(L5): Heisenberg and Schrödinger's Representations (or Pictures)

So far we have looked at QM from the point of view of the evolution of the states. In this picture, known as the Schrödinger's Picture, the states evolve in time following the Schrödinger Equation

$$i\hbar \frac{\partial}{\partial t} |\psi_s(t)\rangle_s = \hat{H} \, |\psi_s(t)\rangle_s$$

while the Observables have no time dependence (except for a possible explicit, parametric time dependence).

In this picture the final state and the original state are related via the evolution operator

$$|\psi_s(t)\rangle = \hat{U}(t, t_0) \, |\psi_s(t_0)\rangle$$

which obeys

$$i\hbar \frac{\partial}{\partial t} \hat{U}(t, t_0) = \hat{H} \, \hat{U}(t, t_0) \qquad \text{(as an operator equation)}$$

~~[Here we are assuming that the system is isolated and thus $\hat{H}$ is time independent.]~~

Then, for $\hat{\Omega}_s$ some operator associated with an observable, we get

$$\frac{d}{dt}\langle \phi_s^*(t)|\hat{\Omega}_s|\psi_s(t)\rangle =$$

$$= \left[\frac{d}{dt}\langle \phi_s^*(t)|\right]\hat{\Omega}_s|\psi_s(t)\rangle + \langle \phi_s(t)|\hat{\Omega}_s \frac{d}{dt}\left[|\psi_s(t)\rangle\right]$$

$$+ \langle \phi_s^*(t)|\frac{\partial \hat{\Omega}_s}{\partial t}|\psi_s(t)\rangle$$

$$= +\frac{i}{\hbar}\langle \phi_s^*(t)|\hat{H}\hat{\Omega}_s|\psi_s(t)\rangle - \frac{i}{\hbar}\langle \phi_s(t)|\hat{\Omega}_s\hat{H}|\psi_s(t)\rangle$$

$$+ \langle \phi_s^*(t)|\frac{\partial \hat{\Omega}_s}{\partial t}|\psi_s(t)\rangle$$

$$= \langle \phi_s^*(t)|\left(\frac{\partial \Omega_s}{\partial t} + \frac{1}{i\hbar}[\hat{\Omega}_s,\hat{H}]\right)|\psi_s(t)\rangle$$

We now observe that since

$$|\psi_s(t)\rangle = e^{-\frac{it\hat{H}}{\hbar}}|\psi_s(0)\rangle \qquad (t_0=0)$$

$$\Rightarrow \frac{d}{dt}\langle \phi_s^*(0)|e^{i\hat{H}t/\hbar}\hat{\Omega}_s e^{-i\hat{H}t/\hbar}|\psi_s(0)\rangle =$$

$$= \langle \phi_s^*(0)|e^{i\hat{H}t/\hbar}\frac{\partial \hat{\Omega}_s}{\partial t}e^{-i\hat{H}t/\hbar}|\psi_s(0)\rangle$$

$$+ \frac{1}{i\hbar}\langle \phi_s(0)|\left[e^{i\hat{H}t/\hbar}\hat{\Omega}_s e^{-i\hat{H}t/\hbar},\hat{H}\right]|\psi_s(0)\rangle$$

We define a set of fixed (time indep.) state vectors

$$|\psi_H(t)\rangle \equiv |\psi_S(0)\rangle \equiv e^{i\hat{H}t/\hbar}\,|\psi_S(t)\rangle$$

and time-dependent operators

$$\hat{\Omega}_H(t) \equiv e^{i\hat{H}t/\hbar}\,\hat{\Omega}_S\,e^{-i\hat{H}t/\hbar}$$

This is the Heisenberg Picture.

$$\Rightarrow \frac{d}{dt}\langle \underbrace{\phi_H}_{\text{Heisenberg}}|\hat{\Omega}_H|\psi_H\rangle \equiv \langle\phi_H|\frac{d\hat{\Omega}}{dt}|\psi_H\rangle$$

$$\Rightarrow \langle\phi_{H}|\frac{d\hat{\Omega}_H}{dt}|\psi_H\rangle = \langle\phi_H|\frac{\partial\hat{\Omega}_H}{\partial t}|\psi_H\rangle + \frac{1}{i\hbar}\langle\phi_H|[\hat{\Omega}_H,\hat{H}]|\psi_H\rangle$$

$$\frac{\partial\hat{\Omega}_H}{\partial t} \equiv \left(\frac{\partial\hat{\Omega}}{\partial t}\right)_H \equiv e^{i\hat{H}t/\hbar}\,\frac{\partial\hat{\Omega}_S}{\partial t}\,e^{-i\hat{H}t/\hbar}$$

$$\Rightarrow \frac{d\hat{\Omega}_H}{dt} = \frac{\partial\hat{\Omega}_H}{\partial t} + \frac{1}{i\hbar}[\hat{\Omega}_H,\hat{H}]$$

[Notice: the Density Matrix evolves with a similar law but with a (−) sign; this is because the D.M. depends on time only in the Schrödinger picture.]

The Interaction Picture:

It is often useful to define a picture which is half-way between the Schrödinger and the Heisenberg Pictures.

The motivation for this is the ~~probl~~ following. In the Schrödinger rep. one has to solve the S.E. first and one can then compute the exp. values of the operators, study the time evolution of the observables etc. On the other hand, in the Heisenberg picture one has to solve the eqns. of motion of the operators and from them one can study observables etc. But both approaches have the practical problem that (a) the exact eigenstates are hard to find and some sort of perturbation theory becomes necessary and (b) the eqns of motion of the operators are generally non-linear and hard to solve. However if the Hamiltonian can be written as

$$H = H_0 + H_{int}$$

where H_0 is "solvable" (i.e. either the eigenstates are known or its eqns of motion can be solved) it is useful to ~~follow~~ adopt the following approach:

(3) Define the Interaction Picture by requiring that the states evolve in time due to the presence of H_{int} while the operators evolve with H_0. In other

words, H_{0s} is the Heisenberg picture of H_0.

