

2.5.5(3): The Effect on Fine Structure of Gravitation

Fine structure of atoms and molecules is very accurately measurable so it is interesting to evaluate the effect of gravitation on the spectra. This can be done most simply by the minimal prescription:

$$E \rightarrow E + m\Phi \quad - (1)$$

where m is the mass of the electron and where Φ is the gravitational potential:

$$\Phi = -\frac{GM}{r} \quad - (2)$$

where G is the Newton constant and where M is a mass that is gravitationally attracted to the mass m . Here r is the vector joining m and M .

Using the minimal prescription (1) in the Einstein energy equation gives:

$$E + m\Phi - mc^2 = \frac{c^2 p^2}{E + m\Phi + mc^2} \quad - (3)$$

so:

$$E = -m\Phi + mc^2 + \frac{1}{2m} p^2 \left(1 + \frac{m\Phi}{2mc^2} \right)^{-1} \quad - (4)$$

The approximation:

$$E \sim mc^2 \quad - (5)$$

Quantizing eq. (4) in the $SU(2)$ basis

gives:

$$H\psi = \left(-m\Phi + mc^2 + \frac{1}{2m} \underline{\sigma} \cdot \underline{p} \left(1 - \frac{n\Phi}{2mc^2} \right) \underline{\sigma} \cdot \underline{p} \right) \psi - (6)$$

in the approximation:

$$m\Phi \ll 2mc^2 - (7)$$

The relevant spin orbit Hamiltonian is:

$$\begin{aligned} H_1\psi &= \frac{i\hbar}{4mc^2} \underline{\sigma} \cdot \underline{\nabla} \Phi \underline{\sigma} \cdot \underline{p} \psi - (8) \\ &= -\frac{i\hbar}{4mc^2} \underline{\sigma} \cdot \underline{g} \underline{\sigma} \cdot \underline{p} \psi \end{aligned}$$

where

$$\underline{g} = -\underline{\nabla} \Phi - (9)$$

is the acceleration due to gravity:

$$\underline{g} = -\frac{MG}{r^3} \underline{r} - (10)$$

It is possible to develop eq. (8) in different ways, including the following:

To consider the effect of the earth's \underline{g} on the electron in an H atom.

To evaluate the effect of the gravitational interaction between an electron and a proton in the H atom.

To develop eqn (1) use:

$$\underline{\sigma} \cdot \underline{p} = \frac{1}{r^2} \underline{\sigma} \cdot \underline{r} \underline{\sigma} \cdot \underline{r} \underline{\sigma} \cdot \underline{p} \quad - (11)$$

$$= \frac{1}{r^2} \underline{\sigma} \cdot \underline{r} (\underline{r} \cdot \underline{p} + i \underline{\sigma} \cdot \underline{L})$$

where

$$\underline{L} = \underline{r} \times \underline{p} \quad - (12)$$

is the classical angular momentum. From eqs. (8) and (11):

$$\text{Real } H_1 \psi = \frac{\hbar}{4mc^2 r^2} \underline{\sigma} \cdot \underline{g} \underline{\sigma} \cdot \underline{r} \underline{\sigma} \cdot \underline{L} \psi \quad - (13)$$

Now use:

$$\underline{\sigma} \cdot \underline{g} \underline{\sigma} \cdot \underline{r} = \underline{g} \cdot \underline{r} + i \underline{\sigma} \cdot \underline{g} \times \underline{r} \quad - (14)$$

so:

$$\text{Real } H_1 \psi = \frac{\hbar \underline{g} \cdot \underline{r}}{4mc^2 r^2} \underline{\sigma} \cdot \underline{L} \psi \quad - (15)$$

In spherical polar coordinates:

$$\underline{r} = r \underline{e}_r \quad - (16)$$

and from eqs. (10) and (16):

$$\underline{g} \cdot \underline{r} = r \underline{g} \cdot \underline{e}_r \quad - (17)$$

However, from eq. (10):

$$4) \quad \underline{g} = -\frac{MG}{r^3} \underline{r} = -\frac{MG}{r^3} r \underline{e}_r \quad - (18)$$

So

$$r \underline{g} \cdot \underline{e}_r = rg \quad - (19)$$

Therefore:

$$\text{Real } H_1 \psi = \frac{\hbar^2 g}{4mc^2 r} \underline{\sigma} \cdot \underline{L} \psi \quad - (20)$$

in which:

$$\underline{\sigma} \cdot \underline{L} = \langle \hat{\underline{\sigma}} \cdot \hat{\underline{L}} \rangle = \hbar(j(j+1) - l(l+1) - s(s+1)) \quad - (21)$$

So

$$\text{Real } H_1 \psi = \frac{\hbar^2 g}{4mc^2 r} (j(j+1) - l(l+1) - s(s+1)) \psi \quad - (22)$$

Units Check

$$\frac{\hbar^2 g}{4mc^2 r} = \frac{\text{J}^2 \text{s}^2 \text{m s}^{-2}}{\text{J m}} = \text{J} \checkmark$$

The energy expectation values from eq. (22) are evaluated as follows:

$$5) \quad E_1 = \frac{\hbar^2 g (j(j+1) - l(l+1) - s(s+1))}{4mc^2} \int \frac{\psi^* \psi}{r} d\tau \quad - (23)$$

For a hydrogenic atom this gives the effect of the earth's gravitational field on the fine structure.

