

Formulari de Física Atòmica i Radiació

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I. ÀTOMS D'UN ELECTRÓ

$$\mu = \frac{m_e M}{m_e + M} \quad \mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1 \quad \mathbf{R} = \frac{M \mathbf{r}_1 + m_e \mathbf{r}_2}{M + m_e}$$

Hamiltonià:

$$\mathcal{H} = -\frac{\hbar^2}{2(M + m_e)} \nabla_{\mathbf{R}_{\text{CM}}}^2 - \frac{\hbar^2}{2\mu} \nabla_{\mathbf{r}}^2 + V(r) = \mathcal{H}_{\text{CM}} + \mathcal{H}_{\mathbf{r}}$$

Moment angular orbital:

$$\mathbf{L} = \frac{1}{\hbar} \mathbf{r} \times \mathbf{p} = -i \mathbf{r} \times \nabla \quad [L_i, L_j] = i \epsilon_{ijk} L_k \quad [L^2, L_i] = 0$$

$$L^2 Y_{\ell m} = \ell(\ell + 1) Y_{\ell m} \quad L_z Y_{\ell m} = m Y_{\ell m}$$

$$\langle Y_{\ell' m'} | Y_{\ell m} \rangle = \delta_{\ell \ell'} \delta_{m m'}$$

$$Y_{\ell m}^* = (-1)^m Y_{\ell -m} \quad Y_{\ell m}(\theta, \phi) = (-1)^{\ell} Y_{\ell m}(\pi - \theta, \pi + \phi)$$

Camp central:

$$\psi_{n\ell m}(r, \theta, \phi) = R_{n\ell}(r) Y_{\ell m}(\theta, \phi) \quad P_{n\ell}(r) = r R_{n\ell}(r)$$

$$-\frac{\hbar^2}{2\mu} \frac{d^2 P_{n\ell}(r)}{dr^2} + \left[\frac{\hbar^2 \ell(\ell + 1)}{2\mu r^2} + V(r) \right] P_{n\ell}(r) = E_{n\ell} P_{n\ell}(r)$$

$$\langle P_{n\ell}(r) | P_{n'\ell}(r) \rangle = \delta_{nn'} \quad n_r = n - \ell - 1 \quad E_n = -\frac{Z^2}{2n^2} m_e c^2 \alpha^2$$

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

Teorema del virial:

$$2\langle T \rangle - \langle \mathbf{r} \cdot \nabla V \rangle = 0$$

$$2\langle T \rangle + \langle V \rangle = 0 \quad \langle T \rangle = -E_n \quad \langle V \rangle = 2E_n$$

$$\frac{\langle v^2 \rangle^{1/2}}{c} = \frac{Z}{n} \alpha$$

Àtoms de Rydberg

$$Z_{\text{ef}} = 1 \quad \langle r \rangle_n \approx n^2 a_0 \quad \Delta E_{n, n+1} \approx \frac{2|E_1|}{n^3}$$

Efecte de massa finita del nucli:

$$E_n = -\frac{Z^2}{2n^2} (\mu \alpha^2 c^2) = \frac{\mu}{m_e} E_n(M = \infty)$$

$$a_\mu = \frac{\hbar^2}{\mu e^2} = \frac{m_e}{\mu} a_0 \quad E_\mu = \frac{\mu}{m_e} E_h$$

Efecte de tamany finit del nucli:

$$\Delta E = \frac{Z^4 e^2}{n^3 a_\mu^3} \frac{2}{5} R_N^2 \delta_{\ell, 0} = \frac{Z^4}{n^3} \frac{2}{5} \left(\frac{R_N}{a_\mu} \right)^2 E_\mu \delta_{\ell, 0}$$

Àtoms exòtics:

(i) **Positroni** (e^+, e^-): $\mu = \frac{m_e}{2}$, $a_\mu = 2a_0$

(ii) **Muoni** (μ^+, e^-)

