the electromagnetism of Maxwell, and *modern* physics.

Faced with incontrovertible evidence for light waves as well as for photons there seemed to be no way out. The established view of the time became that it had to be both, with light propagating as waves and being emitted and absorbed as photons. It didn't seem to make sense, but no one knew how to resolve the dilemma. There was good reason to believe that important elements to understanding were missing, but that is easier said looking back from our present vantage point.

Complementarity

Bohr tried to transform ignorance into virtue by enshrining it in a new philosophical principle called *complementarity*. He said that both aspects of light exist. They represent *complementary* views that are different and even opposite and incompatible. Only by looking from different viewpoints and accepting both can the whole range of phenomena surrounding the concept of light be seen and understood.

Having established a principle meant that it could, perhaps, be applied to other phenomena. Bohr tried to do this. He pointed to complementary approaches in realms far from physics. There is reason and emotion, thought and sentiment, justice and love. The roles of actor and spectator are complementary, in that it seems that you can only be one or the other, but with a fuller view resulting from being both. And think about being both a student and a teacher! Bohr suggested that different cultures are complementary, in that differences in background lead to profound differences in points of view, with a higher synthesis coming with knowledge and experience of the complementary modes of life and thought.

The photons and their guide

Today we can make a beam of light with such small intensity that what we observe is only one, or just a few photons. Each can be separately detected by a *counter*.

Is light really just photons, or is it photons sometimes and waves at other times? Bohr said that both were necessary, and represented complementary points of view. Only with the inclusion of both apparently incompatible sets of phenomena could the full range and meaning of the concept of light be understood.

Today there is a better answer, consistent with all observations and free of the earlier contradictions. This, then, is the synthesis of the wave and particle descriptions: light is an electromagnetic wave. It moves through space as a vibration of electric and magnetic fields. The electric and magnetic fields travel together just as Maxwell described them. The experimental evidence consists of Young's double slit experiment and all the other phenomena that are the result of interference effects.

What Maxwell didn't know is that the field is *quantized*. When it interacts with a screen or anything else, it can do so only in definite amounts, each of which is a quantum of the electromagnetic field. *The photon is a quantum of the electromagnetic field.*

We don't know where a photon will appear on the screen. If there is only one it can be anywhere. Only when there are many of them can we predict what the pattern on the screen will be.

The intensity of light can be described and calculated from the wave theory just as was true before photons were ever thought of. Maxwell showed it to be proportional to the square of the electric field. Now, however, we have to interpret the intensity as telling us how many photons are likely to be observed: *the square of the electric field at any point on the screen is proportional to the probability that a photon can be observed there.* We need both concepts. *The wave tells us where the photons are likely to be.*

The electromagnetic wave, with its propagating electric and magnetic fields, is a ghostly presence, guiding and deciding what can be "seen," but it is not itself directly observed. What we observe are the photons, the quanta of the field. Whenever the wave hits something, as for example in the photoelectric effect, it can lose energy. But it can do so only in pieces, in the *quanta* of the field. We then observe photons, with their definite energy and momentum.

We can't tell precisely where any one of them will be. But together they form the patterns that can be calculated from the wave theory, and that Maxwell had described and calculated earlier.

The fields are continuous. The photons are not. They are discrete. They are the *quanta* of the electromagnetic field.

Are the photons there before they are observed, before the interaction takes place? No, only the wave propagates. It fills space and can go through two slits at the same time. Light is not a beam of photons. They are there only when the wave loses energy by hitting a screen or some other material.

So is light still sometimes a wave and sometimes a particle? Is it still "both"? In some ways it may still seem to be so, but what we have now is a description that encompasses the properties of waves *and* particles. It is neither of the two, but more than both. The new picture that we have of what happens is more complex, and richer than either one or than the two taken separately.

Beyond light: electron waves and the new synthesis

The reconciliation of photons with electromagnetic waves received its greatest impetus from the realization that the same considerations apply to electrons, and even further, to parts of atoms, and eventually to all particles and their combinations.

Before 1905 light had been thought to consist of electromagnetic waves. From then on it became clear that it also had the attributes normally associated with *particles*. Now (from 1925 on) electrons, the quintessential particles, were seen to have the wave attributes that had never before been considered appropriate for them.

We called an electromagnetic wave a ghostly presence that can exchange energy only in quanta. Similarly there are waves that describe the behavior of the electrons. They are no more and no less ghostly than the electromagnetic waves that we are so familiar with, and that we have come to know and learned to use in their various forms.

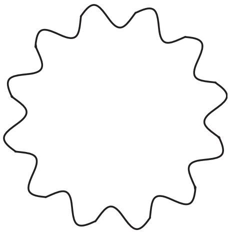
We can make double-slit experiments, just like Young's double-slit experiment, with electrons. This time again there is a wave that travels through space and through the two slits. Again there is a field—this time it is the "electron field." We can observe it when it interacts with a counter or with a television screen. And again the field can transfer energy only in discrete amounts, as the quanta that we call electrons.

We are so used to electromagnetic waves that in spite of what we have called their ghostly nature, we don't think of them as particularly mysterious or obscure. Perhaps it's time we gave equal rights and recognition to the waves that guide the observation of electrons and other particles of matter. Our mistrust is shown by the fact that we don't even have a good name for them. They are sometimes called *matter waves*. Today's materials science, the physics and chemistry that shapes our lives, is unthinkable without a knowledge of these waves. After more than three quarters of a century they are part of our common heritage, but still not part of common awareness and knowledge.

The quantum-mechanical description requires a new attitude toward the physical universe, incorporating uncertainty and probability in essential, inescapable ways. Some of the physicists most closely identified with bringing about the new view battled against this feature, including Einstein, Schrödinger, and de Broglie. In this they were largely unsuccessful, but many physicists today believe that the last word may not yet have been written about this question.

Let's see how the great change in attitudes began. We're back in 1924. We know about photons with their energy, E, equal to hf, and momentum, p, equal to $\frac{E}{c}$, so that for them $E = pc$. We also know that we can talk about the wavelength, λ, of the radiation, equal to $\frac{c}{f}$. This leads to $E = hf = \frac{hc}{\lambda}$. We can combine the two expressions for E to give $pc = \frac{hc}{\lambda}$ or $\lambda = \frac{h}{p}$.

Along comes graduate student Louis de Broglie who says suppose, just suppose, that this relationship works not only for photons but also for electrons. No one had ever considered the possibility that wave phenomena and a wavelength could conceivably be associated with electrons. And we wouldn't remember this stab in the dark either if it hadn't turned out to be one of the great seminal ideas of the twentieth century. De Broglie got his Ph.D. and a Nobel Prize, and h/p is called the de Broglie wavelength.



Did de Broglie have any evidence? Yes he did, of a sort. He said that if there are waves associated with electrons, then they can form standing waves around a proton at a distance r from the proton if the circumference, $2\pi r$, is equal to a whole number of wavelengths. Imagine a wave traveling around the proton. It goes around once. It goes around a second time. If the second time around the maxima and minima are exactly where they were the first time (are *in phase*), the waves will add, i.e., *interfere constructively*. If, on the other hand, the second time around, the wave's maxima fall behind the previous ones, they will fall further behind the next time, and the next time, until they cancel, i.e., *interfere destructively*. Only when the circumference, $2\pi r$, is exactly equal to a whole number of wavelengths, $n\lambda$, where n is a whole number, can the wave continue as a *standing wave*, as in the figure. Since $\lambda = \frac{h}{p}$ or $\frac{h}{mv}$, the criterion can also be written as $2\pi r = \frac{nh}{mv}$ or $mvr = n\hbar$, exactly the quantization condition that Bohr had written down in 1913 when he invented his model.

Where did Bohr get this relation? There was an attempt at justification, but by itself it would hardly have seemed convincing, except that *it worked*, which means that combined with some elementary mechanics and Coulomb's law it led to a set of values for the possible energies of a hydrogen atom which were *correct*, which were, in other words, experimentally observed. De Broglie's hypothesis led to the same relation. This suggested, at the very least, that there might be something to de Broglie's radically new approach.

Further evidence followed: Clinton Davisson and Lester Germer, working at the Bell Telephone Laboratories, then in New York City, saw some strange peaks in the intensity of an electron beam reflected from a nickel crystal when the angle was varied. These were soon interpreted as being the result of interference between the reflections from successive atomic planes of waves whose wavelength was $\frac{h}{p}$. In other words, they observed the interference pattern of electron waves as they were reflected from different planes of nickel atoms.

Shortly afterward George P. Thomson demonstrated what we now know as *electron diffraction*, the pattern produced by an electron beam when it passes through a thin crystal. (G. P.'s father, J. J. Thomson, is credited with the discovery of the electron by showing that a beam of electrons has a definite ratio, $\frac{e}{m_e}$, of charge to mass. It is sometimes said that he described the particle properties of electrons while his son demonstrated the electron's wave properties.)

The beams used by Davisson and Germer and by G. P. Thomson were *monochromatic*, i.e., they consisted of electrons of a single energy and momentum, and the experiments showed them to correspond to a single wavelength.

Even in the simplest atoms the electrons do not all have the same energy. In fact, what seemed to be de Broglie's strongest point, the explanation of the quantization condition, turned out to be, at best, suggestive of a better approach. The attempts to take the Bohr model and its quantization condition further had already limped along for more than a decade. But now everything was about to change, when following de Broglie, quantum mechanics was developed.

From de Broglie to Schrödinger

De Broglie's hypothesis worked perfectly for the electron beams of Davisson and Germer, and G. P. Thomson, with their single wavelengths, single momentum, and single energy. But Bohr had already shown that in atoms the electrons can have different energies and exist in different quantized energy levels. Was there now a way to describe the atomic electrons using de Broglie waves?

