

El Hamiltoniano de estructura fina

$$H_f = -\frac{P^4}{8m^3c^2} + \frac{e^2}{2m^2c^2} \frac{1}{R^3} \mathbf{L} \cdot \mathbf{S} + \frac{\pi e^2 \hbar^2}{2m^2c^2} \delta(\mathbf{R})$$

El Hamiltoniano de estructura hiperfina

El potencial y campo creado por el dipolo magnético μ_p del protón (Jackson 5.64):

$$\mathbf{A}_p(\mathbf{r}) = \frac{\boldsymbol{\mu}_p \times \mathbf{r}}{r^3} \quad \mathbf{B}_p(\mathbf{r}) = \nabla \times \mathbf{A}_p = \left[\frac{3\mathbf{r}(\mathbf{r} \cdot \boldsymbol{\mu}_p)}{r^5} - \frac{\boldsymbol{\mu}_p}{r^3} \right] + \frac{8\pi}{3} \boldsymbol{\mu}_p \delta(\mathbf{r})$$

El hamiltoniano del electrón en presencia de \mathbf{A}_p y \mathbf{B}_p :

$$H = \frac{1}{2m} (\mathbf{P} - \frac{q_e}{c} \mathbf{A}_p)^2 - \boldsymbol{\mu}_e \cdot \mathbf{B}_p$$

$$\begin{aligned} (\mathbf{P} - \frac{q_e}{c} \mathbf{A}_p)^2 &= P^2 - \frac{q_e}{c} (\mathbf{P} \cdot \mathbf{A}_p + \mathbf{A}_p \cdot \mathbf{P}) + \frac{q_e^2}{c^2} A_p^2 \\ &= P^2 - \frac{q_e}{c} [\mathbf{P} \cdot (\boldsymbol{\mu}_p \times \mathbf{R}) + (\boldsymbol{\mu}_p \times \mathbf{R}) \cdot \mathbf{P}] \frac{1}{R^3} = P^2 - \frac{2q_e}{c} \frac{\boldsymbol{\mu}_p \cdot \mathbf{L}}{R^3} \end{aligned}$$

donde $\mathbf{P} \cdot (\boldsymbol{\mu}_p \times \mathbf{R}) = -\mathbf{P} \cdot (\mathbf{R} \times \boldsymbol{\mu}_p) = -(\mathbf{P} \times \mathbf{R}) \cdot \boldsymbol{\mu}_p = (\mathbf{R} \times \mathbf{P}) \cdot \boldsymbol{\mu}_p = \boldsymbol{\mu}_p \cdot \mathbf{L}$

El hamiltoniano hiperfino describe la interacción de q_e y $\boldsymbol{\mu}_e$ del electrón con $\boldsymbol{\mu}_p$:

$$H_{\text{hf}} = -\frac{q_e}{mc R^3} \boldsymbol{\mu}_p \cdot \mathbf{L} - \left[\frac{3(\mathbf{R} \cdot \boldsymbol{\mu}_e)(\mathbf{R} \cdot \boldsymbol{\mu}_p)}{R^5} - \frac{\boldsymbol{\mu}_e \cdot \boldsymbol{\mu}_p}{R^3} \right] - \frac{8\pi}{3} \boldsymbol{\mu}_e \cdot \boldsymbol{\mu}_p \delta(\mathbf{R})$$

Representación de interacción

Ecuación de Schrödinger en presencia de una “perturbación”:

$$i\hbar \frac{d|\psi, t\rangle}{dt} = (H_0 + V(t)) |\psi, t\rangle$$

Transformamos kets y operadores via $U(t) = e^{\frac{i}{\hbar}H_0t}$:

$$|\psi', t\rangle = U(t)|\psi, t\rangle \quad V'(t) = U(t) V(t) U^\dagger(t)$$

Evolución de kets:

$$\begin{aligned} i\hbar \frac{d|\psi', t\rangle}{dt} &= i\hbar \frac{dU(t)}{dt} |\psi, t\rangle + U(t) i\hbar \frac{d|\psi, t\rangle}{dt} \\ &= -H_0 U(t) |\psi, t\rangle + U(t)(H_0 + V(t)) |\psi, t\rangle \\ &= U(t) V(t) |\psi, t\rangle = U(t) V(t) U^\dagger(t) U(t) |\psi, t\rangle \end{aligned}$$

$$i\hbar \frac{d|\psi', t\rangle}{dt} = V'(t)|\psi', t\rangle$$

Evolución de operadores:

$$A'(t) = U(t) A(t) U^\dagger(t) \quad \longrightarrow \quad \frac{dA'}{dt} = \frac{1}{i\hbar} [A'(t), H_0] + \frac{\partial A'}{\partial t}$$

El operador evolución en la representación de interacción

Remplazando $|\psi', t\rangle = T'(t) |\psi', 0\rangle$ en $i\hbar \frac{d|\psi', t\rangle}{dt} = V'(t)|\psi', t\rangle$:

$$\boxed{i\hbar \frac{dT'}{dt} = V'(t) T'(t)} \quad \longrightarrow \quad T'(t) = 1 - \frac{i}{\hbar} \int_0^t V'(t_1) T'(t_1) dt_1$$

