

The Schrödinger Equation for the Hydrogen-Like Atom

$$-\frac{h^2}{8\pi^2\mu}\nabla^2\psi - \frac{Ze^2}{r}\psi = E\psi$$

$$\nabla^2\psi + \frac{8\pi^2\mu Ze^2}{h^2r}\psi + \frac{8\pi^2\mu E}{h^2}\psi = 0$$

$$\frac{1}{\mu} = \frac{1}{m} + \frac{1}{M} = \frac{M+m}{mM}$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$r = \sqrt{x^2 + y^2 + z^2}$$

$$x = r \sin \vartheta \cos \varphi$$

$$y = r \sin \vartheta \sin \varphi$$

$$z = r \cos \vartheta$$

$$dx = \sin \vartheta \cos \varphi dr + r \cos \vartheta \cos \varphi d\vartheta - r \sin \vartheta \sin \varphi d\varphi$$

$$dy = \sin \vartheta \sin \varphi dr + r \cos \vartheta \sin \varphi d\vartheta + r \sin \vartheta \cos \varphi d\varphi$$

$$dz = \cos \vartheta dr - r \sin \vartheta d\vartheta$$

$$\begin{aligned}(dx)^2 &= (\sin \vartheta)^2 (\cos \varphi)^2 (dr)^2 + r^2 (\cos \vartheta)^2 (\cos \varphi)^2 (d\vartheta)^2 + r^2 (\sin \vartheta)^2 (\sin \varphi)^2 (d\varphi)^2 \\ &\quad + 2r \sin \vartheta \cos \vartheta (\cos \varphi)^2 dr d\vartheta - 2r (\sin \vartheta)^2 \cos \varphi \sin \varphi dr d\varphi \\ &\quad - 2r^2 \cos \vartheta \sin \vartheta \cos \varphi \sin \varphi d\vartheta d\varphi\end{aligned}$$

$$\begin{aligned}(dy)^2 &= (\sin \vartheta)^2 (\sin \varphi)^2 (dr)^2 + r^2 (\cos \vartheta)^2 (\sin \varphi)^2 (d\vartheta)^2 + r^2 (\sin \vartheta)^2 (\cos \varphi)^2 (d\varphi)^2 \\ &\quad + 2r \sin \vartheta \cos \vartheta (\sin \varphi)^2 dr d\vartheta + 2r (\sin \vartheta)^2 \cos \varphi \sin \varphi dr d\varphi \\ &\quad + 2r^2 \cos \vartheta \sin \vartheta \cos \varphi \sin \varphi d\vartheta d\varphi\end{aligned}$$

$$(dz)^2 = (\cos \vartheta)^2 (dr)^2 + r^2 (\sin \vartheta)^2 (d\vartheta)^2 - 2r \cos \vartheta \sin \vartheta dr d\vartheta$$

$$\begin{aligned}(ds)^2 &= (dx)^2 + (dy)^2 + (dz)^2 \\ &= (\sin \vartheta)^2 [(\cos \varphi)^2 + (\sin \varphi)^2] (dr)^2 + (\cos \vartheta)^2 (dr)^2 \\ &\quad + r^2 (\cos \vartheta)^2 [(\cos \varphi)^2 + (\sin \varphi)^2] (d\vartheta)^2 + r^2 (\sin \vartheta)^2 (d\vartheta)^2 \\ &\quad + r^2 (\sin \vartheta)^2 [(\sin \varphi)^2 + (\cos \varphi)^2] (d\varphi)^2 = (dr)^2 + r^2 (d\vartheta)^2 + r^2 (\sin \vartheta)^2 (d\varphi)^2\end{aligned}$$

$$h_r = 1, h_\vartheta = r, h_\varphi = r \sin \vartheta$$

$$\begin{aligned}
\nabla^2 &= \frac{1}{h_r h_\vartheta h_\varphi} \left[\frac{\partial}{\partial r} \left(\frac{h_\vartheta h_\varphi}{h_r} \frac{\partial}{\partial r} \right) + \frac{\partial}{\partial \vartheta} \left(\frac{h_r h_\varphi}{h_\vartheta} \frac{\partial}{\partial \vartheta} \right) + \frac{\partial}{\partial \varphi} \left(\frac{h_r h_\vartheta}{h_\varphi} \frac{\partial}{\partial \varphi} \right) \right] \\
&= \frac{1}{r^2 \sin \vartheta} \left[\frac{\partial}{\partial r} \left(r^2 \sin \vartheta \frac{\partial}{\partial r} \right) + \frac{\partial}{\partial \vartheta} \left(\frac{r \sin \vartheta}{r} \frac{\partial}{\partial \vartheta} \right) + \frac{\partial}{\partial \varphi} \left(\frac{r}{r \sin \vartheta} \frac{\partial}{\partial \varphi} \right) \right] \\
&= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \vartheta} \frac{\partial}{\partial \vartheta} \left(\sin \vartheta \frac{\partial}{\partial \vartheta} \right) + \frac{1}{r^2 (\sin \vartheta)^2} \frac{\partial^2}{\partial \varphi^2}
\end{aligned}$$