This is the step that Erwin Schrödinger took in 1925, opening up the field of *quantum mechanics*, the vastly successful framework for all modern theories of matter.

De Broglie's waves, with their single wavelength, momentum, and energy, represent motion without interactions, motion in accord with Newton's first law. Schrödinger's leap into the unknown created an analog to Newton's second law. He showed how the electrons behave when they interact with other particles. In the hydrogen atom, for example, the electron interacts with the proton as a result of their electric interaction. Instead of the concept of forces, however, Schrödinger used that of potential energy. For forces like the gravitational and electric forces that depend only on position, we can use force or potential energy. Either of the two concepts, whichever is more convenient in a particular situation, can be used to describe what happens. In the hydrogen atom, for example, the force between the electron and the proton is $\frac{ke^2}{r^2}$ and the potential energy is $-\frac{ke^2}{r}$, where k is the constant in Coulomb's law, e is the magnitude of the charge on the electron and on the proton, and r is the distance between the two. (For the potential energy we have, as usual, taken the reference level to be where r becomes infinitely large, i.e., where $\frac{1}{r} = 0$.)

Schrödinger started with a relation, or "wave equation," that describes the de Broglie waves. It is usually expressed in terms of the wavelength, λ, but because the wavelength is related to the momentum, p, by $\lambda = \frac{h}{p}$, it can also be expressed in terms of the momentum, or in terms of the kinetic energy, $K = \frac{p^2}{2m}$.

With de Broglie waves we are still talking about electrons moving with constant wavelength, momentum, and kinetic energy, unaffected by forces. But at this point we can ask whether a similar kind of relation, a new wave equation, might work when there are forces, and a potential energy, U. This is the crucial step that Schrödinger took. He said that if there are both a kinetic energy, K, and a potential energy, U, than the total energy is $E = K + U$, and we can substitute the quantity $E - U$ for K in the former wave equation.

The resulting equation is the *Schrödinger equation*, and it created a revolution.

How does the Schrödinger equation work? What can it do?

Our objective is to show you the Schrödinger equation and how it leads to results. Most of what we know about atoms (not just hydrogen atoms), as well as about molecules and solids and a lot more is obtained this way. We won't do any of the calculations for atoms and more complicated systems, but we will show examples that use some of the methods and illustrate the nature of the results that can be obtained.

Suppose we want to know about the hydrogen atom. We'll assume that the nucleus is fixed and concentrate on the electron. The "input" is the relation between potential energy and position, which for the electron in the hydrogen atom is $U = -\frac{ke^2}{r}$. We substitute this relation for U in the Schrödinger equation. The equation now leads to the "output" or "solution." That's a *wave function* with an amplitude that's usually called Ψ (capital Greek *Psi*). It tells you where the electron is likely to be. We can't find out where it is *exactly*. We can only determine the probability of finding it in a given region.

It turns out that the equation has such solutions only for certain values of the total energy, and these turn out to be the allowed, quantized energy levels of the hydrogen atom that we are looking for! In other words, we can find out as much as it is possible to know about where the electron is for each value of the energy, and we can find the *spectrum* of the possible energy levels.

Not only that, but the values of the orbital angular momentum come out right this time, and once we learn how to deal with the equation and add a few extra features, so do all the other atomic and molecular properties. Every place where the Bohr theory was stuck now becomes accessible. This includes the description of atoms beyond hydrogen in the periodic table of elements, for which the potential energy is no longer simple because there is then more than one electron.

To follow our program we will first review how all kinds of waves can be represented by sine functions. We will then apply this knowledge to electron waves by substituting the de Broglie wavelength $\lambda = \frac{h}{p}$, and show how this leads to the Schrödinger equation. Finally we will show for some examples how the Schrödinger equation leads to the wave functions and the energy levels, i.e., to the knowledge about where a particle is and what energy values it can have.

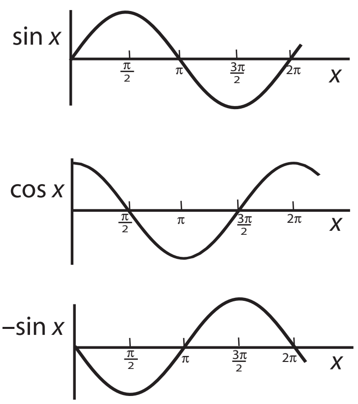
The main difficulty is that there are symbols that you are probably not used to (like Ψ). Don't be put off by them! There is some algebra, but you will see that it isn't any more difficult than what you have already worked with. We would like to encourage all of you to read the following sections before you go on to the Heisenberg

Uncertainty Principle. Some of you may not go through all the details, but we think that you will be happy to see that some of the most modern ideas in physics are not at all mysterious.

We have not yet written down the famous equation, so that our talk about it is so far somewhat vague. We now want to get more serious. This wonderful part of physics, which plays such a profound role in all we know about the world of atoms, and in much of modern technology, has largely remained hidden from a majority of the population. We would like you to take a closer look at it, and although it may mean some courage on your part, you won't want to miss it.

Representing waves

The Schrödinger equation is a *wave equation*, and before we develop it in detail we will review the way waves of all kinds are described mathematically and with graphs. We already know how to represent waves that repeat in space after one wavelength with sines and cosines. (We won't deal with the repetition in time.) The figure shows a graph of sin x as a function of x. Below it is the graph of cos x as a function of x, which looks the same, except that the starting point is different. And below it is a graph of $-\sin x$, i.e., the first graph upside down.



We can see that a special feature of the first two graphs is that at every value of x the middle graph gives the slope of the graph above it. We see, for example, that when sin x is horizontal, so that its slope is zero, at $\pi/2, 3\pi/2$, etc., cos x is zero. When sin x is zero, its slope is one, and so is the value of cos x. The slope of sin x vs. x is cos x vs. x.

Another way of saying exactly the same thing is "the derivative with respect to x of sin x is cos x."

Underneath both graphs is the graph of $-\sin x$ vs. x, and you can see that it gives the slope of the graph just above it, of cos x. This can also be expressed by saying that the derivative with respect to x of cos x is $-\sin x$. It is also the "second derivative" of sin x. We see that the function sin x has the property that its second derivative (the slope of the slope) is equal to the negative of itself.

There is a special notation for these statements. For the first derivatives, $\frac{d}{dx}(\sin x) = \cos x$ and $\frac{d}{dx}(\cos x) = -\sin x$. For the second derivative of sin x, $\frac{d^2}{dx^2}(\sin x) = -\sin x$ (read $d2dx^2$ of $sin x = -sin x$.) And if $y = \sin x$, $\frac{d^2y}{dx^2} = -y$. You can stay with "slope" instead of "derivative," and "slope of the slope" for the second derivative. They mean the same thing.

For our electron wave we'll need the slightly more general function $y = A \sin kx$. The amplitude, A, and the *wave number*, k, can have values to suit the particular wave that we want to consider. For this function the slope is $kA \cos kx$. We can write the relation between the function and its slope as $\frac{dy}{dx} = kA \cos kx$. We can now look at the slope of $kA \cos kx$. It is $-k^2 A \sin kx$, which we see to be $-k^2 y$. This is the first derivative of $kA \cos kx$ and the second derivative of $y = A \sin kx$. We can write it as $\frac{d^2y}{dx^2} = -k^2 y$.

These functions repeat when kx is increased by 2π. In other words, $A \sin kx = A \sin (kx + 2\pi)$ or $A \sin kx = A \sin k(x + \frac{2\pi}{k})$. This shows that the function repeats when x is increased by $\frac{2\pi}{k}$.

But this is just what we mean by a wavelength. We see that the wavelength, λ, is equal to $\frac{2\pi}{k}$. The quantity k is called the wave number. (The symbol is the same as the one we use for the constant in Coulomb's law, but it is a quite different quantity. It should be easy to see from the context which one we're talking about at any one time.)

That's it for the mathematics. The rest is just some talk and playing around with what you already know.

First the talk. $\frac{d^2y}{dx^2} = -k^2 y$ is a relation between a function (y) and its second derivative ($\frac{d^2y}{dx^2}$). It's an equation. We can call it the wave equation. It contains a derivative, so it's called a *differential equation*. $y = A \sin kx$ is one function that is a solution of this equation. What does that mean? Only that if you substitute $A \sin kx$ for y in the equation, the left-hand side is equal to the right-hand side.

All this was well known long before the twentieth century, and had been used successfully to describe all kinds of waves, such as waves on a string as on a violin or guitar, or sound waves, or light waves.

Finally the best we have: the Schrödinger equation

What is it that oscillates in an electron wave? There is nothing that moves, as on the string or in the sound wave. There isn't a simply observable physical property that changes, as the pressure does in a sound wave and the electric and magnetic fields in an electromagnetic wave. The electron wave tells us where the electron is. Not exactly, but, after we square it, it tells us what the probability is of observing the electron in a given spot.

Part of the mystery that still seems to surround the concept of electron waves comes from the fact that we have never found a good word for whatever it is that changes. It continues to be called *the wave function*. It would be nice to have a symbol that would make the waves seem less remote, but that hasn't happened either. The symbol that is universally used for them is Ψ, the Greek *psi*.

Now for the playing around. For all waves $k = \frac{2\pi}{\lambda}$. For the de Broglie waves we also have $\lambda = \frac{h}{p}$, so that $k = \frac{2\pi p}{h}$ or $\frac{p}{\hbar}$ and $p = \hbar k$.

We need the k that appears in the wave equation, but we want to express it in terms of the kinetic energy, K, which is $\frac{1}{2}mv^2$ or $\frac{p^2}{2m}$. For the de Broglie waves we can write it as $K = \frac{\hbar^2 k^2}{2m}$, so that $k^2 = \frac{2mK}{\hbar^2}$.

