8. Considere a equação de onda para o sistema electrão-protão dada por

$$\left\{-\frac{\hbar^2}{2m_e r}\frac{d^2}{dr^2}r \;+\; \frac{\hbar^2\,\ell(\ell+1)}{2m_e r^2} \;-\; \frac{e^2}{4\pi\epsilon_0 r}\right\} R_{n\ell}(r) \;=\; E_n\, R_{n\ell}(r) \quad .$$

Mostre que as seguintes expressões $R_{n\ell}(r)$ para diversos valores de n ($n = 1$, 2, 3, ...) e de ℓ ($\ell = 0$, 1, 2, ... $\leq n-1$), são soluções dessa equação e determine os respectivos valores próprios E_n.

a $\quad R_{10}(r) = 2\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$

b $\quad R_{20}(r) = \left(\frac{1}{2a_0}\right)^{3/2}\left\{2 - \frac{r}{a_0}\right\} e^{-r/2a_0}$

c $\quad R_{21}(r) = \frac{1}{\sqrt{3}}\left(\frac{1}{2a_0}\right)^{3/2}\left\{\frac{r}{a_0}\right\} e^{-r/2a_0}$

d $\quad R_{30}(r) = 2\left(\frac{1}{3a_0}\right)^{3/2}\left\{1 - \frac{2}{3}\frac{r}{a_0} + \frac{2}{27}\left(\frac{r}{a_0}\right)^2\right\} e^{-r/3a_0}$

e $\quad R_{31}(r) = \frac{3}{4}\sqrt{2}\left(\frac{1}{3a_0}\right)^{3/2}\left\{1 - \frac{1}{6}\frac{r}{a_0}\right\}\frac{r}{a_0}\, e^{-r/3a_0}$

f $\quad R_{32}(r) = \frac{2}{27}\sqrt{\frac{2}{5}}\left(\frac{1}{3a_0}\right)^{3/2}\left\{\left(\frac{r}{a_0}\right)^2\right\} e^{-r/3a_0}$

onde a_0 represente o raio de Bohr dado por

$$a_0 \;=\; \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} \quad .$$

Solution:

Using the definition for the Bohr radius, we may simplify the differential operator to

$$-\frac{\hbar^2}{2m_e r}\frac{d^2}{dr^2}r \;+\; \frac{\hbar^2\,\ell(\ell+1)}{2m_e r^2} \;-\; \frac{e^2}{4\pi\epsilon_0 r} \;=\; -\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}r \;-\; \frac{\ell(\ell+1)}{r} \;+\; \frac{2}{a_0}\right\} \quad .$$

a: $\boldsymbol{R_{n=1,\ell=0}(r) = 2\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}}$.

Since $\ell = 0$, we obtain for the differential operator $-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2} r + \frac{2}{a_0}\right\}$. Hence, we must determine

$$\frac{d^2}{dr^2} r\, e^{-r/a_0} = \frac{d}{dr}\left\{e^{-r/a_0} + r\left[-\frac{1}{a_0}e^{-r/a_0}\right]\right\} = \frac{d}{dr}\left\{1 - \frac{r}{a_0}\right\} e^{-r/a_0}$$

$$= -\frac{1}{a_0}e^{-r/a_0} + \left\{1 - \frac{r}{a_0}\right\}\left[-\frac{1}{a_0}e^{-r/a_0}\right] = \left\{-\frac{2}{a_0} + \frac{r}{a_0^2}\right\} e^{-r/a_0}$$

We find then

$$-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2} r + \frac{2}{a_0}\right\} R_{10}(r) =$$

$$= -\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2} r + \frac{2}{a_0}\right\} 2\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0} = -\frac{\hbar^2}{2m_e r} 2\left(\frac{1}{a_0}\right)^{3/2}\left\{\frac{d^2}{dr^2} r e^{-r/a_0} + \frac{2}{a_0}e^{-r/a_0}\right\}$$

$$= -\frac{\hbar^2}{2m_e r} 2\left(\frac{1}{a_0}\right)^{3/2}\left\{\left[-\frac{2}{a_0} + \frac{r}{a_0^2}\right] e^{-r/a_0} + \frac{2}{a_0}e^{-r/a_0}\right\}$$

$$= -\frac{\hbar^2}{2m_e r} 2\left(\frac{1}{a_0}\right)^{3/2}\left\{-\frac{2}{a_0} + \frac{r}{a_0^2} + \frac{2}{a_0}\right\} e^{-r/a_0}$$

$$= -\frac{\hbar^2}{2m_e r} 2\left(\frac{1}{a_0}\right)^{3/2} \frac{r}{a_0^2} e^{-r/a_0} = -\frac{\hbar^2}{2m_e a_0^2} 2\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0} = -\frac{\hbar^2}{2m_e a_0^2} R_{10}(r) \quad .$$

