$$\hat{U}_I(t,t_0) = \hat{U}_0^\dagger(t,t_0)\hat{U}(t,t_0)$$

$$i\hbar\frac{\partial}{\partial t}\hat{U}_I(t,t_0) = i\hbar\left(\frac{\partial}{\partial t}\hat{U}_0^\dagger(t,t_0)\right)\hat{U}(t,t_0) + i\hbar\,\hat{U}_0^\dagger(t,t_0)\left(\frac{\partial}{\partial t}\hat{U}(t,t_0)\right)$$

$$= \left(-\hat{U}_0^\dagger(t,t_0)\hat{H}_0\right)\hat{U}(t,t_0) + \hat{U}_0^\dagger(t,t_0)\hat{H}(t)\hat{U}(t,t_0)$$

$$= \hat{U}_0^\dagger(t,t_0)\left(-\hat{H}_0\hat{U}(t,t_0) + \hat{H}(t)\hat{U}(t,t_0)\right)$$

$$= \hat{U}_0^\dagger(t,t_0)\left(-\hat{H}_0 + \hat{H}(t)\right)\hat{U}(t,t_0)$$

$$= \hat{U}_0^\dagger(t,t_0)\hat{V}(t)\hat{U}(t,t_0)$$

$$= \underbrace{\hat{U}_0^\dagger(t,t_0)\hat{V}(t)\hat{U}_0(t,t_0)}_{\hat{V}_I(t)}\hat{U}_I(t,t_0)$$

$$= \hat{V}_I(t)\hat{U}_I(t,t_0)$$

$$\boxed{i\hbar\frac{\partial}{\partial t}\hat{U}_I(t,t_0) = \hat{V}_I(t)\hat{U}_I(t,t_0)}$$

— interaction picture ('I' for interaction)

cf. $i\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0) = \hat{H}(t)\hat{U}(t,t_0)$

Interaction picture

Expectation value of an arbitrary observable at time t is

$$\underbrace{\langle\psi(t)|\hat{O}(t)|\psi(t)\rangle}_{\text{Schrödinger}} = \langle\psi(t_0)|\overbrace{\underbrace{\hat{U}^\dagger(t,t_0)}_{\langle\psi(t)|}\hat{O}(t)\underbrace{\hat{U}(t,t_0)}_{|\psi(t)\rangle}}^{\text{Heisenberg operator}}|\psi(t_0)\rangle$$

State in Heisenberg representation

$$= \langle\psi(t_0)|\underbrace{\hat{U}_I^\dagger(t,t_0)}_{\langle\psi_I(t)|}\underbrace{\hat{U}_0^\dagger(t,t_0)\hat{O}(t)\hat{U}_0(t,t_0)}_{\hat{O}_I(t)}\underbrace{\hat{U}_I(t,t_0)|\psi(t_0)\rangle}_{|\psi_I(t)\rangle}$$

$$= \langle\psi_I(t)|\hat{O}_I(t)|\psi_I(t)\rangle$$

$\langle \psi_I(t) | \hat{O}_I(t) | \psi_I(t) \rangle$ where $|\psi_I(t)\rangle \equiv \hat{U}_I(t,t_0)|\psi(t_0)\rangle$

$$\hat{O}_I(t) \equiv \hat{U}_0^\dagger(t,t_0)\hat{O}(t)\hat{U}_0(t,t_0)$$

interaction picture (useful for time-dependent perturbation theory)

$$i\hbar \frac{\partial}{\partial t}\hat{U}_I(t,t_0) = \hat{V}_I(t)\hat{U}_I(t,t_0)$$

$$\hat{H}(t) = \hat{H}_0 + \hat{V}(t) \; ; \quad \hat{U}(t,t_0) = \hat{U}_0(t,t_0)\hat{U}_I(t,t_0)$$

$$i\hbar \frac{\partial}{\partial t}\hat{U}_I(t,t_0) = \hat{V}_I(t)\hat{U}_I(t,t_0)$$

$$\Rightarrow \quad \hat{U}_I(t,t_0) = \mathbb{1} + \frac{1}{i\hbar}\int_{t_0}^{t} \underbrace{\hat{V}_I(t_1)\hat{U}_I(t_1,t_0)}_{\text{dummy variable}} dt_1 \qquad -(1)$$

Everything here is exact.
There have been no approximations.