The same old differential equation can now be written to say that the slope of the slope, or the second derivative, $\frac{d^2\Psi}{dx^2}$, is equal to $-k^2\Psi$, i.e., $\frac{d^2\Psi}{dx^2} = -\frac{2mK}{\hbar^2}\Psi$ or $-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} = K\Psi$.

This is all just playing around with symbols, and has so far accomplished nothing except to recast the wave equation for a noninteracting electron. Now, however, comes the leap of faith. Let the electron interact with other charged particles, e.g., a positively charged nucleus, so that there is a potential energy. What happens if we assume that the equation also holds when there is such a potential energy, U, so that the total energy, E, is $K + U$, and K is equal to $E - U$? We rewrite the relation once more, but with $E - U$ instead of K. That gives us $-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} = (E - U)\Psi$, which we can also write as $-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + U\Psi = E\Psi$.

This is what we've been leading up to. *This is the Schrödinger equation.*

What does the Schrödinger equation tell us?

The Schrödinger equation doesn't look anything like Newton's second law, but that is what it corresponds to. It looks, in fact, more like the law of conservation of energy. If we think of the term with the derivatives as representing the kinetic energy, then it says "K"$\Psi + U\Psi = E\Psi$, which looks reassuringly familiar. Newton's second law comes to life when we say what the forces are. The same thing happens here when we specify the potential energy. Here is our prime example: let $U = \frac{-ke^2}{r}$, so that it describes the potential energy of an electron in the field of a proton. (Before we can do that we have to generalize our one-dimensional Schrödinger equation to three dimensions by adding derivatives with respect to y and to z.) The equation now becomes the key that unlocks the secrets of the hydrogen atom.

That key is so different from the classical, Newtonian one that it took a while to figure out how to use it, and there are aspects of the procedure and the results that remain controversial to this day.

Let's go back for a moment to the waves on a guitar string. For them $y = A\ sin\ kx$. We saw that $k = \frac{2\pi}{\lambda}$. Now we know, quite without any new ideas, that if the string has a definite length, waves on the string can exist only with certain definite wavelengths, corresponding to definite musical notes.

The situation is similar for the Schrödinger equation. First put in the potential energy. The solutions are a set of wave functions, Ψ, now not just sines and cosines. They are still functions of the space coordinates. The wave function tells us whatever there is to know about where the particle that the equation describes is located. That information is different and less exact than in the classical case. It tells us the probability of finding the particle at any given place or in any given region.

There is a second piece of information that we get. There are solutions only for certain definite values of the quantity E, the total energy. Each value of E corresponds to a possible, allowed value of the energy, i.e., to an energy level of the system.

For the hydrogen atom the allowed energies come out to be exactly those of the Bohr model, but the angular momentum which Bohr had wrong is now correct, and a whole lot of other stuff, which Bohr couldn't even get close to, is also there. Most importantly, we can describe the properties of the other, more complicated, atoms as well as combinations of atoms in molecules or solids.

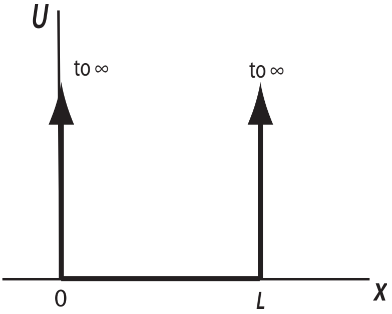
How does the wave function tell us where the particle that it describes is to be found? For a wave on a string the energy is proportional to the square of the amplitude. For an electromagnetic wave, in which the electric field varies in time and space, the energy is proportional to the square of the magnitude of the field. When an electromagnetic wave hits something, the square of the electric field in any small region of space is proportional to the number of photons to be found there. It is proportional to the probability of finding a photon there. That is also the way to use the wave functions that are the solutions of the Schrödinger equation. When the matter wave interacts with a screen or with a counter or with anything else, the square of the magnitude of the wave function, Ψ^2, in a given region is proportional to the probability of finding our particle in that region.

Here, once more, is what we need to do to determine how a particle moves when there are forces on it. We represent the forces by the way the potential energy changes as the particle moves. For the electron in the hydrogen atom, for example, it is $-\frac{ke^2}{r}$. For electrons in other atoms it cannot be written down so simply because there are other electrons, but there is still some function that describes the electric potential energy. We put the appropriate potential energy in the Schrödinger equation and try to find a function that is a solution to the equation. This also gets us the values of the energy, E, for which solutions exist. They are the values of the energy levels. For each such value there is a *solution* (or perhaps several). It is a function, the *wave function*, that when substituted in the equation makes the right-hand side equal to the left-hand side. When we square this function we get another function of position, and this is the function that gives us the probability that we can find the electron in any given region.

The information that we get about the position of our particle is not exact. We get only a probability. That's the best that we can do. But it's a lot. It allows us to describe the structure of atoms, their combinations, and much more. Quantum mechanics is the framework on which our knowledge of the structure of matter is built.

EXAMPLE 7

The "square well"



An electron can be represented as being in an *energy well* that is described by $U = 0$ between $x = 0$ and $x = L$ and by $U = \infty$ outside the well, everywhere else. This may seem like an unrealistic problem. It is, however, the simplest model for a number of physical situations. It can, for example, be used for the nucleus, with nucleons replacing the electrons. To keep the problem as simple as possible we limit it to one dimension. The extension to three dimensions is straightforward. The problem also illustrates that the quantization comes from the confinement of particles to a limited region of space.

(a) What are the wave functions?

(b) Sketch the wave functions for the first three energy levels.

(c) What are the energy levels of the system?

(d) Draw an energy level diagram.

Ans.:

(a) The particle cannot be outside the well, where the potential energy is infinitely large. The wave function must therefore go to zero at the well's boundaries. Inside the well the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} = E\Psi$$

where we have used the x component only, and the potential energy $U = 0$.

Since $U = 0$, there is only kinetic energy, and $E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$. We can therefore write the equation as $\frac{d^2\Psi}{dx^2} = -\frac{2mE}{\hbar^2}\Psi$, where the right-hand side is equal to $-\frac{p^2}{\hbar^2}$, which is equal to $-k^2$, where k is the wave number $\frac{2\pi}{\lambda}$, i.e., the equation is $\frac{d^2\Psi}{dx^2} = -k^2\Psi$.

We know that this equation has solutions that are sine and cosine functions. Both have the property that the slope of the slope (the second derivative) is proportional to the negative of the function itself. We need a function that is equal to zero at $x = 0$. We cannot use the cosine function since $\cos 0 = 1$. The sine function, $\sin x$, on the other hand, is zero at $x = 0$. The wave functions therefore have the form $\Psi = A \sin kx$, where we still have to determine the possible values of k.

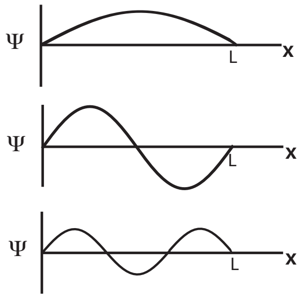
The wave function also has to go to zero at $x = L$. We can therefore immediately see what the wave functions are. They are sine functions that have the value zero at both ends of the well. There is no restriction on how often they can go to zero inside the well, so there is an infinite number of such wave functions. The largest wavelength is such that half the wavelength is equal to L, i.e., that $L = \frac{1}{2}\lambda$. For the next one $L = \lambda$. For all of them $L = n\frac{\lambda}{2}$. Each wave function is described by a value of the *quantum number n*. Since $k = \frac{2\pi}{\lambda}$ and $\lambda = \frac{2\pi}{k}$, $L = \frac{n}{2}\frac{2\pi}{k}$ or $k = \frac{n\pi}{L}$.

We can see that also from the relation for the value zero of the wave function at $x = L$, $\sin kL = 0$. This is so for $kL = 0$ and also for $kL = \pi$, or 2π, 3π, or, in general, $n\pi$. Since $k = \frac{2\pi}{\lambda}$, this gives $\frac{2\pi}{\lambda}L = n\pi$, or $L = n\frac{\lambda}{2}$, and $k = \frac{n\pi}{L}$, as before.

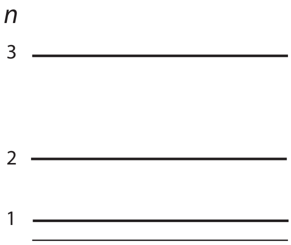
We can now write the wave functions as $\Psi = A \sin \frac{n\pi}{L}x$. There is a different one for each value of n.

(c) To see the values of the energies, we have to go back to E. $E = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{\hbar^2k^2}{2m}$. We can now substitute the quantized values of k, $k = \frac{n\pi}{L}$, to get $E = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{L^2}$ or $E = n^2\frac{\hbar^2\pi^2}{2mL^2}$.

(b)

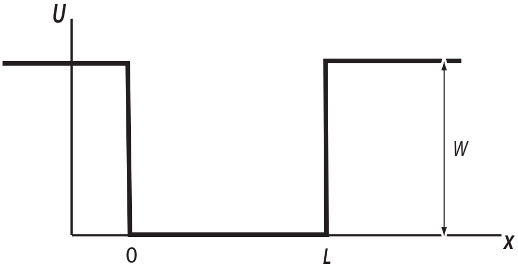


(d)



For a particle with a mass m and a well of width L, the energy levels are n^2E_1, where E_1 is the energy of the lowest state (the ground state) $E_1 = \frac{\hbar^2\pi^2}{2mL^2}$. Since the problem specifies that $U = 0$ inside the well, this energy is entirely kinetic.

