

## part 2

## Spin Orbit Coupling

ELECTRON SPIN

The theory of the atom developed cannot account for a number of well-known experimental observations. One is the fact that many spectral lines actually consist of two separate lines that are very close together.

Another failure of the simple quantum-mechanical theory of the atom occurs in the Zeeman Effect. There we saw that the spectral lines of an atom in a magnetic field should each be split into the three components specified. While the normal Zeeman Effect is indeed observed in the spectra of a few elements under certain circumstances, four, six, or even more components may appear, and even when three components are present their spacing may not agree with .

Fig. 7 are shown several anomalous Zeeman patterns.

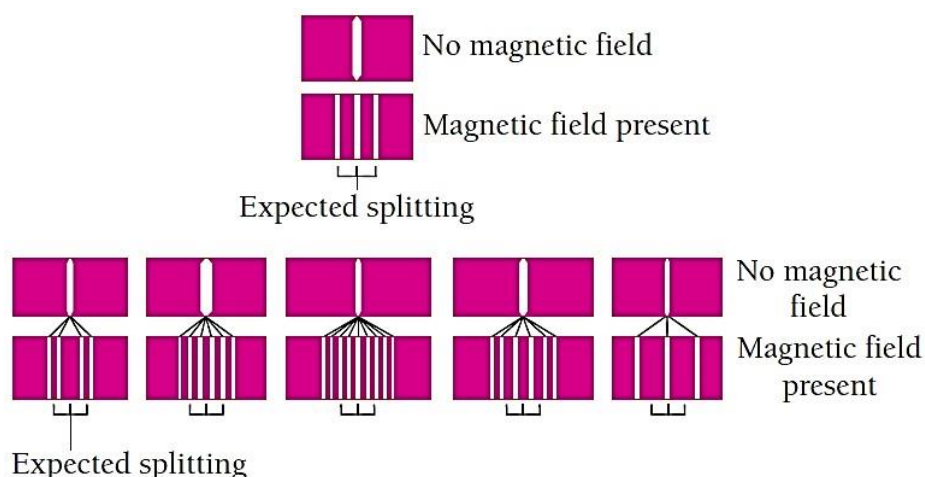


Figure 7. The normal and anomalous Zeeman effects in various spectral lines.

In order to account for both fine structure in spectral lines and the anomalous Zeeman Effect two Dutch graduate students, *Samuel Goudsmit and George Uhlenbeck*, proposed in 1925 that:-

"Every electron has an intrinsic angular momentum, called spin, whose magnitude is the same for all electrons. Associated with this angular momentum is a magnetic moment".

The quantum number  $s$  describes the spin angular momentum of the electron. The only value  $s$  can have is  $\frac{1}{2}$ . The magnitude  $S$  of the angular momentum due to electron spin is given in terms of the spin quantum number  $s$  by:-

$$S = \sqrt{s(s+1)}\hbar = \frac{\sqrt{3}}{2}\hbar \dots \dots (35)$$

This is the same formula as that giving the magnitude  $L$  of the orbital angular momentum in terms of the orbital quantum number  $l$ .  $L = \sqrt{l(l+1)}\hbar$ .

The space quantization of electron spin is described by the spin magnetic quantum number  $m_s$ . We recall that the orbital angular momentum vector can have the  $(2l+1)$  orientations in a magnetic field from  $+l$  to  $-l$ . Similarly the spin angular momentum vector can have the  $2s+1=2$  orientations specified by  $m_s = \frac{1}{2}$  ("spin up") and  $m_s = -\frac{1}{2}$  ("spin down"), as in Fig 8.

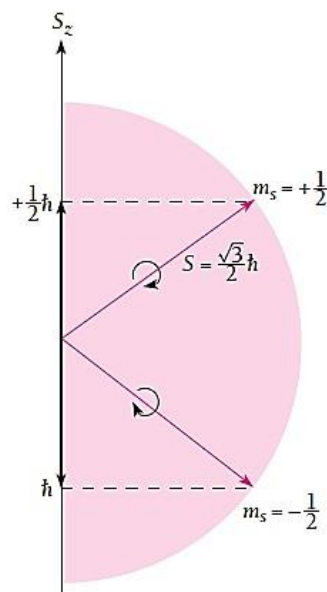


Figure 8:-The two possible orientations of the spin angular momentum vector are

“spin up ”and “spin down”

The component  $S_z$  of the spin angular momentum of an electron along a magnetic field in the  $z$  direction is determined by the spin magnetic quantum number, so that

$$S_z = m_s \hbar = \pm \frac{1}{2} \hbar \dots \dots \dots (36)$$

The gyromagnetic ratio for electron orbital motion is  $(-\frac{e}{2m})$ . The gyromagnetic ratio characteristic of electron spin is almost exactly **twice** that characteristic of electron orbital motion. Taking this ratio as equal to 2, the spin magnetic moment  $\mu_s$  of an electron is related to its spin angular momentum  $\mathbf{S}$  by:-

$$\mu_s = -\frac{e}{m} s \dots \dots \dots (37)$$

The possible components of  $\mu_s$  along any axis, say the  $z$  axis are therefore limited to

$$\mu_{sz} = \pm \frac{e\hbar}{2m} = \pm \mu_B \dots \dots \dots (38)$$

Where  $\mu_B$  is the Bohr magneton =  $9.274 \times 10^{-24}$  J/T =  $5.788 \times 10^{-5}$  eV/T.

