05(3): Gravitationally affected wave functions of the H Atom

As in the previous note the Schroedinger equation in the presence of the earth's gravitational field is:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} + V_1\right)\phi = E\phi \quad -(1)$$

where

$$V_1 = -m_2 MG / R \quad -(2)$$

So:

$$\langle E \rangle = \int \phi^* E \phi \, d\tau$$

$$= \int \phi^* \left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r} + V_1\right)\phi \, d\tau \quad -(3)$$

$$= -\left(\frac{me^4}{32\pi^2\epsilon_0^2\hbar^2}\right)\frac{1}{n^2} - \frac{m_2 MG}{R}$$

This means that the absolute values of the energy levels are shifted by V_1. The atomic spectrum is not affected because it depends on transitions between different n.

However eq. (1) provides additional theoretical information about the H atom in the gravitational field as follows.

First write the potential term in eq (1) in terms of a coordinate r_1 defined as:

2)
$$\frac{e^2}{4\pi\epsilon_0 r_1} = \frac{e^2}{4\pi\epsilon_0 r} + V_1 \quad -(4)$$

So:
$$\frac{1}{r_1} = \frac{1}{r} + x \quad -(5)$$

where
$$x = \frac{4\pi\epsilon_0}{e^2} \frac{m_2 M G}{R} \quad -(6)$$

So:
$$\boxed{r_1 = \frac{r}{1 + xr}} \quad -(7)$$

From eq. (6):
$$x = 4.5346 \times 10^8 \, m^{-1} \quad -(8)$$

Now consider the Schroedinger equation in the coordinate system (r_1, θ, ϕ). It is
$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r_1^2} - \frac{e^2}{4\pi\epsilon_0 r_1} \right) \psi_1 = E_1 \psi_1 \quad -(9)$$

for which
$$E_1 = -\left(\frac{m e^4}{32\pi^2 \epsilon_0^2 \hbar^2} \right) \frac{1}{n^2} \quad -(10)$$

The use of the coordinate system (r_1, θ, ϕ) has the effect of giving the hydrogenic energy levels (10) in the presence of the earth's gravitational field. The wavefunctions of eq. (9) are:

3)

$$\psi(r_1, \theta, \phi) = R(r_1) Y(\theta, \phi) \quad -(11)$$

where:

$$R_{nl}(r_1) = \left(\frac{2Z}{na}\right)\left[\frac{(n-l-1)!}{2n[(n+l)!]^3}\right]\rho_1^l L_{n+l}^{2l+1}(\rho_1) \exp\left(-\frac{\rho_1}{2}\right) \quad -(12)$$

where:

$$\rho_1 = \left(\frac{2Z}{na}\right) r_1 \quad -(13)$$

Here a is the Bohr radius and Z the atomic number.

The expectation value is defined by:

$$\langle E_1 \rangle = \int \psi_1^* E_1 \psi_1 \, d\tau_1 \quad -(14)$$

$$= \int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi}\int_{r_1=0}^{\infty} \psi_1^* E_1 \psi_1 r_1^2 \sin\theta \, dr_1 \, d\theta \, d\phi$$

Therefore r of the usual Schroedinger equation:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0 r}\right)\psi = E\psi \quad -(15)$$

is replaced by r_1 defined from eq. (1).

This procedure gives the same energy levels (10) both from eq. (9) and eq. (15), but the wave functions of eq. (9) are different. The wave functions in the coordinate system (r_1, θ, ϕ) can be expressed in terms of r using eq. (7). The first few radial wave functions

4) of the coordinate system (r_1, θ, ϕ) are as follows.

1s Orbital, $n=1$, $\ell = 0$

$$R_{10}(r) = \left(\frac{1}{a}\right)^{3/2} \exp\left(-\frac{\rho_1}{2}\right) \quad -(16)$$

where

$$\rho_1 = \frac{2Z}{na}\left(\frac{r}{1+xr}\right) \quad -(17)$$

2s Orbital, $n=2$, $\ell=0$

$$R_{20}(r) = \left(\frac{1}{a}\right)^{3/2}\left(\frac{1}{2\sqrt{2}}\right)(2-\rho_1)\exp\left(-\frac{\rho_1}{2}\right) \quad -(18)$$

2p Orbital, $n=2$, $\ell=1$

$$R_{21}(r) = \left(\frac{1}{a}\right)^{3/2}\left(\frac{1}{2\sqrt{6}}\right)\rho_1 \exp\left(-\frac{\rho_1}{2}\right) \quad -(19)$$

3s Orbital $n=3$, $\ell=0$

$$R_{30}(r) = \left(\frac{1}{a}\right)^{3/2}\left(\frac{1}{9\sqrt{3}}\right)(6-6\rho_1+\rho_1^2)\exp\left(-\frac{\rho_1}{2}\right) \quad -(20)$$

3p Orbital $n=3$, $\ell=1$

$$R_{31}(r) = \left(\frac{1}{a}\right)^{3/2}\left(\frac{1}{9\sqrt{6}}\right)(4-\rho_1)\rho_1 \exp\left(-\frac{\rho_1}{2}\right) \quad -(21)$$

3d Orbital $n=3$, $\ell=2$

$$R_{32}(r) = \left(\frac{1}{a}\right)^{3/2}\left(\frac{1}{9\sqrt{30}}\right)\rho_1^2 \exp\left(-\frac{\rho_1}{2}\right) \quad -(22)$$

5) The complete wave functions are given in each of eqs. (16) to (22) by:

$$\psi_1 = R(r_1)\, Y(\theta, \phi) \quad -(23)$$

$$= R\left(\frac{r}{1+xr}\right) Y(\theta, \phi)$$

Eqs. (16) to (22) can be plotted by computer and give entirely new information about the H atom in the gravitational field of an object of mass M. This is true for all atoms and molecules.

The energy expectation values are:

$$\langle E_1 \rangle = \int \psi_1 E_1 \psi_1^* \, d\tau_1 \quad -(24)$$

$$= -\left(\frac{m e^4}{32\pi^2 \epsilon_0^2 \hbar^2}\right)\frac{1}{n^2} \quad -(25)$$

where:

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r_1} - \frac{e^2}{4\pi\epsilon_0 r_1}\right)\psi_1 = E_1\psi_1$$

These are the same as the energy expectation values of

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r} - \frac{e^2}{4\pi\epsilon_0 r}\right)\psi = E\psi \quad -(26)$$