Clase 23

7.3. Aplicación: Estructura fina e hiperfina del átomo de Hidrógeno

7.3.1. Átomo de Hidrógeno

(P7E91)

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} - \frac{e^2}{r}$$

m: masa del e^-

$e \equiv \frac{q}{\sqrt{4\pi\varepsilon_0}}$, q: carga del e^-

$$\hat{H}_0 \phi = E\phi \Rightarrow \dots \Rightarrow$$

polinomios asociados de Laguerre

$$\Rightarrow \begin{cases} \underbrace{\phi_{n\ell m}}_{|n,\ell,m\rangle}(\bar{r}) = \dfrac{2^{\ell+1}}{a_0^{3/2}\, n^{\ell+2}} \sqrt{\dfrac{(n-\ell-1)!}{(n+\ell)!}} \left(\dfrac{r}{a_0}\right)^{\ell} e^{-r/(na_0)}\, L_{n-\ell-1}^{2\ell+1}\left(\dfrac{2r}{a_0 n}\right) Y_{\ell m}(\theta,\varphi) \\[2ex] E_{n\ell m} = -\dfrac{E_I}{n^2} \equiv E_n \end{cases}$$

$\leftarrow$ hay degeneración en los niveles de energía

$$= -\frac{E_I}{(K+\ell)^2} \qquad K = 1,2,3,\dots \; ; \quad n \equiv K+\ell \quad (n = 1,2,3,\dots)$$

$$\ell = 0,1,2,\dots$$

radio de Bohr

$$a_0 \equiv \frac{\hbar^2}{me^2} \approx 5.29\times10^{-11}\,\text{m}$$

$$E_I \equiv \frac{me^4}{2\hbar^2} = \frac{1}{2}mc^2\left(\frac{e^2}{\hbar c}\right)^2$$

$\alpha \equiv \frac{e^2}{\hbar c}$

(α: constante de estructura fina)

$\left(\alpha \approx \frac{1}{137}\right)$

Algunos autoestados:

$$\phi_{100}(\bar{r}) = \frac{e^{-r/a_0}}{(\pi a_0^3)^{1/2}}$$

$$\phi_{211}(\bar{r}) = -\frac{1}{8(\pi a_0^3)^{1/2}} \left(\frac{r}{a_0}\right) e^{-r/(2a_0)} \sin\theta\, e^{i\varphi}$$

¿Degeneración de niveles?

$$n=3 \qquad \left.\begin{array}{c|ccc} & K & \ell & m \\ & 1 & 2 & 2,1,0,-1,-2 \\ & 2 & 1 & 1,0,-1 \\ n=K+\ell & 3 & 0 & 0 \end{array}\right\} \deg(E_3) = 5+3+1 = 9$$

$$\deg(E_n) = \sum_{\ell=0}^{n-1} (2\ell+1) = n^2$$

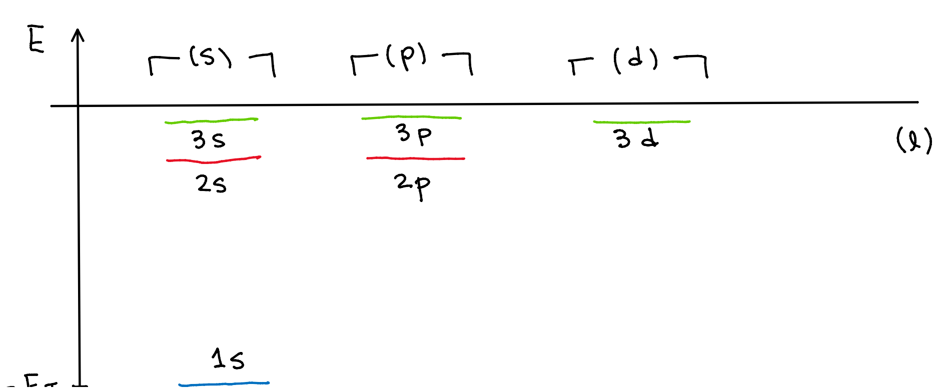
Notación espectroscópica: se da n seguido de una letra que identifica el valor de ℓ:

