Orientation:

now: standard time-dependent perturbation theory

$\downarrow$ application

bound states

→ shift: result here is equivalent to time-independent pert. theory

→ additionally: decay of probability of initially occupied state

next chapter: more formal approach to time-dependent perturbation theory (Dirac interaction picture)

$\downarrow$ application

scattering states

→ cross-section

→ s-wave scattering

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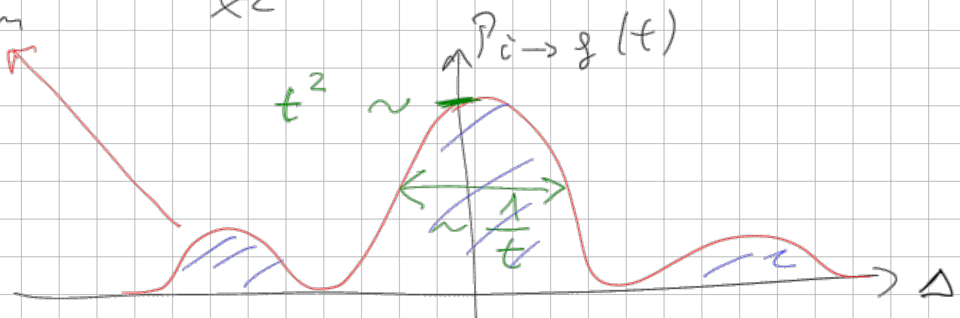
result from last time:

$$P_{i\to f}(t) = \frac{|\vec{d}_{fi}\cdot\vec{E}_0|^2}{\hbar^2}\underbrace{\frac{\sin^2(\Delta t/2)}{\Delta^2}}_{\hat{=}\ \text{diffraction function}}$$

detuning $\Delta = \omega - \omega_{fi}$

$\frac{\sin^2 x}{x^2}$



$$\int_{-\infty}^{+\infty} d\Delta \ \frac{\sin^2(\Delta t/2)}{\Delta^2} = \frac{t}{2}\int_{-\infty}^{+\infty} dx\ \frac{\sin^2 x}{x^2}$$

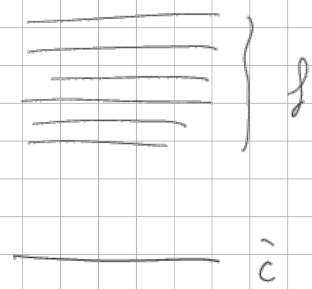
$$= t\ \frac{\pi}{2}$$

conclusion:
$$\frac{\sin^2(\Delta t/2)}{\Delta^2} \overset{t\to\infty}{=} \frac{\pi}{2}\, t\ \delta(\Delta)$$

transition rate $\quad w_{i\to f}(t) = \frac{d}{dt} W_{i\to f}(t) = \frac{\pi}{2} \frac{|\vec{d}_{fi}\cdot\vec{E}_0|^2}{\hbar^2}\,\delta(\omega-\omega_{fi})$

$$w_{i\to[f]}(t) = \frac{\pi}{2}\sum_{[f]} \frac{|\vec{d}_{fi}\cdot\vec{E}_0|^2}{\hbar^2}\,\delta(\omega-\omega_{fi})$$

Fermi's golden rule



extension: incoming light consists of many frequencies

$$\frac{dP_{i\to f}(t)}{dt} = \frac{1}{\hbar^2}\int_{-\infty}^{+\infty} d\omega\, \underbrace{|\vec{d}_{fi}\cdot\vec{E}_0(\omega)|^2}_{\text{varying slowly in frequency around } \omega_{fi}}\ \underbrace{\frac{\sin^2(\omega-\omega_{fi})t/2}{(\omega-\omega_{fi})^2 t}}_{\simeq\ \frac{1}{2}\,\delta(\omega-\omega_{fi})}$$

$$\overset{t\to\infty}{=} \frac{\pi}{2\hbar}\,|\vec{d}_{fi}\cdot\vec{E}_0(\omega_{fi})|^2$$

Wigner-Weißkopf Formula: Recovering time independent P.T.