Thus

$$|\psi_I(t)\rangle \equiv e^{i\hat{H}_{0s}t/\hbar}\,|\psi_s(t)\rangle$$

$$\hat{\Omega}_I(t) \equiv e^{i\hat{H}_{0s}t/\hbar}\,\hat{\Omega}_s\,e^{-i\hat{H}_{0s}t/\hbar}$$

$$\Rightarrow\quad i\hbar\frac{d}{dt}|\psi_I(t)\rangle = i\hbar\frac{d}{dt}\left(e^{i\hat{H}_{0s}t/\hbar}|\psi_s(t)\rangle\right)$$

$$= -\hat{H}_{0s}\,e^{i\hat{H}_{0s}t/\hbar}|\psi_s(t)\rangle + i\hbar\,e^{i\hat{H}_{0s}t/\hbar}\frac{d}{dt}|\psi_s(t)\rangle$$

$$= -H_{0s}\,e^{i\hat{H}_0 t/\hbar}|\psi_s(t)\rangle +$$

$$+\,e^{i\hat{H}_{0s}t/\hbar}\,\hat{H}_s|\psi_s(t)\rangle$$

$$= e^{i\hat{H}_{0s}t/\hbar}\,\hat{H}_{int_s}|\psi_s(t)\rangle$$

$$\Rightarrow\quad \boxed{i\hbar\frac{d}{dt}|\psi_I(t)\rangle = (\hat{H}_{int})_I\,|\psi_I(t)\rangle}$$

i.e. the states evolve with $\hat{H}_{int}$

$$(\hat{H}_{int})_I = e^{iH_0t/\hbar}\,\hat{H}_{int}\,e^{-iH_0t/\hbar}$$

(i.e. the ops. evolve with H_{0I})

Similarly, we can show

$$\boxed{\frac{d\hat{\Omega}_I}{dt} = \frac{\partial\hat{\Omega}_I}{\partial t} + \frac{1}{i\hbar}[\hat{\Omega}_I, \hat{H}_{0s}] = \frac{\partial\Omega_I}{\partial t} + \frac{1}{i\hbar}[\hat{\Omega}_I, \hat{H}_{0I}]}$$

However, H_{0I} and $(H_{int})_I$ are <u>time-dependent</u>

$\Rightarrow$ the evolution operator $\hat{U}_I(t)$

$$|\psi_I(t)\rangle = \hat{U}_I(t)\,|\psi_I(0)\rangle$$

is not a simple exponential of H_I. Indeed we find

$$i\hbar \frac{\partial}{\partial t}|\psi_I\rangle = i\hbar \frac{\partial U_I}{\partial t}|\psi_I(0)\rangle$$

$$H_I|\psi_I\rangle = H_I U_I |\psi_I(0)\rangle$$

$\Rightarrow$ U_I satisfies

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

We can integrate both sides as

$$\int_0^t dt'\, i\hbar \frac{\partial U_I}{\partial t'} = \int_0^t dt'\, H_I(t')\, U_I(t')$$

$$\Rightarrow\quad i\hbar\,[U_I(t) - U_I(0)] = \int_0^t dt'\, H_I(t')\, U_I(t')$$

But $U_I(0) = \hat{I}$ $\Rightarrow$

$$\boxed{U_I(t) = \hat{I} - \frac{i}{\hbar}\int_0^t dt'\, H_I(t')\, U_I(t')}$$

<u>Time-Dependent Perturbation Theory</u>:

This <u>integral equation</u> can be solved formally by iteration:

$$U_I(t) = \hat{I} - \frac{i}{\hbar}\int_0^t dt' \, H_I(t') + \left(\frac{i}{\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt'' \, H_I(t') H_I(t'')$$

$$+ \cdots + \left(-\frac{i}{\hbar}\right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \; H_I(t_1) \cdots H_I(t_n) + \cdots$$

It is convenient to define the time ordered product of two operators $\hat{A}(t)$, $\hat{B}(t)$ as

$$T \hat{A}(t) \hat{B}(t') \equiv \Theta(t-t') \hat{A}(t) \hat{B}(t') + \Theta(t'-t) \hat{B}(t') \hat{A}(t)$$

It is easy to check that

$$T\left(\int_0^t dt' \, \hat{H}_I(t')\right)^2 = T \int_0^t dt_1 \int_0^t dt_2 \; \hat{H}_I(t_1) \hat{H}_I(t_2)$$

$$= \int_0^t dt_1 \int_0^{t_1} dt_2 \; H_I(t_1) H_I(t_2)$$

$$+ \int_0^t dt_2 \int_0^{t_2} dt_1 \; H_I(t_2) H_I(t_1)$$

$$= 2 \int_0^t dt_1 \int_0^{t_1} dt_2 \; H_I(t_1) H_I(t_2)$$

Likewise

$$T\left(\int_0^t dt' \, H_I(t')\right)^n = n! \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \; H_I(t_1) \cdots H_I(t_n)$$

$\Rightarrow$ We can write

$$\hat{U}_I(t) = T \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar}\right)^n \left[\int_0^t dt' \, H_I(t')\right]^n$$

$$\Rightarrow \boxed{\hat{U}_I(t) = T \, e^{-\frac{i}{\hbar}\int_0^t dt' \, \hat{H}_I(t')}}$$ formal solution

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What does this tell us about the Schrödinger states $|\psi_S(t)\rangle$?

Recall that

$$|\psi_S(t)\rangle = e^{-iH_0 t/\hbar}\,|\psi_I(t)\rangle$$

and that

$$|\psi_I(t)\rangle = U_I(t)\,|\psi_I(0)\rangle$$

$$\Rightarrow |\psi_S(t)\rangle = e^{-iH_0 t/\hbar}\,U_I(t)\,|\psi_I(0)\rangle$$

$$\left(|\psi_I(0)\rangle = |\psi_S(0)\rangle\right)$$

Hence $\quad U(t,0) = e^{-iH_0 t/\hbar}\,U_I(t)$

where $\quad U_I(t) = T\, e^{-\frac{i}{\hbar}\int_0^t dt'\, H_I(t')}$

$$\equiv \sum_{n=0}^{\infty}\left(\frac{-i}{\hbar}\right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n\; H_I(t_1)\cdots H_I(t_n)$$

Using that

$$H_I(t) = e^{iH_0 t/\hbar}\, H_{int}\, e^{-iH_0 t/\hbar}$$

we get

$$U_I(t) = \sum_{n=0}^{\infty}\left(\frac{-i}{\hbar}\right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \prod_{j=1}^{n}\left[e^{\frac{i}{\hbar}H_0 t_j} H_{int}(t_j)\, e^{-i\frac{H_0 t_j}{\hbar}}\right]$$

Since $\quad |\psi_s(t)\rangle = \hat{U}(t)\,|\psi_s(0)\rangle \equiv \hat{U}_s(t;0)\,|\psi_s(0)\rangle$

and

$$|\psi_s(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}_0 t}\,|\psi_I(t)\rangle \equiv \hat{U}_0(t,0)\,|\psi_I(t)\rangle$$

