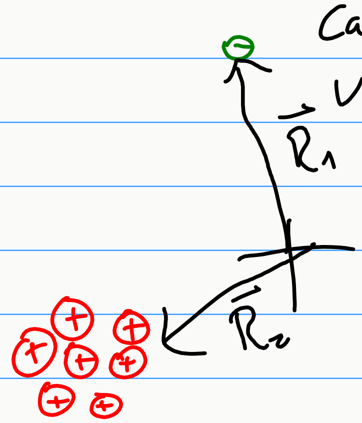
Átomo hidrogenoide

- núcleo y electrón puntuales
- no relativista

carga $-e$
masa m_1



carga Ze
masa m_2

$$H = \frac{P_1^2}{2m_1} + \frac{P_2^2}{2m_2} + V(\vec{R}_1 - \vec{R}_2)$$

Coulomb

- 2 cuerpos a 1 cuerpo

$$\vec{R}_{cm} = \frac{m_1 \vec{R}_1 + m_2 \vec{R}_2}{m_1 + m_2} \qquad \vec{R} = \vec{R}_1 - \vec{R}_2$$

$$\vec{P}_{cm} = \vec{P}_1 + \vec{P}_2 \qquad \vec{P} = \frac{m_2 \vec{P}_1 - m_1 \vec{P}_2}{m_1 + m_2}$$

$$M = m_1 + m_2 \qquad \frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$$

Sabemos $[X_1, P_{1x}] = i\hbar$ y $[X_2, P_{2x}] = i\hbar$

$$[X_{cm}, P_{cm_x}] = \left[\frac{m_1 X_1 + m_2 X_2}{m_1 + m_2}, P_{1x} + P_{2x}\right]$$

$$= \left[\frac{m_1 X_1}{m_1 + m_2}, P_{1x}\right] + \left[\frac{m_2 X_2}{m_1 + m_2}, P_{2x}\right]$$

$$= \left(\frac{m_1}{m_1 + m_2} + \frac{m_2}{m_1 + m_2}\right) i\hbar = i\hbar$$

Con esto podemos reescribir H como

$$H = \frac{P_{CM}^2}{2M} + \frac{P^2}{2\mu} + V(\vec{R})$$

$$H = H_{cm} + H_{int} = H_{cm} \otimes \mathbb{1} + \mathbb{1} \otimes H_{int}$$

interno

Los grados de libertad del centro de masa e internos están desacoplados.

$$[H_{cm}, H_{int}] = 0$$

$$H_{cm} |\varphi\rangle = E_{cm} |\varphi\rangle$$

$$H_{int} |\varphi\rangle = E_{int} |\varphi\rangle$$

Notación
e.v. eigenvalor
e.V. eigenvector

$$H|\varphi\rangle = (E_{cm} + E_{int}) |\varphi\rangle$$

Usando la base de e.V. de $\vec{R}_{cm}$ y $\vec{R}$:

$$\{ |\vec{r}_{cm}, \vec{r}_{int}\rangle \} \qquad \vec{P}_{int} = -i\hbar \vec{\nabla}_{int} \qquad \vec{P}_{cm} = -i\hbar \vec{\nabla}_{cm}$$

$$-\frac{\hbar^2}{2M} \nabla_{cm}^2 \varphi_{cm}(\vec{r}_{cm}) = E_{cm} \varphi_{cm}(\vec{r}_{cm})$$

$$\left[-\frac{\hbar^2}{2\mu} \nabla_{int}^2 + V(\vec{r}) \right] \varphi_{int}(\vec{r}_{int}) = E_{int} \varphi_{int}(\vec{r}_{int})$$

$$\langle \vec{r}_{cm}, \vec{r}_{int} | \varphi \rangle = \varphi(\vec{r}_{cm}, \vec{r}_{int}) = \varphi_{cm}(\vec{r}_{cm})\, \varphi_{int}(\vec{r}_{int})$$

$$\varphi_{cm}(\vec{r}_{cm}) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{k}\cdot\vec{r}_{cm}} \quad \text{con} \quad E_{cm} = \frac{\hbar^2 k^2}{2M}$$

