Lecture 13

Spin

Oct. 22, 2007

Review: Radial Part of Wave Function

$$\left(-\frac{\hbar^2}{2m}\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{2}{r}\frac{\mathrm{d}}{\mathrm{d}r}\right]+\frac{l(l+1)\hbar^2}{2mr^2}-\frac{e^2}{4\pi\epsilon_0 r}-E\right)R(r)=0$$

Solution for large values of r:

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2}R(r)=\frac{2m|E|}{\hbar^2}R(r) \qquad R(r)=Ce^{-r/na_0}$$

Solution for small values of r:

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{2}{r}\frac{\mathrm{d}}{\mathrm{d}r}-\frac{l(l+1)}{r^2}\right)R(r)=0 \qquad R(r)=Cr^l$$

The Radial Wave Functions

$R(r)$ depends on the quantum numbers n and l

The general solutions are of the form:

$$R_{nl}(r) \;=\; \left(\frac{r}{a_0}\right)^l \left(\text{polynomial in } \;\frac{r}{a_0}\; \text{ of order } \; n-l-1\right) e^{-r/na_0}$$

The first few R's:

$$R_{10}(r) = 2\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$$

$$R_{20}(r) = 2\left(\frac{1}{2a_0}\right)^{3/2} \left(1 - \frac{r}{2a_0}\right) e^{-r/2a_0}$$

$$R_{21}(r) = \frac{1}{\sqrt{3}}\left(\frac{1}{2a_0}\right)^{3/2} \left(\frac{r}{a_0}\right) e^{-r/2a_0}$$

Quantized Energies

When the radial equation is solved it's found that solutions exist only for certain quantized values of the energy

$$E = -\frac{1}{2}mc^2\left(\frac{e^2}{4\pi\epsilon_0\hbar c}\right)^2\frac{1}{(n_r+l+1)^2} \qquad \text{with} \qquad n_r = 0,\ 1,\ 2,\ \cdots$$

Define: $n = n_r + l + 1$

$$E = -\frac{1}{2}mc^2\left(\frac{e^2}{4\pi\epsilon_0\hbar c}\right)^2\frac{1}{n^2} = -\frac{1}{2}mc^2\alpha^2\frac{1}{n^2}$$

with $n = 1,\ 2,\ 3,\ \cdots$ and $l \leq n-1$

Summary

$$u(r,\theta,\phi) = R_{nl}(r)Y_{lm}(\theta,\phi)$$

$$E = -\frac{1}{2}mc^2\left(\frac{e^2}{4\pi\epsilon_0\hbar c}\right)^2\frac{1}{n^2} \qquad n = 1,\ 2,\ 3,\ \cdots$$

$$|\vec{L}| = \sqrt{l(l+1)}\hbar \qquad l = 0,\ 1,\ 2,\ \cdots,\ n-1$$

$$L_z = m\hbar \qquad m = -l,\ \cdots,1,\ 0,\ 1,\ \cdots,\ l$$

Energy Levels and Degenracy

Energy depends only upon n.

$$E = -\frac{1}{2} mc^2 \left(\frac{e^2}{4\pi\epsilon_0 \hbar c} \right)^2 \frac{1}{n^2} \qquad n = 1,\ 2,\ 3,\ \cdots$$

For each value of n there are n possible values of l.

$$l = 0,\ 1,\ 2,\ \cdots,\ n-1$$

For each value of l there are $2l+1$ possible values of m.

$$m = -l,\ \cdots,1,\ 0,\ 1,\ \cdots,\ l$$

$\Rightarrow$ degeneracy of the nth level is $\displaystyle\sum_{l=0}^{n-1} (2l+1) = n^2$

