Notes for Lectures in Quantum Mechanics *

Observed Fine Structure of Hydrogen Atom

A. K. Kapoor http://0space.org/users/kapoor

akkapoor@cmi.ac.in; akkhcu@gmail.com

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1 Observed structure of H atom energy levels

The first successful attempt to explain the H atom levels was by Bohr. In quantum mechanics the results are derived by solving the Schr $\ddot{}$ odinger equation. The energy of a level with principal quantum number n is given by

$$En = \frac{\alpha^2 mc^2}{2n^2} \tag{1}$$

where $\alpha = e^2/(4\pi\epsilon_0)$ in SI units, and is known as the fine structure constant. It is dimensionless and has a value 1/137.07. The Schrödinger theory predicts that for a fixed value of the principal quantum number n, the angular momentum can take values $\ell = 0, 1, (n1)$ and for each ℓ the z component of the angular momentum has $(2\ell + 1)$ values $m_{\ell} = \ell, \ell + 1, \ell$. For each level corresponding to these combinations of $n\ell, m_{\ell}$ quantum numbers, the component of the spin of the electron along a specified directions can have two possible values to $\pm 1/2$. The energy depends only on n and hence there is a degeneracy of $2n^2$. For a few energy levels we schemetically show the set of quantum numbers in figure below.

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Boh r Levels : Quantum Numbers and Fine Structure Splitting Fig. 1 Quantum numbers and fine structure

1 Fine structure of H atom

Bohr's theory predicted spectral lines for hydrogen atom correctly. However, precise experiments showed that what was seen as a single spectral line in fact had a fine structure; most of the lines consist of several closely packed spectral lines. Translated in terms of energy levels, the fine structure refers to a 'fine' splitting of energy levels, which is smaller approximately by a factor of α^2 as compared with the differences in Bohr levels with different n.

The experimental results on fine structure of hydrogen atom energy levels can be summarized as follows.

The exact energies depend on j but do not depend on ℓ . Thus the H- atom levels, with the same n but different j, get split by small amounts. However, the levels having same set of values for nj quantum numbers and different $\ell = j \pm 1/2$ remain degenerate, see Fig.4.1(d) Of course, there is no splitting between levels with different m_j (or m_s) values but same nj quantum numbers. So, for example, the structure of lowest three levels is as follows.

• The ground state level, n = 1, having $\ell = 0, j = 1/2$ only, receives corrections but there is no splitting as there is only one j value (=1/2) corresponding to n = 1.

- For $n = 2, \ell$ has values 0, 1 and corresponding values of j are 1/2, 3/2. In the spectroscopic notation, nl_j , these levels are denoted by $2s_{\frac{1}{2}}, 2p_{\frac{1}{2}}, 2p_{\frac{3}{2}}$. The levels $2s_{\frac{1}{2}}$ and $2p_{\frac{1}{2}}$ remain degenerate but $2p_{\frac{3}{2}}$ receives a different correction and splits from the other levels. Thus n = 2 level splits into two levels corresponding to j = 1/2, 3/2.
- Similarly, for n = 3 in Schrödinger theory the levels $3s_{\frac{1}{2}}, 3p_{\frac{1}{2}}, 3p_{\frac{3}{2}}, 3d_{\frac{3}{2}}, 3d_{\frac{5}{2}}$ are all degenerate. These are seen to split into three groups of levels labelled by j values as given below.

(a)
$$3s_{\frac{1}{2}}$$
 and $3p_{\frac{1}{2}}$ (b) $3p_{\frac{3}{2}}, 3d_{\frac{3}{2}}$ (c) $3d_{\frac{5}{2}}$

The results described above are shown in figure, not to the scale, below. As already noted all the above splittings are small and are of the order of $\alpha^4 mc^2$. Lamb shift The Lamb shift refers to a very tiny splitting of energy levels with same nj and different ℓ values. The Lamb shift is of the order of $\alpha^5 mc^2$. For example, experimentally the levels $2s_{\frac{1}{2}}$ and $2p_{\frac{1}{2}}$ are not degenerate and the energy difference is given by

$$E(2s_{\frac{1}{2}}) - E(2p_{\frac{1}{2}}) \approx 1057 \text{MHz.}$$
 (2)

2 Hyperfine structure

The energy levels of Hydrogen atom after taking into account of the fine structure and the Lamb shift appear as shown in figure below. Each of these levels have a hyperfine structure; each level splits further into two levels with energy differences $\sim \frac{m}{M} \alpha^4 mc^2$ where M is the proton mass. Order of magnitudes of various observed energy level splittings can be summarised as follows.

Bohr levels	Fine splitting	Lamb shift	Hyperfine splitting
$\alpha^2 mc^2$	$\alpha^4 mc^2$	$\alpha^5 mc^2$	$\left(\frac{m_e}{m_p}\right) \alpha^4 mc^2$
\sim a few eV	$\sim 104~{\rm eV}$	\sim 106 eV	\sim 107 eV

The energy level diagram showing the fine structure, Lamb shift and the hyperfine structure, drawn schematically, is given below.



(a) Bohr Levels (b) Fine Structure (c) Lamb shift (d) Hyperfine Structure

Fig. $\mathbf{2}$

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