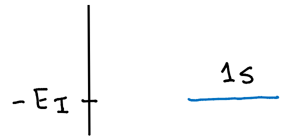
$$\begin{array}{ccc} \ell=0 & \leftrightarrow & s \\ \ell=1 & \leftrightarrow & p \\ \ell=2 & \leftrightarrow & d \\ \ell=3 & \leftrightarrow & f \\ \ell=4 & \leftrightarrow & g \\ & \vdots & \end{array}$$

Subcapa 1s $(n=1,\ \ell=0)$: $\{\phi_{100}(\vec{r})\}$] NIVEL $n=1$

Subcapa 2s $(n=2,\ \ell=0)$: $\{\phi_{200}(\vec{r})\}$

Subcapa 2p $(n=2,\ \ell=1)$: $\{\phi_{211}(\vec{r}),\ \phi_{210}(\vec{r}),\ \phi_{21-1}(\vec{r})\}$] NIVEL $n=2$





7.3.2. Estructura fina del átomo de Hidrógeno

(P7E92)

$$\hat{H} = \hat{H}_0 + \underbrace{mc^2}_{\text{cte, no nos interesa}} + \underbrace{\hat{W}_{mv} + \hat{W}_{so} + \hat{W}_D}_{\hat{W}_f}$$

$\hat{W}_f$ ← términos de estructura fina

$$\hat{W}_{mv} = -\frac{\hat{\bar{p}}^4}{8m^3c^2}$$

(mv)

← corrige energía cinética del e^- (rel. especial)

$$\left[E = c\sqrt{\bar{p}^2 + m^2c^2} \approx \approx mc^2 + \frac{\bar{p}^2}{2m} - \frac{\bar{p}^4}{8m^3c^2} + \dots \right.$$

$$\hat{W}_{so} = \frac{e^2}{m^2c^2} \cdot \frac{\hat{\bar{L}} \cdot \hat{\bar{S}}}{r^3}$$

(espín-órbita)

← interacción entre el campo magnético generado por el e^- y su espín

$$\hat{W}_D = \frac{\pi e^2 \hbar^2}{2m^2c^2} \delta(\bar{r})$$

(Darwin)

← corrige pot. del núcleo por las oscilaciones rápidas del electrón

- Nivel $n = 1$

Veamos cómo afectan los términos de $\hat{W}_f$ a la energía del nivel $n=1$.

$E_1 = -E_I$, tiene degeneración $\overset{\text{para } \hat{H}_0}{\uparrow}$ $\deg(E_1) = 2$ $\quad \{ |1,0,0\rangle \otimes |+\rangle , |1,0,0\rangle \otimes |-\rangle \}$

(debido al espín)

Para hallar las correcciones a la energía hay que diagonalizar $\hat{W}_f$ en el subespacio degenerado.

$$* \quad \hat{W}_{so} = \left(\frac{e}{mc}\right)^2 \frac{1}{r^3} \hat{\bar{L}} \cdot \hat{\bar{S}} \underset{(\ell=0)}{\Longrightarrow} \boxed{[\hat{W}_{so}]_{1s} = 0_{2\times 2}}$$

$$* \quad \hat{W}_D = \frac{\pi e^2 \hbar^2}{2m^2c^2} \delta(\bar{r}) \otimes \hat{\mathbb{1}}_{espín}$$

$$\boxed{[\hat{W}_D]_{1s}} = \langle 1,0,0| \frac{\pi e^2\hbar^2}{2m^2c^2} \delta(\bar{r}) |1,0,0\rangle \cdot \mathbb{1}_{2\times 2} =$$

$$= \int_{\mathbb{R}^3} d^3\bar{r} \; |\phi_{1,0,0}(\bar{r})|^2 \cdot \frac{\pi e^2\hbar^2}{2m^2c^2} \delta(\bar{r}) \cdot \mathbb{1}_{2\times 2} =$$

$$= \frac{\pi e^2\hbar^2}{2m^2c^2} \underbrace{|\phi_{1,0,0}(\bar{0})|^2}_{\frac{1}{\pi a_0^3} = \frac{m^3e^6}{\pi\hbar^6}} = \boxed{\frac{me^8}{2\hbar^4c^2} \cdot \mathbb{1}_{2\times 2}}$$

$$* \quad \hat{W}_{mv} = -\frac{\hat{\bar{p}}^4}{8m^3c^2} \otimes \hat{\mathbb{1}}_{espín}$$

