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Biophysics Department
Modern Physics-Fourth Stage

Lecture Two
Atomic Physics

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The Quantum Model of the Hydrogen Atom

As we mentioned in the last lecture the Bohr model combines both classical and quantum concepts. This treatment can not explain all the experimental results. To do this we should go to:

Full quantum model (Schrödinger equation) to describe hydrogen atom

If we take a look for Schrödinger equation (in 3D):

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + U\psi = E\psi$$

We can see that we just need to know the potential energy function (U) and then solve the second differential equation which is an electrical interaction between the electron and the proton given by:

$$U(r) = -k_e \frac{e^2}{r}$$

r -dependent only

Before solving Schrödinger equation, it is very important to convert equation from Cartesian coordinates (x, y, z) to polar coordinates (r, θ, ϕ) since it is easy to deal with it in solving the problem

Also the wave function of the H-atom can be written in polar coordinates : $\psi(r, \theta, \phi)$

$$z = r \cos \theta$$

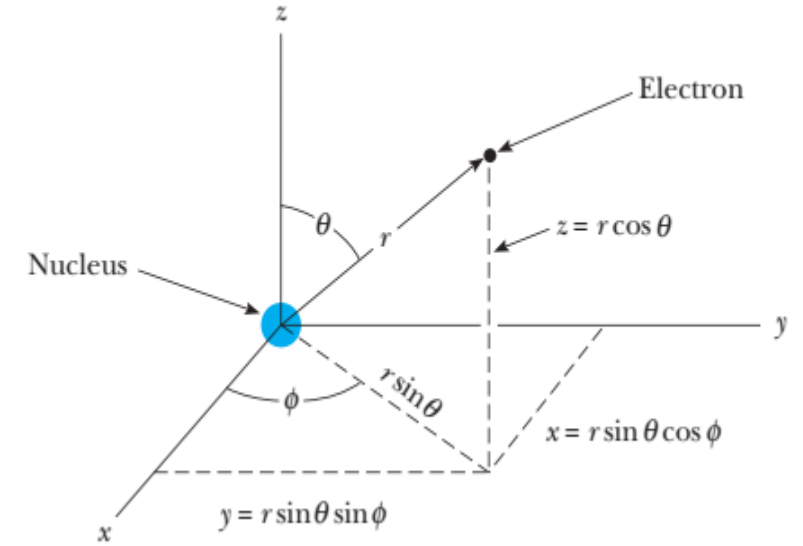
$$x = r \sin \theta \cos \phi$$

$$y = r \sin \theta \sin \phi$$

$$r = \{x^2 + y^2 + z^2\}^{1/2}$$

$$\cos \theta = \frac{z}{r} = z\{x^2 + y^2 + z^2\}^{-1/2}$$

$$\tan \phi = \frac{y}{x}$$



the hydrogen atom wave function can be separated by writing the wave function as a product of functions of each single variable: (very important mathematical tools used to solve Schrödinger equation)

$$\psi(\mathbf{r}) = \psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)$$

What is the boundary conditions of these separated functions?

When the full set of boundary conditions is applied to all three functions, **three different quantum numbers are found** for each allowed state of the hydrogen atom, one for each of the separate differential equations.

➤ **principal quantum number** (n) \longrightarrow related to $R(r)$ which represent probability of finding the electron at a certain radial distance from the nucleus.

$$E_n = -\left(\frac{k_e e^2}{2a_0}\right) \frac{1}{n^2} = -\frac{13.606 \text{ eV}}{n^2} \quad n = 1, 2, 3, \dots$$

➤ **orbital quantum number** (ℓ) comes from the differential equation for $f(\theta)$ and is associated with the orbital angular momentum of the electron.

➤ **orbital magnetic quantum number** (m), arises from the differential equation for $g(\phi)$

The values of n are integers that can range from 1 to ∞ .

The values of ℓ are integers that can range from 0 to $n - 1$.

The values of m_ℓ are integers that can range from $-\ell$ to ℓ .

