

435(2): The Time Dependent Schrodinger equation of Hydrogen Atom in  $\phi$  Frame  $(r_1, \theta, \phi)$

The equation is:

$$E_1 = i\hbar \frac{d\psi_1}{dt_1} = H_1 \psi_1 \quad (1)$$

where all quantities are expressed in frame  $(r_1, \theta, \phi)$  of spherical polar coordinates. Assume that:

$$\psi_1(r_1, t_1) = \exp(-i\omega_1 t_1) \psi_1(r_1) \quad (2)$$

then  $\langle H_1 \rangle = \hbar \omega_1 \int \psi_1^* \psi_1 d\tau_1 \quad (3)$

the infinitesimal volume element  $d\tau_1$  in frame  $(r_1, \theta, \phi)$  is:

$$d\tau_1 = r_1^2 \sin\theta dr_1 d\theta d\phi \quad (4)$$

The hydrogenic wave functions are:

$$\psi_1 = R_{nl}(r_1) Y(\theta, \phi) \quad (5)$$

Define:  $\rho_1 = \left( \frac{2Z}{na} \right) r_1 \quad (6)$

where  $Z$  is the atomic number ( $Z=1$  for H),  $a$  is the Bohr radius and  $n$  is the principal quantum number, then:

$$R_{nl}(r_1) = - \left( \frac{2Z}{na} \right) \left[ \frac{(n-l+1)!}{2n(n+l)!} \right] \rho_1^{l+1} L_{n+l}(\rho_1) \exp\left(-\frac{\rho_1}{2}\right) \quad (7)$$

where  $L_{n+l}(\rho_1)$  are the modified Laguerre polynomials. The spherical harmonics  $Y(\theta, \phi)$  are the same in frames  $(r_1, \theta, \phi)$  and  $(r, \theta, \phi)$ .

The Laplacian in frame  $(r_1, \theta, \phi)$  is:

$$\nabla_1^2 \psi_1 = \frac{1}{r_1} \frac{\partial^2 (r_1 \psi_1)}{\partial r_1^2} + \frac{1}{r_1^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \psi_1}{\partial \theta} \right)$$

$$+ \frac{1}{r_1^2 \sin^2 \theta} \frac{\partial^2 \psi_1}{\partial \phi^2} \quad - (8)$$

So the Laplacian  $\nabla_1^2$  acts on the wavefunction  $\psi_1$  in the same frame  $(r_1, \theta, \phi)$ .

This means that the computation is tractable. The classical Hamiltonian  $H_1$  in frame

$$(r_1, \theta, \phi) \text{ is: } H_1 = \frac{p_1^2}{2m} - \frac{e^2}{4\pi \epsilon_0 r_1} \quad - (9)$$

The relevant Schrodinger quantization is:

$$p_1^2 \psi_1 = -\hbar^2 \nabla_1^2 \psi_1 \quad - (10)$$

The expectation value of  $H_1$  is:

$$E_1 = \langle H_1 \rangle = -\frac{\hbar^2}{2m} \int \psi_1^* \nabla_1^2 \psi_1 d\tau_1 - \frac{e^2}{4\pi \epsilon_0} \int \psi_1^* \frac{1}{r_1} \psi_1 d\tau_1 \quad - (11)$$

From eq. (3):

$$\langle H_1 \rangle = \hbar \omega_1 \int \psi_1^* \psi_1 d\tau_1 \quad - (12)$$

The hydrogen-like radial wavefunctions are changed in space. The function for  $n=1$ ,  $l=0$  is:

$$R_{10} = 2 \left( \frac{Z}{a} \right)^{3/2} \exp \left( -\frac{r_1}{2} \right) \quad (13)$$

where

$$p_1 = \left( \frac{2Z}{na} \right) r_1 \quad (14)$$

so

$$p_1 = \left( \frac{2Z}{na} \right) \frac{r}{n(r)^{1/2}} \quad (15)$$

and there is a range of values for  $p_1$  when Sack transformed to the frame  $(r, \theta, \phi)$ .

Similarly the Hamiltonian in frame  $(r_1, \theta, \phi)$ , Eq. (9), is of some form, mathematically, as the usual Hamiltonian:

$$H = \frac{p^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r} \quad (16)$$

but  $H_1$  has a range of values defined by:

$$H_1 = \frac{p^2}{2m(n(r))} - \frac{n(r)^{1/2} e^2}{4\pi\epsilon_0 r} \quad (17)$$

The Hamiltonian (16) gives:

$$E = \langle H \rangle = -\frac{\mu e^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^3} \quad (18)$$

The Hamiltonian:

$$H = \frac{p_1^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r_1} \quad (19)$$

of result (18) in frame  $(r_1, \theta, \phi)$  but when transformed into frame  $(r, \theta, \phi)$  many new energy levels appear.