There is another, somewhat more general way to test whether the adiabatic approximation is appropriate.

You saw in the first order result for

$$d_f(t) = \delta_{fi} - \frac{i}{\hbar}\int_0^t \underline{\langle f^0 | \underset{\sim}{H}'(t') | n^0 \rangle} \, e^{i\omega_{fn} t'} dt'$$

changes on a time scale τ

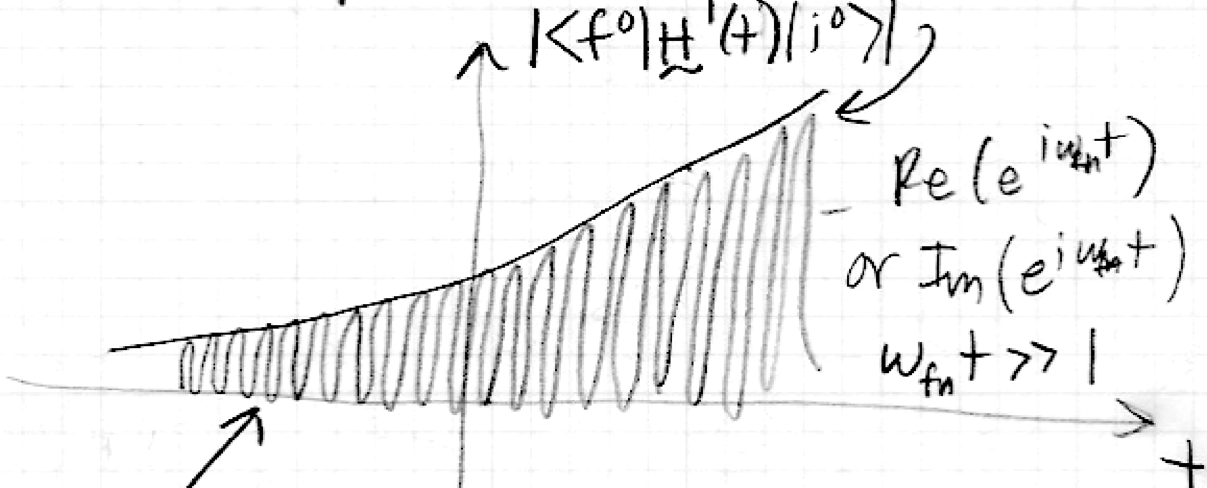
question is, how many cycles does "system" get through in time τ

when $\omega_{fn}\tau \gg 1$ system can respond to perturbation

$$\tau \gg \frac{1}{\omega_{fn}}$$

← choose minimum ω_{fn} to be sure

Pictorially:



tends to wash out integral; tends to allow system to react and stay in the eigenstate (which "tracks" as system changes")

Periodic Perturbation

$t \geq 0: \quad \underset{\sim}{H}'(t) = \underset{\sim}{H}' e^{-i\omega t}$ $\qquad \underset{\sim}{H}' \Rightarrow$ constant

$t < 0: \quad H'(t) = 0$ $\qquad$ occurs experimentally "AC" applied ...

$$d_f(t) = \left(\frac{-i}{\hbar}\right)\int_0^t \langle f^0|\underset{\sim}{H}'|\underset{\text{initial}}{i^0}\rangle e^{i\omega_{fi}t'}dt' \qquad \omega_{fi} = \frac{E_f^0 - E_i^0}{\hbar}$$

$f \neq i$

$$= \left(\frac{-i}{\hbar}\right)\langle f^0|\underset{\sim}{H}'|i^0\rangle \int_0^t dt' e^{i(\omega_{fi}-\omega)t'}$$