Consequently, we find for R_{10} the eigenvalue $E_1 = -\hbar^2/\left(2m_e a_0^2\right)$ under the action of the differential operator. Also using the definition $\alpha = e^2/(4\pi\epsilon_0\hbar c) = \hbar/(m_e a_0 c)$, we obtain $E_1 = -\alpha^2 m_e c^2/2$, which is indeed the expression for the Hydrogen ground state energy we have obtained before.

b: $\boldsymbol{R_{n=2,\ell=0}(r) = \left(\frac{1}{2a_0}\right)^{3/2} \left\{2 - \frac{r}{a_0}\right\} e^{-r/2a_0}}$.

Since $\ell = 0$, we again obtain for the differential operator $-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}\, r \;+\; \frac{2}{a_0}\right\}$. Here, we determine, using the substitution $a_0 \to 2a_0$ in the result of **a**,

$$\frac{d^2}{dr^2}\, r\, e^{-r/2a_0} \;=\; \left\{-\frac{2}{2a_0} + \frac{r}{4a_0^2}\right\} e^{-r/2a_0} \;=\; \left\{-\frac{1}{a_0} + \frac{r}{4a_0^2}\right\} e^{-r/2a_0}$$

Furthermore, we must determine

$$\frac{d^2}{dr^2}\, r^2\, e^{-r/2a_0} \;=\; \frac{d}{dr}\left\{2re^{-r/2a_0} + r^2\left[-\frac{1}{2a_0}e^{-r/2a_0}\right]\right\} \;=\; \frac{d}{dr}\left\{2r - \frac{r^2}{2a_0}\right\} e^{-r/2a_0}$$

$$= \left\{2 - \frac{2r}{2a_0}\right\} e^{-r/2a_0} + \left\{2r - \frac{r^2}{2a_0}\right\}\left[-\frac{1}{2a_0}e^{-r/2a_0}\right] \;=\; \left\{2 - \frac{2r}{a_0} + \frac{r^2}{4a_0^2}\right\} e^{-r/2a_0} \quad .$$

We find then

$$-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}\, r \;+\; \frac{2}{a_0}\right\} R_{20}(r) \;=$$

$$= \;-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2} r + \frac{2}{a_0}\right\}\left(\frac{1}{2a_0}\right)^{3/2}\left\{2 - \frac{r}{a_0}\right\} e^{-r/2a_0}$$

$$= \;-\frac{\hbar^2}{2m_e r}\left(\frac{1}{2a_0}\right)^{3/2}\left\{2\frac{d^2}{dr^2} r e^{-r/2a_0} - \frac{1}{a_0}\frac{d^2}{dr^2} r^2 e^{-r/2a_0} + \frac{4}{a_0}e^{-r/2a_0} - \frac{2r}{a_0^2}e^{-r/2a_0}\right\}$$

$$= \;-\frac{\hbar^2}{2m_e r}\left(\frac{1}{2a_0}\right)^{3/2}\left\{2\left[-\frac{1}{a_0} + \frac{r}{4a_0^2}\right] e^{-r/2a_0} \;-\frac{1}{a_0}\left[2 - \frac{2r}{a_0} + \frac{r^2}{4a_0^2}\right] e^{-r/2a_0} \;+\right.$$

$$\left. + \frac{4}{a_0}e^{-r/2a_0} - \frac{2r}{a_0^2}e^{-r/2a_0}\right\}$$

$$= \;-\frac{\hbar^2}{2m_e r}\left(\frac{1}{2a_0}\right)^{3/2}\left\{-\frac{2}{a_0} + \frac{r}{2a_0^2} - \frac{2}{a_0} + \frac{2r}{a_0^2} - \frac{r^2}{4a_0^3} + \frac{4}{a_0} - \frac{2r}{a_0^2}\right\} e^{-r/2a_0}$$

$$= \;-\frac{\hbar^2}{2m_e r}\left(\frac{1}{2a_0}\right)^{3/2}\left\{\frac{r}{2a_0^2} - \frac{r^2}{4a_0^3}\right\} e^{-r/2a_0} \;=\; -\frac{\hbar^2}{8m_e a_0^2}\, R_{20}(r) \quad .$$

Consequently, we find for R_{20} the eigenvalue $E_2 = -\hbar^2/\left(8m_e a_0^2\right) = -\alpha^2 m_e c^2/8 = E_1/4$ under the action of the differential operator.

c: $\boldsymbol{R_{n=2,\ell=1}(r) = \frac{1}{\sqrt{3}} \left(\frac{1}{2a_0}\right)^{3/2} \left\{\frac{r}{a_0}\right\} e^{-r/2a_0}}$.