Solución iterativa:

$$T'(t) = 1 + \left(-\frac{i}{\hbar}\right) \int_0^t dt_1 V'(t_1) T'(t_1)$$

$$T'(t) = 1 + \left(-\frac{i}{\hbar}\right) \int_0^t dt_1 V'(t_1) + \left(-\frac{i}{\hbar}\right)^2 \int_0^t dt_1 \int_0^{t_1} dt_2 V'(t_1) V'(t_2) T'(t_2)$$

$$T'(t) = 1 + \left(-\frac{i}{\hbar}\right) \int_0^t dt_1 V'(t_1) + \left(-\frac{i}{\hbar}\right)^2 \int_0^t dt_1 \int_0^{t_1} dt_2 V'(t_1) V'(t_2) + \left(-\frac{i}{\hbar}\right)^3 \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 V'(t_1) V'(t_2) V'(t_3) T'(t_3)$$

$$T'(t) = 1 + \left(-\frac{i}{\hbar}\right) \int_0^t dt_1 V'(t_1) + \left(-\frac{i}{\hbar}\right)^2 \int_0^t dt_1 \int_0^{t_1} dt_2 V'(t_1) V'(t_2) + \left(-\frac{i}{\hbar}\right)^3 \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 V'(t_1) V'(t_2) V'(t_3) + \dots$$

$$\text{Formalmente: } T'(t) = \mathcal{T} \left[e^{-\frac{i}{\hbar} \int_0^t V(t_1) dt_1} \right] \quad \text{con} \quad \mathcal{T} [A(t_1) B(t_2)] = \begin{cases} A(t_1) B(t_2) & t_1 \geq t_2 \\ B(t_2) A(t_1) & t_1 < t_2 \end{cases}$$

Transiciones a primer orden entre autoestados de H_0

$$P_{if}(t) = |\langle f | T'(t) | i \rangle|^2 \quad \text{con} \quad T'(t) = 1 - \frac{i}{\hbar} \int_0^t V'(t_1) dt_1$$

$$\langle f | T'(t) | i \rangle = -\frac{i}{\hbar} \int_0^t \langle f | V'(t_1) | i \rangle dt_1 = -\frac{i}{\hbar} \int_0^t \langle f | V(t_1) | i \rangle e^{i\omega_{fi}t_1} dt_1 \quad \text{con} \quad \omega_{fi} \equiv \frac{E_f - E_i}{\hbar}$$

pues $\langle f | V'(t) | i \rangle = \langle f | e^{\frac{i}{\hbar}H_0t} V(t) e^{-\frac{i}{\hbar}H_0t} | i \rangle = \langle f | e^{\frac{i}{\hbar}E_f t} V(t) e^{-\frac{i}{\hbar}E_i t} | i \rangle = \langle f | V(t) | i \rangle e^{i\omega_{fi}t}$

$$P_{if}(t) = \frac{1}{\hbar^2} \left| \int_0^t \langle f | V(t') | i \rangle e^{i\omega_{fi}t'} dt' \right|^2$$

Perturbación sinusoidal

$$V(t) = V \cos \omega t = V \frac{1}{2} (e^{+i\omega t} + e^{-i\omega t})$$

$$P_{if}(t) = \frac{|\langle f | V | i \rangle|^2}{4\hbar^2} \left| \int_0^t \left(e^{i(\omega_{fi} + \omega)t'} + e^{i(\omega_{fi} - \omega)t'} \right) dt' \right|^2$$

$$P_{if}(t) = \frac{|\langle f | V | i \rangle|^2}{4\hbar^2} \left| \frac{1 - e^{i(\omega_{fi} + \omega)t}}{\omega_{fi} + \omega} + \frac{1 - e^{i(\omega_{fi} - \omega)t}}{\omega_{fi} - \omega} \right|^2$$

Si $\omega = 0 \rightarrow V(t) = V \rightarrow P_{if}(t) = \frac{|\langle f | V | i \rangle|^2}{\hbar^2} \left| \frac{1 - e^{i\omega_{fi}t}}{\omega_{fi}} \right|^2 = \frac{|\langle f | V | i \rangle|^2}{\hbar^2} F(t, \omega_{fi})$

con $F(t, \omega_{fi}) \equiv \left| \frac{1 - e^{i\omega_{fi}t}}{\omega_{fi}} \right|^2 = \left| \frac{e^{i\omega_{fi}t/2} - e^{-i\omega_{fi}t/2}}{2i \omega_{fi}/2} \right|^2 = \left[\frac{\sin(\omega_{fi}t/2)}{\omega_{fi}/2} \right]^2$

$$P_{if}(t) = \frac{|\langle f | V | i \rangle|^2}{\hbar^2} \left[\frac{\sin(\omega_{fi}t/2)}{\omega_{fi}/2} \right]^2$$