Shell and Subshell

Shell Notations

n	Shell Symbol
1	K
2	L
3	M
4	N
5	O
6	P

Subshell Notations

ℓ	Subshell Symbol
0	<i>s</i>
1	<i>p</i>
2	<i>d</i>
3	<i>f</i>
4	<i>g</i>
5	<i>h</i>

Example 42.2

The $n = 2$ Level of Hydrogen

For a hydrogen atom, determine the allowed states corresponding to the principal quantum number $n = 2$ and calculate the energies of these states.

SOLUTION

Conceptualize Think about the atom in the $n = 2$ quantum state. There is only one such state in the Bohr theory, but our discussion of the quantum theory allows for more states because of the possible values of ℓ and m_ℓ .

Categorize We evaluate the results using rules discussed in this section, so we categorize this example as a substitution problem.

From Table 42.1, we find that when $n = 2$, ℓ can be 0 or

$$\ell = 0 \rightarrow m_\ell = 0$$

1. Find the possible values of m_ℓ from Table 42.1:

$$\ell = 1 \rightarrow m_\ell = -1, 0, \text{ or } 1$$

Hence, we have one state, designated as the $2s$ state, that is associated with the quantum numbers $n = 2$, $\ell = 0$, and $m_\ell = 0$, and we have three states, designated as $2p$ states, for which the quantum numbers are $n = 2$, $\ell = 1$, and $m_\ell = -1$; $n = 2$, $\ell = 1$, and $m_\ell = 0$; and $n = 2$, $\ell = 1$, and $m_\ell = 1$.

Find the energy for all four of these states with $n = 2$ from Equation 42.21:

$$E_2 = -\frac{13.606 \text{ eV}}{2^2} = -3.401 \text{ eV}$$

Quick Quiz 42.3 How many possible subshells are there for the $n = 4$ level of hydrogen? (a) 5 (b) 4 (c) 3 (d) 2 (e) 1

Quick Quiz 42.4 When the principal quantum number is $n = 5$, how many different values of (a) ℓ and (b) m_ℓ are possible?

The Wave Functions for Hydrogen

Since the potential energy of the H-atom depends only on the **radial distance** r between nucleus and electron, some of the allowed states for this atom can be represented by wave functions that depend only on r . **For these states, $f(\theta)$ and $g(\phi)$ are constants.** The ground state for H-atom and the next-simplest wave functions:

$$\psi_{1s}(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

$$\psi_{2s}(r) = \frac{1}{4\sqrt{2\pi}} \left(\frac{1}{a_0}\right)^{3/2} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$$

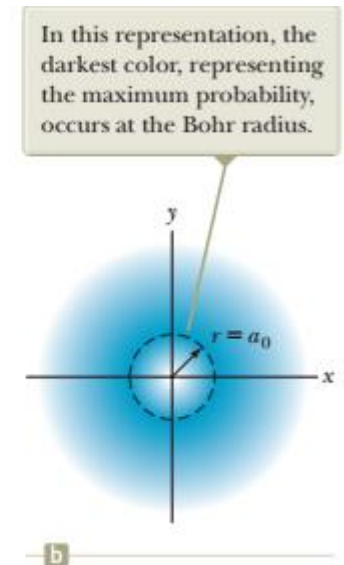
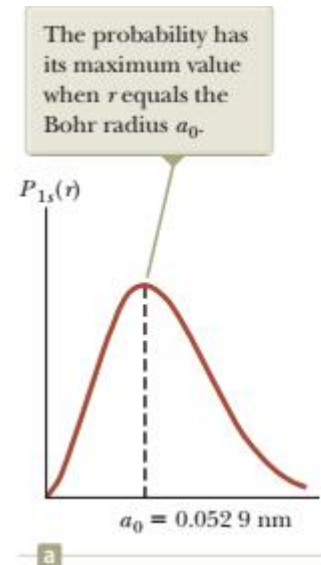
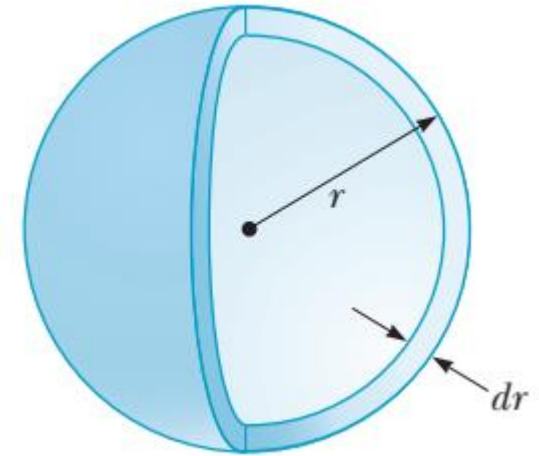
Spherical
symmetry