We find that we can reconstruct the evolution op. in the Schrödinger picture $\hat{U}_s(t,0)$ as

$$U_s(t,0) = \hat{U}_0(t,0)\,\hat{U}_I(t)\,\cancel{|\psi_I(0)\rangle}$$

$$\Rightarrow \hat{U}_s(t,0) = e^{-\frac{i}{\hbar}\hat{H}_0 t}\; T\, e^{-\frac{i}{\hbar}\int_0^t dt'\, H_I(t')}$$

where

$$H_I(t') = e^{iH_0 t'/\hbar}\, H_{int}(t')\, e^{-iH_0 t'/\hbar}$$

Using the def. of T-ordered product and the fact that $\quad e^{iH_0 t_n/\hbar}\, e^{-iH_0 t_{n+1}/\hbar} = U_0^{+}(t_n, t_{n+1})$

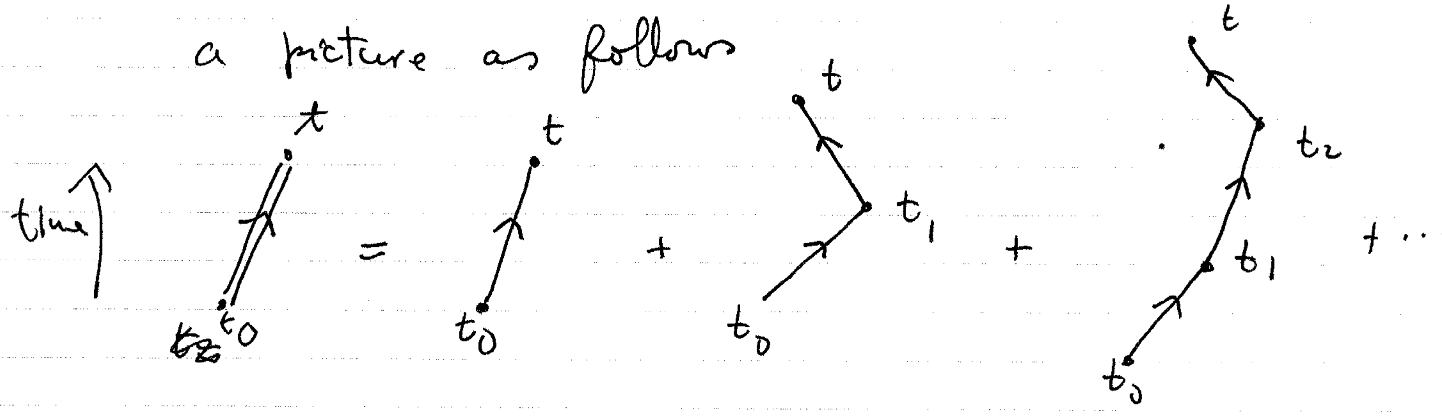
we write

$$\hat{U}_s(t,0) = \sum_{n=0}^{\infty}\left(\frac{-i}{\hbar}\right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \ldots \int_0^{t_{n-1}} dt_n$$

$$\hat{U}_s^0(t,t_1)\,\hat{H}_{int}(t_1)\,\hat{U}_s^0(t_1,t_2)\,\hat{H}_{int}(t_2)\ldots\hat{H}_{int}(t_n)\,\hat{U}_s^0(t_n,0)$$

There is a nice and illustrative pictorial representation of this series.

Let us denote by an arrow the action of $\hat{U}^0_S$ and by a double arrow the full $\hat{U}_S$. Then we can represent each term in the series by a picture as follows



At each intermediate time t_k the interaction term of the Hamiltonian acts.

Suppose that at $t=0$ the system is in the (unperturbed) initial state $|i_0\rangle$ we may now ask for the amplitude that at time t it will be in the final unperturbed state $|f_0\rangle$

The amplitude is

$$\langle f_0(t) | i_0(0)\rangle = \langle f_0 | \hat{U}(t,0) | i_0\rangle$$

Let's evaluate this expression order by order in perturbation theory, i.e in the expansion in powers of H_{int}.

since the unperturbed state $|n^0\rangle$ are a complete set

$$I = \sum_n |n^0\rangle\langle n^0|$$

and the unperturbed evolution operator $\hat{U}_0$ is diagonal in this basis

$$\hat{U}_0 = e^{-iH_0 t/\hbar} = \sum_n e^{-iE_n^0 t/\hbar} |n^0\rangle\langle n^0|$$

we can write the expansion as follows:

$$\langle f_0|\hat{U}(t,0)|i_0\rangle = \langle f_0|\hat{U}_0(t,0)|i_0\rangle +$$

$$+ \left(\frac{-i}{\hbar}\right)\int_0^t dt_1 \, \langle f_0|\hat{U}_0(t,t_1)\hat{H}_{int}(t_1)\hat{U}_0(t_1,0)|i_0\rangle$$

$$+ \left(\frac{-i}{\hbar}\right)^2\int_0^t dt_1\int_0^{t_1} dt_2 \, \langle f_0|\hat{U}_0(t,t_1)\hat{H}_{int}(t_1)\hat{U}_0(t_1,t_2)\hat{H}_{int}(t_2)\hat{U}_0(t_2,0)|i_0\rangle$$

$+ \ldots$

$(t_0=0)$ $\Big|$ $\cancel{= \langle f_0|\hat{U}_0(t,0)|i_0\rangle} +$

$\cancel{+\left(\frac{-i}{\hbar}\right)\sum_{n_1^0, n_1'^0}\int_0^t dt_1}$

$$\langle f^0(t)|i^0(0)\rangle = \delta_{fi}\, e^{-iE_f^0 t/\hbar} + \left(\frac{-i}{\hbar}\right)\int_0^t dt_1 \, e^{-\frac{i}{\hbar}E_f^0(t-t_1)}\langle f^0|\hat{H}_{int}(t_1)|i^0\rangle e^{-\frac{i}{\hbar}E_i^0 t_1}$$

$$+ \left(\frac{-i}{\hbar}\right)^2\int_0^t dt_1\int_0^{t_1} dt_2 \sum_{n^0} e^{-\frac{i}{\hbar}E_f^0(t-t_1)}\langle f^0|\hat{H}_{int}(t_1)|n^0\rangle e^{-\frac{i}{\hbar}E_n^0(t_1-t_2)} \langle n^0|\hat{H}_{int}(t_2)|i^0\rangle e^{-\frac{i}{\hbar}E_i^0 t_2} + \ldots$$

(a) First Order Processes: Born Approximation

To first order (in H_{int}) we get the result

$$\langle f(t) | i(0)\rangle = \delta_{fi}\, e^{-\frac{i}{\hbar}E_f^0 t} +$$

$$+ \left(\frac{-i}{\hbar}\right) \int_0^t dt_1\; e^{-\frac{i}{\hbar}E_f^0 t}\; e^{\frac{i}{\hbar}(E_f^0 - E_i^0)t_1} \langle f^0 | \hat{H}_{int}(t_1) | i^0\rangle$$

Consider the situation that we want to study the case in which $|f\rangle \neq |i\rangle \Rightarrow$

$$\langle f(t) | i(0)\rangle = \left(\frac{-i}{\hbar}\right) e^{-\frac{i}{\hbar}E_f^0 t} \int_0^t dt_1\; e^{\frac{i}{\hbar}(E_f^0 - E_i^0)t_1} \langle f^0 | \hat{H}_{int}(t_1) | i^0\rangle$$

(Born App.)