(iii) **Àtoms muònics** ($e^- \leftrightarrow \mu^-$)

(iv) **Àtoms hadrònics** ($e^- \leftrightarrow \text{hadró}^-$)

Moment angular d'spin

$$\mathbf{S} = \frac{\sigma}{2} \quad \chi_{m_s} \equiv |s, m_s\rangle$$

$$S^2 |s, m_s\rangle = s(s + 1) |s, m_s\rangle \quad S_z |s, m_s\rangle = m_s |s, m_s\rangle$$

Moment angular generalitzat

$$J^2 |j, m\rangle = j(j + 1) |j, m\rangle \quad J_z |j, m\rangle = m |j, m\rangle$$

Acoblament de dos moments angulars:

$$J^2 = J_1^2 + J_2^2 + 2\mathbf{J}_1 \cdot \mathbf{J}_2 \quad J_z = J_{1z} + J_{2z}$$

$$m = m_1 + m_2 \quad j = |j_1 - j_2|, \dots, j_1 + j_2 \quad m = -j, \dots, j$$

$$|j_1, j_2, m_1, m_2\rangle \rightarrow |j_1, j_2, j, m\rangle$$

Acoblament de L i S:

$$|\ell, s, m_\ell, m_s\rangle = Y_{\ell m_\ell} \chi_{s m_s}$$

$$[J^2, L_z + S_z] = 0 \quad [J^2, L_z] \neq 0 \quad [J^2, S_z] \neq 0$$

$$|l, s, j, m\rangle \equiv \Omega_{jm}^\ell(\theta, \phi) \quad \langle \Omega_{j'm'}^{\ell'} | \Omega_{jm}^\ell \rangle = \delta_{jj'} \delta_{mm'} \delta_{\ell\ell'}$$

$$\mathbf{L} \cdot \mathbf{S} |j, m\rangle = \frac{1}{2} [j(j + 1) - \ell(\ell + 1) - s(s + 1)] |j, m\rangle$$

Moments dipolars magnètics:

$$\boldsymbol{\mu}_L = -\mu_B \mathbf{L} \quad \boldsymbol{\mu}_S = -g_s \mu_B \mathbf{S} \quad U = -\boldsymbol{\mu} \cdot \mathbf{B}$$

Equació de Pauli

$$\mathcal{H}_P = \frac{1}{2m} \left(\mathbf{p} + \frac{e}{c} \mathbf{A} \right)^2 - e\varphi - \boldsymbol{\mu}_S \cdot \mathbf{B}$$

$$\psi_{n\ell m_\ell m_s}(r, \theta, \phi) = R_{n\ell}(r) Y_{\ell m_\ell}(\theta, \phi) \chi_{s m_s}$$

Estructura fina:

$$\mathcal{H}_D = \boldsymbol{\alpha} \cdot (\mathbf{p}c - q\mathbf{A}) + \beta mc^2 + q\varphi$$

$$\mathcal{H}_m = -\frac{p^4}{8m^3 c^2} \mathbb{I}_2 \quad \mathcal{H}_{SO} = -\frac{e\hbar}{2m^2 c^2} \mathbf{S} \cdot (\nabla\varphi \times \mathbf{p})$$

$$H_{Dw} = -\frac{e\hbar}{2m^2 c^2} \nabla^2 \varphi \mathbb{I}_2 = \frac{\pi \hbar^2 e^2 Z}{2m^2 c} \delta(\mathbf{r}) \mathbb{I}_2$$

Total:

$$\Delta E_{nj} = E_n \left(\frac{Z\alpha}{n} \right)^2 \left(\frac{n}{j + \frac{1}{2}} - \frac{3}{4} \right) < 0$$

$$\left| \frac{\Delta E_{nj}}{E_n} \right| \approx 5 \times 10^{-5} \frac{Z^2}{n^2} \quad j = \ell \pm \frac{1}{2} \quad Z \leq 30$$

