F 789 – Mecânica Quântica II

1º Semestre de 2023
15/05/2023
Aula 19

Aula passada

Hamiltoniano do átomo de hidrogênio analisado no cap. 6:

$$H_0 = \frac{\mathbf{P}^2}{2m} + V(R) \qquad V(R) = -\frac{q^2}{4\pi\epsilon_0}\frac{1}{R} = -\frac{e^2}{R}$$

Velocidades típicas: $\frac{v}{c} \sim \alpha \equiv \frac{e^2}{\hbar c} = \frac{1}{137} \approx 10^{-2}$

Correções relativísticas da ordem de $\alpha^2 H_0$

$$W_f = W_{mv} + W_{SO} + W_D$$

$$W_{mv} = -\frac{\mathbf{P}^4}{8m^3c^2}$$ (correção à energia cinética)

$$W_{SO} = \frac{1}{2m^2c^2}\frac{1}{R}\frac{dV(R)}{dR}\mathbf{L}\cdot\mathbf{S} = \frac{e^2}{2m^2c^2}\frac{1}{R^3}\mathbf{L}\cdot\mathbf{S}$$ (interação spin-órbita)

$$W_D = \frac{\hbar^2}{8m^2c^2}\nabla^2 V(R) = \frac{\pi e^2\hbar^2}{2m^2c^2}\delta^{(3)}(\mathbf{R})$$ (interação de contato de Darwin)

Aula passada

Efeitos do spin do próton **I**:

$$\mathbf{M}_I = g_p \frac{\mu_n}{\hbar}\mathbf{I}$$

$$g_p \approx 5.585$$

$$\mu_n = \frac{q\hbar}{2M_p}$$

$$\mu_B = \frac{q\hbar}{2m_e}$$

$$M_p \approx 1800\ m$$

Hamiltoniano hiperfino: $W_{hf} = W_{hf}^{(1)} + W_{hf}^{(2)} + W_{hf}^{(3)}$

$$W_{hf}^{(1)} = \frac{\mu_0}{4\pi}\frac{q}{mR^3}\mathbf{L}\cdot\mathbf{M}_I$$

(campo magnético criado pelo movimento orbital do elétron atuando no momento magnético do próton)

$$W_{hf}^{(2)} = -\frac{\mu_0}{4\pi}\frac{1}{R^3}\left[3\left(\mathbf{M}\cdot\hat{\mathbf{n}}\right)\left(\mathbf{M}_I\cdot\hat{\mathbf{n}}\right) - \mathbf{M}\cdot\mathbf{M}_I\right]$$

(campo magnético criado pelo dipolo magnético do spin do elétron atuando no momento magnético do próton)

$$W_{hf}^{(3)} = -\frac{2\mu_0}{3}\mathbf{M}\cdot\mathbf{M}_I\delta^{(3)}\left(\mathbf{R}\right)$$

(interação do dipolo magnético do elétron com o campo magnético dentro do próton)

$$\boxed{W_{hf} \sim \frac{m}{M_p}W_f \approx 10^{-3}W_f}$$

Estrutura fina do nível n=2

$$W_{mv} = -\frac{\mathbf{P}^4}{8m^3c^2}$$

$$W_{SO} = \frac{1}{2m^2c^2}\frac{1}{R}\frac{dV(R)}{dR}\mathbf{L}\cdot\mathbf{S} = \frac{e^2}{2m^2c^2}\frac{1}{R^3}\mathbf{L}\cdot\mathbf{S}$$

$$W_D = \frac{\hbar^2}{8m^2c^2}\nabla^2 V(R) = \frac{\pi e^2\hbar^2}{2m^2c^2}\delta^{(3)}(\mathbf{R})$$

NÍVEL $n=2$: $\ell=0, m=0, m_s=\pm\frac{1}{2}$

$\ell=1, m=0,\pm1, m_s=\pm\frac{1}{2}$

DEGENERESCÊNCIA TOTAL: $2+6=8$

$$E(n=2) = -\frac{E_I}{n^2} = -\frac{E_I}{4} = -\frac{13{,}6}{4}\,eV$$

TEORIA DE PERTURBAÇÃO DEGENERADA.