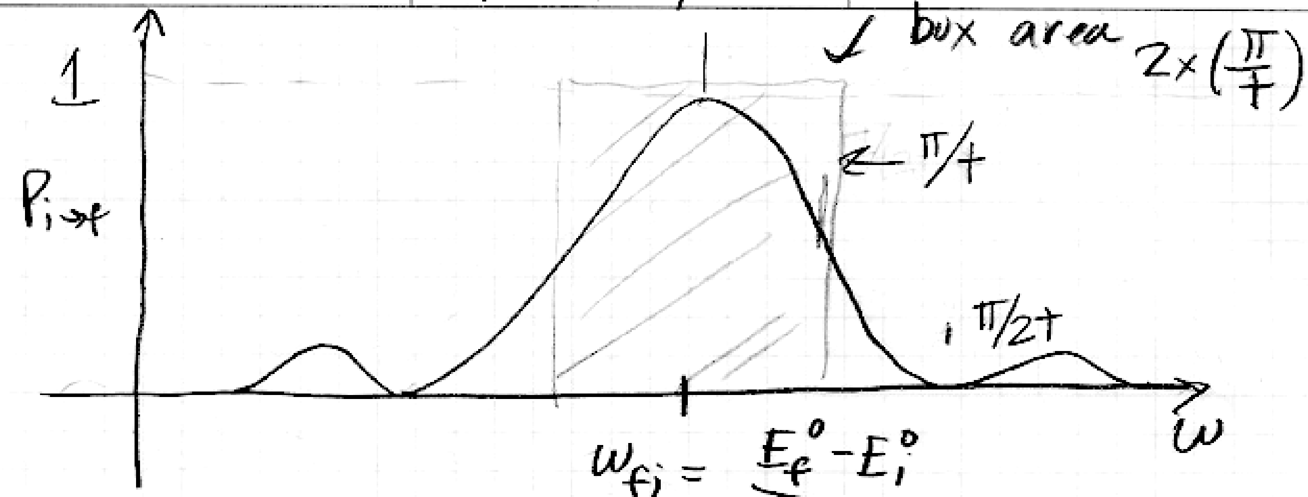
$$= \frac{-i}{\hbar}\langle f^0|\underset{\sim}{H}'|i^0\rangle \underbrace{\frac{e^{i(\omega_{fi}-\omega)t}-1}{i(\omega_{fi}-\omega)}}_{\frac{2e^{i(\omega_{fi}-\omega)t/2}}{\omega_{fi}-\omega}\underbrace{\left(\frac{e^{i(\omega_{fi}-\omega)t/2}-e^{-i(\omega_{fi}-\omega)t/2}}{2i}\right)}_{\sin[(\omega_{fi}-\omega)t/2]}}$$

$$P_{i\to f} = |d_f(t)|^2$$

$$= \frac{1}{\hbar^2}|\langle f^0|\underset{\sim}{H}'|i^0\rangle|^2 \cdot \underbrace{\left\{\frac{\sin\frac{(\omega_{fi}-\omega)t}{2}}{(\omega_{fi}-\omega)\cdot t/2}\right\}^2}_{\text{study this } [f(\omega)]^2} \times t^2$$

1) at $\omega_{fi} = \omega$, $= 1$

2) "width" $\left(\frac{\omega_{fi}-\omega}{2}\right)t \simeq \frac{\pi}{2}$, $\omega_{fi} - \omega \simeq \frac{\pi}{t}$



as $t \to \infty$, this function has area $\simeq 2\times\left(\frac{\pi}{t}\right)$, very peaked at $\omega = \omega_{fi}$

as $t \to \infty$

$$P_{i\to f} = \frac{2\pi}{\hbar^2} |\langle f^0 | \underset{\sim}{H}' | i^0 \rangle|^2 \frac{1}{\cancel{t}} \times \cancel{t^2}^{\,t}\, \delta(\omega - \omega_{fi})$$

or

$$R_{i\to f} = \text{rate of transition} = \frac{dP_{i\to f}}{dt} = \frac{2\pi}{\hbar^2} |\langle f^0 | \underset{\sim}{H}' | i^0 \rangle|^2 \delta(\omega - \omega_{fi})$$

1) $\delta(E - E_{fi}) = \delta(\hbar(\omega - \omega_{fi})) = \frac{1}{\hbar}\delta(\omega - \omega_{fi})$

2) sometimes degeneracy dN_f in the energy interval dE about E_{fi}

then $$\boxed{R_{i\to f} = \frac{2\pi}{\hbar} |\langle f^0 | \underset{\sim}{H}' | i^0 \rangle|^2 \delta(E - E_{fi})\, dN_f}$$

Fermi's Golden Rule (often integrate over E)

Higher Orders - "Pictures"

Usual "picture" → kets (+ bras) move as a function of time.