Since $\ell = 1$, we obtain now for the differential operator $-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}r - \frac{2}{r} + \frac{2}{a_0}\right\}$. Also using the results of **b**, we find then

$$-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}r - \frac{2}{r} + \frac{2}{a_0}\right\} R_{21}(r) =$$

$$= -\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}r - \frac{2}{r} + \frac{2}{a_0}\right\}\frac{1}{\sqrt{3}}\left(\frac{1}{2a_0}\right)^{3/2}\left\{\frac{r}{a_0}\right\} e^{-r/2a_0}$$

$$= -\frac{\hbar^2}{2m_e r}\frac{1}{\sqrt{3}}\left(\frac{1}{2a_0}\right)^{3/2}\left\{\frac{1}{a_0}\frac{d^2}{dr^2}r^2 e^{-r/2a_0} - \frac{2}{r}\frac{r}{a_0}e^{-r/2a_0} + \frac{2}{a_0}\frac{r}{a_0}e^{-r/2a_0}\right\}$$

$$= -\frac{\hbar^2}{2m_e r}\frac{1}{\sqrt{3}}\left(\frac{1}{2a_0}\right)^{3/2}\left\{\frac{1}{a_0}\left[2 - \frac{2r}{a_0} + \frac{r^2}{4a_0^2}\right]e^{-r/2a_0} - \frac{2}{a_0}e^{-r/2a_0} + \frac{2r}{a_0^2}e^{-r/2a_0}\right\}$$

$$= -\frac{\hbar^2}{2m_e r}\left(\frac{1}{2a_0}\right)^{3/2}\left\{\frac{2}{a_0} - \frac{2r}{a_0^2} + \frac{r^2}{4a_0^3} - \frac{2}{a_0} + \frac{2r}{a_0^2}\right\} e^{-r/2a_0}$$

$$= -\frac{\hbar^2}{2m_e r}\frac{1}{\sqrt{3}}\left(\frac{1}{2a_0}\right)^{3/2}\left\{\frac{r^2}{4a_0^3}\right\} e^{-r/2a_0} = -\frac{\hbar^2}{8m_e a_0^2} R_{21}(r) \quad .$$

Consequently, we find for R_{21} the eigenvalue $E_2 = -\hbar^2/\left(8m_e a_0^2\right) = -\alpha^2 m_e c^2/8 = E_1/4$ under the action of the differential operator. This is the same eigenvalue as for R_{20}. Why?

d: $\boldsymbol{R_{n=3,\ell=0}(r) = 2\left(\frac{1}{3a_0}\right)^{3/2}\left\{1-\frac{2}{3}\frac{r}{a_0}+\frac{2}{27}\left(\frac{r}{a_0}\right)^2\right\}e^{-r/3a_0}}$.

Since $\ell = 0$, we again obtain for the differential operator $-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}r + \frac{2}{a_0}\right\}$. Here, we determine, using the substitution $a_0 \to 3a_0$ in the result of **a**,

$$\frac{d^2}{dr^2} r\, e^{-r/3a_0} = \left\{-\frac{2}{3a_0}+\frac{r}{9a_0^2}\right\} e^{-r/3a_0}$$

Furthermore, using the substitution $2a_0 \to 3a_0$ in the result of **b**,

$$\frac{d^2}{dr^2} r^2\, e^{-r/3a_0} = \left\{2-\frac{4r}{3a_0}+\frac{r^2}{9a_0^2}\right\} e^{-r/3a_0} \quad .$$

Finally, we must determine

$$\frac{d^2}{dr^2} r^3\, e^{-r/3a_0} = \frac{d}{dr}\left\{3r^2 e^{-r/3a_0} + r^3\left[-\frac{1}{3a_0}e^{-r/3a_0}\right]\right\} = \frac{d}{dr}\left\{3r^2 - \frac{r^3}{3a_0}\right\} e^{-r/3a_0}$$

$$= \left\{6r - \frac{3r^2}{3a_0}\right\} e^{-r/3a_0} + \left\{3r^2 - \frac{r^3}{3a_0}\right\}\left[-\frac{1}{3a_0}e^{-r/3a_0}\right] = \left\{6r - \frac{2r^2}{a_0} + \frac{r^3}{9a_0^2}\right\} e^{-r/3a_0} \quad .$$

