ACT; Sheet 7; Marc Hauer, Angelo Brade; 24.11.2024

Exercise 3:

1.)

As $\vec{\varepsilon}\cdot\vec{x}_e$ is just a function and spherical symmetrical around the nucleus, it can be expanded in spherical coordinates:

$$\vec{\varepsilon}\cdot\vec{x}_e = \sum_{l}^{\infty}\sum_{m=-l}^{l} c_{lm}\, r^l\, Y_{lm}(\theta,\varphi)$$

Further $\vec{\varepsilon}$ is const., so that $\vec{x}_e$ is the only coordinate dependend term:

$$= \sum_{l}^{\infty}\sum_{m=-l}^{l} c_{lm}\, r_e^l\, Y_{lm}(\theta_e,\varphi_e)$$

If we now consider to lay $\vec{e}_z \parallel r_e$ we get:

$\vec{\varepsilon}\cdot\vec{x}_e \propto \cos(\theta)$, which limits $l=1$ for Y_{lm}.

Thus we finally can justify:

$$\vec{\varepsilon}\cdot\vec{x}_e = r_e \sum_m c_m Y_{1m}(\theta_e,\varphi_e).$$

$\square$

2.) $\vec{A}_{rad}\cdot\hat{\vec{p}}$ has non degenerated eigenvalues with $|x\rangle$ in $|x,s\rangle = |x\rangle\otimes|s\rangle$.

Thus $\vec{A}_{rad}\cdot\hat{\vec{p}}$ can transition from $E_i \to E_f$ with $E_i \neq E_f \Rightarrow \Gamma_{fi} \neq 0$.

As $\vec{A}_{rad}\cdot\hat{\vec{p}}$ has only degenerated eigenvalues with $|s\rangle$ in $|x,s\rangle$:

$E_i = E_f \Rightarrow \Gamma_{fi} = 0$ (no transition for spin).

Now with $\hat{\vec{\mu}}_e\cdot\vec{B}$ having non degenerated eigenvalues with $|s\rangle$ in $|x,s\rangle$, the $E_i \to E_f$ transition yealds $E_i \neq E_f \Rightarrow \Gamma_{fi} \neq 0$.

$\square$

3.) $\vec{A}_{rad}^{(abs)}(\vec{x},t) = \sqrt{\frac{N_\gamma \hbar}{2\varepsilon_0 V\omega}}\,\vec{\varepsilon}\cdot e^{i(\vec{k}\cdot\vec{x}-\omega t)}$

Absorbtion: $N_\gamma \to I_\gamma(\omega)$, such that $\int I_\gamma(\omega)\,d\omega = N_\gamma$

Thus with $\hat{H}(\vec{x},t) = \frac{1}{2m_e}(\hat{\vec{p}}+e\hat{\vec{A}}(\hat{\vec{x}},t)) - e\hat{U}(\hat{\vec{x}})$ and $[\hat{\vec{P}},\vec{A}_{rad}] = [\hat{\vec{P}},\hat{\vec{A}}] = 0$ follows:

$$\Rightarrow \hat{H}_1(\hat{x},t) = \frac{e}{m_e}\sqrt{\frac{I(\omega)\hbar}{2\varepsilon_0 V\omega}}\, e^{-i(\vec{k}\vec{x}-\omega t)}\, i\hbar\,\vec{\varepsilon}\cdot\vec{\nabla}$$

With $R_{fi}^{(1)} = \frac{2\pi}{\hbar}|\langle f^{(0)}|\hat{H}_1|i^{(0)}\rangle|^2\,\delta(E_f^{(0)}-E_i^{(0)}-\hbar\omega)$ follows:

$$R_{fi}^{(1)} = \frac{\pi e^2}{m_e^2}\frac{I_\gamma(\omega)\hbar^2}{\varepsilon_0 V\omega}\,|\langle f^{(0)}|\, e^{-i(\vec{k}\cdot\vec{x}-\omega t)}\,\vec{\varepsilon}\cdot\vec{\nabla}|i\rangle|^2\,\delta(E_f - E_i - \hbar\omega)$$

Periodic boundary conditions $\vec{A}(x_i + L) = \vec{A}(x_i)$ give $d^3k = \left(\frac{2\pi}{L}\right)^3 \Delta n_x \Delta n_y \Delta n_z$ with $k_i = \frac{2\pi}{L} n_i$.