Name	Symbol	Possible Values	Quantity Determined
Principal	$n$	1, 2, 3, .....	Electron energy
Orbital	$l$	0,1,2,.....(n-1)	Orbital angular-momentum magnitude
Magnetic	$m_l$	-l, ....., 0, ....., +l	Orbital angular-momentum direction
Spin magnetic	$m_s$	$+\frac{1}{2}, -\frac{1}{2}$	Electron spin direction

**SPIN-ORBIT COUPLING**

The fine-structure doubling of spectral lines arises from a magnetic interaction between the spin and orbital angular momenta of an atomic electron called **spin orbit coupling**.

Spin-orbit coupling can be understood in terms of a straight forward classical model.

An electron revolving about a nucleus finds itself in a magnetic field because in its own frame of reference, the nucleus is circling about it Fig.9. This magnetic field then acts upon the electron's own spin magnetic moment to produce a kind of internal Zeeman Effect.

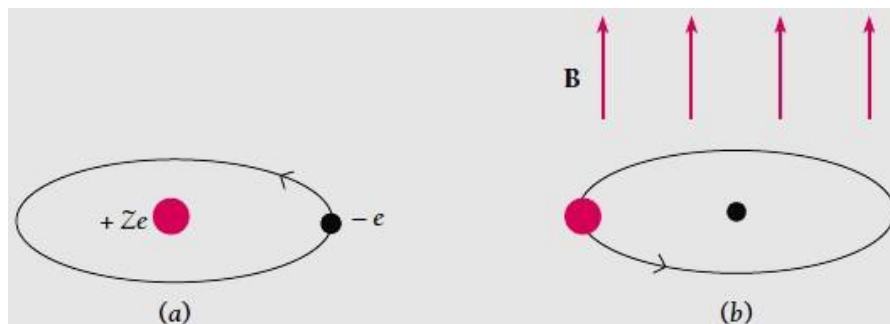


Figure 9 (a) An electron circles an atomic nucleus, as viewed from the frame of reference of the nucleus. (b) From the electron's frame of reference, the nucleus is circling it. The magnetic field the electron experiences as a result is directed upward from the plane of the orbit.

The potential energy  $V_m$  of a magnetic dipole of moment  $\mu$  in a magnetic field  $\mathbf{B}$  as we know:-

$$V_m = -\mu B \cos \theta \dots \dots \dots (39)$$

Where  $\theta$  is the angle between  $\mu$  and  $\mathbf{B}$ . The quantity  $\mu \cos \theta$  is the component of  $\mu$  parallel to  $\mathbf{B}$ . In the case of the spin magnetic moment of the electron this component is  $\mu_{sz} = \pm \mu_B$ . Hence

$$\mu \cos \theta = \pm \mu_B$$

And so **Spin-orbit coupling**

$$V_m = \pm \mu_B B \dots \dots \dots (40)$$

Depending on the orientation of its spin vector **S**, the energy of an atomic electron will be higher or lower by  $\mu_B$  than its energy without spin-orbit coupling. The result is that every quantum state (except *s* states in which there is no orbital angular momentum) is split into two substrates.

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**Example /** Find the minimum magnetic field needed for the Zeeman effect to be observed in spectral lines of 400nm wavelength when a spectrometer whose resolution is ( $\Delta \lambda = 0.01 \text{ nm}$ ) is used.

**Solution/**

$$\begin{array}{ccc}
 \lambda_2 & \lambda_1 + \Delta \lambda & \lambda_1 = 400 \text{ nm} \\
 | & | & | \\
 \nu_2 = \nu_0 - \frac{e}{4\pi m} B & \nu_0 & \nu_1 = \nu_0 + \frac{e}{4\pi m} B
 \end{array}$$

$$\nu_1 - \nu_0 = \nu_0 + \frac{e}{4\pi m} B - \nu_0$$

$$\frac{c}{\lambda_1} - \frac{c}{\lambda_0} = \frac{e}{4\pi m} B$$

$$\left( \frac{c}{400 \times 10^{-9}} - \frac{c}{(400 + 0.01) \times 10^{-9}} \right) = \frac{e}{4\pi m} B$$

$$(62.498) c = \frac{e}{4\pi m} B$$

$$B = \frac{(62.498) (3 \times 10^8) (4\pi) (9.1 \times 10^{-31})}{(1.6 \times 10^{-19})}$$

