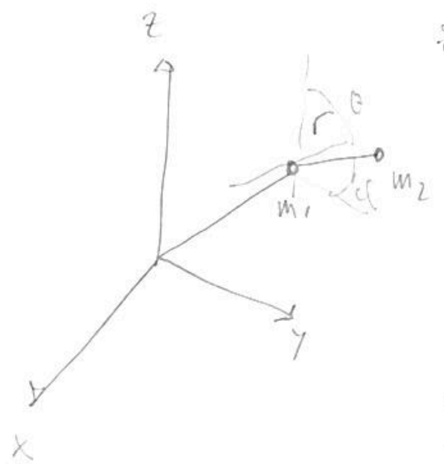

$Z=1$ átomo de hidrógeno

Como $m_1 >> m_2$ r distancia a m_1 y en los hechos c m.

$$X_{cm} = (m_1 x_1 + m_2 x_2)/(m_1+m_2)$$
$$Y_{cm}$$
$$Z_{cm}$$

$$x_2 - x_1 = r \operatorname{sen}\theta \cos\varphi$$
$$y_2 - y_1 = r \operatorname{sen}\theta \operatorname{sen}\varphi$$
$$z_2 - z_1 = r \cos\theta$$

$V(r)$ potencial central

Las posiciones son $\bar{r}_T = \bar{r}_{cm} + \bar{r}$

$$-\frac{\hbar^2}{2(m_1+m_2)} \nabla^2 \Psi_T + V(r)\Psi_T = E_T \Psi_T$$

definimos $\mu = \frac{m_1 m_2}{m_1+m_2}$ y $V(r) = -\frac{Ze^2}{r}$

Proponemos $\Psi = \Psi_{cm}(x,y,z)\,\psi(r,\theta,\varphi)$

$$\Rightarrow \boxed{E_{cm} = -\frac{\hbar^2}{2(m_1+m_2)}\frac{1}{\Psi_{cm}}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\Psi_{cm}}$$

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

$$\Rightarrow \boxed{E_T = E_{cm} + E}$$

ψ se puede escribir como:

$$\psi(r,\theta,\varphi) = R(r)\,\Theta(\theta)\,\Phi(\phi) = R(r)\,Y^l_m(\theta,\varphi)$$

$$Y^l_m(\theta,\varphi) = A\,e^{im\phi}\,P^m_l(\cos\theta)$$

La parte radial queda:

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{2\mu r^2}{\hbar^2}\left[E - V(r)\right] = l(l+1)$$

se puede expresar en términos de los polinomios de Laguerre con la sustitución

de las fuerzas centrales elegimos interacción coulombiana

$$\rho = 2\beta r \quad ; \quad \beta = -\frac{2\mu E}{\hbar^2} \quad ; \quad \gamma = \frac{\mu z e^2}{\hbar^2 \beta}$$

$$\frac{1}{\rho^2}\frac{\partial}{\partial\rho}\left(\rho^2\frac{\partial R(\rho)}{\partial\rho}\right) + \left\{-\frac{1}{4} - \frac{l(l+1)}{\rho^2} + \frac{\gamma}{\rho}\right\}R(\rho) = 0$$

$$\Rightarrow \quad R_{nl}(\rho) = e^{-\rho/2}\rho^l G_n(\rho)$$

$$\psi_{nlm}(r,\theta,\varphi) = R_{nl}(r)\, Y^l_m(\theta,\varphi)$$

$$\psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{z}{a_0}\right)^{3/2} e^{-zr/a_0} \qquad a_0 \equiv \frac{\hbar^2}{\mu e^2} \simeq 0{,}529 \cdot 10^{-8}\ \text{cm}$$

$$\psi_{200} = \frac{1}{4\sqrt{2\pi}}\left(\frac{z}{a_0}\right)^{3/2}\left(2 - z\frac{r}{a_0}\right) e^{-\frac{zr}{2a_0}}$$

$$\psi_{210} = \frac{1}{4\sqrt{2\pi}}\left(\frac{z}{a_0}\right)^{3/2} z\frac{r}{a_0}\, e^{-\frac{zr}{2a_0}} \cos\theta$$

