quantenmechanische Motivation der Dipolübergangsmatrixelemente

$H\psi = E\psi$ stat. Schr. gl. / Eigenwert Problem

$H\psi = -\frac{\hbar}{i}\frac{\partial \psi}{\partial t}$ zeitabh. Schr. gl.

Nehme $H = H_0 + V'(x,t)$

$\uparrow$ Störpotential z.B. $V' = eAx\cos(\omega t)$

$F_x = -\frac{\partial V'}{\partial x}$

$H_0 = -\frac{\hbar^2}{2m}\Delta + V(x)$ ungest. Problem

$H_0 u_\alpha = E_\alpha u_\alpha$

$H_0 u_\beta = E_\beta u_\beta$

$\psi_{\alpha,\beta} = u_{\alpha,\beta}(x,y,z)\cdot e^{-\frac{i}{\hbar}E_{\alpha,\beta}t}$ Lsg. zeitabh. Schr.

Ansatz: $\Psi = c_\alpha \psi_\alpha + c_\beta \psi_\beta$, $c_\alpha = c_\alpha(t)$ auch Lsg. von $H_0\Psi = -\frac{\hbar}{i}\frac{\partial \Psi}{\partial t}$ aber nicht von H

finde Näherungslösung $\rightarrow$ Übung $\overset{*}{\Rightarrow}$

* mehr Annahme:
- ebene Welle
- nur $\vec{E}$-Feld (nicht $\vec{B}$)
- $\vec{E}$ Feld homogen ($\lambda >> a_0$)
- Übergang von $\psi_\alpha \rightarrow \psi_\beta$ $\leftarrow$ stat. Endzustand

$\uparrow$ stat. Anfangsz.

$\omega_{\beta\alpha} := \frac{E_\beta - E_\alpha}{\hbar}$

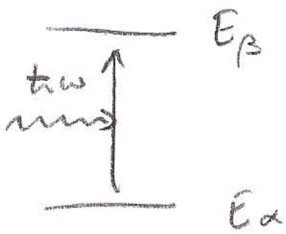
$$\frac{dc_\beta}{dt} \approx \frac{i}{\hbar} e^{\frac{i}{\hbar}(E_\beta - E_\alpha)t} E_0 \cos(\omega t) M_{\beta\alpha} \qquad M_{\beta\alpha} = \int d\vec{r}\, u_\beta^* x u_\alpha$$

$$= \frac{i}{2\hbar} E_0 M_{\beta\alpha}\left(e^{i(\omega_{\beta\alpha}+\omega)t} + e^{i(\omega_{\beta\alpha}-\omega)t}\right)$$

$$c_\beta(t) = \int_0^t \frac{dc_\beta}{dt}dt = \frac{E_0}{2\hbar} M_{\beta\alpha}\left\{\frac{e^{i(\omega_{\alpha\beta}+\omega)t}-1}{(\omega_{\alpha\beta}+\omega)} + \frac{e^{i(\omega_{\beta\alpha}-\omega)t}-1}{(\omega_{\beta\alpha}-\omega)}\right\}$$

B

Absorption



$$\omega_{\beta\alpha} = \frac{E_\beta - E_\alpha}{\hbar} > 0$$

$$\rightarrow \quad |\omega_{\beta\alpha} + \omega| \gg |\omega_{\beta\alpha} - \omega| = \Delta\omega$$

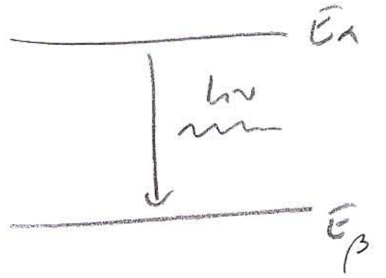
$$c_\beta(t) \cong \frac{E_0}{2\hbar} M_{\beta\alpha} \frac{e^{i(\omega_{\beta\alpha}-\omega)t} - 1}{\omega_{\beta\alpha} - \omega}$$

calculate $c_\beta^* c_\beta$, use $(e^{i\alpha} - 1)(e^{-i\alpha} - 1)$

$$= 2(1 - \cos(\alpha)) = 4\sin^2\left(\frac{\alpha}{2}\right)$$

$$|c_\beta(t)|^2 \sim \frac{E_0^2}{\hbar^2} |M_{\beta\alpha}|^2 \frac{\sin^2(\frac{1}{2}\Delta\omega t)}{(\Delta\omega)^2}$$