CALCULAR A MATRIZ DE W_f NO SUB-ESPAÇO DE $n=2$

ESTADOS: $|\ell, m, m_s\rangle \rightarrow |\ell=0, m=0, m_s=\pm\frac{1}{2}\rangle$

$|\ell=1, m=0,\pm1; m_s=\pm 1/2\rangle$

W_f comuta com L^2

- $[W_{mv}, \vec{L}^2] \propto [\vec{p}^4, \vec{L}^2] = \vec{p}^2[\vec{p}^2, \vec{L}^2] + [\vec{p}^2, \vec{L}^2]\vec{p}^2 = 0$

DO ÁTOMO DE HIDROGÊNIO $[H_0, L^2] = 0 \Rightarrow [p^2, L^2] = 0$

- $[W_D, \vec{L}^2] \propto [\delta(R), L^2] = 0$, POIS L^2 SÓ ATUA NOS ÂNGULOS ESFÉRICOS (θ, ϕ).

- $[W_{SO}, \vec{L}^2] \propto [f(R)\vec{L}\cdot\vec{S}, \vec{L}^2] = f(R)[\vec{L}\cdot\vec{S}, \vec{L}^2]$

$[\vec{L}\cdot\vec{S}, \vec{L}^2] = \sum_{i=1}^{3}[L_i S_i, \vec{L}^2] = \sum_i \overbrace{[L_i, \vec{L}^2]}^{0} S_i = 0$

$\Rightarrow \boxed{[W_f, \vec{L}^2] = 0}$

SE $[A, B] = 0$, ENTÃO NA BASE DE AUTO-ESTADOS DE B

$\langle b_i | A | b_j \rangle = 0$ SE $b_i \neq b_j$

$\Rightarrow \langle \ell = 0, \ldots | W_f | \ell = 1, \ldots \rangle = 0$

W_f é bloco-diagonal

$$(W_f)_{n=2} = \begin{array}{cc} & \begin{array}{cc} \quad 2s \quad & \qquad 2p \qquad \end{array} \\ \begin{array}{c} 2s \\ \\ 2p \end{array} & \left(\begin{array}{c|c} \begin{matrix} \cdot\cdot & \cdot\cdot \\ \cdot\cdot & \cdot\cdot \end{matrix} & 0 \\ \hline 0 & \begin{matrix} \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot \\ \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot \\ \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot \\ \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot \\ \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot \\ \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot \end{matrix} \end{array}\right) \end{array}$$

PRECISAMOS AGORA DE W_f NOS SUBESPAÇOS

$2s$ E $2p$

W_f no sub-espaço $2s$

$\Rightarrow |\ell=0, m=0, m_s=\pm 1/2\rangle \longrightarrow R_{2,0}(r)\, Y_{00}(\theta,\phi)$

$W_{mv} \propto \vec{p}^{\,4}$ E $W_D \propto \delta(R)$ SÃO PURAMENTE ORBITAIS:

$$\langle m_s' | W_{mv} | m_s\rangle_{2s} = \langle \ell=0, m=0 | -\frac{p^4}{8m^3c^2} | \ell=0, m=0\rangle \delta_{m_s', m_s}$$

$$= -\frac{13}{128} mc^2\alpha^4\, \delta_{m_s', m_s}$$ (COMPLEMENTO B_{XII})

$$\langle m_s' | W_D | m_s\rangle_{2s} = \frac{1}{16} mc^2\alpha^4\, \delta_{m_s', m_s}$$

$$\langle \ell=0, m=0, m_s' | f(R)\, \vec{L}\cdot\vec{S} | \ell=0, m=0, m_s\rangle = 0$$

PORQUE $L_i | \ell=0, m=0, m_s\rangle = 0$

$$\langle m_s' | W_f | m_s\rangle_{2s} = -\frac{5}{128} mc^2\alpha^4\, \delta_{m_s', m_s}$$

W_f no sub-espaço $2p$

$|\ell=1, m, m_s\rangle \qquad m = 0, \pm 1 \quad \text{E} \quad m_s = \pm 1/2$

- $[W_{m,v}, L_i] = 0 \quad [W_D, L_i] = 0 \qquad i = x, y, z$

L_i SÓ ATUAM NOS ÂNGULOS (θ, ϕ) E $W_D \propto \delta(R)$

JÁ $W_{mv} \propto \vec{P}^2 \vec{P}^2$ E $\vec{P}^2 \propto \nabla^2 = \frac{1}{r}\frac{d^2}{dr^2}[r\ ] + \frac{L^2}{\hbar^2 r^2}$