Thus $\Gamma_{fi} = \sum_{n_x, n_y, n_z} R_{fi}$ becomes with $L \to \infty$:

$$\Gamma_{fi} = V \int \frac{d^3 p_\gamma}{(2\pi\hbar)^3} R_{fi} \quad \text{with } \vec{p}_\gamma = \hbar \vec{k} \quad | \; d^3 p_\gamma = d\Omega_\gamma \left(\frac{\hbar\omega}{c}\right)^2 d\left(\frac{\hbar\omega}{c}\right) \text{ in spherical coordinates}$$

$$= \frac{V}{(2\pi\hbar)^3} \frac{\pi e^2}{m_e^2} \frac{\hbar^2}{\varepsilon_0 V} \int d\Omega_\gamma \int \left(\frac{\hbar\omega}{c}\right)^2 d\left(\frac{\hbar\omega}{c}\right) \frac{I_\gamma(\omega)}{\omega} |\langle f^{(0)}| e^{-i(\vec{k}\cdot\vec{x} - \omega t)} \vec{\varepsilon}\cdot\vec{\nabla} |i\rangle|^2 \delta(E_f - E_i - \hbar\omega)$$

$$= \frac{V}{(2\pi\hbar)^3} \frac{\pi e^2}{m_e^2} \frac{\hbar^2}{\varepsilon_0 V} \int d\Omega_\gamma \int d\omega \frac{\hbar^3}{c^3} \omega I_\gamma(\omega) \frac{1}{\hbar} \delta\left(\frac{E_f - E_i}{\hbar} - \omega\right) |\langle f^{(0)}| e^{-i(\vec{k}\cdot\vec{x} - \omega t)} \vec{\varepsilon}\cdot\vec{\nabla} |i\rangle|^2$$

$$= \frac{e^2 \hbar^2}{8\pi^2 m_e^2 \varepsilon_0 c^3} \int d\Omega_\gamma \int d\omega \, \omega I_\gamma(\omega) \delta\left(\frac{E_f - E_i}{\hbar} - \omega\right) |\langle f^{(0)}| e^{-i(\vec{k}\cdot\vec{x} - \omega t)} \vec{\varepsilon}\cdot\vec{\nabla} |i\rangle|^2$$

With $\alpha_{em} = \frac{e^2}{4\pi\varepsilon_0 \hbar c}$ and $\omega_{fi} = \frac{E_f - E_i}{\hbar}$:

$$= \frac{\alpha_{em} \cdot \hbar}{2\pi} \omega_{fi} \cdot I_\gamma(\omega_{fi}) \underbrace{\int d\Omega_\gamma \left| \frac{\hbar}{m_e c} \langle f^{(0)}| e^{-i(\vec{k}\cdot\vec{x} - \omega t)} \vec{\varepsilon}\cdot\vec{\nabla} |i\rangle \right|^2}_{M_{fi}} \qquad \square$$

Quickies

Q1) i) sudden perturbation: $\delta t \ll \frac{1}{\omega_{fi}}$ (fast)

adiabatic perturbation: $T = \frac{1}{\omega_{min}}$ (slow) $\rightarrow$ no transitions

ii) If the unperturbed system has degenerate eigenstates, there is not a clear assigment of the eigenvalues to one eigenstate. A pertubation could cancel the degeneration. This leads in an transition, which is not possible in an adiabatic pertubation.

Q2) i) $\hat{O}_I(t) = \hat{U}_s^\dagger(t,t_0) \hat{O}_s(t) \hat{U}(t,t_0)$

ii) Show: $\hat{H}_{0,I} = \hat{H}_{0s}$

$\cdot \; \hat{H}_{0I} = U_s^\dagger(t,t_0) \hat{H}_{0,s} \hat{U}_s(t,t_0) = U_s^\dagger(t,t_0) U_s(t,t_0) \hat{H}_{0,s} = \hat{H}_{0,s} \quad \square$