Summary: previous result

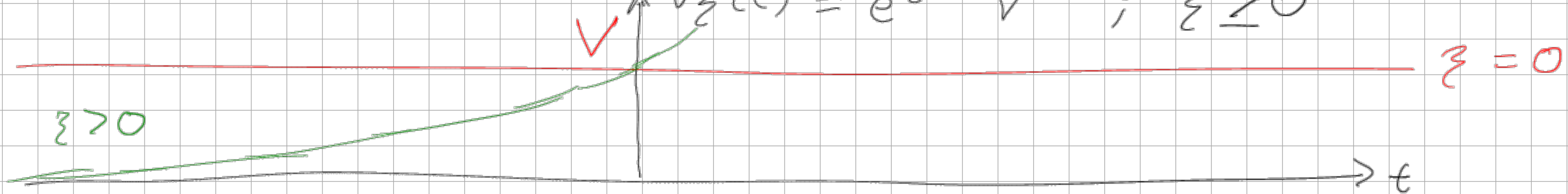
$$c_n^{(0)}(t) = \delta_{ni} \quad ; \quad \omega_{ni}^{(0)} = \frac{E_n^{(0)} - E_i^{(0)}}{\hbar}$$

$$\rightarrow c_n^{(1)}(t) = -\frac{i}{\hbar}\int_{t_0}^{t} dt'\, e^{i\omega_{ni}^{(0)} t'}\, V_{ni}(t') \quad ; \quad V_{ni}(t) = \langle \psi_n^{(0)} | \hat{V}(t) | \psi_i^{(0)} \rangle$$

t_0 ← NOTE

$$c_n^{(2)}(t) = \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \sum_m e^{i\omega_{nm}^{(0)} t'}\, V_{nm}(t')\, e^{i\omega_{mi}^{(0)} t''}\, V_{mi}(t'')$$

$$V_\zeta(t) = e^{\zeta t}\, V \quad ; \quad \zeta \geq 0$$



$$\lim_{t\to-\infty} V_\xi(t) = 0 \xrightarrow{\text{adiabatic switching on of perturbation}} \lim_{t\to 0} V_\xi(t)\ V$$

unperturbed — adiabatic switching on of perturbation — perturbed

$$V_{nm}(t) = e^{\xi t} V_{nm} \quad ; \quad V_{nm} = \langle \psi_n^{(0)} | \hat V | \psi_m^{(0)} \rangle$$

$n \neq i$: 1. order

$$\boxed{c_n^{(1)}(t) = -\frac{i}{\hbar}\int_{\underbrace{-\infty}_{=t_0}}^{t} dt'\, e^{i\omega_{ni}^{(0)} t'} e^{\xi t'} V_{ni} = -\frac{i}{\hbar}\frac{e^{(i\omega_{ni}^{(0)}+\xi)t}}{i\omega_{ni}+\xi} V_{ni}}$$

$$P_{i\to f}(t) = |c_f^{(1)}(t) + \ldots|^2 = \frac{|V_{fi}|^2}{\hbar^2}\frac{e^{2\xi t}}{\omega_{fi}^{(0)2} + \xi^2}$$

transition probabilities

$$\lim_{t\to\infty} W_{i\to f}(t) = \lim_{t\to\infty}\frac{d}{dt}\left(P_{i\to f}(t)\right) = \frac{2\pi|V_{fi}|^2}{\hbar^2}\underbrace{\frac{1}{\pi}\frac{\xi}{\xi^2+\omega_{fi}^{(0)2}}}_{\xrightarrow{\xi \to 0}\ \delta(\omega_{fi}^{(0)})}\ \underbrace{e^{2\xi t}}_{\xrightarrow{\xi\downarrow 0}\ 1}$$

$\Rightarrow$ Fermi's golden rule in the case $\omega = 0$

$$\delta(\omega_{fi}^{(0)}) = \hbar\,\delta(E_f^{(0)} - E_i^{(0)})$$

Now: $n = i$, 2nd order

$$c_i^{(0)}(t) = 1 \quad , \quad c_i^{(1)}(t) = -\frac{i}{\hbar}\frac{e^{\xi t}}{\xi} V_{ii}$$

$$c_i^{(2)}(t) = -\frac{i}{\hbar}\int_{-\infty}^{t} dt' \sum_m e^{i\omega_{im}^{(0)} t'} e^{\xi t'} V_{im}\, \boxed{c_m^{(1)}(t')}$$