COMO $[L_i, L^2] = 0$ E $[L_i, f(r)] = 0 \Rightarrow [L_i, \nabla^2] = 0$

$\Rightarrow [L_i, \vec{P}^2] = 0 \Rightarrow [L_i, \vec{P}^2\vec{P}^2] = 0$

ALÉM DISSO, $[W_{mv}, S_i] = 0 = [W_D, S_i] \quad i = x, y, z$

SEGUE QUE (VER NOTAS):

$$\langle m', m_s' | \begin{Bmatrix} W_{mv} \\ W_D \end{Bmatrix} | m, m_s\rangle = \begin{Bmatrix} C_{mv} \\ C_D \end{Bmatrix} \delta_{m',m}\, \delta_{m_s', m_s}$$

ONDE :

$$C_{mv} = -\frac{7}{384} mc^2\alpha^4$$

$$C_D = 0 \quad (\text{JÁ QUE } \propto R_{2,\ell=1}(0) = 0)$$

W_{SO} no sub-espaço $2p$

$$W_{SO} = \frac{e^2}{2m^2c^2}\frac{1}{R^3}\vec{L}\cdot\vec{S}$$

$|\ell=1, m, m_s\rangle \rightarrow R_{2,1}(r)Y_{1m}(\theta,\phi)$

PARTE RADIAL: $\xi_{2p} = \dfrac{e^2}{2m^2c^2}\displaystyle\int_0^\infty r^2 dr \frac{|R_{2,1}(r)|^2}{r^3} = \frac{mc^2\alpha^4}{48\hbar^2}$

$$\langle m', m_s' | W_{SO} | m, m_s\rangle = \xi_{2p}\langle m', m_s' | \vec{L}\cdot\vec{S} | m, m_s\rangle$$

BASE "NÃO SOMADA": $|\ell=1, s=1/2; m, m_s\rangle$

MUDAR PARA A BASE "SOMADA": $|\ell=1, s=1/2, j, m_j\rangle$

ONDE $j = \frac{1}{2}$ OU $\frac{3}{2}$

USANDO: $\vec{J} = \vec{L}+\vec{S} \Rightarrow \vec{J}^2 = (\vec{L}^2+\vec{S}^2+2\vec{L}\cdot\vec{S}) \Rightarrow \vec{L}\cdot\vec{S} = \frac{1}{2}\left[\vec{J}^2 - \vec{L}^2 - \vec{S}^2\right]$

$$\Rightarrow \langle j', m_j' | \vec{L}\cdot\vec{S} | j, m_j \rangle = \frac{1}{2} \langle j', m_j' | [\vec{J}^2 - \vec{L}^2 - \vec{S}^2] | j, m_j \rangle$$

$$= \frac{\hbar^2}{2} [j(j+1) - l(l+1) - s(s+1)] \delta_{j,j'} \delta_{m_j', m_j}$$

$$= \frac{\hbar^2}{2} [j(j+1) - 2 - \frac{3}{4}] \delta_{j,j'} \delta_{m_j', m_j}$$

$$= \frac{\hbar^2}{2} [j(j+1) - \frac{11}{4}] \delta_{j,j'} \delta_{m_j', m_j}$$

$j = 1/2$: $\langle j=1/2, m_j' | W_{so} | j=1/2, m_j \rangle = -\frac{mc^2}{48} \alpha^4 \delta_{m_j', m_j}$

$j = 3/2$: $\langle j=3/2, m_j' | W_{so} | j=3/2, m_j \rangle = \frac{mc^2}{96} \alpha^4 \delta_{m_j', m_j}$

$j = 1/2$: $W_{mv} + W_{so} = -\underbrace{\left(\frac{7}{384} + \frac{1}{48}\right)}_{\frac{5}{128}} mc^2 \alpha^4 \delta_{m_j', m_j}$

A estrutura fina do nível $n=2$

$2s_{1/2}$

$\ell=0,\ s=1/2 \Rightarrow j=1/2$

$2p_{1/2}$

$$W_f^{(2)} = mc^2\alpha^4 \left(\begin{array}{cc|cc|cccc}
-\frac{5}{128} & 0 & & & & & & \\
0 & -\frac{5}{128} & \multicolumn{2}{c|}{0} & \multicolumn{4}{c}{0} \\
\hline
& & -\frac{5}{128} & 0 & & & & \\
\multicolumn{2}{c|}{0} & 0 & -\frac{5}{128} & \multicolumn{4}{c}{0} \\
\hline
& & & & -\frac{1}{128} & 0 & 0 & 0 \\
\multicolumn{2}{c|}{0} & \multicolumn{2}{c|}{0} & 0 & -\frac{1}{128} & 0 & 0 \\
& & & & 0 & 0 & -\frac{1}{128} & 0 \\
& & & & 0 & 0 & 0 & -\frac{1}{128}
\end{array}\right)$$