Q3) $\Gamma_{stim} \propto N_\gamma$

1) Transition between General States

$\hat{O}|\alpha\rangle = o_\alpha|\alpha\rangle \;\wedge\; \hat{O}|\beta\rangle = o_\beta|\beta\rangle \;,\quad \hat{H}(t) = \hat{H}_0 + \hat{H}_\lambda(t) \;\wedge\; \hat{H}_0|n\rangle = E_n|n\rangle$

1) $|\alpha\rangle = \sum_n c_n^\alpha(t)|n\rangle \;\wedge\; |\beta\rangle = \sum_n c_n^\beta(t)|n\rangle$ with $c_n^i(t) = \langle n|i\rangle \quad (i \in \{\alpha, \beta\})$

$\cdot \; \delta_{\alpha\beta} = \langle\alpha|\beta\rangle = \left(\sum_n \langle n| \bar{c}_n^\alpha\right)\left(\sum_n c_n^\beta |n\rangle\right) = \sum_n \left(\bar{c}_n^\alpha c_n^\beta\right)$

2) Show: $|\langle\beta|\psi_s(t)\rangle|^2 \neq 0 \quad \forall t > t_0$ if $[\hat{H}_0, \hat{O}_s] \neq 0$

$\cdot \; |\langle\beta|\psi_s(t)\rangle|^2 = |\langle\beta|\hat{U}_s(t,t_0)|\alpha\rangle|^2$ where $|\alpha\rangle = |\psi_s(t_0)\rangle$

$$= |\langle\beta|\exp[-\tfrac{i}{\hbar}\hat{H}_s\cdot(t-t_0)]|\alpha\rangle|^2$$

$$\neq |\langle\beta|\exp[-\tfrac{i}{\hbar}E_\alpha(t-t_0)]|\alpha\rangle|^2 \quad (\forall t > t_0)$$

$$= \delta_{\alpha\beta} = 0 \quad \forall \alpha\neq\beta \quad \square$$

| $[\hat{H}_0, \hat{O}_s] \neq 0 \Rightarrow [\hat{H}_s, \hat{O}_s] \neq 0 \Rightarrow |\alpha\rangle \wedge |\beta\rangle$ can't be eigenstates of $\hat{H}$, even if $\hat{H}_1 = 0$?

3) Show: $|\langle\beta|\Psi_I(t)\rangle|^2 = 0$ for $\hat{H}_1 = 0 \wedge \alpha\neq\beta$

$$\cdot\ |\langle\beta|\Psi_I(t)\rangle|^2 = |\langle\beta|\hat{U}_s^+(t,t_0)|\Psi_s(t)\rangle|^2$$

$$= |\langle\beta|\hat{U}_s^+(t,t_0)\hat{U}_s(t,t_0)|\alpha\rangle|^2$$

$$= |\langle\beta|\alpha\rangle|^2$$

$$= \delta_{\alpha\beta} = 0 \quad \forall\alpha\neq\beta \quad \square$$

4) Show: $P_{\beta\alpha} = \left|\sum_{i,f}\langle i|\alpha\rangle\langle\beta|f\rangle\tilde{A}_{fi}(t-t_0)\right|^2$ where $\tilde{A}_{fi} = \langle f|\hat{U}_s(t,t_0)|i\rangle$

$$\cdot\ \langle\hat{O}\rangle = \langle\Psi_s(t)|\hat{O}_s|\Psi_s(t)\rangle$$

$$= \sum_{\alpha,\beta}\langle\Psi_s(t)|\alpha\rangle\langle\alpha|\hat{O}|\beta\rangle\langle\beta|\Psi_s(t)\rangle$$

$$= \sum_\beta o_\beta\langle\Psi_s(t)|\alpha\rangle\langle\beta|\Psi_s(t)\rangle\delta_{\alpha\beta}$$

$$= \sum_\beta o_\beta \underbrace{|\langle\beta|\Psi_s(t)\rangle|^2}_{\text{probability for }\beta}$$

$$P_{\alpha\beta} = |\langle\beta|\Psi_s(t)\rangle|^2$$

$$= |\langle\beta|\hat{U}_s(t,t_0)|\alpha\rangle|^2$$

$$= \left|\sum_{i,f}\langle\beta|f\rangle\langle f|\hat{U}_s(t,t_0)|i\rangle\langle i|\alpha\rangle\right|^2$$

$$= \left|\sum_{i,f}\langle i|\alpha\rangle\langle\beta|f\rangle\tilde{A}_{if}(t-t_0)\right|^2 \quad \text{where } \tilde{A}_{if}(t-t_0) = \langle f|\hat{U}_s(t,t_0)|i\rangle \quad \square$$