Los únicos elementos de matriz no nulos en el subespacio 1s son:

$$\langle 1,0,0| \otimes \langle \pm| \; \hat{W}_{mv} \; |1,0,0\rangle \otimes |\pm\rangle = -\frac{1}{8m^3c^2} \langle 1,0,0| \hat{\bar{p}}^4 |1,0,0\rangle$$

¿Cómo hallar $\langle n,\ell,m | \hat{\bar{p}}^4 | n,\ell,m\rangle$ de forma sencilla?

$$\hat{H}_0 = \frac{\hat{\bar{p}}^2}{2m} \underbrace{- \frac{e^2}{r}}_{\hat{}} \Rightarrow \hat{\bar{p}}^2 = 2m(\hat{H}_0 - \hat{V}) \Rightarrow$$

Truco

$$\underbrace{\qquad\qquad}_{\hat{V}}$$

$$\Longrightarrow \quad \hat{p}^4 = 4m^2 \left(\hat{H}_0^2 + \hat{V}^2 - \hat{H}_0 \hat{V} - \hat{V} \hat{H}_0 \right)$$

$$\langle \hat{p}^4 \rangle_{|n,l,m\rangle} = 4m^2 \left[E_n^2 + e^4 \left\langle \frac{1}{r^2} \right\rangle_{|n,l,m\rangle} + 2e^2 E_n \left\langle \frac{1}{r} \right\rangle_{|n,l,m\rangle} \right]$$

$$\left\langle \frac{1}{r} \right\rangle_{|1,0,0\rangle} = \int_{\mathbb{R}^3} d^3\bar{r} \cdot \frac{1}{r} \left| \phi_{1,0,0}(\bar{r}) \right|^2 = \dots = \frac{me^2}{\hbar^2}$$

$$\left\langle \frac{1}{r^2} \right\rangle_{|1,0,0\rangle} = \int_{\mathbb{R}^3} d^3\bar{r} \cdot \frac{1}{r^2} \left| \phi_{1,0,0}(\bar{r}) \right|^2 = \dots = \frac{2m^2 e^4}{\hbar^4}$$

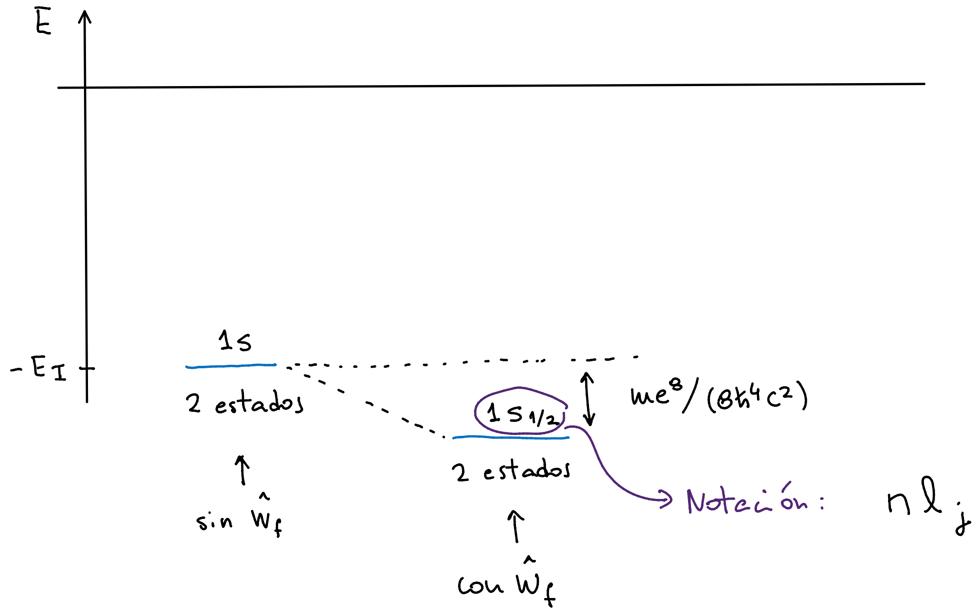
$$\langle \bar{p}^4 \rangle_{|1,0,0\rangle} = \frac{5m^4 e^8}{\hbar^4}$$

$$\boxed{\left[\hat{W}_{mv}\right]_{1s} = -\frac{5me^8}{8\hbar^4 c^2} \cdot \mathbb{1}_{2\times 2}}$$

$$\therefore \quad \boxed{\left[\hat{W}_f\right]_{1s} = -\frac{me^8}{8\hbar^4 c^2} \cdot \mathbb{1}_{2\times 2}}$$