Particulars:

$$\Delta E_m = E_n \left(\frac{Z\alpha}{n} \right)^2 \left(\frac{n}{\ell + \frac{1}{2}} - \frac{3}{4} \right)$$

$$\Delta E_{Dw} = -\frac{Z\alpha^2}{n} E_n \delta_{\ell,0}$$

$$\Delta E_{SO} = -E_n \frac{(Z\alpha)^2}{2n(j + \frac{1}{2})(\ell + \frac{1}{2})} \cdot \begin{cases} +1 & j = \ell + \frac{1}{2} \\ 0 & j = 0 \\ -1 & j = \ell - \frac{1}{2} \end{cases}$$

Estructura hiperfina:

$$\boldsymbol{\mu} = g_I \mu_N \mathbf{I} \quad \mathbf{F} = \mathbf{J} + \mathbf{I} \quad F = |j - I|, \dots, j + I$$

$$\Delta E_{\text{hip}} = C \langle \mathbf{J} \cdot \mathbf{I} \rangle = C \frac{1}{2} [F(F+1) - j(j+1) - I(I+1)]$$

$$\Delta E_{F+1} - \Delta E_F = C(F+1)$$

II. ÀTOMS MULTIELECTRÒNICS

$$\mathcal{H} = -\frac{\hbar^2}{2m} \nabla_{\mathbf{R}_0}^2 - \sum_{i=1}^N \frac{\hbar^2}{2m_e} \nabla_{\mathbf{R}_i}^2 - \sum_{i=1}^N \frac{Ze^2}{r_i} + \sum_{i<j} \frac{e^2}{r_{ij}}$$

$$\mathcal{H}_{CM} = -\frac{\hbar^2}{2(M + Nm_e)} \nabla_{\mathbf{R}}^2$$

$$\mathcal{H}_{\text{rel}} = -\frac{\hbar^2}{2\mu} \sum_{i=1}^N \nabla_{\mathbf{r}_i}^2 - \frac{\hbar^2}{2M} \sum_{i<j} \nabla_{\mathbf{r}_i} \cdot \nabla_{\mathbf{r}_j} - \sum_{i=1}^N \frac{Ze^2}{r_i} + \sum_{i<j} \frac{e^2}{r_{ij}}$$

Sistema de partícules idèntiques

$$[T_{ij}, \mathcal{H}] = 0 \quad T_{ij} \psi = \pm \psi$$

$$[\mathcal{H}, P] = 0$$

$$\text{TS: } T_{ij} \psi_S = \psi_S \quad \forall i, j \Leftrightarrow P \psi_S = \psi_S \quad \forall P$$

$$\text{TA: } T_{ij} \psi_A = -\psi_A \quad \forall i, j \Leftrightarrow P \psi_A = (-1)^P \psi_A \quad \forall P$$

$$S_N = \sum_p \frac{p}{N!} = S_N^\dagger = S_N^2 \quad A_N = \sum_p (-1)^p \frac{p}{N!} = A_N^\dagger = A_N^2$$

Fermions sense interacció

$$\mathcal{H}_0 \varphi_i = E_i \varphi_i \Rightarrow E = \sum_i E_i \quad \psi = \prod_i \varphi_i$$

Determinant d'Slater:

$$\psi_A(x_1, \dots, x_N) = \frac{1}{\sqrt{N!}} \sum_p (-1)^p \varphi_1(x_{p1}) \cdots \varphi_N(x_{pN})$$

Model de partícules independents per l'àtom (MPI)

$$\mathcal{H}^{\text{MPI}} = \sum_{i=1}^N \left(-\frac{\hbar^2}{2\mu} \nabla_i^2 + V_{\text{ef}}(r) \right) \quad V_{\text{ef}}(r) = -\frac{Ze^2}{r} + S(r)$$