We now start on the perturbative approach to approximate quantities.

Iterative approach $\hat{V}(t)$ "small".

$$H(t) = H_0 + V(t) \approx H_0$$

$$\hat{U}(t,t_0) = \hat{U}_0(t,t_0)\hat{U}_I(t,t_0) \approx \hat{U}_0(t,t_0)$$

captures evolution due to H_0

ie. $\hat{U}_I(t,t_0) \approx \mathbb{1}$.

To zeroth order in V,

$$\hat{U}_I(t,t_0) \approx \mathbb{1}.$$

To get the 1st order result, substitute zeroth order result in the RHS of (1):

$$\hat{U}_I(t,t_0) = \mathbb{1} + \frac{1}{i\hbar}\int_{t_0}^{t} \hat{V}_I(t_1)\mathbb{1}\, dt_1$$

1st order expression for $\hat{U}_I$

$$= \mathbb{1} + \frac{1}{i\hbar}\int_{t_0}^{t} \hat{V}_I(t_1)\, dt_1$$

exp... for $\hat{U}_I$

$$\underbrace{1}_{\substack{\text{zeroth}\\ \text{order}\\ \hat{U}_I}} + \underbrace{\frac{1}{i\hbar}\int_{t_0} \cdots}_{\text{1st order correction to } \hat{U}_I}$$

"linear response"

To get the 2nd order approx to $\hat{U}_I$, sub. the 1st order result in RHS of (1):

$$\hat{U}_I(t,t_0) = \mathbb{1} + \frac{1}{i\hbar}\int_{t_0}^{t} \hat{V}_I(t_1)\underbrace{\left(\mathbb{1} + \frac{1}{i\hbar}\int_{t_0}^{t_1}\hat{V}_I(t_2)\,dt_2\right)}_{\hat{U}_I(t_1,t_0)}dt_1$$

$$= \underbrace{\mathbb{1}}_{\substack{\text{zeroth}\\ \text{order}\\ \text{term}}} + \underbrace{\frac{1}{i\hbar}\int_{t_0}^{t}\hat{V}_I(t_1)\,dt_1}_{\text{1st order correction}} + \underbrace{\left(\frac{1}{i\hbar}\right)^2\int_{t_0}^{t}\hat{V}_I(t_1)\int_{t_0}^{t_1}\hat{V}_I(t_2)\,dt_2\,dt_1}_{\text{2nd order correction}}$$

time-ordered sequence $t_2 \leq t_1$

Dyson series. $t_1 \leq t$

Not in exams

$$\hat{U}_I(t,t_0) = \sum_{n=0}^{\infty}\left(\frac{1}{i\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n\, \hat{V}_I(t_1)\hat{V}_I(t_2)\cdots\hat{V}_I(t_n)$$

$$\equiv \underbrace{\mathcal{T}}_{\text{time-ordered}} \exp\left(\frac{1}{i\hbar}\int_{t_0}^{t} V_I(t')\,dt'\right)$$

in general, $\hat{V}_I(t)$ at different times do not commute

Application

First order transition amplitudes and probabilities

$|e\rangle$ ——

$|g\rangle$ ——   ... $|e\rangle$

$|g\rangle$ ———

$\boxed{H_0}$ $+ V(t)$

Probability of transition from $|g\rangle$ to $|e\rangle$ or $|e\rangle$ to $|g\rangle$?

With no $V(t)$, $|g\rangle$ and $|e\rangle$ are stationary states of H_0.

expectation values of observables are time-independent.

not examinable

(In practice, no such thing as H_0 by itself. Because of that, the excited state $|e\rangle$ will decay to the ground state $|g\rangle$ after some time.)

(spontaneous emission — interaction with vacuum field)

General

Eg

Probability of transition from state $|\psi_m^0\rangle$ to $|\psi_n^0\rangle$ at time t.

eigenstates of H_0.