EXAMPLE 8



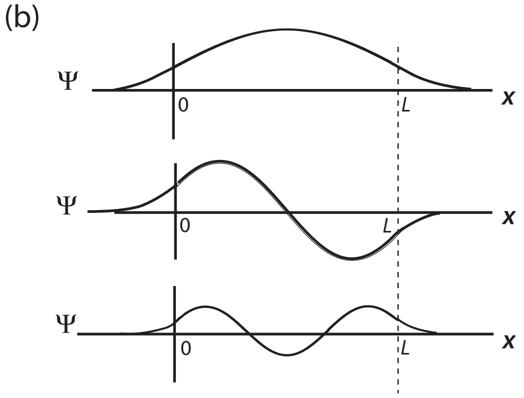
An electron is in an energy well that is described by $U = 0$ between $x = 0$ and $x = L$, and by $U = W$, where W is constant, outside the well, everywhere else.

(a) Describe the form of the wave functions inside and outside the well for values of the energy less than W.

(b) Sketch the wave functions for the first three energy levels.

Ans.:

(a) Inside the well the wave functions are similar to the ones in the previous example, but this time the values at $x = 0$ and $x = L$ are not zero. They can be a combination of sines and cosines. We can see this from the fact that there is, this time, a Schrödinger equation with a different kind of solution also outside the well.



Outside the well the Schrödinger equation is $-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + W = E\Psi$. Since E is smaller than W, we can write this as $\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} = (W - E)\Psi$, where both sides are positive.

This time, outside the well, we need a function for which the slope of the slope (the second derivative) is proportional to the function itself and not its negative. Such a function is e^{ax}. The function e^x has the property that its slope is equal to the function itself. For e^{ax} the slope is ae^{ax} and the slope of the slope is a^2e^{ax}.

Since a can be either positive or negative, the wave function outside the well can either increase or decrease exponentially. We have to discard the exponential increase, which goes to infinity and would lead to unphysical results. (The particle would be infinitely far away all the time.) What remains is the exponential decrease. It has to be fitted to the sinusoidal wave function inside the well in such a way that the function and its slope are continuous, in other words that there are no breaks and no kinks. (A break in the wave function would mean that it would have two values and therefore two probabilities there. A kink would mean two values for the slope, and hence two possible values for other physical quantities.)

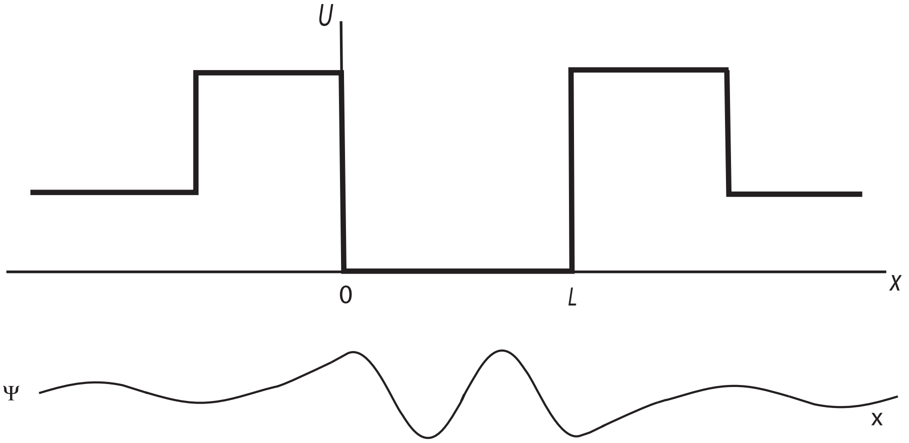
This result is quite different from the classical result. Newtonian mechanics cannot envision a situation where the potential energy is larger than the total energy so that there is a negative kinetic energy. Here there is a rapidly decreasing but finite probability that this occurs. If we think of the "well" as a box, we see that the particle has a finite probability of being outside the box for all finite heights of the box.

EXAMPLE 9

This time there is a "box" with a finite "wall," as in the previous example, but further outside the energy E is larger than the potential energy U. Draw a sketch of a possible wave function.

Ans.:
In the well or box the wave functions for energies less than the height of the walls are sines as before. In the wall section they are exponentials as in the previous example. There is now a third region, farther outside. Since E is greater then U in this region, the wave functions are again sinusoidal, but with a smaller amplitude.

The fact that there is a solution outside, in this third region, means that there is some chance that



the particle can be found there. In other words, the particle can "leak out" or "tunnel" out of the box.

This could not occur in Newtonian mechanics. Since the particle could never be in the wall region, where U is greater than E, corresponding to a negative kinetic energy, there is no way for the particle to overcome the barrier represented by the wall of the box, and it would have to stay inside. The tunneling out is possible according to quantum mechanics. The observation of tunneling is a strong confirmation of the correctness of quantum mechanics. It describes the tunneling of alpha particles from the nucleus in radioactive decay and the overcoming of barriers by electrons in solids.

EXAMPLE 10

What is the Schrödinger equation for a particle in simple harmonic motion?

Ans.:
The potential energy of a particle moving along the x-axis in simple harmonic motion is $\frac{1}{2}kx^2$.

This potential energy is substituted for U in the Schrödinger equation (using only the x component) to get

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2}+\frac{1}{2}kx^2\Psi=E\Psi$$

The solution leads to the energy levels $(n+\frac{1}{2})hf$. The spacing of the levels is the same as that of Planck, but the lowest level is not at $E=0$, but at $E=\frac{1}{2}hf$. That there is a lowest energy that is not zero (a "zero-point energy") is characteristic for quantum mechanics. It shows that there is some motion even at the lowest possible energy.

Heisenberg and the uncertainty principle

Quantum mechanics was developed almost at the same time, independently, by two people. Werner Heisenberg used mathematical methods quite different from those of Schrödinger, and at first it seemed that the two approaches had little in common. Shortly afterward, however, Schrödinger showed that in spite of the fact that they look so different, the two theories are, in fact, equivalent.

Heisenberg emphasized a feature of quantum mechanics that has come to be known as the *Heisenberg uncertainty principle*. Consider first a de Broglie wave with a single wavelength, λ. It is not possible to say where the wave is. It extends through space. The momentum, on the other hand, equal to $\frac{h}{\lambda}$, is precisely known.

It is possible to add waves with different wavelengths, and so to construct a "wave packet" that is in a limited region of space. To do this it is necessary to use waves with different wavelengths and the wave's momentum is then no longer known exactly. With an infinite series of waves, each with a different wavelength, it is possible to describe a localized particle exactly, but the wavelength, and hence the momentum, is then completely unknown.

Now let's look at what happens between these two extremes. Suppose you try to measure the position of an electron. You can shine light on it, i.e., you can send a photon toward it. By seeing the photon bounce off the electron you can determine the electron's position. But with light of wavelength λ, the position can be determined only with an uncertainty Δx of about λ. (With a microscope you can't see anything smaller than the wavelength of the light that you are using. You don't know where a wave is, closer than with an uncertainty of about its wavelength.) The photon that strikes the electron has a momentum $\frac{h}{\lambda}$, and therefore transfers an amount of momentum of about this magnitude to the electron. The momentum it gives up can be this much or less, depending on the angle. The momentum of the electron, Δp, is therefore uncertain to about this extent. We see that the product of the two uncertainties is equal to about h. This is a general result. Light with a smaller wavelength will reduce Δx, but the photon will have more momentum, and so increase Δp. The product $\Delta x\Delta p$ remains the same.

Note that the uncertainty here is intrinsic, i.e., it is not related to just how we measure the quantities. There is no way to get around the limitations of the Heisenberg uncertainty principle.

EXAMPLE 11

Show that the ground-state energy of the hydrogen atom is determined approximately by the uncertainty principle.

Ans.:
To show this we will look at the extent of the electron's wave function as the uncertainty in the

distance. In other words, we will take Δx to be about equal to the radius r. We will use the Bohr model to estimate r. (Of course the Bohr model was developed more than a decade before the uncertainty principle, and was considered to be definite.) The lowest possible magnitude of the electron's momentum is its value in the ground state. We don't know its direction, and can consider the uncertainty Δp to be equal to the magnitude of the momentum in the ground state. The kinetic energy is equal to the negative of the total energy, $K = -E = \frac{k^2me^4}{2\hbar^2}$. K is equal to $\frac{p^2}{2m}$, so that $p^2 = \frac{k^2m^2e^4}{\hbar^2}$ and $p = \Delta p = \frac{kme^2}{\hbar}$. For r we will use the smallest Bohr radius, $\frac{\hbar^2}{kme^2}$, and we see that $\Delta x \Delta p = \hbar$, in keeping with the expectation from the uncertainty principle.

We have to remember that the uncertainty principle is itself not exact. The product $\Delta x \Delta p$ is *of the order* of h, but may be larger or smaller. It has been shown that the smallest value that the product can have is $\frac{\hbar}{2}$.

12.3 Order in the universe: the elements

The beginning: hydrogen and its quantum numbers

We now know how to write down the Schrödinger equation for the hydrogen atom. We use $\frac{-ke^2}{r}$ for the potential energy, U, in it. We are not going to go through the solution process here, but we will write down some of the results.

The energy of the hydrogen atom depends only on the quantum number n, and is equal to $\frac{E_1}{n^2}$, where $E_1 = -13.6\,\text{eV}$.

The orbital angular momentum was already quantized in the Bohr model by his quantization condition $mvr = n\hbar$. The solution of the Schrödinger equation for the hydrogen atom also leads to the conclusion that it is quantized, but with a different relation. It is related to a second quantum number, ℓ, and the orbital angular momentum is equal to $\hbar\sqrt{\ell(\ell+l)}$.