2) Selection Rules

$$[\hat{H}_0, \hat{O}] = 0 \Rightarrow \hat{H}_0|i^{(0)}, o_i\rangle = E_i^{(0)}|i^{(0)}, o_i\rangle \wedge \hat{O}|i^{(0)}, o_i\rangle = o_i|i^{(0)}, o_i\rangle$$

1) Show: $[\hat{H}_1, \hat{O}] = 0 \Rightarrow \langle f^{(0)}, o_f|\hat{H}_1|i^{(0)}, o_i\rangle = 0$ if $o_f \neq o_i$

$$\cdot\ 0 = [\hat{H}_1, \hat{O}]$$

$$\Rightarrow 0 = \langle f^{(0)}, o_f|[\hat{H}_1, \hat{O}]|i^{(0)}, o_i\rangle = \langle f^{(0)}, o_f|\hat{H}_1\hat{O}|i^{(0)}, o_i\rangle - \langle f^{(0)}, o_f|\hat{O}\hat{H}_1|i^{(0)}, o_i\rangle = (o_i - o_f)\langle f^{(0)}, o_f|\hat{H}_1|i^{(0)}, o_i\rangle$$

$$\Rightarrow \langle f^{(0)}, o_f|\hat{H}_1|i^{(0)}, o_i\rangle = 0 \quad \text{if} \quad o_f \neq o_i \quad \square$$

2)
$$\tilde{A}_{fi}^{(n)} = \exp[-\tfrac{i}{\hbar}E_f^{(0)}(t-t_0)]\cdot\Big\{\delta_{fi} - \frac{i}{\hbar}\int_{t_0}^{t}dt'\, e^{i\omega_{fi}(t'-t_0)}\underbrace{\cancel{\langle f^{(0)}, o_f|\hat{H}_1|i^{(0)}, o_i\rangle}}_{\to 0\ (\text{if } o_f\neq o_i)}$$

$$+ \left(-\frac{i}{\hbar}\right)^2\sum_n\int_{t_0}^{t}dt'\int_{t_0}^{t'}dt''\, e^{i\omega_{fn}(t'-t_0)}\cancel{\langle f^{(0)}, o_f|\hat{H}_1|n^{(0)}, o_n\rangle}^{\to 0}\, e^{i\omega_{ni}(t''-t_0)}\cancel{\langle n^{(0)}, o_n|\hat{H}_1|i^{(0)}, o_i\rangle}^{\to 0}$$

$$+ \cancel{(\ldots)}^{\to 0}\Big\}$$

↳ same argument for each term

at least one term goes to 0 [if $o_f \neq o_i \Rightarrow (o_f \neq o_n) \vee (o_i \neq o_n)$]

$$\Rightarrow P_{fi} = 0 \quad \text{if} \quad o_i \neq o_f$$

3) $[\hat{H}_0, \hat{\vec{L}}] = 0$

i) $\hat{H}_1 = f(\hat{z}, t) \Rightarrow \begin{cases}[\hat{H}_1, \hat{L}_z] \wedge [\hat{z}, \hat{L}_z] = 0 & \Rightarrow \Delta m = 0 \\ [\hat{H}_1, \hat{L}^2] \wedge [\hat{z}, \hat{L}^2] = 0 & \Rightarrow \Delta l = 0\end{cases}$

ii) $\hat{H}_1 = g(|\hat{\vec{x}}|, t) \Rightarrow \begin{cases}[\hat{H}_1, \hat{L}_z] \wedge [|\hat{\vec{x}}|, \hat{L}_z] = 0 & \Rightarrow \Delta m = 0 \\ [\hat{H}_1, \hat{\vec{L}}^2] \wedge [|\hat{\vec{x}}|, \hat{\vec{L}}^2] = 0 & \Rightarrow \Delta l = 0\end{cases}$