$$\psi(r, \vartheta, \varphi) = R(r)Y(\vartheta, \varphi)$$

$$\frac{Y}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{R}{r^2 \sin \vartheta} \frac{\partial}{\partial \vartheta} \left(\sin \vartheta \frac{\partial Y}{\partial \vartheta} \right) + \frac{R}{r^2 (\sin \vartheta)^2} \frac{\partial^2 Y}{\partial \varphi^2} + \frac{8\pi^2 \mu Z e^2}{h^2 r} R Y + \frac{8\pi^2 \mu E}{h^2} R Y = 0$$

$$\frac{1}{R r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{1}{Y r^2 \sin \vartheta} \frac{\partial}{\partial \vartheta} \left(\sin \vartheta \frac{\partial Y}{\partial \vartheta} \right) + \frac{1}{Y r^2 (\sin \vartheta)^2} \frac{\partial^2 Y}{\partial \varphi^2} + \frac{8\pi^2 \mu Z e^2}{h^2 r} + \frac{8\pi^2 \mu E}{h^2} = 0$$

$$\frac{1}{R} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{1}{Y \sin \vartheta} \frac{\partial}{\partial \vartheta} \left(\sin \vartheta \frac{\partial Y}{\partial \vartheta} \right) + \frac{1}{Y (\sin \vartheta)^2} \frac{\partial^2 Y}{\partial \varphi^2} + \frac{8\pi^2 \mu Z e^2}{h^2} r + \frac{8\pi^2 \mu E}{h^2} r^2 = 0$$

$$\frac{1}{R} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{8\pi^2 \mu Z e^2}{h^2} r + \frac{8\pi^2 \mu E}{h^2} r^2 = -\frac{1}{Y \sin \vartheta} \frac{\partial}{\partial \vartheta} \left(\sin \vartheta \frac{\partial Y}{\partial \vartheta} \right) - \frac{1}{Y (\sin \vartheta)^2} \frac{\partial^2 Y}{\partial \varphi^2} = \lambda^2$$

$$\frac{1}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{8\pi^2 \mu Z e^2}{h^2} r + \frac{8\pi^2 \mu E}{h^2} r^2 - \lambda^2 = 0$$

$$-\frac{1}{Y \sin \vartheta} \frac{\partial}{\partial \vartheta} \left(\sin \vartheta \frac{\partial Y}{\partial \vartheta} \right) - \frac{1}{Y (\sin \vartheta)^2} \frac{\partial^2 Y}{\partial \varphi^2} - \lambda^2 = 0$$

$$\frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{8\pi^2 \mu Z e^2}{h^2} r R + \frac{8\pi^2 \mu E}{h^2} r^2 R - \lambda^2 R = 0$$

$$-\frac{1}{\sin \vartheta} \frac{\partial}{\partial \vartheta} \left(\sin \vartheta \frac{\partial Y}{\partial \vartheta} \right) - \frac{1}{(\sin \vartheta)^2} \frac{\partial^2 Y}{\partial \varphi^2} - \lambda^2 Y = 0$$

$$\frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) - \left(\lambda^2 - \frac{8\pi^2 \mu Z e^2}{h^2} r - \frac{\mu E}{h^2} r^2 \right) R = 0$$

$$Y(\vartheta, \varphi) = \Theta(\vartheta)\Phi(\varphi)$$

$$-\frac{\Phi}{\sin \vartheta} \frac{\partial}{\partial \vartheta} \left(\sin \vartheta \frac{\partial \Theta}{\partial \vartheta} \right) - \frac{\Theta}{(\sin \vartheta)^2} \frac{\partial^2 \Phi}{\partial \varphi^2} - \lambda^2 \Theta \Phi = 0$$

$$-\frac{1}{\Theta \sin \vartheta} \frac{\partial}{\partial \vartheta} \left(\sin \vartheta \frac{\partial \Theta}{\partial \vartheta} \right) - \frac{1}{\Phi (\sin \vartheta)^2} \frac{\partial^2 \Phi}{\partial \varphi^2} - \lambda^2 = 0$$