Nos enfocamos ahora en los grados internos de libertad (quitamos etiqueta "int") $\varphi_{int} = \psi$

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(\vec{r})\right]\psi(\vec{r}) = E\psi(\vec{r})$$

$$V(\vec{r}) = -\frac{Ze^2}{4\pi\epsilon_0 r}$$

Potencial central

$$V(\vec{r}) = V(r)$$

Por simetría conviene usar coordenadas esféricas

operador de momento angular

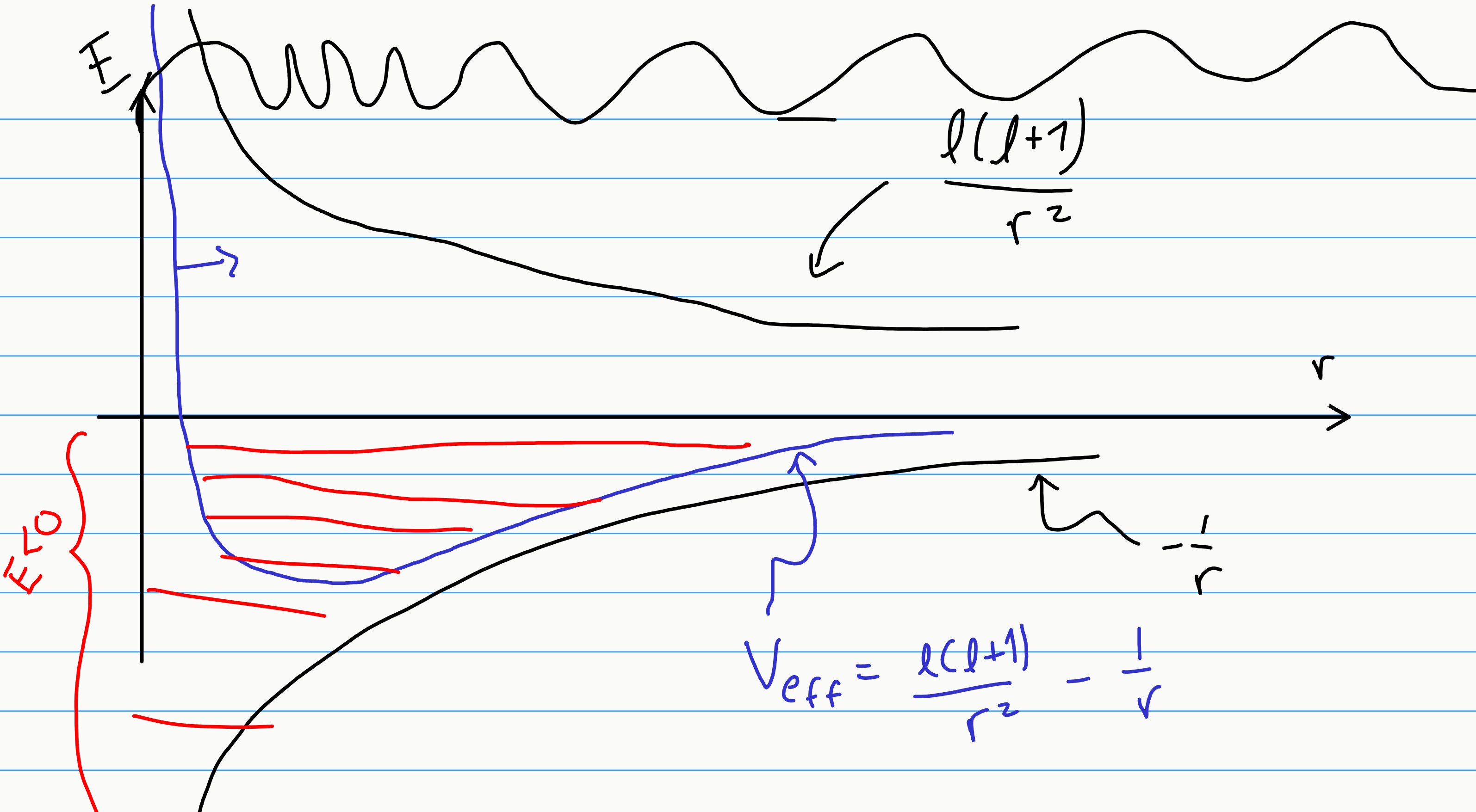
$$H = -\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2} r + \frac{L^2}{2\mu r^2} + V(r)$$