We find then

$$-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}r + \frac{2}{a_0}\right\} R_{30}(r) = -\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}r + \frac{2}{a_0}\right\} 2\left(\frac{1}{3a_0}\right)^{3/2}\left\{1-\frac{2}{3}\frac{r}{a_0}+\frac{2}{27}\left(\frac{r}{a_0}\right)^2\right\} e^{-r/3a_0}$$

$$= -\frac{\hbar^2}{2m_e r} 2\left(\frac{1}{3a_0}\right)^{3/2}\left\{\frac{d^2}{dr^2}re^{-r/3a_0} - \frac{2}{3a_0}\frac{d^2}{dr^2}r^2e^{-r/3a_0} + \right.$$

$$\left. + \frac{2}{27a_0^2}\frac{d^2}{dr^2}r^3e^{-r/3a_0} + \frac{2}{a_0}e^{-r/3a_0} - \frac{4r}{3a_0^2}e^{-r/3a_0} + \frac{4r^2}{27a_0^3}e^{-r/3a_0}\right\}$$

$$= -\frac{\hbar^2}{2m_e r} 2\left(\frac{1}{3a_0}\right)^{3/2}\left\{\left[-\frac{2}{3a_0}+\frac{r}{9a_0^2}\right]e^{-r/3a_0} - \frac{2}{3a_0}\left[2-\frac{4r}{3a_0}+\frac{r^2}{9a_0^2}\right]e^{-r/3a_0} + \right.$$

$$\left. + \frac{2}{27a_0^2}\left[6r - \frac{2r^2}{a_0} + \frac{r^3}{9a_0^2}\right]e^{-r/3a_0} + \frac{2}{a_0}e^{-r/3a_0} - \frac{4r}{3a_0^2}e^{-r/3a_0} + \frac{4r^2}{27a_0^3}e^{-r/3a_0}\right\}$$

$$= -\frac{\hbar^2}{2m_e r} 2\left(\frac{1}{3a_0}\right)^{3/2}\left\{-\frac{2}{3a_0}+\frac{r}{9a_0^2}-\frac{4}{3a_0}+\frac{8r}{9a_0^2}-\frac{2r^2}{27a_0^3}+\frac{4r}{9a_0^2}-\frac{4r^2}{27a_0^3}+\frac{2r^3}{27\times 9a_0^4} + \right.$$

$$\left. + \frac{2}{a_0} - \frac{4r}{3a_0^2} + \frac{4r^2}{27a_0^3}\right\} e^{-r/3a_0}$$

$$= -\frac{\hbar^2}{2m_e r} 2\left(\frac{1}{3a_0}\right)^{3/2}\left\{\frac{r}{9a_0^2} - \frac{2r^2}{27a_0^3} + \frac{2r^3}{27\times 9a_0^4}\right\} e^{-r/3a_0} = -\frac{\hbar^2}{18m_e a_0^2} R_{30}(r) \quad .$$

Consequently, we find for R_{30} the eigenvalue $E_3 = -\hbar^2/(18m_e a_0^2) = -\alpha^2 m_e c^2/18 = E_1/9$ under the action of the differential operator.

e: $R_{n=3,\ell=1}(r) = \frac{3}{4}\sqrt{2}\left(\frac{1}{3a_0}\right)^{3/2}\left\{1 - \frac{1}{6}\frac{r}{a_0}\right\}\frac{r}{a_0}\, e^{-r/3a_0}$.

Since $\ell = 1$, we obtain for the differential operator $-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}r - \frac{2}{r} + \frac{2}{a_0}\right\}$. Also using the results of **d**, we find then

$$-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}r - \frac{2}{r} + \frac{2}{a_0}\right\}R_{31}(r) =$$

$$= -\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}r - \frac{2}{r} + \frac{2}{a_0}\right\}\frac{3}{4}\sqrt{2}\left(\frac{1}{3a_0}\right)^{3/2}\left\{1 - \frac{1}{6}\frac{r}{a_0}\right\}\frac{r}{a_0}e^{-r/3a_0}$$

$$= -\frac{\hbar^2}{2m_e r}\frac{3}{4}\sqrt{2}\left(\frac{1}{3a_0}\right)^{3/2}\left\{\frac{1}{a_0}\frac{d^2}{dr^2}r^2 e^{-r/3a_0} - \frac{1}{6a_0^2}\frac{d^2}{dr^2}r^3 e^{-r/3a_0} + \right.$$

$$\left. + \left[-\frac{2}{r} + \frac{2}{a_0}\right]\left[1 - \frac{1}{6}\frac{r}{a_0}\right]\frac{r}{a_0}e^{-r/3a_0}\right\}$$