$\therefore$ E_1 cambia a $\displaystyle -E_I - \frac{me^8}{8\hbar^4 c^2} = -\frac{me^4}{2\hbar^2} - \frac{me^8}{8\hbar^4c^2}$

Noten que: $\displaystyle \frac{me^8/8\hbar^4c^2}{me^4/2\hbar^2} = \frac{1}{4}\left(\frac{e^4}{\hbar^2c^2}\right) = \frac{1}{4} \cdot \underbrace{\alpha^2}_{(1/137)^2 \ll 1} \ll 1$

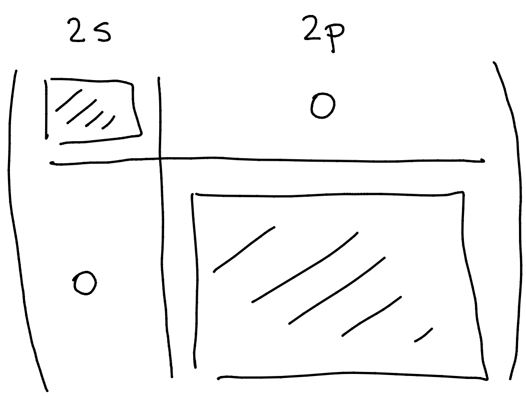


• Nivel $n=2$

$\deg(E_2) = 2 \cdot 2^2 = 8$ → tenemos que diagonalizar una matriz de 8×8

$$E_2 = -\frac{E_I}{4} = -\frac{me^4}{8\hbar^2}$$

$[\hat{W}_f]_{(n=2)} =$



$|2,0,0\rangle \otimes |+\rangle$
$|2,0,0\rangle \otimes |-\rangle$
$|2,1,1\rangle \otimes |+\rangle$
$|2,1,1\rangle \otimes |-\rangle$
$|2,1,0\rangle \otimes |+\rangle$
$|2,1,0\rangle \otimes |-\rangle$
$|2,1,-1\rangle \otimes |+\rangle$
$|2,1,-1\rangle \otimes |-\rangle$

¿Cómo vemos esto?

↓

$$[\hat{L}^2, \hat{W}_f] = 0$$

$$\langle 2p | \hat{W}_f | 2s \rangle = \langle 2p | \frac{\hat{L}^2}{2\hbar^2} \hat{W}_f | 2s \rangle \overset{[\hat{L}^2, \hat{W}_f]}{=} \frac{1}{2\hbar^2} \langle 2p | \hat{W}_f \hat{L}^2 | 2s \rangle = 0$$

$$\langle 2p|\hat{W}_f|2s\rangle = \langle 2p|\frac{\hat{L}^2}{2\hbar^2}\hat{W}_f|2s\rangle \overset{\uparrow}{=} \frac{1}{2\hbar^2}\langle 2p|\hat{W}_f\underbrace{\hat{L}^2|2s\rangle}_{\hbar^2\,0.(0+1)|2s\rangle} = 0$$

$$\therefore \langle 2p|\hat{W}_f|2s\rangle = 0$$

$\therefore$ El elemento de matriz de $\hat{W}_f$ entre en un estado con $l=0$ y otro con $l=1$ es cero.

- Bloque 2s (TAREA)

$$\boxed{[\hat{W}_f]_{2s} = -\frac{5mc^2\alpha^4}{128}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}}$$

- Bloque 2p

$*$ $[\hat{W}_{mv}]_{2p} = ?$

$\langle 2,1,m|\hat{p}^4|2,1,m'\rangle \leftarrow$ independiente de m, m' } Basta con calcularlo para algún m

$$\hat{p}^4 = (\hat{p}^2)^2 = \left(-\hbar^2\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{\hat{L}^2}{r^2}\right)^2$$

$$\therefore \boxed{[\hat{W}_{mv}]_{2p} = -\frac{7}{387}mc^2\alpha^4 \cdot \mathbb{1}_{6\times 6}}$$

