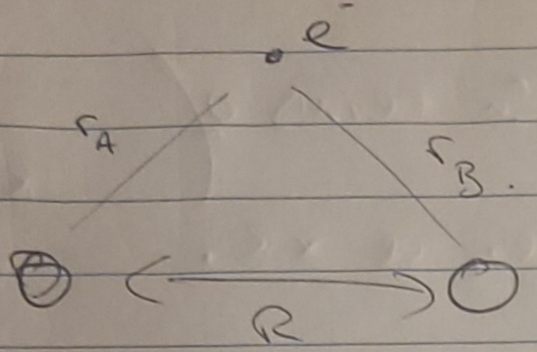

$$V(r) = -2e^2\left(\frac{1}{r_A} + \frac{1}{r_B}\right) \qquad \text{CGS units}$$

TISE:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi = E\psi.$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 - 2e^2\left(\frac{1}{r_A} + \frac{1}{r_B}\right)\right]\psi = E\psi.$$

Introducing $\lambda = \frac{r_A + r_B}{R}$ & $\mu = \frac{r_A - r_B}{R}$.

$$\frac{1}{r_A} + \frac{1}{r_B} = \frac{4}{R}\,\frac{\lambda}{\lambda^2-\mu^2}. \qquad (*)$$

The Laplacian is

$$\nabla^2 = \frac{4}{R^2(\lambda^2-\mu^2)}\left\{\frac{\partial}{\partial\lambda}\left[(\lambda^2-1)\frac{\partial}{\partial\lambda}\right] + \frac{\partial}{\partial\mu}\left[(1-\mu^2)\frac{\partial}{\partial\mu}\right] + \left[\frac{1}{\lambda^2-1} + \frac{1}{1-\mu^2}\right]\frac{\partial^2}{\partial\varphi^2}\right\}.$$

Taking from Ref (5)

Proceeding in "natural units", i.e., $\hbar = m = e = 1$.
This means plots & sols would be in the natural unit

Subbing in, ∇^2 and $(\star)$:

$-\frac{\hbar^2}{2m}\frac{4}{R^2(\lambda^2-\mu^2)}$ inside the $\left[\text{ in TISE} \right]$ without - negative

$$\Rightarrow \underbrace{\frac{4}{R^2(\lambda^2-\mu^2)}}\left\{\frac{\partial}{\partial\lambda}\left[(\lambda^2-1)\frac{\partial}{\partial\lambda}\right]+\frac{\partial}{\partial\mu}\left[(1-\mu^2)\frac{\partial}{\partial\mu}\right]\right.$$

$$\left.+\left[\frac{1}{\lambda^2-1}+\frac{1}{1-\mu^2}\right]\frac{\partial^2}{\partial\varphi^2}\right\}+\frac{4}{R}\underbrace{\frac{\lambda}{\lambda^2-\mu^2}}\cdot 2$$

Can Collect almost.

By Bringing ~~it~~ everything to RHS, we eliminate negative terms, and set $=0$: Now the TISE reads,

$\neq 0$ So cancel.

$$\frac{4}{R^2(\lambda^2-\mu^2)}\left\{\frac{\partial}{\partial\lambda}\left[(\lambda^2-1)\frac{\partial}{\partial\lambda}\right]+\frac{\partial}{\partial\mu}\left[(1-\mu^2)\frac{\partial}{\partial\mu}\right]+\left[\frac{1}{\lambda^2-1}+\frac{1}{1-\mu^2}\right]\frac{\partial^2}{\partial\varphi^2}\right.$$

$$\left.+2R\lambda+\frac{1}{4}ER^2(\lambda^2-\mu^2)\right\}\psi=0.$$

$$\Rightarrow \frac{\partial}{\partial\lambda}\left[(\lambda^2-1)\frac{\partial\psi}{\partial\lambda}\right]+\frac{\partial}{\partial\mu}\left[(1-\mu^2)\frac{\partial\psi}{\partial\mu}\right]+\left[\frac{1}{\lambda^2-1}+\frac{1}{1-\mu^2}\right]\frac{\partial^2\psi}{\partial\varphi^2}$$

$$+\left[c^2(\lambda^2-\mu^2)+2R\lambda\right]\psi=0$$

where $c^2=\frac{1}{4}ER^2$.

Now we ~~have~~ seek Solution in form $\Psi = \Lambda(\lambda) M(\mu) \Phi(\varphi)$, ~~solve~~

We know that $\Phi(\varphi) = e^{im\varphi}$, (Seperation constant m^2) which comes from mono H atom solution, readily available in all textbooks. (Eq^n 4 in report.)