Transition probability:

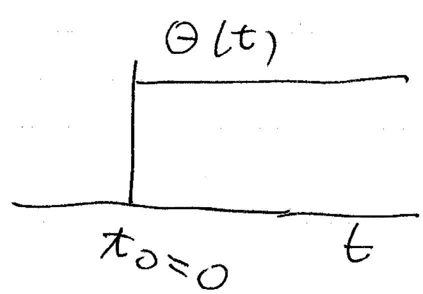
$$P_{i\to f}(t) = |\langle f(t) | i(0)\rangle|^2$$

$$= \left| \frac{1}{i\hbar} e^{-\frac{i}{\hbar}E_f^0 t} \int_0^t dt_1\; e^{\frac{i}{\hbar}(E_f^0 - E_i^0)t_1} \langle f^0 | \hat{H}_{int}(t_1) | i^0\rangle \right|^2$$

$$\equiv \left| \frac{1}{i\hbar} \int_0^t dt_1\; e^{\frac{i}{\hbar}(E_f^0 - E_i^0)t_1} \langle f^0 | \hat{H}_{int}(t_1) | i^0\rangle \right|^2$$

Let us consider a few examples

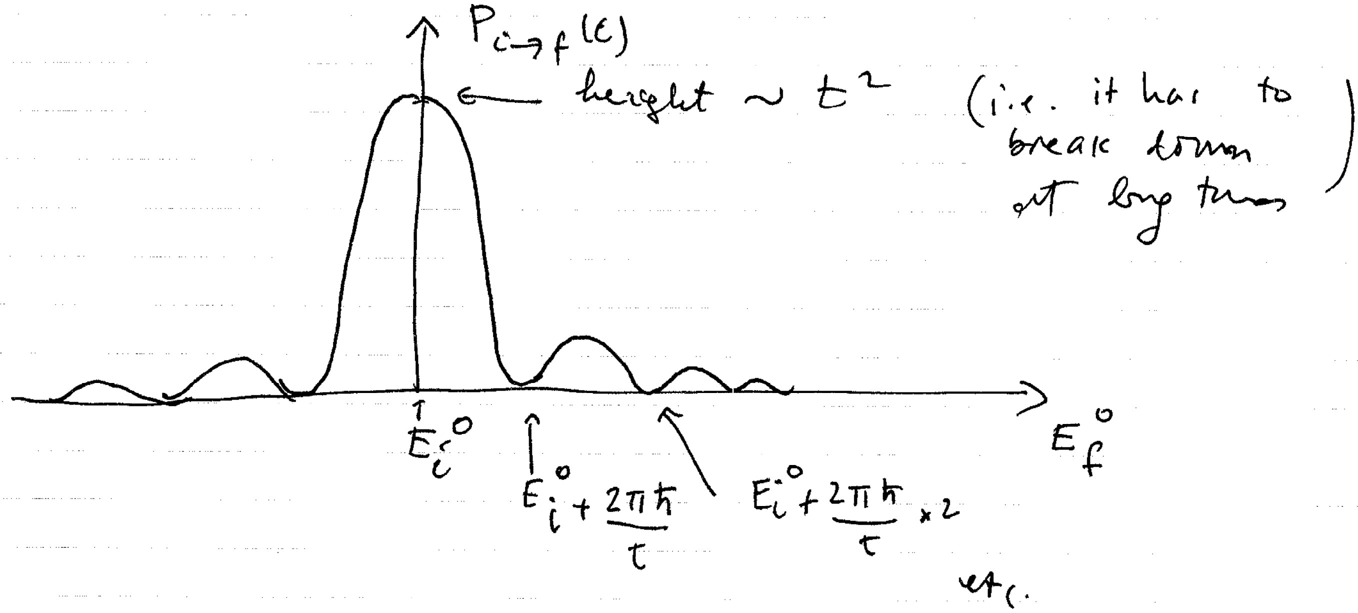
(a) $\hat{H}_{int}(t) = \hat{V}\,\Theta(t)$



$$\Rightarrow \quad P_{i\to f}(t) = \frac{1}{\hbar^2}\left|\int_0^t dt_1\, e^{\frac{i}{\hbar}(E_f^0 - E_i^0)t_1}\, V_{fi}\right|^2$$

$$V_{fi} = \langle f^0 |\, \hat{V} \,| i^0 \rangle$$

$$\Rightarrow \quad P_{i\to f}(t) = |\langle f | \hat{V} | i \rangle|^2 \left[\frac{\sin\left((E_f^0 - E_i^0)t/2\hbar\right)}{(E_f^0 - E_i^0)/2}\right]^2$$



For short times ($t \ll \frac{2\hbar}{E_f^0 - E_i^0}$)

$$P_{i\to f}(t) \sim |\langle f^0 | V | i^0 \rangle|^2 \, \frac{t^2}{\hbar^2} = \left|\frac{\langle f^0 | V | i^0\rangle}{\hbar}\right|^2 t^2$$

[this is also the probability as $E_f^0 \to E_i^0$ at t fixed]

For long times, only those states within $E_i^0 \pm \Delta E$ ($\Delta E \sim \frac{2\pi\hbar}{t}$) will have an appreciable probability.

Area under bump = integrated probab. $\approx |\langle f^0 | \hat{V} | i^0 \rangle|^2 \left|\frac{t}{\hbar}\right|^2 \frac{2\pi\hbar}{t} \sim |V_{fi}|^2 2\pi \frac{t}{\hbar}$

L9 What happens if there are many states within ΔE ?