$$= -\frac{\hbar^2}{2m_e r}\frac{3}{4}\sqrt{2}\left(\frac{1}{3a_0}\right)^{3/2}\left\{\frac{1}{a_0}\left\{2 - \frac{4r}{3a_0} + \frac{r^2}{9a_0^2}\right\}e^{-r/3a_0} - \frac{1}{6a_0^2}\left\{6r - \frac{2r^2}{a_0} + \frac{r^3}{9a_0^2}\right\}e^{-r/3a_0} + \right.$$

$$\left. + \left[-\frac{2}{r} + \frac{2}{a_0}\right]\left[1 - \frac{1}{6}\frac{r}{a_0}\right]\frac{r}{a_0}e^{-r/3a_0}\right\}$$

$$= -\frac{\hbar^2}{2m_e r}\frac{3}{4}\sqrt{2}\left(\frac{1}{3a_0}\right)^{3/2}\left\{\frac{2}{a_0} - \frac{4r}{3a_0^2} + \frac{r^2}{9a_0^3} - \frac{r}{a_0^2} + \frac{r^2}{3a_0^3} - \frac{r^3}{54a_0^4} - \frac{2}{a_0} + \frac{r}{3a_0^2} + \frac{2r}{a_0^2} - \frac{r^2}{3a_0^3}\right\}e^{-r/3a_0}$$

$$= -\frac{\hbar^2}{2m_e r}\frac{3}{4}\sqrt{2}\left(\frac{1}{3a_0}\right)^{3/2}\left\{\frac{r^2}{9a_0^3} - \frac{r^3}{54a_0^4}\right\}e^{-r/3a_0} = -\frac{\hbar^2}{18m_e a_0^2}R_{31}(r) \quad .$$

Consequently, we find for R_{31} the eigenvalue $E_3 = -\hbar^2/\left(18m_e a_0^2\right) = -\alpha^2 m_e c^2/18 = E_1/9$ under the action of the differential operator. This is the same eigenvalue as for R_{30}. Why?

f: $\boldsymbol{R_{n=3,\ell=2}(r) = \frac{2}{27}\sqrt{\frac{2}{5}}\left(\frac{1}{3a_0}\right)^{3/2}\left\{\left(\frac{r}{a_0}\right)^2\right\} e^{-r/3a_0}}$.

Since $\ell = 2$, we obtain for the differential operator $-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}r - \frac{6}{r} + \frac{2}{a_0}\right\}$. Also using the results of **d**, we find then

$$-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}r - \frac{6}{r} + \frac{2}{a_0}\right\}R_{32}(r) =$$

$$= -\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}r - \frac{6}{r} + \frac{2}{a_0}\right\}\frac{2}{27}\sqrt{\frac{2}{5}}\left(\frac{1}{3a_0}\right)^{3/2}\left\{\left(\frac{r}{a_0}\right)^2\right\} e^{-r/3a_0}$$

$$= -\frac{\hbar^2}{2m_e r}\frac{2}{27}\sqrt{\frac{2}{5}}\left(\frac{1}{3a_0}\right)^{3/2}\left\{\frac{1}{a_0^2}\frac{d^2}{dr^2}r^3 e^{-r/3a_0} + \left[-\frac{6}{r} + \frac{2}{a_0}\right]\left(\frac{r}{a_0}\right)^2 e^{-r/3a_0}\right\}$$

$$= -\frac{\hbar^2}{2m_e r}\frac{2}{27}\sqrt{\frac{2}{5}}\left(\frac{1}{3a_0}\right)^{3/2}\left\{\frac{1}{a_0^2}\left\{6r - \frac{2r^2}{a_0} + \frac{r^3}{9a_0^2}\right\}e^{-r/3a_0} + \left[-\frac{6}{r} + \frac{2}{a_0}\right]\left(\frac{r}{a_0}\right)^2 e^{-r/3a_0}\right\}$$

$$= -\frac{\hbar^2}{2m_e r}\frac{2}{27}\sqrt{\frac{2}{5}}\left(\frac{1}{3a_0}\right)^{3/2}\left\{\frac{6r}{a_0^2} - \frac{2r^2}{a_0^3} + \frac{r^3}{9a_0^4} - \frac{6r}{a_0^2} + \frac{2r^2}{a_0^3}\right\}e^{-r/3a_0}$$

$$= -\frac{\hbar^2}{2m_e r}\frac{2}{27}\sqrt{\frac{2}{5}}\left(\frac{1}{3a_0}\right)^{3/2}\left\{-\frac{r^3}{9a_0^4}\right\}e^{-r/3a_0} = -\frac{\hbar^2}{18m_e a_0^2}R_{32}(r) \quad .$$

Consequently, we find for R_{32} the eigenvalue $E_3 = -\hbar^2/\left(18m_e a_0^2\right) = -\alpha^2 m_e c^2/18 = E_1/9$ under the action of the differential operator. This is the same eigenvalue as for R_{30}. Why?

