An Electron in an Electromagnetic Field

The hamiltonian for a particle in an EM field is

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

in which

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

and q is the charge of the particle of mass m. Here we remain in SI units, and

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

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

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

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

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

We keep

$$q\,u(\vec{r},t) = -e^2/r = -\frac{q^2}{4\pi\epsilon_0 r} \qquad (6)$$

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

$$p \cdot A = A \cdot p \tag{7}$$

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

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

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

where

$$\vec{L} = \vec{r} \times \vec{p} \tag{11}$$

is the orbital angular momentum.

So H is

$$H = \frac{\vec{p}^2}{2m} - \frac{q}{m} p \cdot A + \frac{q^2}{2m} \vec{A}^2 - \frac{q^2}{4\pi\epsilon_0 r} - \frac{q}{m} S \cdot B \tag{12}$$

or with $q = -\sqrt{4\pi\epsilon_0}\, e$

$$H = \frac{p^2}{2m} - \frac{q}{2m} L \cdot B + \frac{q^2}{2m} \vec{A}^2 - \frac{e^2}{r} - \frac{q}{m} S \cdot B. \tag{13}$$

Note that $\vec{S}$ couples to $\vec{B}$ twice as strongly as $\vec{L}$.

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

$$A^2 = \frac{1}{4}(r \times B)\cdot(r \times B)$$

$$= \frac{1}{4}\sum_{ijk\ell m=1}^{3} \epsilon_{ijk} r_j B_k \, \epsilon_{i\ell m} r_\ell B_m$$

$$= \frac{1}{4}\sum_{jk\ell m}\left[\delta_{j\ell}\,\delta_{km} - \delta_{jm}\,\delta_{k\ell}\right] r_j B_k r_\ell B_m$$

$$= \frac{1}{4}\left[\vec{r}^{\,2}\vec{B}^2 - (\vec{r}\cdot\vec{B})^2\right]. \tag{14}$$

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

$$\vec{r}^{\,2}\vec{B}^2 - (\vec{r}\cdot\vec{B})^2 = B^2(\vec{r}^{\,2} - r_3^2) = B^2(r_1^2 + r_2^2)$$

$$= B^2(x^2+y^2). \tag{15}$$

So with $\mu_B = q\hbar/(2m_e) = -9.27\times10^{-24}\,\frac{J}{T}$, our H is

$$H = \frac{\vec{p}^{\,2}}{2m} - \frac{q}{2m}BL_z + \frac{q^2B^2}{8m}(x^2+y^2) - \frac{e^2}{r} - \frac{q}{m}BS_z \tag{16}$$

$$= \underbrace{\frac{p^2}{2m} - \frac{e^2}{r}}_{H_0} \underbrace{- \frac{\mu_B}{\hbar}BL_z - 2\frac{\mu_B}{\hbar}BS_z}_{H_1} + \frac{q^2B^2}{8m}(x^2+y^2). \tag{17}$$

$$= H_0 + H_1 + H_2$$

Incidentally, $\omega_L = -\frac{qB}{2m}$ is the Larmor angular velocity.

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

$$|n \ell m \sigma_z\rangle \tag{18}$$

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

$$\left(\frac{p^2}{2m_e} - \frac{e^2}{r} - \frac{\mu_B}{\hbar} B L_z - 2\frac{\mu_B}{\hbar} B S_z\right)|n\ell m \sigma_z\rangle \tag{19}$$

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

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

in which

$$\mu_B = \frac{q\hbar}{2m_e} = -\frac{\sqrt{4\pi\epsilon_0}\, e\hbar}{2m_e} = -9.27 \times 10^{-24} \frac{J}{T} \tag{20}$$

is the Bohr magneton. Note that the energy shift due to B in the state $|n\ell m \pm 1\rangle$ is

$$\Delta E = \mu_B B (m \pm 1) \tag{21}$$

So the spin of the electron contributes twice its $\frac{S_z}{\hbar}$ while L_z contributes just $L_z/\hbar$. One says that the gyromagnetic ratio of the electron's spin is 2 to lowest order.

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

$$H_1 = -\mu_B \frac{B}{\hbar} \left(L_z + 2 S_z \right). \qquad (22)$$

How big are these terms?

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

and

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

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

$$\mu_B = \frac{e\hbar}{2m_e} = 5.788 \times 10^{-11} \frac{\text{MeV}}{\text{T}} = 5.788 \times 10^{-5} \frac{\text{eV}}{\text{T}} \qquad (25)$$

in which T = 1 tesla = 10^4 gauss. Fields people can make rarely exceed 10 T, so

$$\left| \mu_B B (m \pm 1) \right| \lesssim 6 \times 10^{-4}\ \text{eV} \qquad (26)$$

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 currently 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

$$\langle | x^2+y^2 | \rangle \sim a_0^2 = \left(\frac{\hbar^2}{mee^2}\right)^2 \qquad (27)$$

where $a_0 = 0.52$ Å.
Thus the ratio of $\langle H_2 \rangle / \langle H_1 \rangle$ is of the order of

$$\frac{E_2}{E_1} \sim \frac{\langle H_2 \rangle}{\langle H_1 \rangle} \sim \frac{q^2 B^2 a_0^2}{me} \cdot \frac{1}{\mu_B B}$$

$$\sim \frac{q^2 B^2 a_0^2}{me} \cdot \frac{me}{q\hbar B} = \frac{q\hbar B}{m} \cdot \frac{1}{\left(\frac{\hbar^2}{ma_0^2}\right)} \qquad (28)$$

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

$$E_0 \sim \frac{\langle p^2 \rangle}{2m} \sim \frac{\hbar^2}{ma_0^2} \qquad (29)$$

Thus

$$\frac{E_2}{E_1} \sim \frac{\mu_B B}{\hbar^2/(ma_0^2)} \sim \frac{E_1}{E_0} . \qquad (30)$$

So $E_2 \sim 10^{-4} E_1 \sim 10^{-8} E_0$. (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 $|n\,l\,m\,\sigma_z\rangle$

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

in which $\sigma_z = \pm 1$ and $\mu_B = q\hbar/(2me)$. Each n, l level will have

$$2(2l+1)$$

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 $\vec{L}^2, \vec{S}^2, L_z, S_z,$ & $L_z + S_z$:

$$\vec{L}^2\,|n\,l\,m\,\sigma_z\rangle = \hbar\, l(l+1)\,|n\,l\,m\,\sigma_z\rangle$$
$$\vec{S}^2\,|n\,l\,m\,\sigma_z\rangle = \hbar\, s(s+1)\,|n\,l\,m\,\sigma_z\rangle = \hbar\frac{3}{4}\,|n\,l\,m\,\sigma_z\rangle$$
$$L_z\,|n\,l\,m\,\sigma_z\rangle = \hbar m\,|n\,l\,m\,\sigma_z\rangle$$
$$S_z\,|n\,l\,m\,\sigma_z\rangle = \frac{\hbar}{2}\sigma_z\,|n\,l\,m\,\sigma_z\rangle$$
$$(L_z + S_z)\,|n\,l\,m\,\sigma_z\rangle = \hbar\left(m + \frac{\sigma_z}{2}\right)|n\,l\,m\,\sigma_z\rangle.$$