Potencial de ionització (per un e^- de valència ns^1)

$$I_p = \frac{Z_{\text{ef}}^2}{2n^2} E_h$$

Àtom d'Heli

$$\mathcal{H} \simeq \left(-\frac{\hbar^2}{2m} \nabla_1^2 - \frac{Ze^2}{r_1} \right) + \left(-\frac{\hbar^2}{2\mu} \nabla_2^2 - \frac{Ze^2}{r_2} \right) + \frac{e^2}{r_{12}}$$

Estat fonamental $1s^2$

Sense interacció: $E = E_{n=1} + E_{n=1}$

Teoria de pertorbacions: $\Delta E = \frac{5}{8} Z$

Mètode variacional: $E = Z_{\text{ef}}^2 - 2Z_{\text{ef}}Z + \frac{5}{8}Z_{\text{ef}}$

$$Z_{\text{ef}} = Z - \frac{5}{16}$$

Nivells excitats ($1s, n\ell$)

$$\Psi = \psi_+ \chi_{00} \quad \Psi = \psi_- \chi_{1M_S}$$

$$\psi_{\pm}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}} [u_{1s}(\mathbf{r}_1) u_{n\ell m}(\mathbf{r}_2) \pm u_{n\ell m}(\mathbf{r}_1) u_{1s}(\mathbf{r}_2)]$$

Sense interacció: $E = E_{1s} + E_{n\ell} = -\frac{Z^2}{2} \left(1 + \frac{1}{n^2} \right)$

Teoria de pertorbacions: $\Delta E = J \pm K$

$$J = \iint |\varphi_{100}(\mathbf{r}_1)|^2 \frac{e^2}{r_{12}} |\varphi_{n\ell m_L}(\mathbf{r}_2)|^2 d\mathbf{r}_1 d\mathbf{r}_2$$

$$K = \iint \varphi_{100}^*(\mathbf{r}_1) \varphi_{n\ell m_L}^*(\mathbf{r}_2) \frac{e^2}{r_{12}} \varphi_{100}(\mathbf{r}_2) \varphi_{n\ell m_L}(\mathbf{r}_1) d\mathbf{r}_1 d\mathbf{r}_2$$

Mètode variacional: $E = I^{(Z_{1s})} + I^{(Z_{n\ell})} + J + K$

Degeneració

$$D(n\ell; q) = \binom{2(2\ell+1)}{q} = \frac{[2(2\ell+1)]!}{[2(2\ell+1)-q]! q!}$$

$$^{2S+1}L \Rightarrow D = \sum_{LS} (2L+1)(2S+1)$$

$$^{2S+1}L_J \Rightarrow D = 2J+1$$

Acoblament LS (o acoblament de Russell-Sanders)

$$\Delta E_{so} = \frac{1}{2} T_{\alpha}(L, S) [J(J+1) - L(L+1) - S(S+1)]$$

Capa menys que semiplena: $T_{\alpha} > 0$

Capa més que semiplena: $T_{\alpha} < 0$

Capa semiplena $T_\alpha = 0$

Regla de l'interval de Landé:

$$E(J+1) - E(J) = T_\alpha(J+1) \Rightarrow \frac{E(J+1) - E(J)}{E(J) - E(J-1)} = \frac{J+1}{J}$$

Paritat

$$\text{Paritat} = (-1)^{\sum_i l_i}$$

III. ÀTOMS EN CAMPS EXTERNES (Efecte Zeeman)

$$\mathcal{H} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{Ze^2}{r} + \mu_B B(L_z + 2S_z) + \frac{\hbar^2}{2m_e^2 c^2} \frac{Ze^2}{r^3} \mathbf{L} \cdot \mathbf{S}$$

Situació en què $\mathcal{H}_B \gg \mathcal{H}_{SO}$

Zeeman Normal

$$E = E_n + \Delta E_{m_\ell + 2m_s} = E_n + \mu_B B(m_\ell + 2m_s)$$

Paschen-Back

$$E_{n\ell m_\ell m_s} = E_n + \Delta E_{m_\ell + 2m_s} - E_n \frac{Z^2 \alpha^2}{n} \frac{m_\ell m_s}{\ell(\ell + \frac{1}{2})(\ell + 1)} (1 - \delta_{\ell 0})$$