$*$ $[\hat{W}_D]_{2p} = ?$

Como $l\neq 0$, resulta $\phi_{2,1,m}(\vec{r}=\vec{0}) = 0$

$$\therefore \quad \boxed{[\hat{W}_D]_{2p} = 0_{6\times 6}}$$

$$* \quad [\hat{W}_{SO}]_{2p} = ?$$

$$\hat{W}_{SO} = f(r)\,\hat{\vec{L}}\cdot\hat{\vec{S}}, \qquad \text{con} \qquad f(r) = \left(\frac{e}{mc}\right)^2 \cdot \frac{1}{r^3}$$

$$\phi_{n,l,m}(\bar{r}) = R_{nl}(r)\,Y_{lm}(\theta,\varphi)$$

$$\left(\langle 2,1,m| \otimes \langle \pm|\right) f(r)\,\hat{\vec{L}}\cdot\hat{\vec{S}} \left(|2,1,m'\rangle \otimes |\pm\rangle\right) =$$

$$= \underbrace{\left[\int_0^\infty dr.\, r^2 f(r)\,|R_{21}(r)|^2\right]}_{= \frac{mc^2}{48\hbar^2}\alpha^4} \cdot \underbrace{\left(\langle l=1,m| \otimes \langle \pm|\right) \hat{\vec{L}}\cdot\hat{\vec{S}} \left(|l=1,m'\rangle \otimes |\pm\rangle\right)}_{\text{La matriz asociada no va a ser diagonal}}$$

$$\hat{\vec{L}}\cdot\hat{\vec{S}} = \frac{1}{2}\left(\hat{\vec{J}}^2 - \hat{\vec{L}}^2 - \hat{\vec{S}}^2\right) \qquad \left(\hat{\vec{J}} \equiv \hat{\vec{L}} + \hat{\vec{S}}\right)$$

es diagonal en la $\underbrace{\text{base de autoestados}}$ comunes a $\hat{\vec{J}}^2, \hat{J}_z, \hat{\vec{L}}^2, \hat{\vec{S}}^2$.

$$\downarrow$$

$$|l=1, s=\tfrac{1}{2}; j, m_j\rangle$$

$$\left.\begin{array}{l} l=1 \\ s=1/2 \end{array}\right\} \Rightarrow \quad j = \frac{1}{2}, \frac{3}{2}$$

A $\hat{L}.\hat{S}$ sólo le importan los valores de j y no los de m_j.

Escribimos $\hat{W}_{so}$ en la base dada por estos estados:

$$\left| l=1,\ s=1/2,\ j=3/2,\ m_j = \begin{Bmatrix} 3/2 \\ 1/2 \\ -1/2 \\ -3/2 \end{Bmatrix} \right\rangle$$

$$\left| l=1,\ s=1/2,\ j=1/2,\ m_j = \begin{Bmatrix} 1/2 \\ -1/2 \end{Bmatrix} \right\rangle$$

$$\langle \hat{L}.\hat{S} \rangle_{j=3/2} = \frac{\hbar^2}{2} \cdot \Big[\underbrace{\tfrac{3}{2}\left(\tfrac{3}{2}+1\right)}_{j(j+1)} - \underbrace{1(1+1)}_{l(l+1)} - \underbrace{\tfrac{1}{2}\left(\tfrac{1}{2}+1\right)}_{s(s+1)} \Big] = \frac{\hbar^2}{2}$$

$$\langle \hat{L}.\hat{S} \rangle_{j=1/2} = \frac{\hbar^2}{2} \cdot \Big[\tfrac{1}{2}\left(\tfrac{1}{2}+1\right) - 1(1+1) - \tfrac{1}{2}\left(\tfrac{1}{2}+1\right) \Big] = -\hbar^2$$

$$\therefore \boxed{ [\hat{W}_{so}]_{2p} = \frac{mc^2}{48h^2} \alpha^4 \left(\begin{array}{c|c} -\hbar^2 . \mathbb{1}_{2\times 2} & 0 \\ \hline 0 & \frac{\hbar^2}{2} \mathbb{1}_{4\times 4} \end{array} \right) }$$