Here:

$$\hbar = 6.62618 \times 10^{-34} \text{ Js}$$

$$g = 9.80665 \text{ m s}^{-2}$$

$$m = 9.10953 \times 10^{-31} \text{ kg}$$

$$c = 2.997925 \times 10^8 \text{ m s}^{-1}$$

$$\text{one joule} = 5.03445 \times 10^{22} \text{ cm}^{-1}$$

Therefore:

$$J_g = \frac{\hbar^2 g}{4mc^2} = 1.31477 \times 10^{-53} \text{ J m}^{-1} \quad - (24)$$

$$= 6.61914 \times 10^{-31} \text{ cm}^{-1} \text{ m}^{-1}$$

is the gravitational fine structure constant. - (25)

Therefore:

$$E_1 = 6.61914 \times 10^{-31} (j(j+1) - l(l+1) - s(s+1)) \int \frac{\psi^* \psi}{r} d\tau$$

ii wave numbers

In a very rough approximation, for hydrogenic orbitals:

$$\int \frac{\psi^* \psi}{r} d\tau \sim \frac{Z}{a_0} \quad (26)$$

here the Bohr radius is:

$$a_0 = 5.29177 \times 10^{-11} \text{ m} \quad (27)$$

so

$$E_1 \sim 1.25084 \times 10^{-20} Z(j(j+1) - l(l+1) - s(s+1))$$

wavenumbers

- (28)

For a 2p electron in H the usual fine structure splitting is 0.365 cm^{-1} .

So the effect of the earth's gravity is about twenty orders of magnitude smaller. This is the result expected from the fact that the electromagnetic field is orders of magnitude stronger than the gravitational field, and explains why the earth's gravitational field has no effect on atomic or molecular fine structure. In order to observe the effect of gravitation on atomic or molecular fine structure the value of g must be maximised. For

the sun, $g_{\text{mass}} \frac{M}{r^2} = 1.9891 \times 10^{30} \text{ kg}$ and radius $r = 6.96342 \times 10^8 \text{ m}$, with $G = 6.6725 \times 10^{-11} \text{ m}^3 \text{ kg}^{-1} \text{ s}^{-2}$. This is still

7) not enough to give a measurable spectroscopic effect. The experiment would consist of light grazing the sun being absorbed by H in the sun's atmosphere and the spectrum recorded on earth.

In order to see an effect, an object must be used of very large mass and very small radius, with an atmosphere that contains atomic hydrogen. Light grazing this object would be absorbed and its spectrum recorded on earth. The spectral splitting might become very large if g were very large, and the spectrum would be different from that recorded on earth.

However a neutron star has a mass of 1.4 to 3.2 solar masses and a typical radius of 12 km. So for a neutron star of twice the solar mass:

$$g = 1.8434 \times 10^{14} \text{ ms}^{-2} \quad - (29)$$

There is also atomic H in the atmosphere of a neutron star, so E_{11} eq. (28) becomes, very roughly:

$$E_1 \sim 1.25084 \times 10^{-7} \sum (j(j+1) - l(l+1) - s(s+1)) \quad - (30)$$

Wavenumbers.

This seems to be within the range of FT Spectrometers.

8) To evaluate the effect of the gravitational interaction between proton and electron eq. (8) is used in the form:

$$H_1 \psi = - \frac{\hbar^2 M G}{4 m c^2 r^3} \underline{\sigma} \cdot \underline{r} \underline{\sigma} \cdot \underline{p} \psi \quad - (31)$$

$$\text{So Real } H_1 \psi = \frac{\hbar^2 M G}{4 m c^2 r^3} \underline{\sigma} \cdot \underline{L} \psi \quad - (32)$$

giving the energy expectation value:

$$E_{1g} = \frac{\hbar^2 M G}{4 m c^2} (j(j+1) - l(l+1) - s(s+1)) \int \frac{\psi^* \psi}{r^3} d\tau \quad - (33)$$

where M is the mass of the proton and m is the mass of the electron. This compares with the electromagnetic result:

$$E_{1em} = \frac{e^2 \hbar^2}{16 \pi \epsilon_0 m^2 c^2} (j(j+1) - l(l+1) - s(s+1)) \int \frac{\psi^* \psi}{r^3} d\tau \quad - (34)$$

The ratio of (33) and (34) is:

$$\frac{E_{1g}}{E_{1em}} = \left(\frac{4 \pi \epsilon_0 G}{e^2} \right) m \underline{M} \quad - (35)$$

$$= 2.89214 \times 10^{-16} m \underline{M}$$

We have:

$$\text{electron mass } m = 9.10953 \times 10^{-31} \text{ kg}$$

$$\text{proton mass } \underline{M} = 1.67265 \times 10^{-27} \text{ kg}$$

9) So:

$$E_{ig} = 2.89214 \times 10^{16} \times 9.10953 \times 10^{-31} \times 1.67265 \times 10^{-27}$$

$$\frac{E_{ig}}{E_{em}} = 4.40677 \times 10^{-41}$$

Therefore the spin orbit coupling due to gravitation is forty one orders of magnitude smaller than that due to electromagnetism in the H atom. Hence the gravitational effect is entirely undetectable by this direct method.

In order to enhance the effect of gravitation a resonance mechanism is necessary.