$\langle \psi_n^0 | \psi_m^0 \rangle = 0$

$$\langle \psi_n^0 | \psi_m(t)\rangle = \langle \psi_n^0 | \underbrace{\hat{U}(t,t_0)|\psi_m^0\rangle}_{|\psi_m(t)\rangle}$$

starting point is $|\psi_m^0\rangle$

transition amplitude $n \leftarrow m$

$$= \langle \psi_n^0 | \hat{U}_0(t,t_0)\, \hat{U}_I(t,t_0) |\psi_m^0\rangle$$

$$\hat{U}_0(t,t_0) = \exp\left(-\frac{i}{\hbar}\hat{H}_0(t-t_0)\right)$$

$$H_0|\psi_n^0\rangle = E_n^0 |\psi_n^0\rangle$$

$$= \underbrace{e^{-\frac{i}{\hbar}E_n^0(t-t_0)}}\, \underline{\langle \psi_n^0 | \hat{U}_I(t,t_0)|\psi_m^0\rangle}$$

factor here is inconsequential if we are only interested in transitions probabilities from m to n.

Now find $\langle \psi_n^0 | \hat{U}_I(t,t_0)|\psi_m^0\rangle$

We start our approximations now

- take the 1st order expression.

$$\hat{U}_I(t,t_0) = \mathbb{1} + \frac{1}{i\hbar}\int_{t_0}^{t} \hat{V}_I(t_1)\,dt_1$$

$$\hat{V}_I(t_1) = \hat{U}_0^\dagger(t_1,t_0)\,\hat{V}(t_1)\,\hat{U}_0(t_1,t_0)$$

To 1st order in V,

$$\langle \psi_n^0 | \hat{U}_I(t,t_0) | \psi_m^0 \rangle$$

$$= \langle \psi_n^0 | \psi_m^0 \rangle + \frac{1}{i\hbar}\langle \psi_n^0 \Big| \int_{t_0}^{t} \hat{U}_0^\dagger(t_1,t_0)\,\hat{V}(t_1)\,\hat{U}_0(t_1,t_0)\,dt_1 \Big| \psi_m^0 \rangle$$

$$= \delta_{nm} + \frac{1}{i\hbar}\int_{t_0}^{t} \langle \psi_n^0 | e^{i\frac{\hat{H}_0}{\hbar}(t_1-t_0)}\,\hat{V}(t_1)\,e^{-\frac{i}{\hbar}\hat{H}_0(t_1-t_0)} | \psi_m^0 \rangle\,dt_1$$

$$= \delta_{nm} + \frac{1}{i\hbar}\int_{t_0}^{t} e^{\frac{i}{\hbar}E_n^0(t_1-t_0)}\langle \psi_n^0 | \hat{V}(t_1) | \psi_m^0 \rangle\, e^{-\frac{i}{\hbar}E_m^0(t_1-t_0)}\,dt_1$$

$$= \delta_{nm} + \frac{1}{i\hbar}\int_{t_0}^{t} \langle \psi_n^0 | \hat{V}(t_1) | \psi_m^0 \rangle\, e^{\frac{i}{\hbar}(E_n^0 - E_m^0)(t_1-t_0)}\,dt_1$$

For $n \neq m$, $\delta_{nm} = 0$

and $$P_{n\leftarrow m}(t) = \left| \langle \psi_n^0 | \hat{U}(t,t_0) | \psi_m^0 \rangle \right|^2$$

$$= \left| \langle \psi_n^0 | \hat{U}_I(t,t_0) | \psi_m^0 \rangle \right|^2$$

$$P_{n\leftarrow m}(t) = \frac{1}{\hbar^2}\left| \int_{t_0}^{t} \langle \psi_n^0 | \hat{V}(t_1) | \psi_m^0 \rangle\, e^{\frac{i}{\hbar}(E_n^0 - E_m^0)(t_1-t_0)}\,dt_1 \right|^2$$

Probability of transition at time t from eigenstate m of H_0 (the unperturbed time-independent Hamiltonian) to a different eigenstate n of H_0, due to the effect of a perturbation V that operates from time t_0 to time t.; to 1st order in V.

$$P_{n\leftarrow m} = P_{m\leftarrow n} \quad \text{(show it)}$$

(" Probability of absorption of photon = Probability of stimulated emission of photon ")

(The above calculation does not account for the occupation of the state.)