$$\psi_{21\pm1} = \frac{1}{8\sqrt{2\pi}}\left(\frac{z}{a_0}\right)^{3/2} z\frac{r}{a_0} \cdot e^{-\frac{zr}{2a_0}} \operatorname{sen}\theta\, e^{\pm i\varphi}$$

$$\psi_{300} = \frac{1}{81\sqrt{3\pi}}\left(\frac{z}{a_0}\right)^{3/2}\left(27 - 18z\frac{r}{a_0} + \frac{2z^2r^2}{a_0^2}\right) e^{-\frac{zr}{3a_0}}$$

$$\psi_{310} = \frac{1}{81}\sqrt{\frac{2}{\pi}}\left(\frac{z}{a_0}\right)^{3/2}\left(6 - \frac{zr}{a_0}\right)\frac{zr}{a_0}\, e^{-\frac{zr}{3a_0}} \cos\theta$$

$$\psi_{31\pm1} = \frac{1}{81\sqrt{\pi}}\left(\frac{z}{a_0}\right)^{3/2}\left(6 - \frac{zr}{a_0}\right)\frac{zr}{a_0}\, e^{-\frac{zr}{3a_0}} \operatorname{sen}\theta\, e^{\pm i\varphi}$$

$$\psi_{320} = \frac{1}{81\sqrt{6\pi}}\left(\frac{Z}{a_0}\right)^{3/2} Z^2 \frac{r^2}{a_0^2}\, e^{-\frac{Zr}{3a_0}} \left(3\cos^2\theta - 1\right)$$

$$\psi_{32\pm1} = \frac{1}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \frac{Z^2 r^2}{a_0^2}\, e^{-\frac{Zr}{3a_0}}\ \mathrm{sen}\,\theta\cos\theta\ e^{\pm i\varphi}$$

$$\psi_{32\pm2} = \frac{1}{162\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \frac{Z^2 r^2}{a_0^2}\, e^{-\frac{Zr}{3a_0}}\ \mathrm{sen}^2\theta\ e^{\pm 2i\varphi}$$

$$E_n = -Z^2\frac{\mu e^4}{2\hbar^2 n^2}$$

$n \in \mathbb{N}$

$\ell = 0, 1, 2, \ldots, n-1$

$m = -\ell, \ldots, \ell$

n	1	2		3		
ℓ	0	0	1	0	1	2
m	0	0	-1, 0, 1	0	-1, 0, 1	-2, -1, 0, 1, 2
deg(ℓ)	1	1	3	1	3	5
deg(m)	1	4		9		

9)

a) El fundamental es el ψ_{100}

Proba de $r > a_0$

$$\int_0^{\pi}\int_0^{2\pi}\int_{a_0}^{\infty} \psi_{100}^* \psi_{100}\, r^2 \operatorname{sen}\theta \, dr\, d\theta\, d\varphi = 2\pi \int_0^{\pi}\int_{a_0}^{\infty} \frac{1}{\pi}\left(\frac{z}{a_0}\right)^3 e^{-2z\frac{r}{a_0}} r^2 \operatorname{sen}\theta \, dr\, d\theta =$$

$$= \boxed{2\left(\frac{z}{a_0}\right)^3 \cdot 2 \int_{a_0}^{\infty} r^2 e^{-\frac{2zr}{a_0}} dr} =$$

Uso que

$$\int x^2 e^{-2ax} dx = \left[-2ax(ax+1) - 1\right] \frac{e^{-2ax}}{4a^3}$$

$$= e^{-2z\frac{r}{a_0}} \left[-2\left(\frac{zr}{a_0}\right)\left(\frac{zr}{a_0}+1\right) - 1\right]\Bigg|_{a_0}^{\infty} \simeq 0,677$$

b) Una distancia mayor a $2a_0$ $\simeq 0,238$ clasicamente es 0

c) Para que se encuentre dentro del protón

$$4\left(\frac{z}{a_0}\right)^3 \int_0^{r_p} r^2 e^{-\frac{2zr}{a_0}} dr = \dots \simeq 1 \cdot 10^{-9} \quad \text{muy poco probable}$$