A third quantum number, m_l, describes how the atom can orient itself in a magnetic field.

These relations are not just pulled out of a magic hat, but are the result of perfectly well-defined mathematical procedures that need to be used to *solve* the Schrödinger equation and that existed and were known long before Schrödinger. The numerological rules for the three quantum numbers, n, ℓ, and m_l, are the unambiguous mathematical consequences of the Schrödinger equation.

There is a fourth quantum number (m_s) for the electron in a hydrogen atom, which is not derivable from the Schrödinger equation. Like the other quantum numbers it is related to a dynamic property, in this case the electron's spin angular momentum. Its existence was discovered, even before the advent of quantum mechanics, when it was realized that there were twice as many possible states (for the two possible spin states) as could be accounted for without it.

Does that mean that it has no theoretical justification or explanation? No, the situation is much more interesting than that. It is also the natural outcome and consequence of an equation, but one that goes beyond the Schrödinger equation. Unlike it, it is consistent with the special theory of relativity. (In the Schrödinger equation we use $K = \frac{1}{2}mv^2$, which is equal to the kinetic energy only when v is much less than c, the speed of light.)

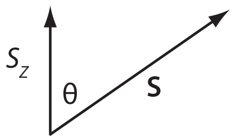
This equation, the Dirac equation, developed by P.A.M. Dirac in 1930, is not a generalization of the Schrödinger equation, but rather a quite different equation whose primary achievement is that it describes properties of the electron, including those that are direct consequences of the theory of relativity. These include the spin angular momentum, the spin magnetic moment, and their ratio, the gyromagnetic ratio. These properties cannot be derived from the Schrödinger equation. If we use the Schrödinger equation to find the energy levels of hydrogen, these properties have to be included separately.

The spin angular momentum of the electron always has the same magnitude. It can be written as $\hbar\sqrt{s(s+1)}$ so as to look like the orbital angular momentum, but s can have only the single value $\frac{1}{2}$. The component of this spin angular momentum along the direction of the magnetic field can take on two values, $m_s\hbar$, where m_s is equal to $+\frac{1}{2}$ or $-\frac{1}{2}$.

EXAMPLE 12

What is the angle between the spin angular momentum and the magnetic field in the ground state of hydrogen?

Ans.:



The spin angular momentum vector is **S**. Its magnitude, S, is $\hbar\sqrt{s(s+1)}$, where s is the quantum number that is always equal to $\frac{1}{2}$, so that $S = \hbar\sqrt{\frac{1}{2}(\frac{1}{2}+1)} = 0.866\hbar$. Its component along the magnetic field is $S_z = \frac{1}{2}\hbar$. The relation between the two is $S \cos\theta = S_z$ or $0.866\hbar \cos\theta = 0.5\hbar$, so that $\cos\theta = \frac{0.5}{0.866}$ or $\theta = cos^{-1}\frac{0.5}{0/866} = 54.7°$.

Let's review the hydrogen atom quantum numbers. Here they are, together with the related mechanical properties:

(1) n can vary from one to infinity. The energy is $\frac{E_1}{n^2}$, where $E_1 = -13.6\,\text{eV}$. The other quantum numbers do not influence the energy. (This is true only in the hydrogen atom!)

(2) ℓ can go from zero to $n-1$. The magnitude of the orbital angular momentum is $\hbar\sqrt{\ell(\ell+1)}$.

(3) m_l can vary between $-l$ and l. It describes the component of the orbital angular momentum along the direction of the magnetic field. This component is equal to $m_l\hbar$.

(4) m_s can be either $\frac{1}{2}$ or $-\frac{1}{2}$. The component of the spin angular momentum in the direction of the magnetic field is $m_s\hbar$.

Each possible set or combination of these quantum numbers distinguishes a particular *state* of the atom with a different wave function. The energies of some of the states may be the same, and this is true in hydrogen (only!) for all of the states with the same value of the quantum number n. Similarly, the orbital angular momentum is the same for all of the states with the same value of the quantum number ℓ.

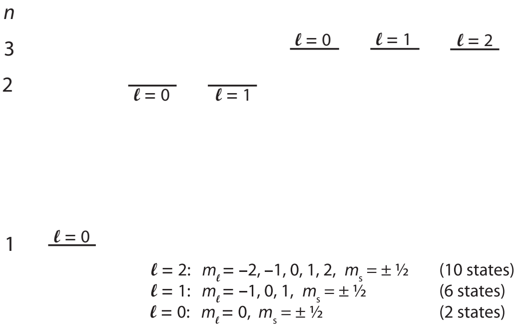
EXAMPLE 13

What is the sequence of energy levels in the hydrogen atom?

Ans.:

In the hydrogen atom the energy is determined only by the quantum number n. But for each value of n there is more than one state, each with its different wave function. For the ground state, with $n = 1$, there are two states, one with $m_s = \frac{1}{2}$ and one with $m_s = -\frac{1}{2}$. Both have $\ell = 0$ and $m_l = 0$. For $n = 2$, ℓ can be zero or one. For $\ell = 0$, $m_l = 0$, and there are again the two states with the two different values of m_s. Still for $n = 2$, there are also the states with $\ell = 1$. For them m_l can take on the values 1, 0, and -1. For each there are the two possible values of m_s, so that there are six states, for a total of eight for this value of n.

The next higher levels are for $n = 3$. In hydrogen all have the same energy, with two states for $\ell = 0$, six states for $\ell = 1$, and 10 states with $\ell = 2$ ($m_l = 2, 1, 0, -1$, and -2, each with the two values of m_s), for a total of 18 states with this value of n. For $n = 4$ there are 14 more states, and so on.



Hydrogen shows the way: the other elements

We can now look at what happens in atoms other than hydrogen. The first obstacle arises immediately. In the hydrogen atom we have just two particles, the proton and the electron. In all other atoms we have a nucleus and more electrons. Even in the old, classical, Newtonian scheme we don't know how to deal with more than two particles at a time. At least we don't know how to do it *exactly*.

What works sufficiently, most of the time, is to use a model that considers just one electron at a time, and to think of it as moving in a steady field, which is the average field whose sources are the nucleus and all of the other electrons. We know that these other electrons are moving around in ways that are impossible to know or to follow, but we will use the blur that they represent as if it were a steady background for the one electron on which we choose to focus. We can then talk about the wave function of that one electron in the field of the nucleus and all the other electrons.

The origin of order: the Pauli exclusion principle

We now have to consider the principle that gives rise to the hierarchy of the elements and leads to their diversity and to their order in the periodic table of the elements. Without it there would not be the vast variety of properties among the elements and their combinations. The world would be a much more homogeneous and bleaker place, without a chance for us to exist. Here it is:

Each electron in an atom must be characterized by a different set of quantum numbers. This is the *Pauli exclusion principle*, discovered by Wolfgang Pauli in 1925.

Without the Pauli principle all of the electrons in an atom could be in the lowest energy level, with the quantum numbers that the electron has in the ground state of the hydrogen atom. The atoms would be much more similar to one another than they actually are. The differences between the atoms would be minor, and combinations between them little different from element to element.

With the Pauli exclusion principle the electrons must have different sets of quantum numbers. They must move at different distances from the nucleus, with different energies and angular momenta, and be differently affected by magnetic fields. This is what underlies the richness among the elements and of their combinations, and the variety and complexity of chemistry and biology.

Atomic structure: beyond the Coulomb field

We can now go to the atoms of the periodic table of elements beyond hydrogen. They have nuclei that have more protons, so that there are also more electrons in the neutral atoms.

Each time a proton is added to the nucleus it changes the electric field and the electric potential for all the electrons. If this were all, we could deal with it very simply, because all that does is to change the amount of charge of the nucleus. The field would still be proportional to $\frac{1}{r^2}$, one that is called a *Coulomb field*. But we also add electrons, in an unknown, complicated way, at some distance from the nucleus.

The electrons exert forces on each other, and as they move, the electric field changes with time in unpredictable ways. If we want to calculate what happens, we have to resort to approximations. The usual approach is to look at one electron at a time, in the field created by the nucleus and all the other electrons. We don't know that field from moment to moment, but we can get a pretty good idea of its average over time and use that. This average field is no longer the Coulomb field of a single charge at the center. It is no longer proportional to $\frac{1}{r^2}$.

EXAMPLE 14

What are the quantum numbers that describe the two electrons in the ground state of the neutral helium atom?

Ans.:

Helium is the second element in the periodic table. Its atomic number is 2. n is still one. ℓ and m_l both have to be zero. Only m_s distinguishes the two electrons. The quantum numbers are $1, 0, 0, \frac{1}{2}$ and $1, 0, 0, -\frac{1}{2}$.

The number of protons in the nucleus (the atomic number, Z) increases by one for each step up the periodic table of elements. For each added proton another electron is added to the neutral atom. Where do these electrons go? The new atom will normally be in its *ground state*, the state with the lowest possible energy. Each added electron will therefore go into the configuration (the *state*) where it has the lowest possible energy, and this is determined by the set of its quantum numbers.