Separación de variables

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

Ecuación radial $\qquad R(r) = \frac{u(r)}{r}$

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr} + \frac{l(l+1)\hbar^2}{2\mu r^2} - \frac{e^2}{4\pi\epsilon_0 r}\right]u = Eu$$



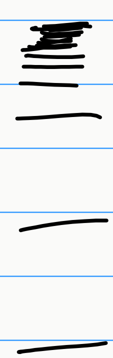
• Si $l > 0$ entonces $u(0) = 0$

Buscamos soluciones para $E < 0$

Encontramos el número principal cuántico "n"

$E_1 = 13.6\,eV$

$$E_n = -\frac{E_1}{n^2}$$

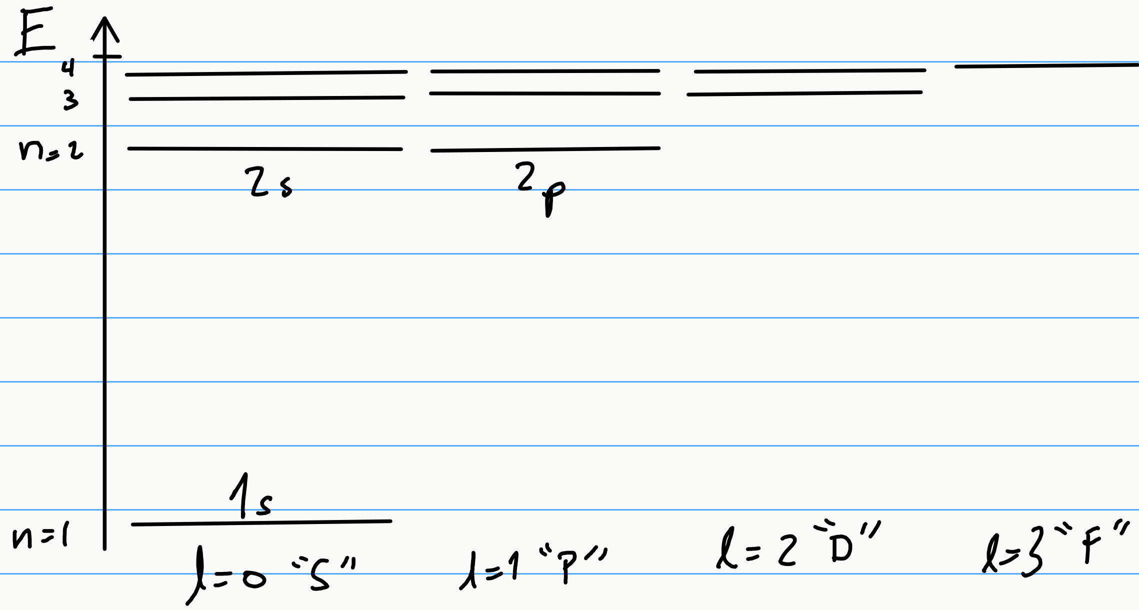


$$E_1 = \frac{\hbar^2}{\mu a_0^2} = \frac{1}{2}\alpha^2 \mu c^2$$

$$a_0 = \frac{\hbar^2 4\pi\epsilon_0}{\mu e^2}$$ radio de Bohr

$$\alpha = \frac{e^2}{4\pi\epsilon_0 \hbar c} \approx \frac{1}{137}$$

- Estructura de niveles:



$n = 1, 2, \dots$

$l = 0, 1, \dots, n-1$ degenerados

$m = -l, \dots, l$ degenerados

$R_{1,0}$ estado base

$\cancel{R_{1,1}}$ l debe ser $< n$