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

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

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

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

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

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

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

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

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 $L\to\infty$:

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

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

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

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

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

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

Quickies

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

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

"sudden" is too fast for transitions to occur

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.

true, but its because $T\sim 1/\Delta E\to+\infty$ so it becomes impossible to have a "slow enough" perturbation.

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

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

- $\hat{H}_{0,I} = U_s^\dagger(t,t_0)\,\hat{H}_{0,s}\,\hat{U}_s(t,t_0) = U_s^\dagger(t,t_0)\,U_s(t,t_0)\,\hat{H}_{0,s} = \hat{H}_{0,s}$ ✓ □

Q3) $\Gamma_{stim}\propto N_\gamma$ ✓

1) Transition between General States

$$\hat{O}|\alpha\rangle=o_\alpha|\alpha\rangle\ \wedge\ \hat{O}|\beta\rangle=o_\beta|\beta\rangle\quad,\quad \hat{H}(t)=\hat{H}_0+\hat{H}_1(t)\ \wedge\ \hat{H}_0|n\rangle=E_n|n\rangle$$

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

- $\delta_{\alpha\beta}=\langle\alpha|\beta\rangle=\left(\sum_n\langle n|\overline{c_n^\alpha}\right)\left(\sum_n c_n^\beta|n\rangle\right)=\sum_n\left(\overline{c_n^\alpha}\,c_n^\beta\right)$ ✓

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

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

$$= |\langle\beta| \exp[-\tfrac{i}{\hbar}\hat{H}_s (t-t_0)] |\alpha\rangle|^2 \qquad \Big| \; [\hat{H}_0, \hat{O}_s] \neq 0 \;\Rightarrow\; [\hat{H}_s, \hat{O}_s] \neq 0 \;\Rightarrow\; |\alpha\rangle \wedge |\beta\rangle \text{ can't be eigenstates of } \hat{H}, \text{ even if } \hat{H}_1 = 0 \text{ ?}$$

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

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

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

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

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

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

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

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 $\tilde{A}_{fi} = \langle f|\hat{U}_s(t,t_0)|i\rangle$

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

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

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

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

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

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

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

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

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 $o_f \neq o_i$

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

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

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

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

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

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

$\hookrightarrow$ same argument for each term

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

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

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

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

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