For $n \neq m$,

$$P_{n \leftarrow m}(t) = \left(\frac{1}{\hbar}\right)^2 \left| \int_{t_0}^{t} \langle \psi_n^0 | \hat{V}(t_1) | \psi_m^0 \rangle e^{\frac{i(E_n^0 - E_m^0)(t_1 - t_0)}{\hbar}} \, dt_1 \right|^2 \quad — (*)$$

General.

We will apply (*) to specific forms of V(t).

V(t) harmonic, applied from $t \geq t_0$.

We can also V(t) independent of time from time $t' = t_0$ to time t. (frequency of harmonic is zero).

Case V(t) is independent of time over the time of application.

time in which e^- feels the potential of the atom.

V(t) is constant during this time.

$$P_{n \leftarrow m}^{n \neq m}(t) = \frac{1}{\hbar^2} \left| \int_{t_0}^{t} V_{nm} \, e^{\frac{i(E_n^0 - E_m^0)}{\hbar}(t_1 - t_0)} \, dt_1 \right|^2, \quad V_{nm} = \langle \psi_n^0 | V | \psi_m^0 \rangle.$$

Define $\omega_{nm} = \frac{E_n^0 - E_m^0}{\hbar}$

called the transition frequency between levels n and m.

$$= \frac{|V_{nm}|^2}{\hbar^2} \left| \int_{t_0}^{t} e^{i\omega_{nm}(t_1 - t_0)} \, dt_1 \right|^2$$

$$= \frac{|V_{nm}|^2}{\hbar^2} \left| \frac{e^{i\omega_{nm}(t - t_0)} - 1}{i\omega_{nm}} \right|^2$$

$|z|^2 = zz^*$.

$$= \frac{|V_{nm}|^2}{\hbar^2} \left| \frac{\quad}{i\omega_{nm}} \right|$$

$|z|^2 = zz^*$.

$$= \frac{|V_{nm}|^2}{\hbar^2 \omega_{nm}^2} \left(e^{i\omega_{nm}(t-t_0)} - 1\right)\left(e^{-i\omega_{nm}(t-t_0)} - 1\right)$$

$$= \frac{|V_{nm}|^2}{\hbar^2 \omega_{nm}^2} \left(1 + 1 - e^{i\omega_{nm}(t-t_0)} - e^{-i\omega_{nm}(t-t_0)}\right)$$

$$= \frac{|V_{nm}|^2}{\hbar^2 \omega_{nm}^2} \left(2 - 2\cos(\omega_{nm}(t-t_0))\right)$$

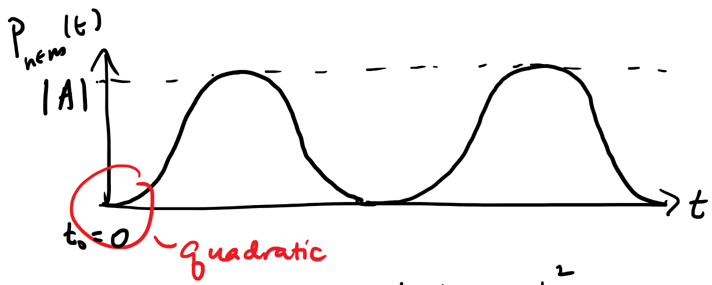
$$= \frac{2|V_{nm}|^2}{\hbar^2 \omega_{nm}^2} \left(2 \sin^2 \frac{\omega_{nm}(t-t_0)}{2}\right)$$

$$= \frac{4|V_{nm}|^2}{\hbar^2 \omega_{nm}^2} \sin^2 \frac{\omega_{nm}(t-t_0)}{2}$$

$$\boxed{P_{n\leftarrow m}(t) = \frac{4|V_{nm}|^2}{\hbar^2 \omega_{nm}^2} \sin^2 \frac{\omega_{nm}(t-t_0)}{2}}$$

, V constant in time during the period of application.

