63(20): Radial Resonance Equation for H Atom

Start with the resonance equation of the Coulomb Law

$$\nabla^2\phi + \underline{\omega}\cdot\underline{\nabla}\,\phi + (\underline{\nabla}\cdot\underline{\omega})\,\phi = -\rho/\epsilon_0 \quad -(1)$$

Consider the radial component in spherical polar co-ordinates

$$\nabla^2\phi = \frac{\partial^2\phi}{\partial r^2} + \frac{2}{r}\frac{\partial\phi}{\partial r} \quad -(2)$$

$$\underline{\omega}\cdot\underline{\nabla}\,\phi = \omega_r\frac{\partial\phi}{\partial r} \quad -(3)$$

$$(\underline{\nabla}\cdot\underline{\omega})\,\phi = \frac{\phi}{r^2}\frac{\partial}{\partial r}\left(r^2\omega_r\right) \quad -(4)$$

Then:

$$\frac{\partial^2\phi}{\partial r^2} + \frac{2}{r}\frac{\partial\phi}{\partial r} + \omega_r\frac{\partial\phi}{\partial r} + \frac{\phi}{r^2}\left(2r\omega_r + r^2\frac{\partial\omega_r}{\partial r}\right) = -\frac{\rho}{\epsilon_0} \quad -(5)$$

Choose a ______ radial spin connection:

$$\omega_r = -1/r \quad -(6)$$

to obtain:

$$\boxed{\frac{\partial^2\phi}{\partial r^2} + \frac{1}{r}\frac{\partial\phi}{\partial r} - \frac{1}{r^2}\phi = -\frac{\rho}{\epsilon_0}} \quad -(7)$$

Alternatively, eqn (7) may be obtained by using:

$$\nabla^2\phi - \underline{\omega}\cdot\underline{\nabla}\,\phi - (\underline{\nabla}\cdot\underline{\omega})\,\phi = -\rho/\epsilon_0 \quad -(8)$$

and:

$$\omega_r = \frac{1}{\ }. \quad -(9)$$

2)

Now assume:

$$\rho = \rho(0) \cos(\kappa_r r). \quad — (10)$$

The radial resonance equation is therefore:

$$\frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r}\frac{\partial \phi}{\partial r} - \frac{1}{r^2}\phi = -\frac{\rho(0)}{\epsilon_0}\cos(\kappa_r r). \quad —(11)$$

Now use the change of variable:

$$\kappa_r r = \exp(i\kappa_r R) \quad — (12)$$

to obtain

$$\boxed{\frac{\partial^2 \phi}{\partial R^2} + \kappa_r^2 \phi = \frac{\rho(0)}{\epsilon_0} \mathrm{Real}\left(e^{2i\kappa_r R}\cos\left(e^{i\kappa_r R}\right)\right)} \quad — (13)$$

where

$$\exp(i\kappa_r R) = \cos(\kappa_r R) + i\sin(\kappa_r R). \quad — (14)$$

Thus:

$$\boxed{R = \frac{1}{\kappa_r}\cos^{-1}(\kappa_r r).} \quad — (15)$$

Now define:

$$A\cos(\kappa' R) := \mathrm{Real}\left(e^{2i\kappa_r R}\cos\left(e^{i\kappa_r R}\right)\right)$$

3) Then a valid particular integral of eq. (13) is

$$\phi_p(R) = \frac{A\rho(0)}{\epsilon_0} \frac{\cos(\kappa' R)}{\kappa_r^2 - \kappa'^2} \quad \text{— (17)}$$

and resonance occurs at:

$$A \cos(\kappa_r R) = \cos(2\kappa_r R)\cos(\cos(\kappa_r R))\cosh(\sin(\kappa_r R)) + \sin(2\kappa_r R)\sin(\cos(\kappa_r R))\sinh(\sin(\kappa_r R)).$$

$$\text{— (18)}$$

These results are now ready for incorporation in code or for the computation of the effect of resonance on the radial wavefunctions of H.