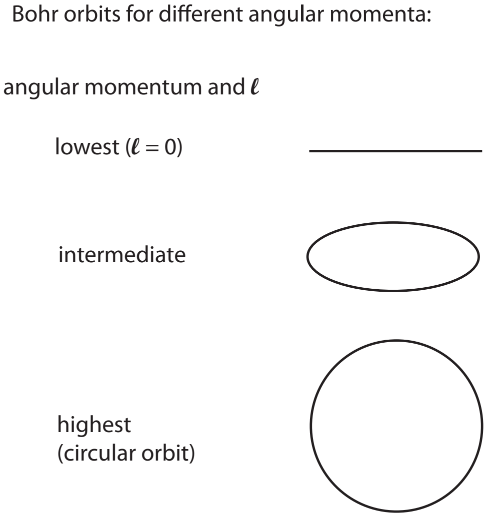
We know what happens when the electric field is exactly that of a single charge. The allowed states are then those of the hydrogen atom. For this case we know the sequence of energy levels. We know that the energy depends only on the quantum number n. The states with the lowest energy are all the possible states with $n = 1$ (2 of them). The next lowest are the eight with $n = 2$, all with the same energy ($\ell = 0$ with two different values of m_s, and $\ell = 1$ with 3 different values of m_l, each with two different values of m_s), and so on.

We have already seen that even with $Z = 2$ the electric field is more complicated than a Coulomb field. We now need to know what the sequence of energy levels is in atoms other than hydrogen. In addition to its dependence on n, the energy will then also depend on the value of the quantum number ℓ. Indeed, this ℓ dependence is fundamental to the structure of the periodic table of the elements.

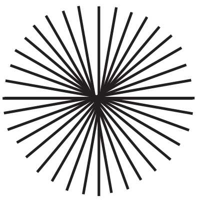
The ℓ dependence and the order of the elements

If all states with a given value of n, or with a given value ℓ, are filled, the resulting distribution of electrons is spherically symmetrical. We talk about a filled *shell* (with a particular value of n) or a filled *subshell* (with a particular value of ℓ). In helium, for example, the $n = 1$ shell is filled with its two electrons. Element number 3, with three protons in its nucleus, is lithium. Look at the third electron. It will have $n = 2$, but which value of ℓ will correspond to the lowest energy, and therefore to the ground state?

Higher angular momentum represents motion farther away from the nucleus. We can see how this comes about by going back to how the Bohr model was extended before quantum mechanics was invented by proposing that the orbits could be elliptical. The "biggest" ellipse is a circle, and circular orbits represent the maximum angular momentum and the highest value of ℓ.



In this description lower angular momentum corresponds to elliptical orbits. But what is an orbit with zero angular momentum and $\ell = 0$? There is then no rotation at all, just back-and-forth motion of the electron. It is straight-line simple harmonic motion right through the nucleus. The fact that the straight-line orbit can be at any angle leads to he conclusion that the state with $\ell = 0$ is spherically symmetrical.



Bohr's way of looking at the atom, with its exact paths for the electrons, is not correct, but it gives a partial view of some of the properties of atoms and provides a picture that can help to clarify some of the concepts.

The following is true in Bohr's model and remains so in the correct quantum-mechanical description. The lower the angular momentum, the more time the electron spends near the nucleus. An electron in the $\ell = 0$ state spends the most time near the nucleus where the attraction is strongest and the energy the lowest. With higher angular momentum the electron spends more time further away. The attraction is then smaller and the energy higher.

This continues to be so as more electrons are added, with each, as always, going to the lowest available energy level. Each time we go from one element to the next, we add a proton to the nucleus. The corresponding added electron goes into the state with the lowest value of angular momentum, i.e., with the lowest value of ℓ that is available.

The sequence is simple, but only up to $Z = 18$ (Ar). By this time we have the two elements with $n = 1$, the two elements with $n = 2$ and $\ell = 0$, the six elements with $n = 2$ and $\ell = 1$, the two elements with $n = 3$ and $\ell = 0$, and the six elements with $n = 3$ and $\ell = 1$. The energies are different from those of the hydrogen atom, not only because the nuclear charge is different, but because of the ℓ-dependence of the energy. Nevertheless the sequence is still that of the energy levels of the hydrogen atom.

The order changes

As we move further along in the periodic table, the sequence changes. We might have expected to go on with $n = 3$, $\ell = 2$, but this does not happen. The low (zero) angular momentum of $n = 4$, $\ell = 0$ causes the next electron to be so close (on the average) to the nucleus, hence so strongly attracted, that this state has the lowest energy, lower than the state with $n = 3$ and $\ell = 2$. It is therefore the one that is filled first. Only after that do we get to the electrons with $n = 3$ and $\ell = 2$.

EXAMPLE 15

(a) What is the sequence of energy levels in the argon atom?

(b) What is the sequence of energy levels in the potassium atom? The calcium atom?

(c) Sketch the sequence of energy level schematically for the elements up to $Z = 36$, showing the dependence of the energy on n and ℓ.

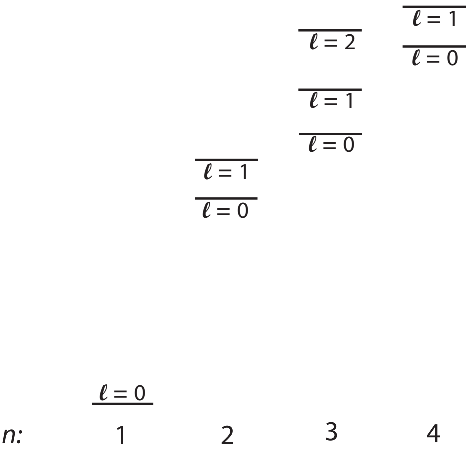
Ans.:

(a) Argon is element number 18. In its ground state its 18 electrons are in the 18 lowest-energy states. First are the two in the shell with $n = 1$. Then there are the eight in the shell with $n = 2$, of which two are in the subshell with $\ell = 0$ and six in the subshell with $\ell = 1$. Then there are eight in the shell with $n = 3$, first two in the subshell with $\ell = 0$ and then six in the subshell with $\ell = 1$.

(b) In potassium ($Z = 19$) the first 18 electrons have the same values of n and ℓ as in argon (but with different energies!). The nineteenth is in the lowest state with $n = 4$, which is the one with $\ell = 0$ (and $m_l = 0$).

The sequence continues with calcium, with the twentieth electron in the second state with the same n and ℓ as potassium (and the other value of m_s). Only then come the 10 elements in which the subshell with $n = 3$ and $\ell = 2$ is gradually filled. After that we go back to the "regular" sequence, with $n = 4$ and $\ell = 1$. That gets us to $Z = 36$.

(c)



$\ell = 2$: $m_\ell = -2, -1, 0, 1, 2$, $m_s = \pm 1/2$ (10 states)
$\ell = 1$: $m_\ell = -1, 0, 1$, $m_s = \pm 1/2$ (6 states)
$\ell = 0$: $m_\ell = 0$, $m_s = \pm 1/2$ (2 states)

The interruption of the sequence of values of n has remarkable consequences. We have gone to states with $n = 4$ before completing the possibilities with $n = 3$. But higher values of n, as in the Bohr model, still correspond to larger (average) radii. Going back to $n = 3$ after already having put electrons in the shell with $n = 4$, with its larger radius, means that an *inner* shell, one with a smaller average radius, is then being filled.

When atoms combine to form molecules or solids, it is the outer electrons (the *valence electrons*) that are primarily involved. Filling an inner shell doesn't affect the outside of the atom very much, so that the way the atom engages in chemical combinations is not much changed. If electrons are added to an inner shell as we go from one element to the next, therefore, the neighbors in the periodic table are much more similar to each other than in the more normal sequence where electrons are added to the outermost shell. They are called *transition* elements.

Another feature of transition elements with an inner shell that is only partially full is that they often have extraordinary magnetic properties. This is because for them the angular momentum and the magnetic moment do not add up to zero as they do for filled shells or subshells.

The first group of transition elements is the one beyond calcium, from scandium ($Z = 21$) to nickel ($Z = 28$). It includes iron ($Z = 26$), the most important magnetic element. A similar situation occurs several times in the periodic table. The rare-earth elements ($Z = 58$ to 71) are chemically so similar to one another that the early investigators couldn't even separate them.

The filling of levels continues. Each successive element has a ground state that represents the lowest available energy consistent with the Pauli principle. Each electron can be described by a solution of the Schrödinger equation (with the spin component added) in the electric field that is created by the nucleus and all the other electrons.

Why does the periodic table end? What causes elements to cease to exist beyond about $Z = 92$? Here we have to leave atomic physics and go to the question of what holds the nucleus together. Already for Z greater than 83 the nuclei are unstable, *radioactive*. Some have very long lifetimes, of the order of billions of years, as is true for two of the uranium isotopes. Others are continually produced as radioactive *daughter products* of these long-lived nuclei. Some elements with values of Z beyond 92 have been produced artificially, most notably neptunium and plutonium (Z equal to 93 and 94), which have also been detected in small quantities in nature. There are about 10 more with higher values of Z, most with extremely short lifetimes, falling apart mostly by the process of spontaneous fission.

We have already touched on this question in the first chapter. The stability of nuclei depends on the competition between the actions of the nuclear force and the electric force. The nuclear force attracts all nucleons to each other, but acts only between neighboring nucleons. The electric force acts only between the protons, and repels them from each other. But its range is longer. Each proton repels all of the others. As we go to larger and larger nuclei, eventually the disruptive electric force wins, and the periodic table of the elements comes to a natural end.

12.4 Summary

At the end of the nineteenth century it seemed reasonable to assume that the basic laws of physics were known. The mechanics of Newton and the electromagnetism of Maxwell were the central parts of what we now call *classical physics*. Together with the laws of force for gravitation, electricity, and magnetism they were expected to describe and "explain" all of the phenomena of the physical world.

The discovery of x-rays (1895), radioactivity (1896), and electrons (1897) pointed in new directions. The Michelson–Morley experiment (1887) and the discovery of quantization by Planck (1900) revealed contradictions with the seemingly established classical laws.

The problem highlighted by the Michelson–Morley experiment was resolved by the Special Theory of Relativity in 1905, which resulted from a fresh examination of the fundamental nature of space and time. It was another 20 years before the quantum theory was put on a firm footing by what is now called *quantum mechanics*. The result was the modern understanding of matter in all its forms.