$$= \left(-\frac{i}{\hbar}\right)^2 \int_{-\infty}^{t} dt' \sum_m e^{(i\cancel{\omega_{im}^{(0)}}+\xi)t'}\ \underbrace{V_{im} V_{mi}}\ \frac{e^{(i\cancel{\omega_{mi}^{(0)}}+\xi)t'}}{i\omega_{mi}^{(0)}+\xi}$$

$$= \left(-\frac{i}{\hbar}\right)^2 \sum_m |V_{im}|^2 \underbrace{\int_{-\infty}^{t} dt'\, e^{2\xi t'}}_{\frac{e^{2\xi t}}{2\xi}} \cdot \frac{1}{i\omega_{mi}^{(0)} + \xi} \quad = |V_{im}|^2$$

$$C_i(t) = \underbrace{1 - \frac{i}{\hbar}\frac{V_{ii}}{\xi} e^{\xi t}} + \left(-\frac{i}{\hbar}\right)^2 \sum_m \frac{|V_{im}|^2}{2\xi(i\omega_{mi}^{(0)} + \xi)} e^{2\xi t} + \dots$$

$$\dot{C}_i(t) = -\frac{i}{\hbar} V_{ii} e^{\xi t} + \left(-\frac{i}{\hbar}\right)^2 \sum_m \frac{|V_{im}|^2}{i\omega_{mi}^{(0)} + \xi} e^{2\xi t} + \dots$$

$$\frac{\dot{C}_i(t)}{C_i(t)} = \frac{-\frac{i}{\hbar}\underline{V_{ii}} e^{\xi t} + \left(-\frac{i}{\hbar}\right)^2 \frac{|V_{ii}|^2}{\xi} e^{2\xi t} + \left(-\frac{i}{\hbar}\right)^2 \sum_{m\neq i} \frac{|V_{im}|^2}{i\omega_{mi}^{(0)} + \xi} e^{2\xi t} + \dots}{1 - \frac{i}{\hbar}\frac{V_{ii}}{\xi} e^{\xi t} + \dots}$$

= expansion up to second order in V

$$= \underline{\cancel{\frac{i}{\hbar}\frac{V_{ii}}{\xi} e^{\xi t} \cdot \left(-\frac{i}{\hbar}\right) V_{ii} e^{\xi t}}} - \frac{i}{\hbar} V_{ii} e^{\xi t} + \underline{\cancel{\left(-\frac{i}{\hbar}\right)^2 \frac{|V_{ii}|^2}{\xi} e^{2\xi t}}}$$

$$\underbrace{\frac{\dot{C}_i(t)}{C_i(t)}} = \underbrace{-\frac{i}{\hbar}\left\{ \underbrace{V_{ii}\, e^{\xi t}}_{\xi \downarrow 0\; = 1} + \sum_{m\neq i} \frac{|V_{im}|^2}{E_i^{(0)} - E_m^{(0)} + i\hbar\xi} \underbrace{e^{2\xi t}}_{\xi \downarrow 0\; = 1} + \dots \right\}}_{\text{independent of time}}$$

$$= \underbrace{-\frac{i}{\hbar}\,\Delta_i}$$

$$c_i(t) = c_i(0)\,\exp\left\{-\underline{\frac{i}{\hbar}E_i^{(0)}t} - \frac{i}{\hbar}\underbrace{\Delta_i}_{\mathrm{Re}\,\Delta_i + i\,\mathrm{Im}\,\Delta_i} t\right\}$$

$$\Delta_i = \underbrace{\Delta_i^{(1)} + \mathrm{Re}\,\Delta_i^{(2)}}_{\text{time-independent perturbative shift of energy}} + \underbrace{i\,\mathrm{Im}\,\Delta_i^{(2)}}_{\text{exponential decay}}$$

time-independent perturbative shift of energy

exponential decay

Note: $\displaystyle \frac{1}{x+i\varepsilon} = \frac{1}{x+i\varepsilon}\cdot\frac{x-i\varepsilon}{x-i\varepsilon} = \frac{x-i\varepsilon}{x^2+\varepsilon^2} = \frac{x}{x^2+\varepsilon^2} \underbrace{- i\pi\,\frac{1}{\pi}\frac{\varepsilon}{x^2+\varepsilon^2}}_{\hat{=}\, i\,\mathrm{Im}\,\Delta_i^{(2)}}$