$$-\frac{\sin \vartheta}{\Theta} \frac{\partial}{\partial \vartheta} \left(\sin \vartheta \frac{\partial \Theta}{\partial \vartheta} \right) - \frac{1}{\Phi} \frac{\partial^2 \Phi}{\partial \varphi^2} - \lambda^2 (\sin \vartheta)^2 = 0$$

$$-\frac{\sin \vartheta}{\Theta} \frac{\partial}{\partial \vartheta} \left(\sin \vartheta \frac{\partial \Theta}{\partial \vartheta} \right) - \lambda^2 (\sin \vartheta)^2 = -\frac{1}{\Phi} \frac{\partial^2 \Phi}{\partial \varphi^2} = \nu^2$$

$$\sin \vartheta \frac{d}{d\vartheta} \left(\sin \vartheta \frac{d\Theta}{d\vartheta} \right) + \lambda^2 (\sin \vartheta)^2 \Theta - \nu^2 \Theta = 0$$

$$\frac{d^2\Phi}{d\varphi^2}+\nu^2\Phi=0$$

$$m=\nu$$

$$\Phi(\varphi)=Ae^{im\varphi}+Be^{-im\varphi},m\neq 0$$

$$\Phi(\varphi)=A+B\varphi,m=0$$

$$\Phi_m(\varphi)=\frac{1}{\sqrt{2\pi}}e^{im\varphi}$$

$$\frac{1}{\sin \vartheta} \frac{d}{d\vartheta} \left(\sin \vartheta \frac{d\Theta}{d\vartheta} \right) + \lambda^2 \Theta - \frac{m^2 \Theta}{(\sin \vartheta)^2} = 0$$

$$x=\cos\vartheta$$

$$\frac{\mathrm{d}\Theta}{\mathrm{d}\vartheta}=\frac{dx}{d\vartheta}\frac{\mathrm{d}\Theta}{dx}=-\sin\vartheta\frac{\mathrm{d}\Theta}{dx}$$

$$\frac{\mathrm{d}}{d\vartheta}=\frac{dx}{d\vartheta}\frac{\mathrm{d}}{dx}=-\sin\vartheta\frac{\mathrm{d}}{dx}$$

$$\frac{\mathrm{d}}{dx}\Big[(1-x^2)\frac{\mathrm{d}\Theta}{dx}\Big]+\Big[\lambda^2-\frac{m^2}{(1-x^2)}\Big]\Theta=0$$

$$Y_{lm}(\vartheta,\varphi)=N_{lm}P_l^m(\cos\vartheta)\Phi_m(\varphi)=\epsilon\sqrt{\frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}P_l^m(\cos\vartheta)\Phi_m(\varphi)$$

$$\epsilon=(-1)^m\forall m>0,\epsilon=1\forall m\leq 0$$

$$Y_{0,0}=\frac{1}{\sqrt{4\pi}}$$

$$Y_{1,0}=\sqrt{\frac{3}{4\pi}}\cos\vartheta$$

$$Y_{1,\pm 1}=\mp \sqrt{\frac{3}{8\pi}}\sin\vartheta\,e^{\pm i\varphi}$$

$$Y_{2,0}=\sqrt{\frac{5}{16\pi}}[3(\cos\vartheta)^2-1]$$

$$Y_{2,\pm 1}=\mp \sqrt{\frac{15}{8\pi}}\sin\vartheta\,\cos\vartheta\,e^{\pm i\varphi}$$

$$Y_{2,\pm 2} = \sqrt{\frac{15}{32\pi}} (\sin \vartheta)^2 e^{\pm 2i\varphi}$$

$$\frac{h^2}{4\pi^2\mu} \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) - \left(\frac{h^2 \lambda^2}{4\pi^2 \mu r^2} - \frac{Ze^2}{r} - E \right) R = 0$$

$$\rho=\alpha r$$

$$\frac{d}{dr}=\frac{d\rho}{dr}\frac{d}{d\rho}=\alpha\frac{d}{d\rho}$$

$$\frac{h^2}{8\pi^2\mu}\frac{\alpha^2}{\rho^2}\alpha\frac{d}{d\rho}\left(\frac{\rho^2}{\alpha^2}\alpha\frac{dR}{d\rho}\right)-\left(\frac{h^2\lambda^2\alpha^2}{8\pi^2\mu\rho^2}-\frac{Ze^2\alpha}{\rho}-E\right)R=0$$