Situació en què $\mathcal{H}_B \ll \mathcal{H}_{SO}$

Sense pertorbar:

$$\Delta E_{SO} = -E_n \frac{(Z\alpha)^2}{2n(j + \frac{1}{2})(\ell + \frac{1}{2})} \cdot \begin{cases} +1 & j = \ell + \frac{1}{2} \\ 0 & j = 0 \\ -1 & j = \ell - \frac{1}{2} \end{cases}$$

Efecte Zeeman Anòmal:

$$\Delta E_B = \mu_B B m_j \left(\frac{2j+1}{2\ell+1} \right) = \mu_B B g_j m_j$$

Fórmula de Landé:

$$g_j = g_\ell \frac{j(j+1) + \ell(\ell+1) - s(s+1)}{2j(j+1)} + g_s \frac{j(j+1) + s(s+1) - \ell(\ell+1)}{2j(j+1)}$$

Àtoms multieletrònics

$$\mathcal{H}'_B = \mu_B B(L_z + 2S_z)$$

Camp B intens:

- Z.N.: $\Delta E_B = \mu_B B(M_L + 2M_S)$
- P.B.: $\Delta E_B = \mu_B B(M_L + 2M_S) + \Delta E_{SO}(B \neq 0)$

Camp B feble:

$$\Delta E_B = g_J \mu_B B M_J$$

Fórmula de Landé:

$$g_J = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$$

IV. RADIACIÓ

Regles de selecció (dipolar elèctric):

Estructura grossa:

$$\Delta \ell = \pm 1, \quad \Delta m_\ell = 0, \pm 1 \quad \Delta m_s = 0$$

Estructura fina:

$$\Delta \ell = \pm 1, \quad \Delta j = 0, \pm 1 \quad \Delta m_j = 0, \pm 1$$

Multieletrònics:

$$\Delta J = 0, \pm 1, \quad \Delta M_J = 0, \pm 1 \quad \pi_f = -\pi_i$$

A. CONSTANTS I UNITATS

$$\alpha = \frac{e^2}{\hbar c} = \frac{e^2}{4\pi\epsilon_0 \hbar c} = \frac{1}{137,036}$$

$$m_e c^2 \alpha^2 = \frac{e^2}{a_0} = \frac{m_e e^4}{\hbar^2} = 27,2114 \text{ eV} \equiv E_h$$

$$a_0 = \frac{\hbar^2}{m_e e^2} = 5,2918 \times 10^{-11} \text{ m}$$

$$\mu_B = \frac{e\hbar}{2m_e c} = \frac{1}{2c} = \frac{\alpha}{2}$$

$$\mu_N = \frac{e\hbar}{2m_p c} = \frac{\mu_B}{1836,15}$$

$$1 \text{ cm}^{-1} = 1,23984 \times 10^{-4} \text{ eV}$$

$$1 \text{ eV} = 8065,54 \text{ cm}^{-1}$$

$$1 \text{ cm}^{-1} = 2,988 \times 10^4 \text{ MHz}$$

B. TEORIA DE PERTORBACIONS

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}' \quad E \approx E_n + \Delta E$$

Sense degeneració: $\Delta E = \langle \psi_0 | \mathcal{H}' | \psi_0 \rangle$

Amb degeneració: $\Delta E = \langle \psi_{0\beta} | \mathcal{H}' | \psi_{0\alpha} \rangle$

C. MÈTODE VARIACIONAL

$$H |\psi_n\rangle = E_n |\psi_n\rangle \quad |\phi\rangle = |\psi_n\rangle \quad E_0 \leq E[\phi] = \frac{\langle \phi | H | \phi \rangle}{\langle \phi | \phi \rangle}$$

$$\delta E[\phi] = 0$$