→ operators ($\underset{\sim}{X}$, $\mathcal{L}$, etc) are time-independent

("Schrödinger Picture")

Actually, though, only expectation values end up being measured. Could stick the time dependence on the operators!

How? Need a concept of the propagator

$$\underbrace{|\Psi_s(t_0)\rangle}_{\text{Schrödinger ket at } t=t_0} \xrightarrow[\text{forward in time}]{\text{lunge}} |\Psi_s(t)\rangle$$

(denote by subscript s)

could say: $|\Psi_s(t)\rangle = \underbrace{\underset{\sim}{U}_s(t,t_0)}_{\text{the propagator (operator)}}|\Psi_s(t_0)\rangle$

properties:

1) want $\langle\Psi_s(t)|\Psi_s(t)\rangle = \langle\Psi_s(t_0)|\Psi_s(t_0)\rangle = 1$

$$\langle\Psi_s(t_0)|\underbrace{\underset{\sim}{U}_s^\dagger(t,t_0)U_s(t,t_0)}_{=\underset{\sim}{\mathbb{1}}}|\Psi_s(t)\rangle = 1$$

"Unitary" $\underset{\sim}{U}^\dagger = \underset{\sim}{U}^{-1}$

2) composition: $\underset{\sim}{U}(t_3,t_2)\underset{\sim}{U}(t_2,t_1) = \underset{\sim}{U}(t_3,t_1)$

3) initial condition: $\underset{\sim}{U}(t,t) = \underset{\sim}{\mathbb{1}}$

4) round trip $\underset{\sim}{U}(t_2,t_1) = \underset{\sim}{U}^{-1}(t_1,t_2)$
$= \underset{\sim}{U}^{\dagger}(t_1,t_2)$ unitary

5) differential equation

$$i\hbar \frac{d}{dt}\left[|\psi_s(t)\rangle\right] = \underset{\sim}{H}_s |\psi_s(t)\rangle$$

"Schrödinger Picture" is what subscript means

$$i\hbar \frac{d}{dt} \underset{\sim}{U}_s(t,t_0) \underbrace{|\psi_s(t_0)\rangle}_{\text{no time dependence.}} = \underset{\sim}{H}_s \underset{\sim}{U}_s(t,t_0) |\psi_s(t_0)\rangle$$

so $$i\hbar \frac{d}{dt} \underset{\sim}{U}_s = \underset{\sim}{H}_s \underset{\sim}{U}_s$$ differential operator equation

most easily solved when $\psi_s(t_0)$ are eigenstates of a static (time independent) hamiltonian, say, $\underset{\sim}{H}_s^0$:

$$\underset{\sim}{H}_s^0 |\psi_s(t_0)\rangle = \underset{\sim}{H}_s^0 |n_s^0\rangle = E_n^0 |n_s^0\rangle$$

since $\underset{\sim}{U}_s(t_0,t_0) = \underset{\sim}{\mathbb{1}}$

$$i\hbar \frac{d}{dt} \underset{\sim}{U}_s(t,t_0)\Big|_{t_0} = \begin{pmatrix} E_1^0 & 0 & 0 & \cdots \\ 0 & E_2^0 & 0 & \\ 0 & 0 & E_3^0 & \\ \vdots & \vdots & & \ddots \end{pmatrix}$$

$$\underset{\sim}{U}_s(t,t_0) = \begin{pmatrix} e^{\frac{-iE_1^0}{\hbar}(t-t_0)} & 0 & 0 & \cdots \\ 0 & e^{\frac{-iE_2^0}{\hbar}(t-t_0)} & 0 & \\ 0 & 0 & e^{\frac{-iE_3^0}{\hbar}(t-t_0)} & \\ \vdots & \vdots & & \end{pmatrix}$$

$$= e^{\frac{-i\underset{\sim}{H}_s^0}{\hbar}(t-t_0)}$$ imaged in the basis of eigenkets of $\underset{\sim}{H}_s^0$.