the probability of finding a particle in any region

$$P(r) dr = |\psi|^2 dV = |\psi|^2 4\pi r^2 dr$$

the radial probability density function for the hydrogen atom in its ground state (1s):

$$P_{1s}(r) = \left(\frac{4r^2}{a_0^3}\right) e^{-2r/a_0}$$



Example 42.3

The Ground State of Hydrogen

(A) Calculate the most probable value of r for an electron in the ground state of the hydrogen atom.

SOLUTION

Conceptualize Do not imagine the electron in orbit around the proton as in the Bohr theory of the hydrogen atom. Instead, imagine the charge of the electron spread out in space around the proton in an electron cloud with spherical symmetry.

Categorize Because the statement of the problem asks for the “most probable value of r ,” we categorize this example as a problem in which the quantum approach is used. (In the Bohr atom, the electron moves in an orbit with an *exact* value of r .)

Analyze The most probable value of r corresponds to the maximum in the plot of $P_{1s}(r)$ versus r . We can evaluate the most probable value of r by setting $dP_{1s}/dr = 0$ and solving for r .

Differentiate Equation 42.25 and set the result equal to zero:

$$\begin{aligned}\frac{dP_{1s}}{dr} &= \frac{d}{dr} \left[\left(\frac{4r^2}{a_0^3} \right) e^{-2r/a_0} \right] = 0 \\ e^{-2r/a_0} \frac{d}{dr} (r^2) + r^2 \frac{d}{dr} (e^{-2r/a_0}) &= 0 \\ 2re^{-2r/a_0} + r^2(-2/a_0)e^{-2r/a_0} &= 0 \\ (1) \quad 2r[1 - (r/a_0)]e^{-2r/a_0} &= 0\end{aligned}$$

Set the bracketed expression equal to zero and solve for r :

$$1 - \frac{r}{a_0} = 0 \rightarrow r = a_0$$

Finalize The most probable value of r is the Bohr radius! Equation (1) is also satisfied at $r = 0$ and as $r \rightarrow \infty$. These points are locations of the *minimum* probability, which is equal to zero as seen in Figure 42.11a.

(B) Calculate the probability that the electron in the ground state of hydrogen will be found outside the Bohr radius.

SOLUTION

Analyze The probability is found by integrating the radial probability density function $P_{1s}(r)$ for this state from the Bohr radius a_0 to ∞ .

Set up this integral using Equation 42.25:

$$P = \int_{a_0}^{\infty} P_{1s}(r) dr = \frac{4}{a_0^3} \int_{a_0}^{\infty} r^2 e^{-2r/a_0} dr$$

Put the integral in dimensionless form by changing variables from r to $z = 2r/a_0$, noting that $z = 2$ when $r = a_0$ and that $dr = (a_0/2) dz$:

$$P = \frac{4}{a_0^3} \int_2^{\infty} \left(\frac{za_0}{2}\right)^2 e^{-z} \left(\frac{a_0}{2}\right) dz = \frac{1}{2} \int_2^{\infty} z^2 e^{-z} dz$$

Evaluate the integral using partial integration (see Appendix B.7):

$$P = -\frac{1}{2}(z^2 + 2z + 2)e^{-z} \Big|_2^{\infty}$$

Evaluate between the limits:

$$P = 0 - \left[-\frac{1}{2}(4 + 4 + 2)e^{-2}\right] = 5e^{-2} = 0.677 \text{ or } 67.7\%$$

Finalize This probability is larger than 50%. The reason for this value is the asymmetry in the radial probability density function (Fig. 42.11a), which has more area to the right of the peak than to the left.

WHAT IF? What if you were asked for the *average* value of r for the electron in the ground state rather than the most probable value?

Answer The average value of r is the same as the expectation value for r .