$$B = 1.339 \text{ T} \quad \text{or } B \approx 1.34 \text{ T}$$

## Independent Perturbation Theory Fine Structure

### Time-Independent Perturbation Theory:

For many reasons it is important to understand the basic level-structure of atomic hydrogen. As the simplest atom, it is a good starting point to understand the various mechanisms at work inside atoms. Early atomic physics was focussed on measuring and explaining the various atomic spectra. In recent years, atomic physics has progressed into new areas such as precision measurement, quantum optics, and even quantum computation. Atomic level structure still plays an important role in modern atomic physics, however, particularly in the rapidly evolving field of laser-cooled and trapped atoms. In solid-state physics, the atomic properties of impurity and dopant atoms play a major role, and the properties of quantum dots (artificial atoms) closely mirror those of real atoms. In nuclear physics, precision atomic spectroscopy allows precise measurements of isotopic masses and other isotopic properties. In addition, as the most abundant element, much astronomical data is based on measuring the spectral lines of hydrogen. Lastly, hydrogen is a system with many degeneracies, in which physically important results can be obtained from low-order degenerate perturbation theory, so it is an excellent area to practice applying what we have learned. We only have time to touch on atomic physics in this course, and we will focus only on the hydrogen atom for the time-being. This ignores the important and rich problem of electron-electron interaction, which dominates most of the periodic table of elements. The results from studying hydrogen, however, are readily generalized to other alkali metal (group I) atoms such as lithium (Li), sodium (Na), potassium (K), rubidium (Rb), cesium (Cs), and Francium (Fr). Because their optical properties are governed by the behavior of a single valence electron, they are currently the predominant elements used in lasercooling and trapping experiments, and all but Francium have been evaporatively cooled into Bose-Einstein condensates, which are many-body states with a single macroscopic wavefunction analogous to laser-light, but with bosonic atomic isotopes taking the place of photons. Singly ionized group II elements (Be, Mg, Ca, Sr, Ba, Ra) are also hydrogen-like, and due to their similar optical properties, are commonly used in trapped-ion experiments, such as trapped-ion quantum computers. Lastly, exotic states such as positronium (electron-positron bound state) and muonic hydrogen (proton-muon bound state) also share the hydrogen level structure. In this section we will consider four basic effects, two based on the response of hydrogen to external fields, and two based based on internal effects related to the intrinsic spin of the electron and proton. These four effects are :

1. DC Stark Effect: response of an atom to an applied static electric field.
2. Atomic Fine-structure: Interaction of the electron spin with the atom's internal magnetic field.
3. Atomic Hyperfine-structure: Interaction of the nuclear spin with the atom's internal magnetic field.
4. Zeeman Effect: response of an atom to an applied static magnetic field.

These lectures are based primarily on the treatment in the well-known quantum text by Griffiths, and 'Quantum Mechanics volume two' by Nobel Laureate Claude Cohen-Tannoudji. We first briefly review the bare hydrogen problem without spin, which was treated last semester. The simplest isotope of hydrogen consists of an electron orbiting a proton, which interact via the coulomb interaction. The bare Hamiltonian for the relative motion of the electron and the nucleus in a hydrogen atom is

$$H_0 = \frac{P^2}{2m_e} + V_c(R), \quad (1)$$

where the coulomb potential is given by

$$V_c(R) = -\frac{e^2}{4\pi\epsilon_0 R}, \quad (2)$$

with  $R$  being the operator for the distance between the electron and the proton. Strictly speaking, the mass is not the electron mass,  $m_e$ , but rather the reduced mass  $\mu = \frac{m_e m_n}{m_e + m_n}$ , where  $m_n$  is the nuclear mass. To good approximation, we have  $\mu \approx m_e$ , but precision atomic spectroscopy can resolve the correction to this  $\mu \approx m_e(1 - m_e/m_n)$ . This leads to a detectable nuclear-mass dependent shift in the atomic spectrum known as the isotope effect. Thus all of the following results can be applied to Deuterium and Tritium, simply by replacing  $m_e$  with the appropriate reduced mass.

It is customary to use as a basis simultaneous eigenstates of  $H_0$ ,  $L^2$  and  $L_z$ . The corresponding eigenvalue equations are then

$$H_0 |n\ell m_\ell^{(0)}\rangle = E_n^{(0)} |n\ell m_\ell^{(0)}\rangle, \quad (3)$$

$$L^2 |n\ell m_\ell^{(0)}\rangle = \hbar^2 \ell(\ell + 1) |n\ell m_\ell^{(0)}\rangle, \quad (4)$$

and

$$L_z |n\ell m_\ell^{(0)}\rangle = \hbar m_\ell |n\ell m_\ell^{(0)}\rangle, \quad (5)$$

where the unperturbed energy eigenvalue is

$$E_n^{(0)} = -\frac{\hbar^2}{2m_e a_0^2} \frac{1}{n^2} = -\frac{13.6 \text{ eV}}{n^2} = -\frac{2.18 \times 10^{-18} \text{ J}}{n^2}, \quad (6)$$

with

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{m_e e^2} \quad (7)$$