In the following table we collect the results of the preceding calculus.

	principal quantum number n and angular momentum ℓ		binding energy
$R_{n\ell}$	n	$\ell < n$	$E_n = -\alpha^2 m_e c^2/2n^2$
R_{10}	1	0	$E_1 = -\alpha^2 m_e c^2/2$
R_{20}	2	0	$E_2 = -\alpha^2 m_e c^2/8$
R_{21}	2	1	$E_2 = -\alpha^2 m_e c^2/8$
R_{30}	3	0	$E_3 = -\alpha^2 m_e c^2/18$
R_{31}	3	1	$E_3 = -\alpha^2 m_e c^2/18$
R_{32}	3	2	$E_3 = -\alpha^2 m_e c^2/18$

9. Considere os resultados dos exercícios (6) e (8).

a Caso $R_{n\ell}(r)$, para $n = 1, 2, 3, \dots$ e $\ell = 0, 1, 2, \dots \leq n-1$, é uma das soluções da equação

$$\left\{ -\frac{\hbar^2}{2m_e r}\frac{d^2}{dr^2}r \; + \; \frac{\hbar^2\,\ell(\ell+1)}{2m_e r^2} \; - \; \frac{e^2}{4\pi\epsilon_0 r} \right\} R_{n\ell}(r) \; = \; E_n\,R_{n\ell}(r) \quad ,$$

e $Y_\ell^m(\vartheta, \varphi)$, para $\ell = 0, 1, 2, \dots$ e $m = -\ell, -\ell+1, \dots, \ell-1, \ell$, uma das soluções da equação

$$L^2\,Y_\ell^m(\vartheta,\varphi) \; = \; \hbar^2\,\ell(\ell+1)\,Y_\ell^m(\vartheta,\varphi)$$

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$$L^2 \; = \; -\hbar^2 \left\{ \frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\frac{\partial}{\partial\vartheta} \; + \; \frac{1}{\sin^2(\vartheta)}\frac{\partial^2}{\partial\varphi^2} \right\} \quad ,$$

então mostre que $\psi_{n\ell m}(\vec{r}) = R_{n\ell}(r)\,Y_\ell^m(\vartheta,\varphi)$ é uma das soluções da equação

$$\left\{ -\frac{\hbar^2}{2m_e}\,\bigtriangledown^2 \; - \; \frac{e^2}{4\pi\epsilon_0 r} \right\} \psi_{n\ell m}(\vec{r}) \; = \; E_n\,\psi_{n\ell m}(\vec{r}) \quad .$$

b Caso $R_{n\ell}(r)$ satisfaz a relação

$$\int_0^\infty r^2 dr\;|R_{n\ell}(r)|^2 \; = \; 1 \quad ,$$

e $Y_\ell^m(\vartheta,\varphi)$ satisfaz a relação

$$\int_0^{2\pi} d\varphi \int_0^\pi \sin(\vartheta) d\vartheta\;|Y_\ell^m(\vartheta,\varphi)|^2 \; = \; 1 \quad ,$$

então mostre que $\psi_{n\ell m}(\vec{r}) = R_{n\ell}(r)\,Y_\ell^m(\vartheta,\varphi)$ satisfaz a relação

$$\int_{-\infty}^\infty dx \int_{-\infty}^\infty dy \int_{-\infty}^\infty dz\;|\psi_{n\ell m}(x,y,z)|^2 \; = \; 1 \quad .$$

Solution:

a. In the lectures it has been shown

$$\hbar^2\bigtriangledown^2 \; = \; \frac{\hbar^2}{r}\frac{d^2}{dr^2}r \; - \; \frac{L^2}{2m_e r^2} \quad .$$