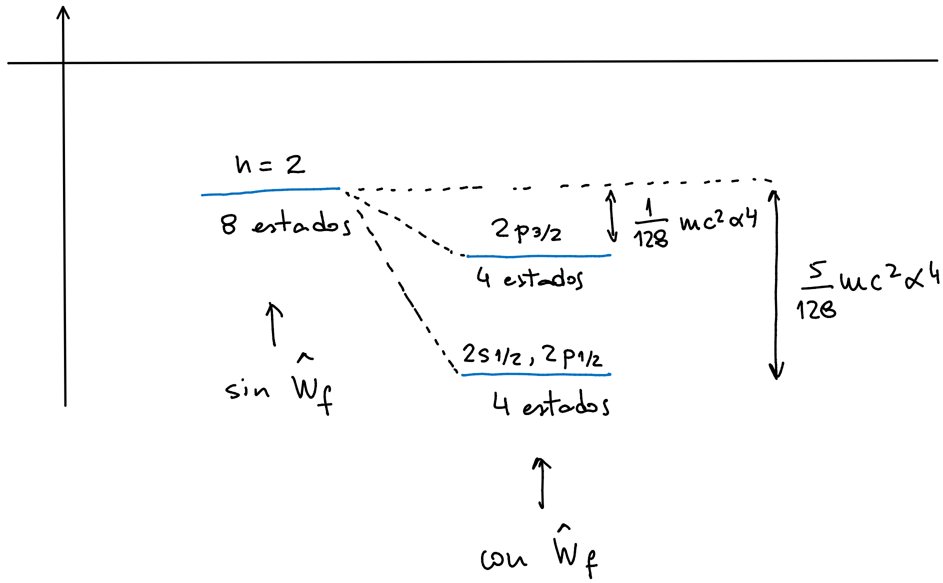
base acoplada o de suma de mom. angular

$$\boxed{ [\hat{W}_f]_{2p} = [\hat{W}_{mv}]_{2p} + [\hat{W}_D]_{2p} + [\hat{W}_{so}]_{2p} }$$

Correcciones a la energía

$$2p \to 2p_{3/2} \longrightarrow -\frac{mc^2}{128}\alpha^4$$

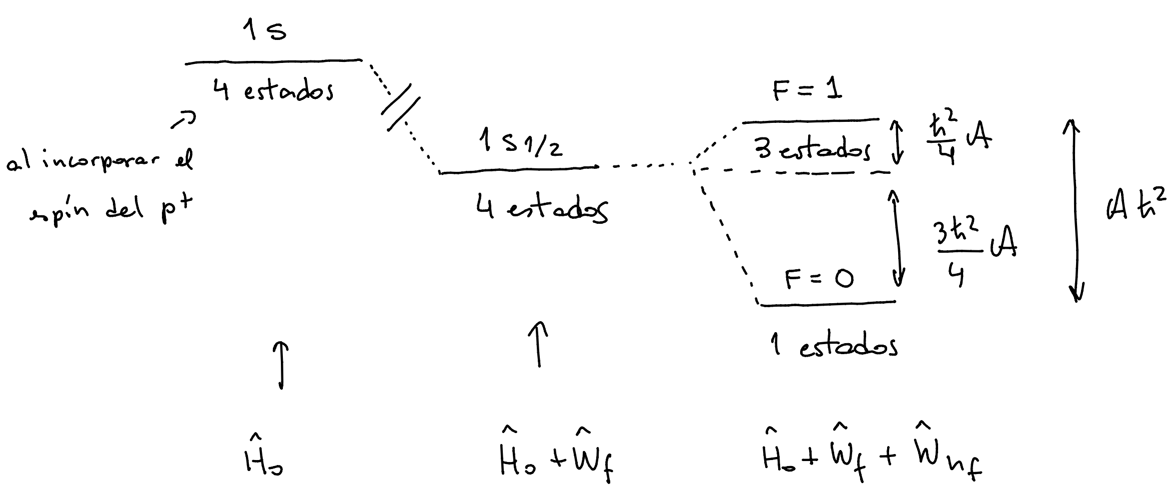
$$2p \to 2p_{1/2} \longrightarrow -\frac{5mc^2}{128}\alpha^4$$



7.3.3. Estructura hiperfina del átomo de Hidrógeno

El protón también tiene espín.

$$\hat{\vec{F}} = \hat{\vec{S}}_{e-} + \hat{\vec{S}}_{p+}$$



$$\frac{A\hbar^2}{2\pi} = 1420405751{,}768 \pm 0{,}001 \text{ Hz}$$

Los átomos de H en el espacio interestelar se detectan en radioastronomía por la radiación que emiten al decaer espontáneamente de $F=1$ a $F=0$ $(\lambda \simeq 21\,\text{cm})$.