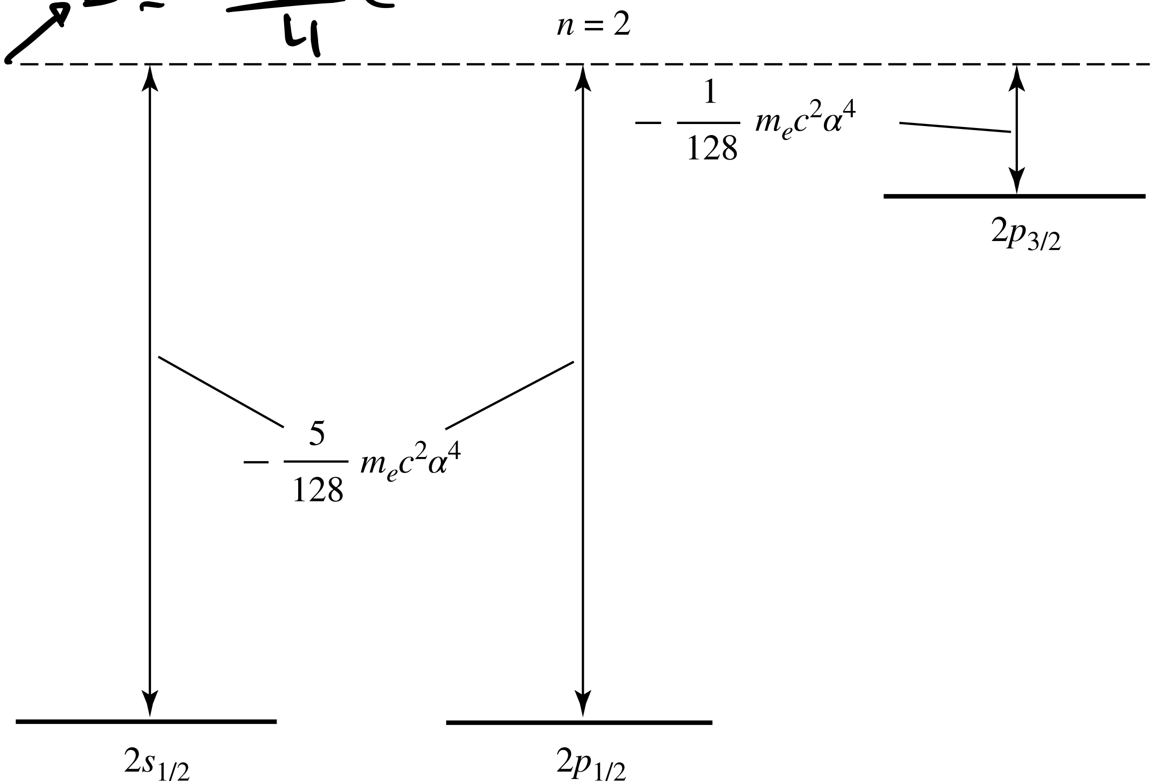
$2p_{3/2}$

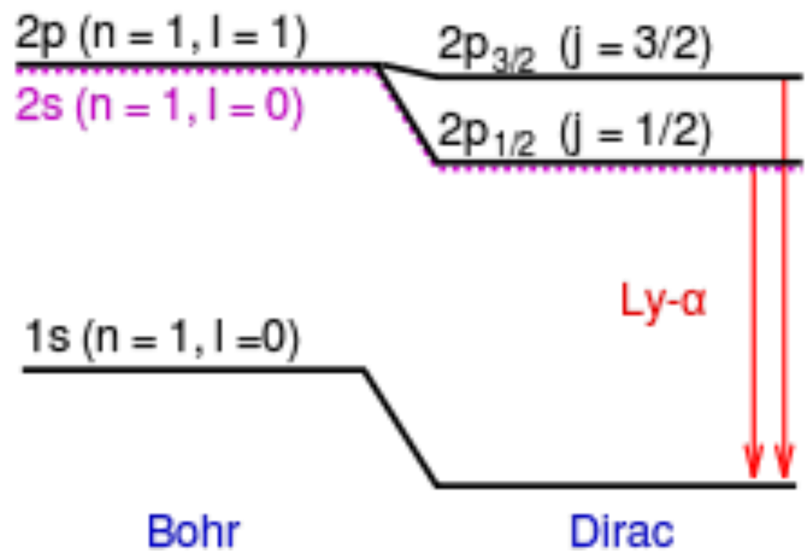
$$\left.\begin{array}{l} 2S_{j=1/2} \\ \\ 2P_{j=1/2,\,3/2} \end{array}\right\} \text{NOTAÇÃO ESPECTROSCÓPICA}$$

$$j=\frac{3}{2}:\ \left(-\frac{7}{384}+\frac{1}{96}\right)mc^2\alpha^4 = -\frac{1}{128}mc^2\alpha^4$$