Let us compute the <u>total</u> probability for such a decay

$$P(t) = \sum_{f \in \Delta E} P_{i \to f}(t)$$

In particular we will assume that $|\langle f|V|i\rangle|^2$ <u>does not change</u> very much (i.e. it is smooth) <u>within that group of states</u> and that the <u># of states</u> in a interval $\Delta \varepsilon$ around E_n^0 <u>is a smooth function</u> $\rho_0(\varepsilon_n)\,\Delta\varepsilon$ where $\rho(\varepsilon)$ is the <u>density of states</u>

$$\Rightarrow \sum_{f \in \Delta E} P_{i \to f}(t) \approx \int_{\text{group}} dE_f\, \rho(\varepsilon_f)\, |\langle f|V|i\rangle|^2 \left| \frac{\sin(\Delta\varepsilon)\frac{t}{2\hbar}}{\frac{\Delta\varepsilon}{2}} \right|^2$$

$$\underset{\substack{\text{(valid at}\\ \text{long times)}}}{\approx} |\langle f|V|i\rangle|^2_{E_f^0}\; \rho_0(E)\Big|_{E_f^0} \underbrace{\int_{-\infty}^{+\infty} dE_f \left(\frac{\sin(\Delta\varepsilon)t/2\hbar}{\frac{\Delta\varepsilon}{2}} \right)^2}_{\frac{2\pi t}{\hbar}}$$

$$\Delta\varepsilon = E_f - E_f^0$$

$$\Rightarrow \sum_{f \in \Delta E} P_{i \to f}(t) \approx |\langle f|V|i\rangle|^2_{E_f^0}\; \rho(E_f^0)\; \frac{2\pi t}{\hbar}$$

$$\equiv \Gamma t$$

where Γ is the <u>transition rate</u>

$$\Gamma = \frac{2\pi}{\hbar}\left[|\langle f| V |i\rangle|^2 \rho(E) \right]_{E=E_i^0}$$

<u>Fermi's Golden Rule</u>

Alternatively we can realize that, as t grows,

$$\frac{4 \sin^2\left[\frac{(E_f^0 - E_i^0)t}{2\hbar}\right]}{(E_f^0 - E_i^0)^2} \sim \frac{2\pi t}{\hbar}\,\delta(E_f^0 - E_i^0)$$

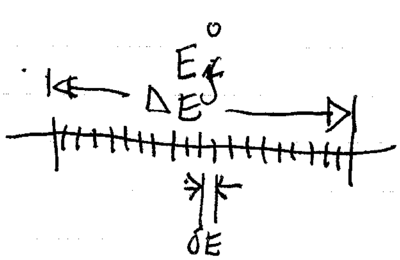
$$\Rightarrow \quad P_{i\to f}(t) \equiv \Gamma_{i\to f}\, t$$

$$\Gamma_{i\to f} = \frac{2\pi}{\hbar} |\langle f|V|i\rangle|^2 \,\delta(E_f^0 - E_i^0)$$

$$\sum_{f\in\Delta E} \Gamma_{i\to f} = \Gamma = \frac{2\pi}{\hbar} \underbrace{\sum_{f\in\Delta E} |\langle f|V|i\rangle|^2 \,\delta(E_f^0 - E_i^0)}_{|\langle f|V|i\rangle|^2 \rho(E_i^0)}$$

Note: The Golden Rule holds only if $t > \frac{2\pi\hbar}{\Delta E}$

but $t \ll \frac{2\pi\hbar}{\delta E}$ (where δE is the level spacing)



$(\Delta E \gg \delta E)$

Application of the Golden Rule

Consider a particle in a momentum state in a box of volume L^3. At some time $t=0$ a potential $V(\vec{r})$ is turned on inside the box. What is the rate at which the particle makes transitions to other momentum states?

Momentum: $\vec{p} = \hbar \vec{k}$

Transitions $|\vec{p}\rangle \rightarrow |\vec{p}\,'\rangle$

$$\langle \vec{k}'|\hat{V}|\vec{k}\rangle = \int \frac{d^3r}{L^{3/2}}\, e^{-i\vec{k}'\cdot\vec{r}}\, V(\vec{r})\, \frac{e^{i\vec{k}\cdot\vec{r}}}{L^{3/2}}$$

$$\left(\Psi(\vec{k}) = \frac{1}{L^{3/2}} e^{i\vec{k}\cdot\vec{r}}\right) \qquad \equiv \frac{1}{L^3} V(\vec{k}-\vec{k}')$$

$$\Rightarrow V(\vec{k}-\vec{k}') = \int d^3r\, V(\vec{r})\, e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}$$

Transition Rate $$\Gamma_{\vec{k}\rightarrow\vec{k}'} = \frac{2\pi}{\hbar} \frac{|V(\vec{k}-\vec{k}')|^2}{(L^3)^2}\, \delta(E^0_{\vec{k}} - E^0_{\vec{k}'})$$

Here $E^0_{\vec{k}} = \dfrac{\hbar^2 \vec{k}^2}{2m}$

Rate for scattering into a small angle $d\Omega$:

$$d\Gamma = \sum_{\vec{k}'\in d\Omega} \Gamma_{\vec{k}\rightarrow\vec{k}'}$$

$\hookrightarrow$ all states $|\vec{k}'\rangle$ inside $d\Omega$

$\#$ of states in $d^3k' = L^3 \dfrac{d^3k'}{(2\pi)^3} = \underbrace{\dfrac{L^3 m k'}{(2\pi)^3 \hbar^2}}_{\substack{\text{\# of states per unit energy}\\ \text{and solid angle}}} d\Omega' \, dE_{k'}$

(recall quantization in a box $k = \dfrac{2\pi n}{L}$)

$\left(\begin{array}{l} E = \dfrac{p^2}{2m} = \dfrac{\hbar^2 k^2}{2m} \Rightarrow dE = \dfrac{\hbar^2}{m} k\,dk \\ d^3k = d\Omega\, k^2 dk \end{array} \right)$

$$\Rightarrow \sum_{\vec{k}' \in d\Omega} \rightarrow d\Omega' \int_0^\infty \frac{L^3 m k'}{(2\pi)^3 \hbar^2} dE_{k'}$$

$$\Rightarrow d\Gamma = d\Omega' \int_0^\infty L^3 \frac{m|\vec{k}'|}{(2\pi)^3 \hbar^2} dE_{k'} \; \frac{2\pi}{\hbar} \frac{|V(\vec{k}-\vec{k}')|^2}{(L^3)^2} \delta(E_k^0 - E_{k'}^0)$$

$$\Rightarrow d\Gamma = \frac{d\Omega'}{L^3} \frac{m|\vec{k}|}{4\pi^2 \hbar^3} |V(\vec{k}-\vec{k}')|^2$$

(here $\vec{k}'$ is a vector in $d\Omega'$ of length k)

<u>Scattering Expt.:</u> beam of particles which scatter into $d\Omega$ at the rate $d\Gamma$ per incident particle in the volume L^3. The flux of particles per incident particle of momentum $\hbar k$ in vol. L^3 is $\dfrac{\hbar|\vec{k}|}{m L^3} \Rightarrow$

$$\text{(diff) cross section} = \frac{\text{rate}}{\text{flux}} = \frac{d\Gamma}{\frac{\hbar|k|}{mL^3} d\Omega} \Rightarrow$$

$$\frac{d\sigma}{d\Omega} = \frac{m^2}{4\pi^2 \hbar^4} |V(\vec{k}-\vec{k}')|^2$$

which is the Born approx. to the diff cross section.