Use Equation 42.25 to evaluate the average value of r :

$$\begin{aligned} r_{\text{avg}} &= \langle r \rangle = \int_0^{\infty} rP(r) dr = \int_0^{\infty} r \left(\frac{4r^2}{a_0^3}\right) e^{-2r/a_0} dr \\ &= \left(\frac{4}{a_0^3}\right) \int_0^{\infty} r^3 e^{-2r/a_0} dr \end{aligned}$$

Evaluate the integral with the help of the first integral listed in Table B.6 in Appendix B:

$$r_{\text{avg}} = \left(\frac{4}{a_0^3}\right) \left(\frac{3!}{(2/a_0)^4}\right) = \frac{3}{2}a_0$$

Physical Interpretation of the Quantum Numbers

The principal quantum number n

The principal quantum number n of a particular state in the hydrogen atom determines the energy of the atom

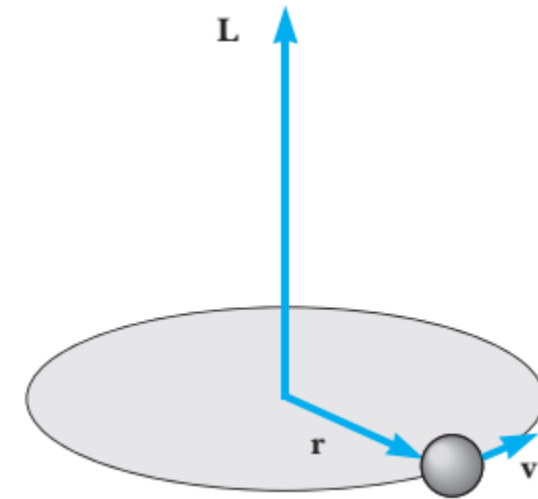
The Orbital Quantum Number ℓ

According to quantum mechanics, an atom in a state whose principal quantum number is n can take on the following discrete values of the magnitude of the orbital angular momentum:

$$L = \sqrt{\ell(\ell + 1)}\hbar \quad \ell = 0, 1, 2, \dots, n - 1$$

The Orbital Magnetic Quantum Number $m\ell$

According to classical physics, the energy of the loop-field system depends on the direction of the magnetic moment of the loop with respect to the magnetic field $UB = -\mu \times B$. Any energy between $-\mu B$ and $+\mu B$ is allowed by classical physics.



According to quantum mechanics, there are *discrete* directions allowed for the magnetic moment vector μ with respect to the magnetic field vector \mathbf{B} . This situation is very different from that in classical physics, in which all directions are allowed.

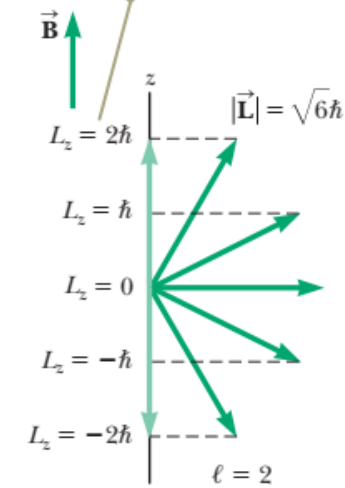
Allowed values of L_z ▶

$$L_z = m_\ell \hbar$$

$$\cos \theta = \frac{L_z}{L} = \frac{m_\ell}{\sqrt{\ell(\ell + 1)}}$$

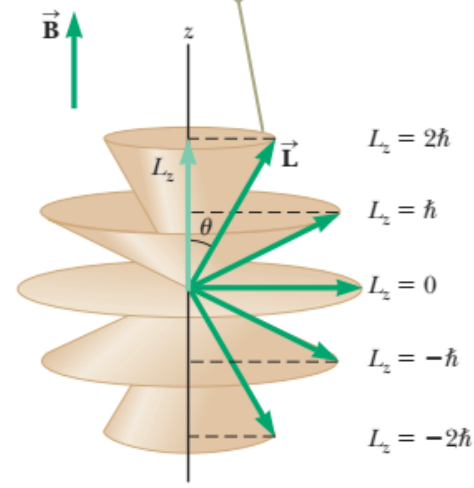
Therefore, in a collection of atoms, there are atoms in all three states and the single spectral line in Figure *a* splits into three spectral lines. This phenomenon is called the *Zeeman effect*.