$$\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{dR}{d\rho}\right)-\left(\frac{\lambda^2}{\rho^2}-\frac{8\pi^2\mu Ze^2}{h^2\alpha\rho}-\frac{8\pi^2\mu E}{h^2\alpha^2}\right)R=0$$

$$-\frac{1}{4}=-\frac{8\pi^2\mu E}{h^2\alpha^2}$$

$$\alpha^2=\frac{8\pi^2\mu|E|}{h^2}$$

$$\beta=\frac{8\pi^2\mu Ze^2}{h^2\alpha}$$

$$\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{dR}{d\rho}\right)+\left(\frac{\beta}{\rho}-\frac{\lambda^2}{\rho^2}-\frac{1}{4}\right)R=0$$

$$R(\rho)=e^{-a\rho}F(\rho)$$

$$\frac{dR}{d\rho}=e^{-a\rho}F'(\rho)-ae^{-a\rho}F(\rho)$$

$$\frac{d^2R}{d\rho^2}=e^{-a\rho}F''(\rho)-2ae^{-a\rho}F'(\rho)+a^2e^{-a\rho}F(\rho)$$

$$\frac{d^2R}{d\rho^2}+\frac{2}{\rho}\frac{dR}{d\rho}+\left(\frac{\beta}{\rho}-\frac{\lambda^2}{\rho^2}-\frac{1}{4}\right)R=0$$

$$\begin{aligned} e^{-a\rho}F''(\rho)-2ae^{-a\rho}F'(\rho)+a^2e^{-a\rho}F(\rho)+\frac{2}{\rho}e^{-a\rho}F'(\rho)-\frac{2}{\rho}ae^{-a\rho}F(\rho)+\left(\frac{\beta}{\rho}-\frac{\lambda^2}{\rho^2}-\frac{1}{4}\right)e^{-a\rho}F(\rho) \\ =0 \end{aligned}$$

$$F''(\rho)-2aF'(\rho)+a^2F(\rho)+\frac{2}{\rho}F'(\rho)-\frac{2}{\rho}aF(\rho)+\left(\frac{\beta}{\rho}-\frac{\lambda^2}{\rho^2}\right)F(\rho)=0$$

$$F''(\rho)+\left(\frac{2}{\rho}-1\right)F'(\rho)+\left(\frac{\beta}{\rho}-\frac{\lambda^2}{\rho^2}\right)F(\rho)=0, a=1/2$$

$$F(\rho)=\rho^sL(\rho)$$

$$F'(\rho) = \rho^s L'(\rho) + s\rho^{s-1}L(\rho)$$

$$F''(\rho) = \rho^s L''(\rho) + 2s\rho^{s-1}L'(\rho) + s(s-1)\rho^{s-2}L(\rho)$$

$$\rho^s L''(\rho) + 2s\rho^{s-1}L'(\rho) + s(s-1)\rho^{s-2}L(\rho) + \left(\frac{2}{\rho} - 1\right)[\rho^s L'(\rho) + s\rho^{s-1}L(\rho)] + \left(\frac{\beta}{\rho} - \frac{\lambda^2}{\rho^2}\right)\rho^s L(\rho)$$

$$= 0$$

$$\rho^2 L'' + 2s\rho L' + s(s-1)L + (2\rho - \rho^2)(L' + s\rho L) + (\beta\rho - \lambda^2)L = 0$$

$$\rho^2 L'' + \rho[2(s+1) - \rho]L' + [\rho(\beta - s - 1) + s(s+1) - \lambda^2]L = 0$$

$$\rho = 0 \rightarrow s(s+1) - \lambda^2 = 0$$

$$\lambda^2 = l(l+1)$$

$$s = l, s = -(l+1)$$

$$\rho^2 L'' + \rho[2(l+1) - \rho]L' + [\rho(\beta - l - 1) + l(l+1) - l(l+1)]L = 0$$

$$\rho L'' + [2(l+1) - \rho]L' + (\beta - l - 1)L = 0$$

$$L(\rho) = \sum_{k=0}^{\infty} a_k \rho^k$$

$$k(k-1)a_k \rho^{k-1} + 2(l+1)ka_k \rho^{k-1} - ka_k \rho^k + (\beta - l - 1)a_k \rho^k = 0$$

$$k(k+1)a_{k+1} \rho^k + 2(l+1)(k+1)a_{k+1} \rho^k + (\beta - l - 1 - k)a_k \rho^k = 0$$

$$a_{k+1} = \frac{k+l+1-\beta}{(k+1)(k+2l+2)} a_k$$