L8

Radioactive Decay of a Nucleus

Consider a nucleus in some state $|i\rangle$ which decays by emission of a particle of momentum $|\hbar\vec{k}\rangle$. Let $|f\rangle$ be the final state of the nucleus (ignoring recoil). Let the matrix element for this transition be $\langle f, \hbar\vec{k}|\hat{V}|i\rangle$ (and assume that it is known). The initial energy is E_i and the final energy is $E_f + \varepsilon_{\vec{k}}$ $\Rightarrow$

The transition rate for a transition with the particle moving out in $d\Omega$ is

$$d\Gamma = d\Omega \int_0^\infty \frac{m|\vec{k}|\,L^3}{(2\pi)^2\hbar^3}\, d\varepsilon_{\vec{k}}\, |\langle f, \hbar\vec{k}|\hat{V}|i\rangle|^2 \delta(E_i - E_f - \varepsilon_k)$$

$$= d\Omega\, \frac{m k L^3}{(2\pi)^2\hbar^3}\, |\langle f, \hbar\vec{k}\,|\hat{V}|i\rangle|^2$$

where $\vec{k}$ points along $d\Omega$ and

$$|\vec{k}| = \sqrt{\frac{2m}{\hbar^2}(E_i - E_f)}$$

$$\text{Total Rate} = \int d\Gamma = \frac{m\,k L^3}{(2\pi)^2\,\hbar^3} \int d\Omega\, |\langle f, \hbar\vec{k}|\hat{V}|i\rangle|^2$$

which is the rate at which the nucleus decays.

Adiabatic Perturbations

Consider now a perturbation which is turned on *slowly*.

For example, let us consider potentials of the form

$$\hat{V}(t) = e^{\eta t}\, \hat{V}$$

with $\eta > 0$. We will let $\eta \to 0$ afterwards.

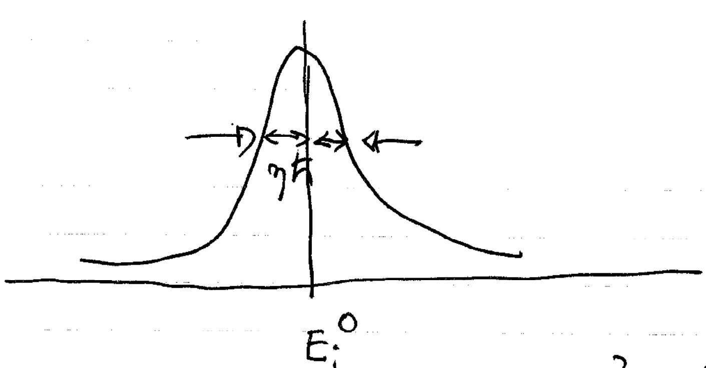
$\Rightarrow$ We have to compute integrals of the form

$$\int_{t_0}^{t} dt'\, e^{\eta t'}\, e^{\frac{i}{\hbar}(E_f^0 - E_i^0)t'} \underset{t_0 \to -\infty}{\approx} \int_{-\infty}^{t} dt'\, e^{\eta t'}\, e^{\frac{i}{\hbar}(E_f^0 - E_i^0)t'}$$

$$= \hbar\, \frac{e^{\eta t + \frac{i}{\hbar}(E_f^0 - E_i^0)t}}{E_i^0 - E_f^0 + i\eta\hbar}$$

The transition probability is

$$P_{i\to f}(t) = |\langle f|\hat{V}|i\rangle|^2\, \frac{e^{2\eta t}}{(E_i^0 - E_f^0)^2 + \eta^2\hbar^2}$$



Clearly only those states with $|E_f^0 - E_i^0| \lesssim \eta\hbar$ will contribute

$$\frac{dP}{dt} = \text{Total rate} = |\langle f|V|i\rangle|^2\, e^{2\eta t}\, \frac{2\eta\hbar}{(E_f^0 - E_i^0)^2 + (\eta\hbar)^2} \underset{\eta\to 0}{\Rightarrow} |\langle f|V|i\rangle|^2 \frac{2\pi}{\hbar}\delta(\Delta E)$$

$\Rightarrow$ the rate is

$$\Gamma_{i\to f} = \frac{2\pi}{\hbar} \, |\langle f|\hat{V}|i\rangle|^2 \, \delta(E_i^0 - E_f^0)$$

Harmonic Perturbations

Consider now the situation in which $\hat{V}(t)$ (up to an adiabatic switching on factor) is harmonic, i.e.

$$\hat{V}(t) = \frac{\hat{V}}{2} e^{\eta t} \left(e^{i\omega t} + e^{-i\omega t}\right)$$

$$\Rightarrow \quad P_{i\to f}(t) = |\langle f|\,\hat{U}(t)\,|i\rangle|^2 \equiv |\langle f|\psi_i(t)\rangle|^2$$

$$P_{i\to f}(t) \approx \left| \frac{1}{i\hbar} e^{-iE_f^0 \frac{t}{\hbar}} \int_{t_0}^{t} dt' \, \frac{e^{\eta t'}}{2} \langle f|\hat{V}|i\rangle \left[e^{i\omega t'} + e^{-i\omega t'}\right] e^{i\Delta E \frac{t'}{\hbar}} \right|^2$$

$$\Delta E = E_f^0 - E_i^0$$

$$\approx \left| \frac{1}{i\hbar} \int_{-\infty}^{t} dt' \, \frac{1}{2} \langle f|\hat{V}|i\rangle \left(e^{\eta t' + i\left(\omega + \frac{\Delta E}{\hbar}\right)t'} + e^{\eta t' + i\left(\frac{\Delta E}{\hbar} - \omega\right)t'} \right) \right|^2$$

$$= \frac{|\langle f|V|i\rangle|^2}{4\hbar^2} \left| \frac{e^{\eta t + i\left(\omega + \frac{\Delta E}{\hbar}\right)t}}{\eta + i\left(\omega + \frac{\Delta E}{\hbar}\right)} + \frac{e^{\eta t + i\left(\frac{\Delta E}{\hbar} - \omega\right)t}}{\eta + i\left(\frac{\Delta E}{\hbar} - \omega\right)} \right|^2$$

$$P_{i\to f}(t) = \frac{|\langle f|\hat{V}|i\rangle|^2}{4\hbar^2}\left\{ \frac{e^{2\eta t}}{\eta^2+\left(\omega+\frac{\Delta E}{\hbar}\right)^2} + \frac{e^{2\eta t}}{\eta^2+\left(\omega-\frac{\Delta E}{\hbar}\right)^2} + \right.$$