When a body is heated its atoms gain energy of vibration. Planck showed that only certain frequencies of vibration are possible, in accord with the relation $E = Nhf$, where N is a whole number and h is a constant, later named Planck's constant.

A photon is a *quantum* of electromagnetic energy. It behaves in many ways like a particle. It has speed c, energy hf, and momentum $\frac{hf}{c}$. In the *photoelectric effect* a photon of energy $E_{\mathrm{ph}} = hf$ hits a material and is absorbed by it. An electron is released if the photon energy is at least as large as the electron's binding energy, E_{B}. Any leftover energy is given to the electron as kinetic energy, $K : E_{\mathrm{ph}} = K + E_{\mathrm{B}}$ or $hf = K + E_{\mathrm{B}}$.

The Bohr model of the atom is part of the "old" quantum theory and leads to some incorrect conclusions. It does, however, lead to the correct spectrum of quantized energies for the hydrogen atom. It was superseded by quantum mechanics in 1925.

It was the first model of an atom consisting of a nucleus surrounded by electrons. It was also the first model to include the quantization of atomic energies and transitions between its *energy levels*. In the transition between levels with energies E_i and E_f the energy difference $E_\mathrm{i} - E_\mathrm{f} = \Delta E$ can be given to a photon with energy $E_\mathrm{ph} = hf$ so that $\Delta E = hf$.

The simplest form of the Bohr model is that of a hydrogen atom with one electron moving in a circle about a nucleus consisting of a single proton. There are two relations that characterize the model. One is the *force equation* $F_\mathrm{e} = k\frac{e^2}{r^2} = m\frac{v^2}{r}$. The other is the *quantization condition* $mvr = n\hbar$. The combination of these two relations leads to expressions for the possible values of the speed, the radius, and the energy of the atom.

The radius is $n^2 r_1$, where $r_1 = 0.53 \times 10^{-10}\,\mathrm{m}$. The energy is $\frac{1}{n^2}E_1$, where $E_1 = -13.6\,\mathrm{eV}$. One electron volt (eV) = 1.6×10^{-19} J. n is a *quantum number* that can take on all integral numbers from one to infinity.

In the Compton effect a photon collides with an electron in an elastic collision, i.e., with the conservation of kinetic energy and momentum. A new photon is created, with a smaller energy and hence smaller frequency and larger wavelength. The wavelength is longer by $\Delta\lambda = \frac{h}{m_\mathrm{e}c}(1 - \cos\theta)$.

The rest energy of an electron is 0.51 MeV. ($1\,\mathrm{MeV} = 10^6\,\mathrm{eV}$). When a photon with energy greater than twice this amount (1.02 MeV) hits a material, it can create an *electron pair*, i.e., an electron and a positron. (A positron is similar to an electron, but with a positive charge.)

Conversely, when a positron comes to rest near an electron, the two annihilate, i.e., they disappear, and their energy is given to two photons. The two photons move in opposite directions in order to conserve momentum.

When electrons with a single kinetic energy, K, hit a target and are decelerated, *continuous x-rays* are emitted, with energies from zero to K. In addition, the electrons can raise the energy of the target atoms to higher levels from which they then fall back to the ground state with the emission of *characteristic x-rays*.

Electromagnetic waves propagate just as Maxwell showed. They can go through two slits and recombine to show *interference effects*. But the electromagnetic field can interchange energy only in discrete amounts, as quanta of the field, called photons.

This synthesis shows that the quantized electromagnetic field accounts both for the propagation as electromagnetic waves and for the emission and absorption of electromagnetic energy as photons.

In Maxwell's theory the *intensity* of an electromagnetic wave is proportional to the square of the amplitude of the wave. We can now interpret the intensity in a region as proportional to the probability of finding a photon in that region.

The same reconciliation and synthesis of the points of view of particles and waves as for electromagnetism applies also to electrons and to other particles. The "particles" propagate as waves and show interference effects, as shown by the groundbreaking experiments of Davisson and Germer and of G. P. Thomson. The field associated with them can interchange energy only in discrete steps, i.e., as *quanta* whose properties are those of particles, i.e., of electrons and the other particles that we know.

Just as the square of the amplitude of an electromagnetic wave in a region is proportional to the probability of finding a photon there, so the square of the amplitude of an "electron wave" is proportional to the probability of finding an electron there. The symbol that is used for the matter wave amplitude is Ψ (Greek capital *psi*).

The general wave equation is $\frac{d_2\Psi}{dx^2} = -k^2\Psi$, where $k = \frac{2\pi}{\lambda}$.

For de Broglie waves: $k = \frac{2\pi}{h}p = \frac{p}{\hbar}$, and since $K = \frac{1}{2}mv^2 = \frac{p^2}{2m}$, $k^2 = \frac{p^2}{\hbar^2} = \frac{2mK}{\hbar^2}$, and the wave equation is $-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} = K\Psi$.

If, with Schrödinger, we let $K = E - U$, we get the Schrödinger equation $-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + U\Psi = E\Psi$.

The value of Ψ^2 in a region is proportional to the probability of finding the electron (or other particle) there. For any expression for the potential energy, U, there are solutions of the Schrödinger equation only for certain values of the energy, E, and these are the allowed values of the energy.

The *Heisenberg uncertainty principle* says that the position and momentum of a particle cannot both be known exactly at the same time. The products of their uncertainties $\Delta x \Delta p$ cannot be less than (approximately) h.

The Schrödinger equation for the hydrogen atom leads to the same energy levels as the Bohr model, $E_n = \frac{1}{n^2}E_1$, with $E_1 = -13.6\,\text{eV}$. Other properties, as for example the angular momentum, are incorrectly predicted by the Bohr model, but the results derived from quantum mechanics are in accord with all observations.

In atoms beyond hydrogen there are more protons in the nucleus and more electrons in the neutral atom. Each energy level of the atom is characterized by a different set of four quantum numbers. The quantum number n determines the energy. The quantum number ℓ determines the orbital angular momentum, which is equal to $\sqrt{\ell(\ell+1)}\hbar$. ℓ can be between zero and $n-1$. There are two more quantum numbers, m_ℓ, which can be from $-\ell$ to ℓ, and m_s, which can be $+\frac{1}{2}$ or $-\frac{1}{2}$.

In the ground state of an atom the energy levels are occupied by electrons, one for each level, starting from the level with the lowest energy. The fact that there can be only one electron occupying a level is called the *Pauli exclusion principle*.

With lower values of the orbital angular momentum (and ℓ) an electron spends more time near the nucleus. It is then more strongly attracted to the nucleus and its energy is lower. Therefore energy levels with lower ℓ are filled first.

In hydrogen only n determines the energy. In other atoms it is both n and ℓ. The quantum number n also determines the size of the atom. In the sequence of atoms in the periodic table of elements the levels are not always filled in the order of values of n. Sometimes inner levels (with lower n) are left empty and filled only in atoms further up in the table of elements (with greater atomic number). This happens for the *transition elements*. Transition elements with partially filled inner levels often have extraordinary magnetic properties.

12.5 Review activities and problems

Guided review

1. Photoelectrons are observed to be emitted by a cesium surface with an energy of 1.5 eV. The work function (the minimum energy to release an electron) of cesium is 2.1 eV. What are the energy, frequency, and wavelength of the photons that give rise to this emission?

2. (a) What are the total energy, the kinetic energy, and the potential energy of a hydrogen atom in the state with $n = 3$, according to the Bohr model?

(b) What are the energy, frequency, and wavelength of the light emitted by a hydrogen atom in the transition from the state with $n = 5$ to the state with $n = 3$?

3. A photon with energy 1 MeV hits a metal surface. It gives rise to a Compton recoil photon, which travels in the direction opposite to that of the original photon. What are the energies of the recoil photon and of the Compton electron?

4. A beam of 1-MeV photons hits a cesium surface.

(a) What is the energy of the photoelectrons?

(b) What are the maximum and minimum energies of the Compton electrons? What is the energy of the Compton electron with the most probable energy?

5. In positron emission tomography the patient is injected with a chemical substance that contains a positron-emitting isotope. The injected substance is designed to travel preferentially to specific parts of the body, e.g., to cancerous regions.

(a) After a positron is emitted, it slows down as a result of collisions with the surrounding atoms. What happens to it after that?

(b) What feature makes it possible to determine by measurements outside the body where the positron emission takes place?

(c) Why does the injected material have to contain positive rather than negative beta rays?

6. In a cathode–ray tube, such as those used in oscilloscopes and in old computer and television monitors, electrons are accelerated by an “electron gun” and then hit a fluorescent screen.

In one tube the electrons are accelerated by a potential difference of 20,000 V. What are the ranges of the energies, frequencies, and wave-lengths of the x-rays produced at the screen?

7. One of the simplest models of a nucleus is that of an energy well whose size is the experimentally known nuclear size. What is the lowest energy of a neutron in a one-dimensional well whose size is 3×10^{-15} m?

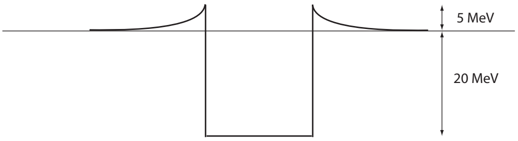
8. (a) The solution of the Schrödinger equation outside a finite well is proportional to $\Psi = e^{-ax}$, so that $\frac{d^2\Psi}{dx^2} = a^2\Psi$. Substitute this solution in the Schrödinger equation, $\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} = (W - E)\Psi$, and so find a in terms of W, E, and m.