The allowed projections on the z axis of the orbital angular momentum \vec{L} are integer multiples of \hbar .



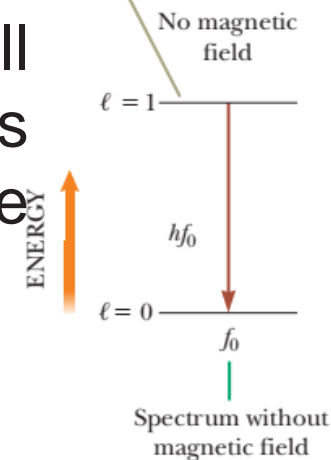
a

Because the x and y components of the orbital angular momentum vector are not quantized, the vector \vec{L} lies on the surface of a cone.



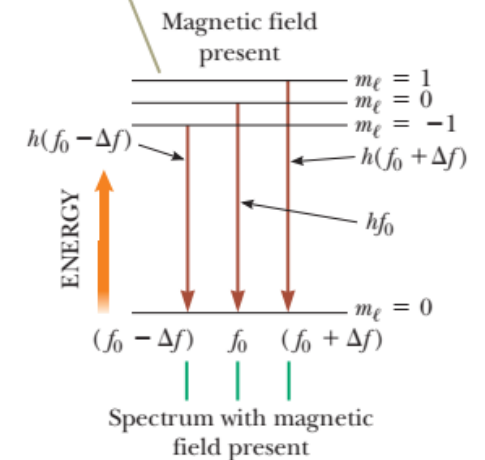
b

When $\vec{B} = 0$, the excited state has a single energy and only a single spectral line at f_0 is observed.



a

Atoms in three excited states decay to the ground state with three different energies, and three spectral lines are observed.



b

Example 42.4**Space Quantization for Hydrogen**

Consider the hydrogen atom in the $\ell = 3$ state. Calculate the magnitude of \vec{L} , the allowed values of L_z , and the corresponding angles θ that \vec{L} makes with the z axis.

SOLUTION

Conceptualize Consider Figure 42.13a, which is a vector model for $\ell = 2$. Draw such a vector model for $\ell = 3$ to help with this problem.

Categorize We evaluate results using equations developed in this section, so we categorize this example as a substitution problem.

Calculate the magnitude of the orbital angular momentum using Equation 42.27:

$$L = \sqrt{\ell(\ell + 1)}\hbar = \sqrt{3(3 + 1)}\hbar = 2\sqrt{3}\hbar$$

Calculate the allowed values of L_z using Equation 42.28 with $m_\ell = -3, -2, -1, 0, 1, 2$, and 3:

$$L_z = -3\hbar, -2\hbar, -\hbar, 0, \hbar, 2\hbar, 3\hbar$$

Calculate the allowed values of $\cos \theta$ using Equation 42.29:

$$\cos \theta = \frac{\pm 3}{2\sqrt{3}} = \pm 0.866 \quad \cos \theta = \frac{\pm 2}{2\sqrt{3}} = \pm 0.577$$

$$\cos \theta = \frac{\pm 1}{2\sqrt{3}} = \pm 0.289 \quad \cos \theta = \frac{0}{2\sqrt{3}} = 0$$

Find the angles corresponding to these values of $\cos \theta$:

$$\theta = 30.0^\circ, 54.7^\circ, 73.2^\circ, 90.0^\circ, 107^\circ, 125^\circ, 150^\circ$$

WHAT IF? What if the value of ℓ is an arbitrary integer? For an arbitrary value of ℓ , how many values of m_ℓ are allowed?

Answer For a given value of ℓ , the values of m_ℓ range from $-\ell$ to $+\ell$ in steps of 1. Therefore, there are 2ℓ nonzero values of m_ℓ (specifically, $\pm 1, \pm 2, \dots, \pm \ell$). In addition, one more value of $m_\ell = 0$ is possible, for a total of $2\ell + 1$ values of m_ℓ . This result is critical in understanding the results of the Stern–Gerlach experiment described below with regard to spin.

THANK YOU
FOR YOUR ATTENTION

Reference

