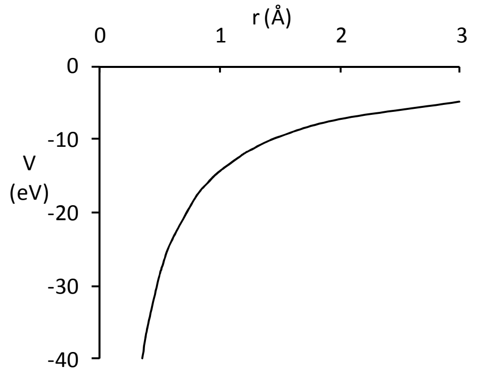
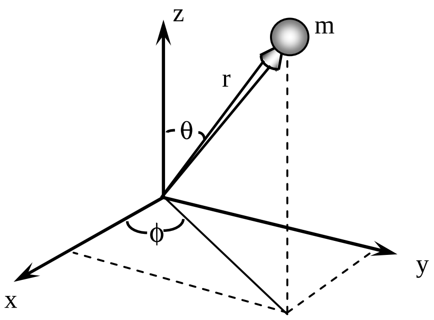
Ground State of the Hydrogen Atom





$$V(r) = \frac{-Z\,e^2}{4\pi\varepsilon_o r} \qquad e = 1.60218\text{x}10^{-19}\text{C}$$

$\varepsilon_o = 8.85419 \text{ x } 10^{-12}\ J^{-1}\ c^2\ m^{-1}$ $\qquad m_e = 9.1093897\text{x}10^{-31}$ kg

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$$-\frac{\hbar^2}{2m}\nabla^2\,\Psi + V\,\Psi = E\,\Psi$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\Psi + \frac{-Z\,e^2}{4\pi\varepsilon_o r}\,\Psi = E\,\Psi$$

$$\nabla^2 = \frac{1}{r}\left(\frac{\partial^2}{\partial r^2}\right) r + \left(\frac{1}{r^2}\right)\Lambda^2 \qquad \Lambda^2 = \frac{1}{\sin^2\theta}\left(\frac{\partial^2}{\partial\phi^2}\right) + \left(\frac{1}{\sin\theta}\right)\left(\frac{\partial}{\partial\theta}\sin\theta\,\frac{\partial}{\partial\theta}\right)$$

$$\Psi = R(r)\ \Theta(\theta)\ \Phi(\phi) = R(r)\ Y_{\ell,m_\ell}$$

$$-\frac{\hbar^2}{2mr^2}\,\frac{\partial^2\Phi}{\partial\phi^2} = -\frac{\hbar^2 m_\ell^2}{2mr^2}\,\Phi \qquad L_z = \hbar\ m_\ell \qquad \Phi(\phi) = \left(\frac{1}{2\pi}\right)^{1/2} e^{im_\ell\phi}$$

$$-\hbar^2\Lambda^2\ Y_{\ell,m_\ell} = \hbar^2\ \ell(\ell+1)\ Y_{\ell,m_\ell}$$

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r}\frac{\partial^2}{\partial r^2}\,r\,R(r)\,Y_{\ell,m_\ell} + \frac{\Lambda^2}{r^2}\,R(r)\,Y_{\ell,m_\ell}\right) - \frac{Z\,e^2}{4\pi\varepsilon_o r}\,R(r)\,Y_{\ell,m_\ell} = E\,R(r)\,Y_{\ell,m_\ell}$$

$$-\frac{\hbar^2}{2m}\left(Y_{\ell,m_\ell}\frac{1}{r}\frac{\partial^2}{\partial r^2}\,r\,R(r) - R(r)\,\frac{\ell(\ell+1)}{r^2}\,Y_{\ell,m_\ell}\right) - \frac{Z\,e^2}{4\pi\varepsilon_o r}\,R(r)\,Y_{\ell,m_\ell} = E\,R(r)\,Y_{\ell,m_\ell}$$