So, we sub in $\Psi = \Lambda(\lambda) M(\mu) e^{im\varphi}$ and divide through by $\Lambda(\lambda) M(\mu) e^{im\varphi}$. and setting $\frac{\partial^2 \Psi}{\partial \varphi^2} = -m^2 \Psi$.

$\Rightarrow \frac{\partial}{\partial \lambda}\left[(\lambda^2-1)\right.$ ~~~~ and setting $\frac{\partial^2 \Psi}{\partial \varphi^2} = -m^2 \Psi$.

Comes from → seperating $c^2(\lambda^2-\mu^2)$

$$\Rightarrow \left\{ \frac{1}{R\Lambda} \frac{\partial}{\partial \lambda}\left[(\lambda^2-1)\frac{\partial \Lambda}{\partial \lambda}\right] - \frac{m^2}{\lambda^2-1} + 2aR\lambda + c^2\lambda^2 \right\}$$

No longer partials!

$$+ \left\{ \frac{1}{M} \frac{\partial}{\partial \mu}\left[(1-\mu^2)\frac{\partial M}{\partial \mu}\right] - \frac{m^2}{1-\mu^2} - c^2\mu^2 \right\} = 0.$$

For this to hold for any value λ and μ, the expressions within the two braces must be constant and of opposite signs

Set the λ part to equal seperation constant β and the μ part to $-\beta$, we have,

$$\frac{d}{d\lambda}\left[(\lambda^2-1)\frac{d\Lambda}{d\lambda}\right] + \left[2R\lambda + c^2\lambda^2 - \frac{m^2}{\lambda^2-1} - \beta\right]R = 0$$

and,

$$\frac{d}{d\mu}\left[(1-\mu^2)\frac{dM}{d\mu}\right] + \left[\beta - \frac{m^2}{1-\mu^2} - c^2\mu^2\right]M = 0.$$

We made use of the ϕ dependency being $\Phi(\phi) = e^{im\phi}$ form, so let's show it for the mono H atom.
The TISE reads.

$$\left[-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r}\right]\Psi = E\Psi.$$

Again, for simplicity, we take our "natural units" to eliminate $\hbar$, m & e from the expression, while also subbing in the Laplacian in polar coordinates,

$$\Rightarrow \left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{\cancel{e^2}1}{r} + E\right]\Psi.$$

By subbing in ~~Ψ and cancelling~~ $\Psi = R(r)\Theta(\theta)\Phi(\phi)$ and dividing by $R\Theta\Phi$, we have,

$$\cancel{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\partial\right.}$$

$$\frac{1}{R}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{1}{\Theta}\frac{1}{r^2\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \frac{1}{\Phi}\frac{1}{r^2\sin^2\theta}\frac{d^2\Phi}{d\phi^2}$$

$$+\frac{1}{r} + E = 0$$

Multiply by $r^2\sin^2\theta$:

$$\sin^2\theta \frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \boxed{\frac{1}{\Phi}\frac{d^2\Phi}{d\phi}}$$

$$+ \frac{1}{r} + E = 0 .$$

$= \alpha^2$ $= -\alpha^2$

dep on r, θ.   dep on Φ only.

for ~~the~~ this to hold true for all r, θ, ϕ both terms must be equal to a constant, we call the seperation constant α^2, such that

$$\frac{d^2\Phi}{d\phi} + \alpha^2\Phi = 0 .$$

$\frac{\partial^2\psi}{\partial\phi^2} = -m^2\psi$ ~~was~~ was used ased.

which has general solution,

$$\Phi = A\cos(\alpha\phi) + B\sin(\alpha\phi)$$

A, B arb constants.

The boundary condition $\Phi(0) = \Phi(2\pi)$, and also the symmetry $\Phi(0) = -\Phi(\pi)$ gives $B=0$ and solution is

$$\cancel{\Phi A(\phi) = A} \quad \Phi(\phi) = A\cos(\alpha\phi) .$$

This can also be represented in the form $Ae^{i\alpha\phi}$.

physically α is the magnetic quantum number m_l.

We therefore have

$$\Phi(\phi) = A\cos m_l\phi \quad \text{or} \quad \Phi(\phi) = Ae^{im_l\phi} .$$

Both are valid. We subbed in $e^{im\phi}$ when solving the molecular ion TISE, but the $\cos m\phi$ is ~~more stra~~ okay too.