$$+ \frac{e^{2\eta t}\, e^{i2\omega t}}{\left(\eta+i\left(\frac{\Delta E}{\hbar}+\omega\right)\right)\left(\eta-i\left(\frac{\Delta E}{\hbar}-\omega\right)\right)} +$$

$$\left. + \frac{e^{2\eta t}\, e^{-i2\omega t}}{\left(\eta-i\left(\frac{\Delta E}{\hbar}+\omega\right)\right)\left(\eta+i\left(\frac{\Delta E}{\hbar}-\omega\right)\right)} \right\}$$

$$\Rightarrow \frac{dP_{i\to f}(t)}{dt} = \frac{|\langle f|\hat{V}|i\rangle|^2}{\cancel{4}_2\hbar^2}\left\{ \frac{\cancel{2}\eta\, e^{2\eta t}}{\eta^2+\left(\omega+\frac{\Delta E}{\hbar}\right)^2} + \frac{\cancel{2}\eta\, e^{2\eta t}}{\eta^2+\left(\omega-\frac{\Delta E}{\hbar}\right)^2} \right.$$

$$\left. + \frac{\cancel{2}(\eta+i\omega)\, e^{2\eta t+i2\omega t}}{\left(\eta+i\left(\frac{\Delta E}{\hbar}+\omega\right)\right)\left(\eta-i\left(\frac{\Delta E}{\hbar}-\omega\right)\right)} + \frac{\cancel{2}(\eta-i\omega)\, e^{2\eta t+i2\omega t}}{\left(\eta-i\left(\frac{\Delta E}{\hbar}+\omega\right)\right)\left(\eta+i\left(\frac{\Delta E}{\hbar}-\omega\right)\right)} \right\}$$

$$\frac{dP_{i\to f}(t)}{dt} = \frac{1}{2} e^{2\eta t}\, |\langle f|\hat{V}|i\rangle|^2 \left\{ \left[\frac{\eta}{(E_i^0-E_f^0+\hbar\omega)^2+(\eta\hbar)^2} + \right.\right.$$

$$\left. + \frac{\eta}{(E_i^0-E_f^0-\hbar\omega)^2+(\eta\hbar)^2} \right] (1-\cos 2\omega t)$$

$$\left. + \sin 2\omega t \left[\frac{E_i^0-E_f^0+\hbar\omega}{(E_i^0-E_f^0+\hbar\omega)^2+(\eta\hbar)^2} + \frac{E_i^0-E_f^0-\hbar\omega}{(E_i^0-E_f^0-\hbar\omega)^2+(\eta\hbar)^2} \right] \right\}$$

Clearly, as $\eta \to 0$ the first two terms become δ-functions which enforce the condition $\Delta E = \pm \hbar\omega$. The last two terms, on the other hand, oscillate very rapidly for $t \gg \frac{2\pi}{\omega}$ and hence average out to zero.

Thus the rate is

$$\Gamma_{0\to f} = \frac{2\pi}{\hbar} |\langle f|\hat{V}|i\rangle|^2 \frac{1}{4} \left[\delta(E_f^0 - E_i^0 + \hbar\omega) + \delta(E_f^0 - E_i^0 - \hbar\omega)\right]$$

Second Order Transitions

What happens if the process is not allowed to first order, (i.e. $\langle f|\hat{V}|i\rangle = 0$)? Clearly we must go to second order in $\hat{V}$. The second order correction is

$$\langle f | \psi_i(t)\rangle^{(2)} = \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \sum_n \langle f|\hat{V}|n\rangle \langle n|\hat{V}|i\rangle \times$$

$$e^{\eta t_1} \times e^{\frac{i}{\hbar}(E_f^0 - E_n^0)t_1} \; e^{\frac{i}{\hbar}(E_n^0 - E_i^0)t_2} \; e^{\eta t_2}$$

$$\underset{t_0 \to -\infty}{\approx} e^{-i(E_i^0 - E_f^0)\frac{t}{\hbar}} \frac{e^{2\eta t}}{E_i^0 - E_f^0 + 2i\eta\hbar} \sum_n \frac{\langle f|\hat{V}|n\rangle \langle n|\hat{V}|i\rangle}{E_i^0 - E_n^0 + i\eta\hbar}$$

Similar arguments tell us that, if $|f\rangle$ is part of a continuum of states, ⇒

$$\Gamma_{0\to f} \approx \frac{2\pi}{\hbar} \left| \sum_n \frac{\langle f|\hat{V}|n\rangle \langle n|\hat{V}|i\rangle}{E_i^0 - E_f^0 + i\eta\hbar} \right|^2 \delta(E_f^0 - E_i^0)$$

↑

"second order matrix element"

L10 Forward Scattering Amplitude

We will now consider the case in which we want to know the amplitude that the final state and the initial states are the same ("forward scattering")

Recall the relation between the states in the Schrödinger and interaction reps.

$$|\psi_s(t)\rangle = e^{-iH_0 t/\hbar} |\psi_I(t)\rangle$$

$$\Rightarrow \langle i|\psi_s(t)\rangle = e^{-iE_i^0 t/\hbar} \langle i|\psi_I(t)\rangle$$

To first order we have

$$|\psi_I(t)\rangle \approx |\psi_I(t_0)\rangle + \frac{1}{i\hbar}\int_{t_0}^{t} dt'\, H_I(t')\, |\psi_I(t_0)\rangle + \dots$$

Let the initial state be $|i\rangle = |\psi_I(t_0)\rangle = |\psi_s(t_0)\rangle$

The states $|\psi_I(t)\rangle$ obey

$$i\hbar \frac{d}{dt} |\psi_I(t)\rangle = H_I(t) |\psi_I(t)\rangle$$

$\Rightarrow$ $\langle i | \psi_I(t)\rangle$ obeys the equation:

$$i\hbar \frac{d}{dt} \langle i | \psi_I(t)\rangle = \langle i | H_I(t) | \psi_I(t)\rangle$$

$$= \sum_n \langle i | H_I(t) | n\rangle \langle n | \psi_I(t)\rangle$$

complete set of states

$$= \langle i | H_I(t) | i\rangle \langle i | \psi_I(t)\rangle +$$

$$+ \sum_{n\neq i} \langle i | H_I(t) | n\rangle \langle n | \psi_I(t)\rangle$$

$$\frac{1}{\langle i | \psi_I(t)\rangle} \frac{d}{dt} \langle i | \psi_I(t)\rangle = \frac{d}{dt} \ln \langle i | \psi_I(t)\rangle$$

$$i\hbar \frac{d}{dt} \ln \langle i | \psi_I(t)\rangle = \langle i | H_I(t) | i\rangle +$$

$$+ \sum_{n\neq i} \langle i | H_I(t) | n\rangle \frac{\langle n | \psi_I(t)\rangle}{\langle i | \psi_I(t)\rangle}$$

