372(1): The Basic Equations of Lagrangian Quantum Mechanics.

With reference to UFT 371:

$$-\hbar^2\nabla^2\psi = p^2\psi = \frac{L^2}{\alpha}\left(\frac{2}{r}-\frac{1}{a}\right)\psi \quad -(1)$$

where

$$\psi = \psi(r)\,\psi(\theta,\phi) \quad -(2)$$

is the wavefunction, a product of the radial and angular wavefunctions. The lagrangian is:

$$\mathcal{L} = \frac{1}{2}m\left(\dot{r}^2 + r^2\dot{\beta}^2\right) - U \quad -(3)$$

where

$$\dot{\beta}^2 = \dot{\theta}^2 + \dot{\phi}^2\sin^2\theta \quad -(4)$$

The proper Lagrange variables are r and β, so there are two Euler Lagrange equations:

$$\frac{\partial\mathcal{L}}{\partial r} = \frac{d}{dt}\left(\frac{\partial\mathcal{L}}{\partial\dot{r}}\right) \quad -(5)$$

and

$$\frac{\partial\mathcal{L}}{\partial\beta} = \frac{d}{dt}\left(\frac{\partial\mathcal{L}}{\partial\dot{\beta}}\right) \quad -(6)$$

For the H atom:

$$U(r) = \frac{-e^2}{4\pi\epsilon_0 r} \quad -(7)$$

in which case:

$$r = \frac{\alpha}{1+\epsilon\cos\beta} \quad -(8)$$

and the classical momentum is:

2)

$$\rho^2 = \frac{L^2}{\alpha}\left(\frac{2}{r} - \frac{1}{a}\right) \quad -(9)$$

The semi major axis of the ellipse (8) is

$$a = \frac{\alpha}{1-\epsilon^2} \quad -(10)$$

Defining

$$U = -\frac{k}{r} \quad -(11)$$

then

$$k = \frac{e^2}{4\pi\epsilon_0} \quad -(12)$$

The half right latitude is:

$$\alpha = \frac{L^2}{mk} = \left(\frac{4\pi\epsilon_0}{e^2}\right)\frac{L^2}{m} \quad -(13)$$

which is Eq. (15) of Note 371(8), $\underline{Q.E.D.}$

Eq. (13) can be expressed as:

$$\alpha = \frac{L^2}{m\hbar c\,\alpha_{fs}} \quad -(14)$$

where the fine structure constant is:

$$\alpha_{fs} = \frac{e^2}{4\pi\hbar c\epsilon_0} \quad -(15)$$

The eccentricity of the three dimensional ellipse (8) is defined as:

$$\epsilon^2 = 1 + \frac{2EL^2}{mk^2} \quad -(16)$$

) where the total energy of the H atom is:

$$E = -\frac{me^4}{32\pi^2\epsilon_0^2\hbar^2 n^2} \quad -(17)$$

where n is the principal quantum number.

Therefore:

$$\epsilon^2 = 1 - \frac{1}{n^2}\left(\frac{L}{\hbar}\right)^2 \quad -(18)$$

The angular momentum quantizes as:

$$L^2\psi = \ell(\ell+1)\hbar^2\psi \quad -(19)$$

where ℓ is the angular momentum quantum number. So the classical L^2 is the expectation value:

$$L^2 = \langle L^2 \rangle = \int \psi^* L^2 \psi \, d\tau = \ell(\ell+1)\hbar^2 \quad -(20)$$

Therefore

$$\alpha = \frac{\lambda_c}{2\pi}\frac{\ell(\ell+1)}{\alpha_{fs}} \quad -(21)$$

and

$$\epsilon = \left(1 - \frac{\ell(\ell+1)}{n^2}\right)^{1/2} \quad -(22)$$

where the Compton wavelength is

$$\lambda_c = \frac{h}{mc} \quad -(23)$$

It follows that:

$$\frac{L^2}{\alpha} = \frac{2\pi}{\lambda_c}\alpha_{fs}\hbar^2 \quad -(24)$$

and that

$$a = \frac{\lambda_c}{2\pi}\frac{n^2}{\alpha_{fs}} \quad -(25)$$

Therefore Eq. (1) becomes:

$$\nabla^2\phi = -\frac{2\pi}{\lambda_c}\alpha_{fs}\left(\frac{2}{r} - \frac{2\pi\alpha_{fs}}{\lambda_c n^2}\right)\phi \quad -(26)$$

Finally note that:

$$\frac{2\pi}{\lambda_c}\alpha_{fs} = \frac{1}{a_0} = \frac{me^2}{4\pi\hbar^2\epsilon_0} \quad -(27)$$

where a_0 is the Bohr radius. So:

$$\boxed{\nabla^2\phi = -\frac{1}{a_0}\left(\frac{2}{r} - \frac{1}{n^2 a_0}\right)\phi} \quad -(28)$$

As shown in Note 371(8):

$$\nabla^2\phi = \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\phi(r)}{dr}\right) - \frac{l(l+1)}{r^2}\phi(r) \quad -(29)$$

So the radial wavefunctions $\phi(r)$ can be obtained directly from eqs. (28) and (29). The angular wavefunctions are the spherical harmonics. The next note will extend this method to other atoms, notably helium.