Consequently,

$$\left\{ -\frac{\hbar^2}{2m_e}\,\bigtriangledown^2 - \frac{e^2}{4\pi\epsilon_0 r} \right\} \psi_{n\ell m}(\vec{r}) \; = \; \left\{ -\frac{\hbar^2}{2m_e r}\frac{d^2}{dr^2}r \; + \; \frac{L^2}{2m_e r^2} \; - \; \frac{e^2}{4\pi\epsilon_0 r} \right\} R_{n\ell}(r)\,Y_\ell^m(\vartheta,\varphi) \; =$$

$$= \; -\frac{\hbar^2}{2m_e r}\frac{d^2}{dr^2}\,r R_{n\ell}(r)\,Y_\ell^m(\vartheta,\varphi) \; + \; \frac{L^2}{2m_e r^2}R_{n\ell}(r)\,Y_\ell^m(\vartheta,\varphi) \; - \; \frac{e^2}{4\pi\epsilon_0 r}R_{n\ell}(r)\,Y_\ell^m(\vartheta,\varphi)$$

$$= -Y_\ell^m(\vartheta,\varphi)\,\frac{\hbar^2}{2m_e r}\,\frac{d^2}{dr^2}\,rR_{n\ell}(r) \;+\; R_{n\ell}(r)\,\frac{L^2}{2m_e r^2}\,Y_\ell^m(\vartheta,\varphi) \;-\; Y_\ell^m(\vartheta,\varphi)\frac{e^2}{4\pi\epsilon_0 r}R_{n\ell}(r)$$

$$= -Y_\ell^m(\vartheta,\varphi)\,\frac{\hbar^2}{2m_e r}\,\frac{d^2}{dr^2}\,rR_{n\ell}(r) \;+\; R_{n\ell}(r)\,\frac{\hbar^2\,\ell(\ell+1)}{2m_e r^2}\,Y_\ell^m(\vartheta,\varphi) \;-\; Y_\ell^m(\vartheta,\varphi)\frac{e^2}{4\pi\epsilon_0 r}R_{n\ell}(r)$$

$$= -Y_\ell^m(\vartheta,\varphi)\,\frac{\hbar^2}{2m_e r}\,\frac{d^2}{dr^2}\,rR_{n\ell}(r) \;+\; Y_\ell^m(\vartheta,\varphi)\,\frac{\hbar^2\,\ell(\ell+1)}{2m_e r^2}\,R_{n\ell}(r) \;-\; Y_\ell^m(\vartheta,\varphi)\frac{e^2}{4\pi\epsilon_0 r}R_{n\ell}(r)$$

$$= Y_\ell^m(\vartheta,\varphi)\,\left\{-\frac{\hbar^2}{2m_e r}\,\frac{d^2}{dr^2}\,rR_{n\ell}(r) \;+\; \frac{\hbar^2\,\ell(\ell+1)}{2m_e r^2}\,R_{n\ell}(r) \;-\; \frac{e^2}{4\pi\epsilon_0 r}R_{n\ell}(r)\right\}$$

$$= Y_\ell^m(\vartheta,\varphi)\,\left\{-\frac{\hbar^2}{2m_e r}\,\frac{d^2}{dr^2}\,r \;+\; \frac{\hbar^2\,\ell(\ell+1)}{2m_e r^2} \;-\; \frac{e^2}{4\pi\epsilon_0 r}\right\}\,R_{n\ell}(r)$$

$$= Y_\ell^m(\vartheta,\varphi)\,E_n\,R_{n\ell}(r) \;=\; E_n\,R_{n\ell}(r)Y_\ell^m(\vartheta,\varphi) \;=\; E_n\,\psi_{n\ell m}(\vec{r}) \quad .$$

b. In the lectures it has been shown

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \;=\; \int_0^\infty r^2 dr \int_0^{2\pi} d\varphi \int_0^\pi \sin(\vartheta) d\vartheta \quad .$$

Consequently,

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \,\left|\psi_{n\ell m}(x,y,z)\right|^2 \;=$$

$$= \int_0^\infty r^2 dr \int_0^{2\pi} d\varphi \int_0^\pi \sin(\vartheta) d\vartheta \;\left|R_{n\ell}(r)\,Y_\ell^m(\vartheta,\varphi)\right|^2$$

$$= \int_0^\infty r^2 dr \int_0^{2\pi} d\varphi \int_0^\pi \sin(\vartheta) d\vartheta \;\left|R_{n\ell}(r)\right|^2\;\left|Y_\ell^m(\vartheta,\varphi)\right|^2$$

$$= \int_0^\infty r^2 dr \;\left|R_{n\ell}(r)\right|^2 \int_0^{2\pi} d\varphi \int_0^\pi \sin(\vartheta) d\vartheta \;\left|Y_\ell^m(\vartheta,\varphi)\right|^2$$

$$= 1 \times 1 \;= 1 \quad .$$

10. Um estado excitado do átomo de hidrogénio pode-se representar por $H(n, \ell, m)$, onde n, ℓ e m representam respectivamente o número quântico principal, o de momento angular orbital e o magnético ($m = -\ell$, $-\ell + 1$, ..., 0, ..., $+\ell$).
No entanto, da solução da equação de onda para o átomo de hidrogénio deduzimos que o espectro de Coulomb é dado por

$$E_n \; = \; -\frac{E_\infty}{n^2} \quad , \quad n = 1,\, 2,\, 3,\, \ldots$$

e ainda a condição $\ell \leq n - 1$ para estados quânticos fisicamente aceitáveis.
Portanto, existem vários estados excitados diferentes com a mesma energia.
Este fenómeno chama-se *degenerescência*.