En el prob 10

$$\langle r \rangle = \frac{3}{2}\frac{a_0}{z}$$

$$\langle r^{-1} \rangle = \frac{z}{a_0}$$

En el prob 11

mas de lo mismo pero como se busca

el mas probable se deriva

$$P(r) = \frac{1}{16}\frac{1}{2\pi}\left(\frac{z}{a_0}\right)^3 \left(2 - z\,r/a_0\right)^2 e^{-zr/a_0} \qquad \frac{\partial P}{\partial r} = 0$$

En el prob 12

$$\bar{J} = \frac{\hbar}{2mi}\left[\psi^* \nabla\psi - \psi\nabla\psi^*\right]$$

$$\left.\begin{array}{l}\psi_{100}\\ \psi_{200}\\ \psi_{210}\end{array}\right\} \rightarrow J = 0. \quad (\text{son reales})$$

pero $\psi_{21\pm1}$ no $\rightarrow \bar{J} = \pm \dfrac{\hbar |\psi|^2}{mr\,\text{sen}\,\theta}\hat{\phi}$

como sale $\hat{\phi}$

$$\nabla\psi = \frac{\partial\psi}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial\psi}{\partial\theta}\hat{\theta} + \frac{1}{r\,\text{sen}\,\theta}\frac{\partial\psi}{\partial\varphi}\hat{\phi}$$

13 - Sea la función de onda de un átomo de hidrógeno: $\psi = A(\varphi_{210} - \varphi_{21-1} + \varphi_{100})$ donde los $\varphi_{n\ell m}$ son las autofunciones normalizadas de $\hat{H}$

a) Normalizar ψ

b) Hacer una tabla con los valores que pueden medirse de E, L^2, L_z y sus probabilidades

c) Calcular $\langle L^2 \rangle$, $\langle L_z \rangle$ y $\langle H \rangle$

d) Hallar ψ para un tiempo t cualquiera y repetir los cálculos de "c" Discutir el resultado.

a) $$1 = A^2 \int (\varphi_{210}^* - \varphi_{21-1}^* + \varphi_{100}^*)(\varphi_{210} - \varphi_{21-1} + \varphi_{100})\, d\bar{x} = A^2\, 3$$

$$\Rightarrow \boxed{A = \frac{1}{\sqrt{3}}}$$

b)

n	ℓ	E_n	$P(E_n)$	L^2	$P(L^2)$	L_z	$P(L_z)$
1	0	E_1	1/3	0	1/3	0	1/3
2	0	E_2	2/3	0	2/3	0	2/3
2	1	E_2	2/3	2	2/3	-1,0,1	2/3

c)

$$\langle L^2 \rangle = \frac{1}{3} \int (\varphi_{210}^* - \varphi_{21-1}^* + \varphi_{100}^*)\, L^2 (\varphi_{210} - \varphi_{21-1} + \varphi_{100})\, d\bar{r}$$

$$\langle L^2 \rangle = \frac{1}{3}\left[\hbar^2 (2 + 2 + 0)\right] = \boxed{\frac{4}{3}\hbar^2 = \langle L^2 \rangle}$$

$$\langle L_z \rangle = \frac{1}{3} \int (\varphi_{210}^* - \varphi_{21-1}^* + \varphi_{100}^*)\, L_z (\varphi_{210} - \varphi_{21-1} + \varphi_{100})\, d\bar{r}$$

$$\langle L_z \rangle = \frac{1}{3}\hbar \left[0 - 1 + 0\right] = \boxed{-\frac{\hbar}{3} = \langle L_z \rangle}$$

$$\langle \hat{H} \rangle = \frac{1}{3}E_1 + \frac{2}{3}E_2 = \frac{1}{3}E_1 + \frac{2}{3}\frac{E_1}{4} = \left(\frac{1}{3} + \frac{1}{6}\right)E_1$$

$$\boxed{\langle \hat{H} \rangle = \frac{E_1}{2} = -\frac{\mu}{4}\frac{z^2 e^4}{\hbar^2}}$$