Fixed pair of m & n states,
How does $P_{n\leftarrow m}(t)$ depend on time?



When θ is small,
$\sin\theta \approx \theta$.

Amplitude $|A| = \dfrac{4|V_{nm}|^2}{\hbar^2 \omega_{nm}^2}$

Period $T = \dfrac{2\pi}{\omega_{nm}}$

$\rightarrow |V_{nm}| \ll \hbar\omega_{nm}$

Conditions of validity? $P_{n\leftarrow m} << 1$ — $(t-t_0)$ small.

When $(t-t_0)$ is small,

$$P_{n\leftarrow m} \approx \frac{4|V_{nm}|^2}{\hbar^2\omega_{nm}^2}\left(\frac{\omega_{nm}(t-t_0)}{2}\right)^2$$

$$= \frac{|V_{nm}|^2}{\hbar^2}(t-t_0)^2$$

(Similarly, if ω_{nm} is small, $P_{n\leftarrow m} \approx \frac{|V_{nm}|^2}{\hbar^2}(t-t_0)^2$)

Next. Fixed time interval for application of V.

How does $P_{n\leftarrow m}$ depend on ω_{nm}?

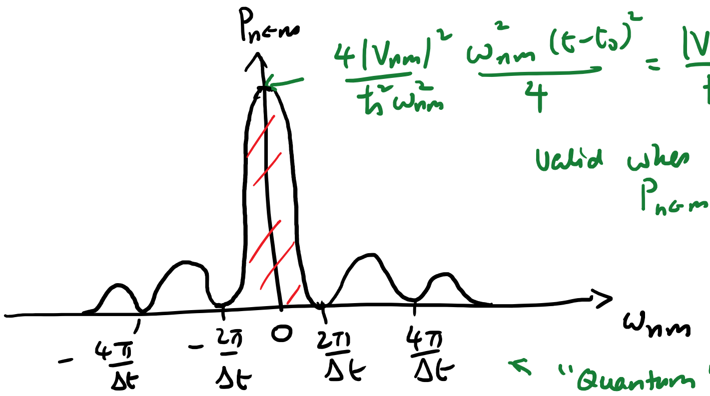
$$P_{n\leftarrow m}(t) = \frac{4|V_{nm}|^2}{\hbar^2\omega_{nm}^2}\sin^2\left(\frac{\omega_{nm}(t-t_0)}{2}\right)$$

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

$x \approx 0$, $\sin x \approx x$

$\frac{\sin x}{x} \approx 1$

$\lim_{x\to 0}\frac{\sin x}{x} = 1$



$\frac{4|V_{nm}|^2}{\hbar^2\omega_{nm}^2}\frac{\omega_{nm}^2(t-t_0)^2}{4} = \frac{|V_{nm}|^2}{\hbar^2}(\Delta t)^2$

Valid when $P_{n\leftarrow m} << 1$.

← "Quantum" nature.

$\Delta t = t - t_0$.

major peak centered at $\omega_{nm} = 0$.

Peak height $\propto (\Delta t)^2$ }
Peak width $\propto \frac{1}{(\Delta t)}$ } Peak area $\propto (\Delta t)^1$

Here, when V is independent of time during the period of application,

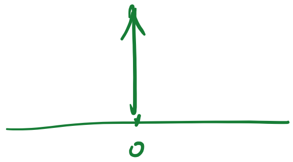
$P_{n\leftarrow m}$ is <u>max</u> when $\omega_{nm} \approx 0$

— "Conservation of energy".

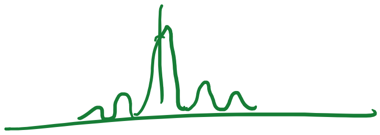
(eg. of scattering in the figure — "elastic scattering")

Classical conservation of energy

Classical conservation of energy



NOT



Roughly speaking,

$P_{n\leftarrow m}$ is significant for $\omega_{nm} \sim \frac{1}{\Delta t}$

$\Delta E \Delta t \sim \hbar$.