A estrutura fina do nível $n=2$

$E^0 = -\frac{13.6}{4}$ eV





A solução exata de Dirac

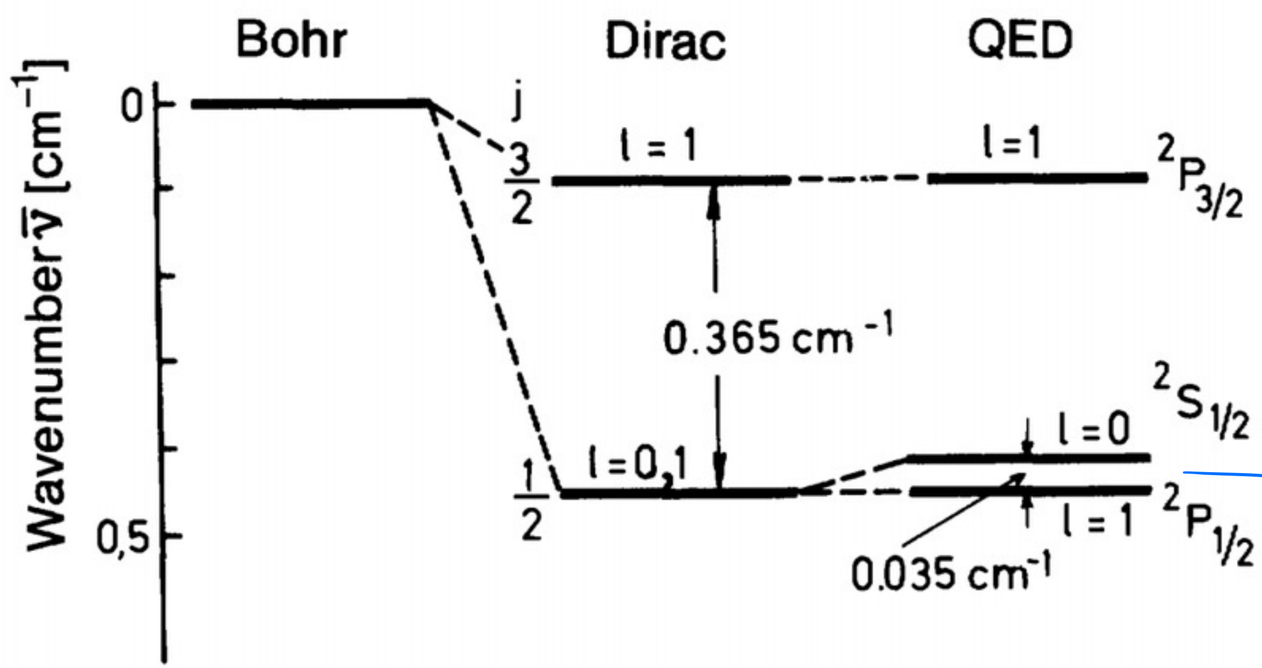
$$\boxed{E_{n,j}^{\text{Dirac}} = mc^2\left[1+\alpha^2\left(n-j-\frac{1}{2}+\sqrt{\left(j+\frac{1}{2}\right)^2-\alpha^2}\right)^{-2}\right]^{-1/2}}$$

Expandindo em potências de α^2:

$$E_{n,j}^{\text{Dirac}} = mc^2 \underbrace{-\frac{1}{2}\frac{mc^2\alpha^2}{n^2}}_{-\frac{E_I}{n^2}} - \frac{mc^2}{2n^4}\left(\frac{n}{j+\frac{1}{2}}-\frac{3}{4}\right)\alpha^4 + \mathcal{O}\left(\alpha^6\right)$$

$E_{2S_{1/2}} = E_{2P_{1/2}}$ É MANTIDA EM TODAS AS ORDENS DE α^2

O “Lamb shift”



EFEITO DE ELETRODINÂMICA QUÂNTICA:

DESLOCAMENTO LAMB

"LAMB SHIFT"