Emission

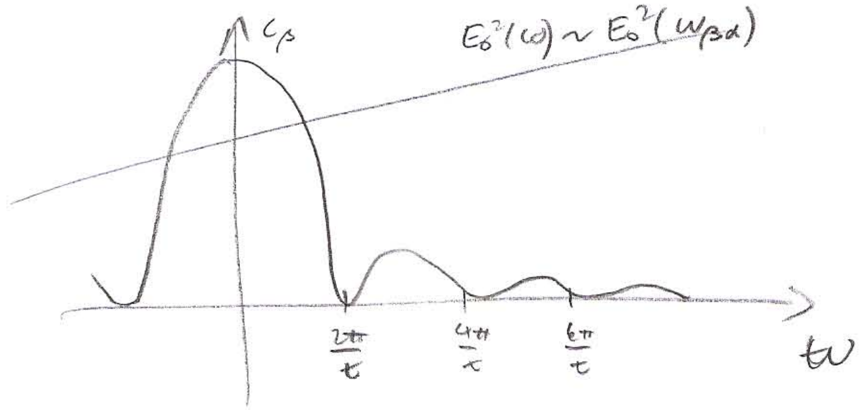


$$\omega_{\beta\alpha} = \frac{E_\beta - E_\alpha}{\hbar} < 0$$

$$|\omega_{\beta\alpha} - \omega| \gg |\omega_{\beta\alpha} + \omega| = \Delta\omega$$

ditto Absorption, i.e. same $|c_\beta(t)|^2$

$\rightarrow$ $\boxed{\text{Absorption = Emission } W_i}$



$$\int_{-\infty}^{\infty} d\Delta\omega \, \frac{E_0^2(\omega_{\beta\alpha}) |M_{\beta\alpha}|^2}{\hbar^2} \frac{\sin^2(\frac{1}{2}\Delta\omega)}{\Delta\omega^2}$$

$$= \frac{E_0^2(\omega_{\beta\alpha})\,|M_{\beta\alpha}|^2}{\hbar^2}\;\frac{t^2}{4}\int_{-\infty}^{\infty}\frac{\sin^2(\frac{1}{2}\Delta\omega t)}{(\frac{1}{2}\Delta\omega t)^2}\,d(\Delta\omega)$$

$$= \frac{E_0^2(\omega_{\beta\alpha})\,|M_{\beta\alpha}|^2}{\hbar^2}\;2t\underbrace{\int_{-\infty}^{\infty}\frac{\sin^2\xi}{\xi^2}\,d\xi}_{\pi} \qquad \frac{1}{2}\Delta\omega t = \xi \quad d\Delta\omega = \frac{2}{t}\,d\xi$$

$$= \frac{\pi E_0^2(\omega_{\beta\alpha})\,|M_{\beta\alpha}|^2}{2\hbar^2}\;t$$

$\uparrow$

Übergangsw. wächst mit t

$$W_{\alpha\beta} = \frac{|c_\beta(t)|^2}{t} = \frac{\pi E_0^2(\omega_{\beta\alpha})\,|M_{\beta\alpha}|^2}{2\hbar^2}$$

$E_0^2 \rightarrow w(\omega_{\beta\alpha})$

thermisches Ggw, isotrop, addiere x, y, z Komp.

$$B_{\beta\alpha} = \frac{\pi}{3\varepsilon_0\hbar^2}\,|M_{\beta\alpha}|^2 \qquad \text{Abs. / stim. Em}$$