(b) Find the value of a for a neutron in a well for which $W = 100$ MeV in an energy level $E = 80$ MeV. (Remember to use SI units for the energies and all other terms.)

(c) What is the ratio of the value of Ψ at $x = 10^{-15}$ m to that at $x = 0$?

(d) What is the ratio of the probabilities of finding the neutron at these two places?

9.



One of the first applications of quantum mechanics to the atomic nucleus was the successful description of alpha–particle radioactivity.

The diagram shows the cross section of a three-dimensional energy well as a model for the nucleus. There is a rectangular part in the center and a part that decreases as $\frac{1}{r}$ outside. The rectangular part represents an approximation to the attraction of a particle inside the nucleus as a result of the nuclear force. The $\frac{1}{r}$ part represents the electrostatic (Coulomb) repulsion outside.

Assume that the nucleus consists of alpha particles inside the well, with the various available energies.

(a) Qualitatively describe the fate of alpha particles in the nucleus as described by this model for the following ranges of the alpha particle energy inside the well:

(i) less than 20 MeV,
(ii) between 20 and 25 MeV,
(iii) more than 25 MeV.

10. (a) Write down the Schrödinger equation for the electron inside the energy well of Examples 7 and 8.

(b) In what way are the wave functions similar in the two cases?

(c) In what way are they different?

11. Show that the ground state energy of the infinite square well (Example 7) is given approximately by the Uncertainty Principle.

12. Define the four quantities **L**, **S**, ℓ, and s.

13. In hydrogen the states with the same value of n and different values of ℓ have the same value of the energy. What is different about them?

14. What are the quantum numbers that describe the electrons in the ground state of the neutral lithium ($Z = 3$) atom?

15. (a) What feature of the figure for Example 15 leads to the fact that the sequence of energy levels is different for hydrogen and for elements with $Z > 20$?

(b) Which level on this diagram represents the transition elements? Explain.

Problems and reasoning skill building

1. What is the smallest energy a photon can have that will allow it to be absorbed by a hydrogen atom in its ground state?

2. Ultraviolet light causes sunburn and damage to the skin. What characteristic is responsible for the fact that this is so for ultraviolet light but not for visible light?

3. An electron and a neutron travel at the same speed. What is the ratio of their de Broglie wavelengths, $\frac{\lambda_e}{\lambda_n}$?

4. The uranium atom has 92 times as many electrons as the hydrogen atom, but its radius is only about $3\frac{1}{2}$ times larger. Explain.

5. Atoms of a certain element have three energy levels. They are observed to emit photons with energies 1 eV, 2 eV, and 3 eV. Draw two possible energy level diagrams.

6. A hypothetical atom has three atomic energy levels. They are at -1.5, -2, and -3 eV.

(a) What is its ground state energy?

(b) What is its ionization energy?

(c) What is the lowest energy of photons that can be emitted by this atom?

(d) What are the energies of photons that can be emitted by this atom when it is in its ground state?

7. Suppose an electron could be in a nucleus whose diameter is 3×10^{-15} m. What would the depth of an energy well have to be to make this possible? To get an approximate answer, calculate the ground-state energy of an electron in an infinite well of this diameter.

8. The diffraction pattern on a screen for a certain setup is the same for an electron beam as for light whose wavelength is 495 nm. What is the speed of the electrons?

9. It takes a photon of 1.4×10^{-18} J to break a certain molecule apart into its atoms. What are the wavelength and frequency of the photon? What kind of photon is this?

10. An electron is accelerated through a potential difference of 300 V.

(a) What is the energy of the electron in eV and in J?

(b) What is its wavelength?

11. An electron's kinetic energy is larger by 1% than $\frac{1}{2}mv^2$.

(a) What is its energy in eV?

(b) What is its wavelength?

12. A photon hits a hydrogen atom and is absorbed. The photon momentum is 6.45×10^{-27} kgm/s. To which energy level (i.e., to which value of n) is the atom raised from its ground state?

13. The lowest binding energy of the electrons in barium (its work function) is 2.48 eV.

(a) What are the threshold energy, frequency, and wavelength of photons that can lead to the emission of photoelectrons from barium?

(b) What is the range of wavelengths of visible light that can give rise to photoelectrons from barium?

14. Sketch the wave functions for each of the three regions of Guided review Question 9.

Multiple choice questions

1. In the annihilation of a positron and an electron at least two photons are produced because of

(a) energy conservation,

(b) momentum conservation,

(c) $E = mc^2$,

(d) the difference in the masses of the positron and the electron.

2. Compared to the initial photon, the photon scattered by the Compton effect has a larger

(a) energy

(b) momentum

(c) frequency

(d) wavelength

3. The number of electrons emitted in the photoelectric effect is proportional to the following characteristic of the incident light:

(a) intensity

(b) energy

(c) momentum

(d) wavelength

4. A hypothetical atom has three energy levels at -1.5, -2, and -3 eV. The atom, in its ground state, can absorb photons with the following energies (in eV):

(a) 1, 1.5, 3

(b) 0.5, 1, 2

(c) 0.5, 1, 1.5, 2, 3

(d) 1, 1.5, 2, 2.5, 3

Synthesis problems and projects

1. Go to the PhET website and open the simulation *Models of the Hydrogen Atom*.

Click on *Experiment*.

Click on the button under "Turn on the gun." You will see "photons" moving toward a "box" that contains hydrogen. Inside the box is a question mark to indicate that we are trying to determine the nature of the hydrogen atoms.

Click on "Show Spectrometer" and "white". Some of the photons that you see moving upward on the screen are absorbed by the hydrogen in the box. The hydrogen then emits new photons. The spectrometer detects the photons that are emitted by the hydrogen and displays their wavelengths. Move the slider at the bottom to "fast" so that the photons accumulate more quickly.

After the spectrum has developed, write down, as best you can, the wavelengths at which photons are detected by the spectrometer. Note that the scale is linear only in the central region, from 380 nm to 780 nm, i.e., in the visible region.

Click on *Predictions*.

Here the question mark is replaced by various models of the atom. For each case you can observe the behavior predicted by the model.

(a) Click on the "Billiard Ball model": the atom is a hard ball without any internal structure. The photons (or any other particles) make only elastic collisions. That means that the total kinetic energy is the same before and after the collision.

Describe why there is or is not any radiation emitted according to this model.

(b) In the "Plum Pudding Model" electrons are embedded (like plums or raisins) in a pudding (or cake) of positive charge. The electrons can be given some energy to move back and forth in the atom. They would radiate this energy away, but not with the spectrum of discrete wavelengths that are registered by the spectrometer.

(c) Rutherford showed that the positive charge is concentrated in a tiny nucleus rather than spread out throughout the atom. (See the simulation "Rutherford Scattering" in the next problem. There is also a description of nuclei in Chapter 1 and at the beginning of Chapter 13.)

Move the slider to its slowest position. Click on the "Classical Solar System" model. Click on "Show electron energy level diagram." Here the electrons move around the nucleus as do planets around the sun. Since the electrons are accelerated ($a = \frac{v^2}{r}$) the electromagnetic theory predicts that they radiate energy rapidly. (To reset, go to an earlier model.)

What happens to the atom? Why?

(d) Now click on the "Bohr model"and look at the prediction. How did Bohr deal with the failure of the Classical Solar System model? What does his model say about the stability of the atom? What does it indicate quantitatively about the angular momentum of the atom? What are the two relations that together let you calculate the energy levels of the atom? How can you calculate the energies that may be emitted by the atoms from the energy levels? How can you calculate the frequencies and wavelengths of the emitted radiation?

(e) Does the de Broglie model change anything that we said in the previous paragraph (d) about the angular momentum and the energy levels? What was de Broglie's contribution?

(f) Which quantity do the Bohr and de Broglie models describe correctly? Which do they describe incorrectly?

(g) What are the predictions of the Schrödinger model about the energy levels? About the angular momentum?

(h) List some other successes that the Schrödinger model has with quantities that the other models either describe incorrectly or cannot deal with.

(i) Look at the line on the spectrum with the largest wavelength in the central region (where the scale is linear). It corresponds to a transition between two energy levels of the atom. Try to identify the values of n of the two energy levels. (You will have to guess what the values are and then calculate to see whether you guessed correctly.)

Do the same for the level pairs that give rise to the radiation at the next lower wavelengths. (Your experience with the first pair should make this easier.)

2. Go to the PhET website and open the simulation *Rutherford Scattering*.

Select "Rutherford Atom" from the tabs at the top. You see a gold atom with its 79 protons and 118 neutrons.

"Turn on the gun" by clicking on the "0" on the left. Alpha particles come from the bottom and are deflected by the nucleus. Click on "Show traces" to see their paths.

Change the alpha-particle energy by moving the slider from "min" to "max." What changes do you observe? Explain.

Change the target nucleus to $^{44}_{20}\mathrm{Ca}$ (20 protons and 24 neutrons). What change to you observe? Explain.

Select “Plum Pudding Atom” from the tabs at the top. Turn on the gun and “Show traces.” What do you observe? Explain your observation and contrast it with the observations for the Rutherford Atom.

The atom is about 14 cm across on the screen. What would be the order of magnitude of the diameter of a gold nucleus on the screen to the same scale?

3. Describe positron emission tomography. (Try the article in newworldencyclopedia.org.)

4. What are the energies, according to the Bohr model, of a singly ionized helium atom, i.e., an alpha particle with a single atomic electron?

5. A muonic hydrogen atom is one in which the atomic electron is replaced by a negative muon. The negative muon has the same charge as the electron, but 207 times the mass. The other properties of the two particles are the same.

What, according to the Bohr model, are the allowed energies?

6. Bohr suggested that truth and clarity are complementary. Explain what he may have meant, with examples.