$$\lim_{\varepsilon \downarrow 0} \frac{1}{x+i\varepsilon} = \frac{1}{x} - i\pi\,\delta(x)$$

$$\Delta_i^{(1)} = V_{ii}, \quad \mathrm{Re}\,\Delta_i^{(2)} \sum_{m\neq i} \frac{|V_{im}|^2}{E_i^{(0)} - E_m^{(0)}} \quad \checkmark$$

$$c_i(t) = \exp\left\{-\frac{i}{\hbar}\left[E_i^{(0)} + \Delta_i^{(1)} + \mathrm{Re}\,\Delta_i^{(2)} - i\pi \underbrace{\sum_{m\neq i} |V_{im}|^2\,\delta(E_i^{(0)} - E_m^{(0)})}_{\frac{\hbar}{2\pi}\sum_{m\neq i} W_{i\to m}}\right]t\right\}$$

Fermi's golden rule

$\hat{=}$ exponential decay

(Wigner-Weisskopf, 1930)

Different Pictures:

Motivation:

- Dirac interaction picture: dynamics for states and operators
- Irrespective of picture: always the same expectation value ($\hat{=}$ measurable quantity)
- 3 different pictures:

	Schrödinger picture	Dirac picture	Heisenberg picture
states	time-dependent	time-dependent due to perturbation	time-independent
operators	time-independent (usually)	time " due to unperturbed Hamilton	time dependent

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application: adiabatic switching on of perturbation in view of scattering

Schrödinger and Heisenberg Picture

Note: simplification → all operators in Schrödinger picture are time-independent

$$\begin{cases} i\hbar \frac{\partial}{\partial t} |\Psi_S(t)\rangle = \hat{H}_S |\Psi_S(t)\rangle \\ i\hbar \frac{\partial}{\partial t} \hat{O}_S = 0 \end{cases}$$

S: Schrödinger picture

formal solution: $|\Psi_S(t)\rangle = \underbrace{e^{-\frac{i}{\hbar}\hat{H}_S t}}_{\text{time evolution operator}} \underbrace{|\Psi_S(0)\rangle}_{=:|\Psi_H\rangle}$

H: Heisenberg picture

$$|\Psi_S(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}_S t} |\Psi_H\rangle \Leftrightarrow |\Psi_H\rangle = e^{\frac{i}{\hbar}\hat{H}_S t} |\Psi_S(t)\rangle$$

$$i\hbar \frac{\partial}{\partial t} |\Psi_H\rangle = \left(-\hat{H}_S + \hat{H}_S\right) e^{\frac{i}{\hbar}\hat{H}_S t} |\Psi_S(t)\rangle \equiv 0$$

$$\langle \psi_S(t) | \hat{O}_S | \psi_S(t) \rangle = \langle \psi_H | \underbrace{\hat{O}_H(t)}_{\text{wanted}} | \psi_H \rangle$$

$$= \langle \psi_H | e^{\frac{i}{\hbar}\hat{H}_S t} \; e^{-\frac{i}{\hbar}\hat{H}_S t} | \psi_H \rangle$$

$$\Rightarrow \hat{O}_H(t) = e^{+\frac{i}{\hbar}\hat{H}_S t} \, \hat{O}_S \, e^{-\frac{i}{\hbar}\hat{H}_S t}$$

example: $\hat{H}_H(t) = e^{\frac{i}{\hbar}\hat{H}_S t} \hat{H}_S e^{-\frac{i}{\hbar}\hat{H}_S t} \equiv \hat{H}_S$ time independent

$$i\hbar \frac{\partial}{\partial t} \hat{O}_H(t) = e^{\frac{i}{\hbar}\hat{H}_S t} \left(-\hat{H}_S \hat{O}_S + \hat{O}_S \hat{H}_S \right) e^{-\frac{i}{\hbar}\hat{H}_S t} \quad \left(\frac{\partial}{\partial t} \hat{O}_S = 0 \right)$$

$$= \left[\hat{O}_H(t), \hat{H}_S \right]_- = \left[\hat{O}_H(t), \hat{H}_H(t) \right]_-$$

Heisenberg equation