But $\langle n | \psi_I(t)\rangle = \frac{1}{i\hbar} \int_{t_0}^{t} dt' \langle n | H_I(t') | i\rangle$

$(n \neq i)$

$$\langle i | \psi_I(t)\rangle = 1 + \frac{1}{i\hbar} \int_{t_0}^{t} dt' \langle i | H_I(t') | i\rangle$$

$\Rightarrow$ to leading order we get

$$i\hbar \frac{d}{dt} \ln \langle i | \psi_I(t) \rangle = \langle i | H_I(t) | i \rangle +$$

$$+ \sum_{n \neq i} \frac{1}{i\hbar} \int_{t_0}^{t} dt' \, \langle i | H_I(t) | n \rangle \langle n | H_I(t') | i \rangle$$

$$+ \cdots$$

<u>Example</u> $\hat{V}(t) = e^{\eta t} \hat{V} \qquad (\eta \to 0)$

$$\hat{H}_I(t) = e^{i \hat{H}_0 t/\hbar} \, \hat{V}(t) \, e^{-i \hat{H}_0 t/\hbar}$$

$$i\hbar \frac{d}{dt} \ln \langle i | \psi_I(t) \rangle = e^{\eta t} \langle i | \hat{V} | i \rangle +$$

$$+ \sum_{n \neq i} \frac{1}{i\hbar} \int_{t_0}^{t} dt' \, \langle i | \hat{V}(t) | n \rangle \langle n | \hat{V}(t') | i \rangle e$$

$$i\hbar \frac{d}{dt} \ln \langle i | \psi_I(t) \rangle = \langle i | \hat{V} | i \rangle +$$

$$+ \sum_{n \neq i} \frac{| \langle i | \hat{V} | n \rangle |^2}{i \eta \hbar + E_i^0 - E_n^0} + \cdots$$

(a) <u>Discrete states:</u> set $\eta \to 0$

$$\Rightarrow i\hbar \frac{d}{dt} \ln \langle i | \psi_I(t) \rangle = \langle i | \hat{V} | i \rangle + \sum_{n \neq i} \frac{| \langle i | \hat{V} | n \rangle |^2}{E_i^0 - E_n^0}$$

Now $| \psi_S(t) \rangle = e^{-i H_0 \frac{t}{\hbar}} | \psi_I(t) \rangle$

$\Rightarrow \langle i | \psi_S(t) \rangle = e^{-i E_0 \frac{t}{\hbar}} \langle i | \psi_I(t) \rangle \Rightarrow$ we get

$$i\hbar \frac{d}{dt} \ln \langle i | \Psi_S(t) \rangle = E_i^0 + \langle i | \hat{V} | i \rangle + \sum_{i \neq n} \frac{|\langle i | \hat{V} | n \rangle|^2}{E_i^0 - E_n^0}$$

We recognize that the r.h.s. is the ~~exx~~ energy of state $|i\rangle$ corrected to 2^{nd} order in pt. theory

$$\Rightarrow \langle i | \Psi_S(t) \rangle = \langle i | \Psi_S(0) \rangle \, e^{-i E_i t/\hbar}$$

$$E_i = E_i^0 + \langle 0 | \hat{V} | i \rangle + \sum_{n \neq i} \frac{|\langle i | \hat{V} | n \rangle|^2}{E_i^0 - E_n^0} + \dots$$

(as it should!) Hence, for discrete states, we rotate the unperturbed states adiabatically into the perturbed states.

(b) Continuum of States $|n\rangle$ in a neighborhood of $|i\rangle$

$$\frac{1}{E_i^0 - E_n^0 + i\eta\hbar} = \frac{E_i^0 - E_n^0}{(E_i^0 - E_n^0)^2 + (\eta\hbar)^2} - \frac{i\eta\hbar}{(E_i^0 - E_n^0)^2 + (\eta\hbar)^2}$$

$$\equiv \mathcal{P} \frac{1}{E_i^0 - E_n^0} - i\pi \, \delta(E_i^0 - E_n^0)$$

$\mathcal{P}$: ppal value.

$$\lim_{\eta \to 0} \int dE_n^0 \frac{(E_i^0 - E_n^0)}{(E_i^0 - E_n^0)^2 + (\eta\hbar)^2} f(E_n^0) \equiv \mathcal{P} \int dE_n^0 \frac{f(E_n^0)}{E_i^0 - E_n^0}$$

$\Rightarrow$ we get

$$\sum_{n\neq i} \frac{|\langle i|\hat{V}|n\rangle|^2}{i\eta\hbar + E_i^0 - E_n^0} \equiv \mathcal{P} \sum_n{}' \frac{|\langle i|\hat{V}|n\rangle|^2}{E_i^0 - E_n^0}$$

$$- i\pi \sum_n{}' \delta(E_i^0 - E_n^0)\, |\langle i|\hat{V}|n\rangle|^2$$

Since $\Gamma_{i\to f} = \frac{2\pi}{\hbar} |\langle n|\hat{V}|i\rangle|^2 \delta(E_i^0 - E_n^0)$

$$\Rightarrow \pi \sum_n{}' |\langle i|\hat{V}|n\rangle|^2 \delta(E_i^0 - E_n^0) =$$

$$= \frac{\hbar}{2} \sum_n{}' \Gamma_{i\to n} \equiv \frac{\hbar}{2}\Gamma$$

total rate out of $|i\rangle$

$\Rightarrow$

$$i\hbar \frac{d}{dt} \ln\langle i|\psi_I(t)\rangle = \langle i|\hat{V}|i\rangle + \mathcal{P}\sum_n{}' \frac{|\langle i|\hat{V}|n\rangle|^2}{E_i^0 - E_n^0}$$

$$- i\frac{\hbar}{2}\Gamma$$

$$\Rightarrow E_i = E_i^0 + \mathcal{P}\sum_n{}' \frac{|\langle i|\hat{V}|n\rangle|^2}{E_i^0 - E_n^0}$$

("complex energy" $E_i - i\frac{\hbar\Gamma}{2}$)

but the state has a width $\frac{\hbar\Gamma}{2}$, i.e.

$$\langle i|\psi_S(t)\rangle \sim \langle i|\psi_S(0)\rangle\, e^{-iE_0\frac{t}{\hbar} - \frac{\Gamma t}{2}}$$

$$\Rightarrow |\langle i|\psi_S(t)\rangle|^2 \sim |\langle i|\psi_S(0)\rangle|^2\, e^{-\Gamma t}$$

rate of probab. decay.