267(5): Effect of Ubiquitous Thomas Precession on the H Atom.

Thomas Precession is ubiquitous because it is the rotation of the Minkowski metric. It appears on all scales and in all situations. In gravitational theory the velocity of the Thomas precession is defined by the equivalence principle:

$$\frac{1}{2} m v_\theta^2 = \frac{mMG}{r} \quad -(1)$$

So

$$v_\theta^2 = \frac{2MG}{r} \quad -(2)$$

In electrostatics:

$$\frac{1}{2} m v_\theta^2 = \frac{e^2}{4\pi\epsilon_0 r} \quad -(3)$$

So

$$\boxed{v_\theta^2 = \frac{e^2}{2\pi\epsilon_0 r m}} \quad -(4)$$

The Thomas precession causes all observable planar orbits to precess to give the planar ellipse:

$$r = \frac{\alpha}{1+\epsilon\cos(x\phi)} \quad -(5)$$

where

$$x = 1 + \frac{3MG}{c^2\alpha} \quad -(6)$$

Arguing in direct analogy:

$$MG \rightarrow \frac{e^2}{4\pi\epsilon_0 m} = \frac{\hbar}{mc}\alpha_f \quad -(7)$$

2) Here α_f is the fine structure constant:

$$\alpha_f = \frac{e^2}{4\pi\hbar c\epsilon_0} = 0.007297351 \quad -(8)$$

and where the Compton wavelength is:

$$\lambda_c = \frac{h}{mc} = 2.426309 \times 10^{-12}\,m \quad -(9)$$

so

$$\frac{\hbar}{mc} = \frac{\lambda_c}{2\pi} \quad -(10)$$

Therefore:

$$\boxed{x = 1 + \frac{3MG}{c^2\alpha} \rightarrow 1 + \frac{3\alpha_f\lambda_c}{2\pi\alpha}} \quad -(11)$$

In both gravitational and electrostatic theory:

$$H = E = T + V \quad -(12)$$

$$= \frac{1}{2}mv^2 - \frac{k}{r}$$

and

$$r = \frac{\alpha}{1 + \epsilon\cos(x\phi)} \quad -(13)$$

In gravitation:

$$k = mMG \quad -(14)$$

and in electrostatics:

$$k = \frac{e^2}{4\pi\epsilon_0} \quad -(15)$$

The velocity in eq. (12) is defined by:

$$v^2 = \left(\frac{dr}{dt}\right)^2 + r^2\left(\frac{d\phi}{dt}\right)^2 \quad -(16)$$

where

$$\omega = \frac{d\phi}{dt} = \frac{L}{mr^2} \quad -(17)$$

The force in both gravitation and electrostatics is defined by:

$$F = m\left(\frac{d^2r}{dt^2} - r\left(\frac{d\phi}{dt}\right)^2\right) = -\frac{L^2}{mr^2}\left(\frac{d^2}{d\phi^2}\left(\frac{1}{r}\right) + \frac{1}{r}\right)$$

$$= -\frac{k}{r^2} \quad -(18)$$

In both cases:

$$m\frac{d^2r}{dt^2} = -\frac{L^2}{mr^2}\frac{d^2}{d\phi^2}\left(\frac{1}{r}\right)$$

$$= -\frac{k}{r^2} + \frac{L^2}{mr^3} \quad -(19)$$

if

$$r = \frac{\alpha}{1+\epsilon\cos\phi} \quad -(20)$$

However, if:

$$r = \frac{\alpha}{1+\epsilon\cos(x\phi)} \quad -(21)$$

then:

4)

$$m\frac{d^2 r}{dt^2} = x^2\left(-\frac{k}{r^2} + \frac{L^2}{mr^3}\right) \quad -(22)$$

and the hamiltonian (12) changes from:

$$H = E = \frac{p^2}{2m} - \frac{k}{r} \quad -(23)$$

to:

$$H = E = \frac{p^2}{2m} - \frac{x^2 k}{r} + (x^2 - 1)\frac{L^2}{2mr^2}$$

$$= \frac{1}{2}m\left(\frac{dr}{dt}\right)^2 + x^2\left(-\frac{k}{r} + \frac{L^2}{2mr^2}\right) \quad -(24)$$

Therefore in general the ubiquitous Thomas precession causes the Schroedinger equation to change from:

$$-\frac{\hbar^2}{2m}\nabla^2\phi = \left(E + \frac{k}{r}\right)\phi \quad -(25)$$

to

$$-\frac{\hbar^2}{2m}\nabla^2\phi = \left(E + x^2\frac{k}{r} - (x^2-1)\frac{L^2}{2mr^2}\right)\phi \quad -(26)$$

where

$$x = 1 + \frac{3\alpha_f \lambda_c}{2\pi r_B n} \quad -(27)$$

where

$$\alpha = r_B = 5.29177 \times 10^{-11}\, m \quad -(28)$$

is the Bohr radius.

5) Therefore the entire structure of computational quantum chemistry is changed by the ubiquitous Thomas precession.

From eq. (27):

$$x = 1 + \frac{0.000159754}{n^2} \quad -(29)$$

if it is assumed that:

$$L = n\hbar \quad -(30)$$

and that

$$\alpha = n^2 r_B = \frac{4\pi\epsilon_0 n^2 \hbar^2}{m e^2} \quad -(31)$$

where

$$n = 1, 2, 3, \ldots \quad -(32)$$

Eq. (30) is Bohr quantization. In Schroedinger quantization:

$$\hat{L}_Z \phi = m_\ell \hbar \phi \quad -(33)$$

where $\hat{L}_Z$ is the orbital angular momentum operator.

Here:

$$m_\ell = L, L-1, \ldots, -L. \quad -(34)$$

The key relation between the Bohr and Schroedinger H atoms is that their energy levels are the same, and defined by n, the principal quantum number. So as a working hypothesis it is assumed that x is defined by eq. (29).

6)

The energy levels of the Bohr and Schroedinger atoms are:

$$E = -\frac{k}{2\alpha} = -\frac{mk^2}{2n^2\hbar^2} \quad -(35)$$

so

$$\frac{1}{n^2} = -\frac{2\hbar^2 E}{mk^2} \quad -(36)$$

Therefore:

$$\boxed{x = 1 - 0.000159754\left(\frac{2\hbar^2 E}{mk^2}\right)} \quad -(37)$$

The solution of eq. (26) needs computational methods in general. However it can be approximated by:

$$-\frac{\hbar^2}{2m}\nabla^2\phi = \left(E + \frac{x^2 k}{r}\right)\phi \quad -(38)$$

The solution of eq. (38) are the same for H as those of the Schroedinger equation, but:

$$k \rightarrow x^2 k \quad -(39)$$

With this rule we can compute:

$$\langle r \rangle = \left\langle \frac{\alpha}{1+\epsilon\cos(x\phi)} \right\rangle \quad -(40)$$

as in note 267(4).