SEPARATION OF VARIABLES IN HYDROGEN ATOMS

1. $$\frac{-\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2}\right]+U(r)\psi=E\psi$$

2. $\psi(r,\ \theta,\ \varphi)=R(r)\Theta(\theta)\Phi(\varphi)$ and $Y(\theta,\ \varphi)=\Theta(\theta)\Phi(\varphi)$

3. Substitute $\psi(r,\ \theta,\ \varphi)$ and multiply by $\dfrac{-2\mu r^2}{\hbar^2\psi(r,\ \theta,\ \varphi)}=\dfrac{-2\mu r^2}{\hbar^2 R(r)Y(\theta,\ \varphi)}$

4. $$\boxed{\frac{1}{R(r)}\frac{\partial}{\partial r}\left(r^2\frac{dR}{dr}\right)}+\frac{1}{Y(\theta,\ \varphi)\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y(\theta,\ \varphi)}{\partial\theta}\right)$$
$$+\frac{1}{Y(\theta,\ \varphi)\sin^2\theta}\frac{\partial^2 Y(\theta,\ \varphi)}{\partial\varphi^2}+\boxed{\frac{2\mu r^2}{\hbar^2}(E-U(r))}=0$$

5. Set the terms in dotted box which depend on r to the constant β and the remainder of $\theta,\ \varphi$ dependent terms to $-\beta$.

6. $$\frac{1}{R(r)}\frac{\partial}{\partial r}\left(r^2\frac{\partial R(r)}{\partial r}\right)+\frac{2\mu r^2}{\hbar^2}(E-U(r))=\beta$$

7. $$\frac{1}{Y(\theta,\ \varphi)\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y(\theta,\ \varphi)}{\partial\theta}\right)+\frac{1}{Y(\theta,\ \varphi)\sin^2\theta}\frac{\partial^2 Y(\theta,\ \varphi)}{\partial\varphi^2}=-\beta$$

8. Multiplying equation 7 by $Y(\theta,\ \varphi)$ we get the rigid-rotor Schrödinger Equation

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y(\theta,\ \varphi)}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y(\theta,\ \varphi)}{\partial\varphi^2}=-\beta Y(\theta,\ \varphi)$$

9. $Y(\theta,\ \varphi)=\Theta(\theta)\Phi(\varphi)$

10. Insert #9 into equation #8 and multiply by $\left(\dfrac{\sin^2\theta}{\Theta(\theta)\Phi(\phi)}\right)$

11. $$\frac{\sin\theta}{\Theta(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta(\theta)}{\partial\theta}\right) + \boxed{\frac{1}{\Phi(\varphi)}\frac{\partial^2\Phi(\varphi)}{\partial\varphi^2}} = -\beta\sin^2\theta$$

12. In equation 11 set the term in dashed box, the φ-dependent term, to $-m^2$ and the θ-dependent terms to m^2.

13. $$\frac{\partial^2\Phi(\varphi)}{\partial\varphi^2} = -m^2\Phi(\varphi)$$

14. $$\sin\theta\left[\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta(\theta)}{\partial\theta}\right)\right] + (\beta\sin^2\theta - m^2)\Theta(\theta) = 0$$

15. Setting $\beta = \ell(\ell+1)$ and $U(r) = \dfrac{-Ze^2}{4\pi\varepsilon_0 r}$ we have

16. R equation: $$\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right) + \left[\frac{2\mu^2 r^2}{\hbar^2}\left(E + \frac{Ze^2}{4\pi\varepsilon_0 r}\right) - \ell(\ell+1)\right]R(r) = 0$$

17. Θ equation: $$\sin\theta\left[\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta(\theta)}{d\theta}\right)\right] + (\ell(\ell+1)\sin^2\theta - m^2)\Theta(\theta) = 0$$

18. Φ equation: $$\frac{d^2\Phi(\varphi)}{d\varphi^2} = -m^2\Phi(\varphi)$$