

## A $\hbar$ Electron in an Electromagnetic Field

The hamiltonian for a particle in an EM field is

$$H = \frac{1}{2m} [\vec{p} - q\vec{A}(\vec{r}, t)]^2 + qU(\vec{r}, t) - \frac{q}{m} \vec{S} \cdot \vec{B}(\vec{r}, t) \quad (1)$$

in which

$$\vec{S} = \frac{\hbar}{2} \vec{\sigma} \quad (2)$$

and  $q$  is the charge of the particle of mass  $m$ . Here

$$\vec{B}(\vec{r}, t) = \vec{\nabla} \times \vec{A}(\vec{r}, t), \quad (3)$$

An important special case is when  $\vec{A}$  represents a constant magnetic field  $\vec{B}$ . This is the case, for instance, if

$$\vec{A}(\vec{r}) = -\frac{1}{2} \vec{r} \times \vec{B}. \quad (4)$$

Here  $(\vec{A}, U)$  is in the Coulomb or radiation gauge because

$$\vec{\nabla} \cdot \vec{A} = -\frac{1}{2} \sum_{ijk} \epsilon_{ijk} \partial_i r_j B_k = 0. \quad (5)$$

We keep

$$qU(\vec{r}, t) = -e^2/r \quad (6)$$

as in the hydrogen atom.

So we are looking at a hydrogen atom in a static constant magnetic field  $B$ .

By (5), the order of  $p$  and  $A$  does not matter

$$p \cdot A = A \cdot p \quad (7)$$

$$= -\frac{1}{2} \sum_{ijk} p_i \epsilon_{ijk} r_j B_k \quad (8)$$

$$= \frac{1}{2} \sum_{ijk} p_i \epsilon_{jik} r_j B_k \quad (9)$$

$$= \frac{1}{2} B \cdot \vec{r} \times \vec{p} = \frac{1}{2} B \cdot \vec{L} \quad (10)$$

where

$$\vec{L} = \vec{r} \times \vec{p} \quad (11)$$

is the orbital angular momentum.

So  $H$  is

$$H = \frac{\vec{p}^2}{2m} - \frac{q}{m} p \cdot A + \frac{q^2}{2m} A^2 - \frac{e^2}{r} - \frac{q\hbar}{2m} \sigma \cdot B \quad (12)$$

with  $q = -e < 0$

$$H = \frac{\vec{p}^2}{2m} + \frac{e}{2m} B \cdot L + \frac{e^2}{2m} A^2 - \frac{e^2}{r} + \frac{e\hbar}{2m} \sigma \cdot B \quad (13)$$

The third term here  $\vec{A}^2$  is

$$\begin{aligned}
 A^2 &= \frac{1}{4} (\vec{v} \times \vec{B}) \cdot (\vec{v} \times \vec{B}) \\
 &= \frac{1}{4} \sum_{ijklm=1}^3 \epsilon_{ijkl} v_j B_k \epsilon_{ilm} v_l B_m \\
 &= \frac{1}{4} \sum_{jklm} [\delta_{jle} \delta_{klm} - \delta_{jlm} \delta_{kle}] v_j B_k v_l B_m \\
 &= \frac{1}{4} [\vec{v}^2 \vec{B}^2 - (\vec{v} \cdot \vec{B})^2] \quad (14)
 \end{aligned}$$

Let's choose our coordinates so that  $\hat{z} = \hat{B}$ .

Then

$$\begin{aligned}
 \vec{v}^2 \vec{B}^2 - (\vec{v} \cdot \vec{B})^2 &= B^2 (\vec{v}^2 - v_3^2) = B^2 (v_1^2 + v_2^2) \\
 &= B^2 (x^2 + y^2) \quad (15)
 \end{aligned}$$

So our H is

$$H = \frac{\vec{p}^2}{2m} + \frac{e}{2m} B L_z + \frac{e^3 B^2}{8m} (x^2 + y^2) - \frac{e^2}{r} + \frac{e\hbar}{2m} B \sigma_z \quad (16)$$

$$\begin{aligned}
 &= \underbrace{\frac{p^2}{2m} - \frac{e^2}{r}}_{H_0} + \underbrace{\frac{eB}{2m} L_z + \frac{e\hbar}{2m} B \sigma_z}_{H_1} + \frac{e^2 B^2}{8m} (x^2 + y^2) \quad (17) \\
 &= H_0 + H_1 + H_2
 \end{aligned}$$

The first four terms  $(H_0 + H_1)$  have the e-vecs

$$|l m \sigma_z\rangle \quad (18)$$

$$(H_0 + H_1) |l m \sigma_z\rangle =$$

$$\left( \frac{p^2}{2m_e} - \frac{e^2}{r} + \frac{eB}{2m_e} L_z + \frac{e\hbar}{2m_e} B \sigma_z \right) |l m \sigma_z\rangle \quad (19)$$

$$= \left( -\frac{1}{2} m_e c^2 \frac{\alpha^2}{n^2} + \frac{e\hbar}{2m_e} B m + \frac{e\hbar}{2m_e} B \sigma_z \right) |l m \sigma_z\rangle.$$

$$= \left[ -\frac{1}{2} m_e c^2 \frac{\alpha^2}{n^2} + \mu_B B (m + \sigma_z) \right] |l m \sigma_z\rangle$$

in which

$$\mu_B = \frac{e\hbar}{2m_e} \quad (20)$$

is the Bohr magneton. Note that the energy shift due to  $B$  in the state  $|l m \sigma_z\rangle$  is

$$\Delta E = \mu_B B (m \pm 1) \quad (21)$$

So the spin of the electron contributes twice its  $S_z$  while  $L_z$  contributes just  $L_z/\hbar$ .