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r}\frac{\partial^2}{\partial r^2}\,r\,R - \frac{\ell(\ell+1)}{r^2}\,R\right) - \frac{Z\,e^2}{4\pi\varepsilon_o r}\,R = E\,R$$

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r}\frac{\partial^2}{\partial r^2}\,r\,R\right) - \frac{Z\,e^2}{4\pi\varepsilon_o r}\,R = E_{gs}\,R$$ for ground state $\ell = 0$

Guess: $R(r) = A\,e^{-\alpha r}$

$$\frac{d}{dr}\, r\, R = r\,\frac{dR}{dr} + R$$

$$\frac{d^2}{dr^2}\, r\, R = \frac{d}{dr}\left(r\,\frac{dR}{dr}\right) + \frac{dR}{dr} \quad = \quad r\,\frac{d^2R}{dr^2} + \frac{dR}{dr} + \frac{dR}{dr} \quad = \quad r\,\frac{d^2R}{dr^2} + 2\frac{dR}{dr}$$

$$-\frac{\hbar^2}{2m}\left(\alpha^2 R - \frac{2\alpha}{r}R\right) - \frac{Z e^2}{4\pi\varepsilon_o r} R = E_{gs} R$$

$$-\frac{\hbar^2\alpha^2}{2m} + \frac{\hbar^2 2\alpha}{2mr} - \frac{Z e^2}{4\pi\varepsilon_o r} = E_{gs}$$

$$E_{gs} = -\frac{\hbar^2\alpha^2}{2m} \qquad\qquad \frac{\hbar^2\alpha}{mr} - \frac{Z e^2}{4\pi\varepsilon_o r} = 0$$

$$\alpha = \frac{\sqrt{-2mE}}{\hbar} \qquad\qquad \alpha = \frac{Z e^2}{4\pi\varepsilon_o}\,\frac{m}{\hbar^2}$$

$$E_{gs} = -\left(\frac{Z^2 e^4 m}{32\pi^2\varepsilon_o^2\,\hbar^2}\right) \qquad E_n = -\left(\frac{e^4 m}{32\pi^2\varepsilon_o^2\hbar^2}\right)\frac{Z^2}{n^2}$$ including excited states

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$$a_o = \frac{4\pi\varepsilon_o\,\hbar^2}{me^2} \qquad E_n = -\frac{\hbar^2}{2ma_o^2}\,\frac{Z^2}{n^2} \qquad \alpha = \frac{Z}{a_o}$$

$a_o = 0.0529$ nm = 0.529 Å

$$E_n = -13.606 \text{ eV}\,\frac{Z^2}{n^2} = -109{,}678.\ \text{cm}^{-1}\,\frac{Z^2}{n^2}$$

$$E_n = -1312 \text{ kJ mol}^{-1}\,\frac{Z^2}{n^2} = -\frac{H}{2}\,\frac{Z^2}{n^2}$$ where 1H= 2625.5 kJ mol^{-1}

Normalize

$$\int_0^\infty\int_0^\pi\int_0^{2\pi} \Psi^2\, r^2 \sin\theta\, dr\, d\theta\, d\phi = A^2 \int_0^\infty\int_0^\pi\int_0^{2\pi} e^{-2Zr/a_o}\, r^2 \sin\theta\, dr\, d\theta\, d\phi = ?$$

$$A^2 \int_0^{2\pi} d\phi \int_0^\pi \sin\theta\, d\theta \int_0^\infty e^{-2Zr/a_o}\, r^2\, dr = A^2\, 4\pi \int_0^\infty e^{-2Zr/a_o}\, r^2\, dr =$$

$$A^2\, 4\pi\left(\frac{2}{(2Z/a_o)^3}\right) = ? \qquad\qquad \int_0^\infty x^n\, e^{-ax}\, dx = \frac{n!}{a^{n+1}}$$

$$A = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_o}\right)^{3/2}$$

$$\Psi_{1s}(r) = \Psi_{100}(r) = R(r) = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_o}\right)^{3/2} e^{-Zr/a_o}$$