a Demostra que o número de estados excitados diferentes com energia E_n, é igual ao quadrado do número quântico principal n.

Do passado existe ainda uma outra classificação dos estados excitados de hidrogénio, classificação em que se consideram como manifestações diferentes do mesmo estado $H(n, \ell)$ (indicado por $n\ell$), os vários estados $H(n, \ell, 0)$, $H(n, \ell, \pm 1)$, $H(n, \ell, \pm 2)$, ..., $H(n, \ell, \pm \ell)$. Neste abordagem o número quântico de momento angular orbital ℓ é representado por uma letra de acordo com o seguinte quadro

ℓ	0	1	2	3	4	5	6	7
letra	s	p	d	f	g	h	i	j

b Faça um quadro para estados quânticos fisicamente aceitáveis onde se indica os estados $H(n, \ell)$ para $n = 1$, ..., 6 e $\ell = 0$, ..., 5.

Solution:

a. For $n = 1$ we only have $\ell = 0$ and $m = 0$. Consequently, for $n = 1$ we find one possible state, the *ground state* $|n = 1, \ell = 0, m = 0\rangle$, with energy $E_1 = -E_\infty/1$.

For $n = 2$ we have $\ell = 0$ with $m = 0$ and $\ell = 1$ with $m = -1$, 0, +1. Consequently, for $n = 2$ we find four ($1 + 3 = 2^2$) possible states, $|n = 2, \ell = 0, m = 0\rangle$, $|n = 2, \ell = 1, m = -1\rangle$, $|n = 2, \ell = 1, m = 0\rangle$, and $|n = 2, \ell = 1, m = +1\rangle$, with energy $E_2 = -E_\infty/4$.

For $n = 3$ we have $\ell = 0$ with $m = 0$, $\ell = 1$ with $m = -1$, 0, +1 and $\ell = 2$ with $m = -2$, -1, 0, +1, +2. Consequently, for $n = 3$ we find nine ($1 + 3 + 5 = 3^2$) possible states, $|n = 3, \ell = 0, m = 0\rangle$, $|n = 3, \ell = 1, m = -1\rangle$, $|n = 3, \ell = 1, m = 0\rangle$, $|n = 3, \ell = 1, m = +1\rangle$, $|n = 3, \ell = 2, m = -2\rangle$, $|n = 3, \ell = 2, m = -1\rangle$, $|n = 3, \ell = 2, m = 0\rangle$, $|n = 3, \ell = 2, m = +1\rangle$, and $|n = 3, \ell = 2, m = +2\rangle$, with energy $E_3 = -E_\infty/9$.

The number of states with the same value for ℓ equals $2\ell + 1$.
The maximum value for ℓ equals $n - 1$.
Hence, the number of states N_n with the same energy E_n, is given by

$$N_n \; = \; 1 \, + \, 3 \, + \, 5 \, + \, \ldots \, + \, (2(n-3)+1) \, + \, (2(n-2)+1) \, + \, (2(n-1)+1) \quad .$$

The trick for adding this series has been found the other day by Carl Friedrich Gauss. Just add it term by term to the same thing but in reversed order. You obtain then

$$N_n + N_n = [1 + 2(n-1) + 1] + [3 + 2(n-2) + 1] + [5 + 2(n-3) + 1] + \dots$$
$$+ \dots + [2(n-3) + 1 + 5] + [2(n-2) + 1 + 3] + [2(n-1) + 1 + 1] \quad .$$

The expressions in between the brackets all add up to $2n$.
Furthermore, there are n terms.
Hence,

$$2N_n = n \times 2n \qquad \rightarrow \qquad N_n = n^2 \quad .$$

Consequently, the degeneracy of the energy level E_n equals n^2.

b.

n	s	p	d	f	g	h
1	1s					
2	2s	2p				
3	3s	3p	3d			
4	4s	4p	4d	4f		
5	5s	5p	5d	5f	5g	
6	6s	6p	6d	6f	6g	6h