One  $\hbar$  says that the gyro magnetic ratio of the electron's spin is 2 to lowest order.

Equivalently, in (17) the third and fourth terms are

$$H_1 = \frac{eB}{2m} L_z + \frac{e\hbar}{2m} B\sigma_z = \frac{eB}{2m} (L_z + 2S_z). \quad (22)$$

How big are these terms?

$$E_n^0 = -\frac{1}{2}mc^2 \frac{\alpha^2}{n^2} = -\frac{13.6 \text{ eV}}{n^2} \quad (23)$$

and

$$\frac{E_n^0}{h} \approx 10^{14} \text{ to } 10^{15} \text{ Hz}. \quad (24)$$

The corrections  $M_B B (m \pm 1)$  due to  $H_1$  are much smaller because

$$M_B = \frac{e\hbar}{2me} = 5.788 \times 10^{-11} \frac{\text{MeV}}{\text{T}} = 5.788 \times 10^{-5} \frac{\text{eV}}{\text{T}} \quad (25)$$

in which  $T = 1 \text{ tesla} = 10^4 \text{ gauss}$ . Fields people can make rarely exceed 10T, so

$$|M_B B (m \pm 1)| \lesssim 6 \times 10^{-4} \text{ eV} \quad (26)$$

or about  $10^4$  (or four orders of magnitude smaller than)  $E_n^0$  the Bohr energy levels.

The fifth term  $H_2$  (in (17)) is still smaller for commonly achievable B's.

To see this, we note that the matrix elements of  $x^2 + y^2$  in the states near the ground state are

$$\langle x^2 + y^2 \rangle \sim a_0^2 = \left( \frac{\hbar^2}{m e e^2} \right)^2. \quad (27)$$

Thus the ratio of  $\langle H_2 \rangle / \langle H_1 \rangle$  is of the order of

$$\begin{aligned} \frac{E_2}{E_1} &\sim \frac{\langle H_2 \rangle}{\langle H_1 \rangle} \sim \frac{e^2 B^2 a_0^3}{m e} \frac{1}{\frac{e \hbar B}{m e}} \\ &= \frac{e B a_0^2}{\hbar}. \end{aligned} \quad (28)$$

But  $\langle p \rangle \sim \hbar / a_0$  and so

$$E_0 \sim \frac{\langle p^2 \rangle}{2m} \sim \frac{\hbar^2}{m a_0^2} \quad (29)$$

Thus

$$\frac{E_2}{E_1} \sim \frac{e \hbar B}{m} \frac{1}{\hbar^2 / (m a_0^2)} \sim \frac{E_1}{E_0}. \quad (30)$$

$$\text{So } E_2 \sim 10^{-4} E_1 \sim 10^{-8} E_0. \quad (31)$$

Thus for laboratory-sized magnetic fields and for H-atoms in the lower Bohr levels  $n=1, 2, \dots, 10$  etc, we can approximate  $H$  as

$$H \sim H_0 + H_1$$

and find its e-vecs as  $|n l m \sigma_z\rangle$

$$(H_0 + H_1) |n l m \sigma_z\rangle = \left[ -\frac{1}{2} m c^2 \frac{\alpha^2}{n^2} + \mu_B B (m + \sigma_z) \right] |n l m \sigma_z\rangle$$

in which  $\sigma_z = \pm 1$  and  $\mu_B = e\hbar/2m_e$ .  
Each  $n, l$  level will have

$$2(l+1)$$

different energy levels. The B-field breaks most, but not all, of the degeneracy.

These states are an example of the simple way of adding two angular momenta  $\vec{L}$  and  $\vec{S}$ . These states are e-vecs of  $\vec{L}^2, \vec{S}^2, L_z, S_z,$  &  $L_z + S_z$ :

$$\vec{L}^2 |n l m \sigma_z\rangle = \hbar^2 l(l+1) |n l m \sigma_z\rangle$$

$$\vec{S}^2 |n l m \sigma_z\rangle = \hbar^2 s(s+1) |n l m \sigma_z\rangle = \hbar^2 \frac{3}{4} |n l m \sigma_z\rangle$$

$$L_z |n l m \sigma_z\rangle = \hbar m |n l m \sigma_z\rangle$$

$$S_z |n l m \sigma_z\rangle = \frac{\hbar}{2} \sigma_z |n l m \sigma_z\rangle$$

$$(L_z + S_z) |n l m \sigma_z\rangle = \hbar \left( m + \frac{\sigma_z}{2} \right) |n l m \sigma_z\rangle.$$