Probability Distributions

In spherical coordinates, the differential volume element is:

$$(r\sin\theta \mathrm{d}\phi)(r\mathrm{d}\theta)(\mathrm{d}\phi) = r^2 \sin\theta \,\mathrm{d}\theta\,\mathrm{d}\phi\,\mathrm{d}r$$

$$P(\theta,\phi) = |Y_{lm}(\theta,\phi)|^2 \sin\theta$$

$$P(r) = r^2 |R_{nl}(r)|^2$$

Normalization:

$$\int_0^{\pi}\int_0^{2\pi} |Y_{lm}(\theta,\phi)|^2 \sin\theta \,\mathrm{d}\theta\,\mathrm{d}\phi = 1$$

$$\int_0^{\infty} r^2 |R_{nl}(r)|^2 \,\mathrm{d}r = 1$$

Magnetic Dipole Moment

A circulating charge produces a magnetic dipole moment

Classically:

$$\mu = I(\text{Area}) = \frac{qv}{2\pi r}\pi r^2$$

$$= -\frac{e m_e v r}{2m_e} = -\frac{e}{2m_e}L$$

In quantum mechanics, even though there is no orbit the relation turns out to be the same.

QM:

$$\vec{\mu} = -\frac{e}{2m_e}\vec{L}$$

$$\mu_z = -\frac{e}{2m_e}L_z = -\frac{e\hbar}{2m_e}m$$

Bohr magneton: $$\mu_B = \frac{e\hbar}{2m_e} = 5.8 \times 10^{-5}\ \text{eV/T}$$

Zeeman Effect

Because of the magnetic moment, states of different m will have different energies when the atom is placed in an external magnetic field. The energy degeneracy is broken.

Energy of magnetic dipole in a magnetic field:

$$U = -\vec{\mu} \cdot \vec{B}$$

$\Rightarrow$ energy is lower when $\vec{\mu}$ and $\vec{B}$ are aligned.

For an applied external magnetic field in the z-direction, the energy of states of same n and l are split.

$$\Delta E = \frac{e\hbar B}{2m_e} m$$

Spin

In addition to mass and electric charge, the electron also carries intrinsic angular momentum.

This is not angular momentum due to motion, it is there even if the electron is standing still.

It is as if the electron were spinning like a top, though how a presumably point particle like the electron can spin is one of the conceptual mysteries of quantum mechanics.

The quantum number associated with this spin is $s = 1/2$ such that the electron has:

magnitude of total angular momentum: $|\vec{S}| = \sqrt{\frac{1}{2}(\frac{1}{2}+1)}\,\hbar = \sqrt{\frac{3}{4}}\,\hbar$

angular momentum along z-axis: $S_z = m_s\hbar = \pm\frac{1}{2}\,\hbar$

Degeneracy

One of the effects of the electron spin is to double the degeneracy of the atomic states. For each state specified by n, l, m the electron can either have spin up $m_s = +1/2$ or spin down $m_s = -1/2$ along the z-axis.

$$u(r, \theta, \phi, \pm) = R_{nl}(r) Y_{lm}(\theta, \phi) \chi_{\pm}$$

The electron spin will also cause further splitting when the atom is in an external magnetic field because of the additional magnetic moment due to the spin.

The g-factor for the Electron

A spinning charge produces a magnetic dipole. For the case of the electron, this is:

$$\vec{\mu} = -g\,\frac{e}{2m_e}\,\vec{S} \qquad \text{with} \qquad g = 2.$$

The reason that $g = 2$ follows from relativistic quantum mechanics (the Dirac equation). That's too hard for us to go into. For now, you'll just have to accept it.
The total energy splitting in an external magnetic field is then:

$$\Delta E = \frac{e\hbar B}{2m_e}\,(m + 2m_s)$$

Each state of n, l, m is further split into two energies depending on whether m_s is + or - 1/2.

Addition of Angular Momentum

There are two contributions to the total angular momentum, $\vec{J}$, of the electron in the hydrogen atom: the electron's orbital angular momentum, $\vec{L}$ and the electron's spin, $\vec{S}$.

$$\vec{J} = \vec{L} + \vec{S}$$

$$J_z = L_z + S_z \qquad \Rightarrow \qquad m_j = m + m_s$$

maximum value of $|\vec{J}|$ when $\vec{L}$ and $\vec{S}$ are aligned. $\Rightarrow$ $j = l + 1/2$

minimum value of $|\vec{J}|$ when $\vec{L}$ and $\vec{S}$ are anti-aligned. $\Rightarrow$ $j = l - 1/2$