The "Picture" Concept

"Schrödinger" Observable $\underset{\sim}{\Omega}_s$ (static in time)

$$\langle\psi_s(t)|\underset{\sim}{\Omega}_s|\psi_s(t)\rangle = \underbrace{\langle\psi_s(t_0)|}_{\text{static bra}}\underbrace{\underset{\sim}{U}_s^{\dagger}(t,t_0)\underset{\sim}{\Omega}_s\underset{\sim}{U}_s(t,t_0)}_{\text{could say, the operator moves.}}\underbrace{|\psi_s(t_0)\rangle}_{\text{static ket}}$$

The "Heisenberg" Picture is:

$$\underset{\sim}{\Omega}_H = \underset{\sim}{U}_s^{\dagger}(t,t_0)\underset{\sim}{\Omega}_s\underset{\sim}{U}_s(t,t_0)$$

very time dependent

usually pretty static like $\hat{X}$, $\hat{P}$

$$|\psi_H\rangle = |\psi_s(t_0)\rangle = \underset{\sim}{U}_s^{-1}(t,t_0)|\psi_s(t)\rangle$$

$$|\psi_H\rangle = \underset{\sim}{U}_s^{\dagger}(t,t_0)|\psi_s(t)\rangle$$

usually pretty static.

very time dependent

The "Interaction" Picture

$$\underset{\sim}{H}_s = \underset{\sim}{H}_s^0 + \underset{\sim}{H}_s^1(t)$$

but work in the picture that would be Heisenberg if $\underset{\sim}{H}_s^1(t) = 0$.

when $\underset{\sim}{H}_s^1(t) \neq 0$, this is called the Interaction Picture:

$$|\psi_I(t)\rangle = \underset{\sim}{U}_s^{0\dagger}(t,t_0)|\psi_s(t)\rangle \quad \left\{\begin{matrix}\text{when } \underset{\sim}{H}_s^1(t)=0 \\ = |\psi_s(t_0)\rangle\end{matrix}\right\}$$

$$i\hbar\frac{d}{dt}|\psi_I(t)\rangle = \underline{i\hbar\frac{d\underset{\sim}{U}_s^{0\dagger}}{dt}}|\psi_s\rangle + \underline{i\hbar\underset{\sim}{U}_s^{0\dagger}\frac{d}{dt}|\psi_s\rangle}$$

$$i\hbar\frac{d}{dt}\underset{\sim}{U}_s^0 = \underset{\sim}{H}_s^0\underset{\sim}{U}_s^0 \qquad \text{dagger it all!}$$

$$-i\hbar\frac{d}{dt}\underset{\sim}{U}_s^{0\dagger} = (\underset{\sim}{H}_s^0\underset{\sim}{U}_s^0)^\dagger = \underset{\sim}{U}_s^{0\dagger}\underset{\sim}{H}_s^{0\dagger} = \underset{\sim}{U}_s^{0\dagger}\underset{\sim}{H}_s^0$$

hermitian

$$\underset{\sim}{U}_s^{0\dagger}(\underset{\sim}{H}_s^0 + \underset{\sim}{H}_s^1(t))|\psi_s\rangle$$

$$= \underset{\sim}{U}_s^{0\dagger}(\underset{\sim}{H}_s^0 + \underset{\sim}{H}_s^1(t))\underset{\sim}{U}_s^0|\psi_I\rangle$$

$$i\hbar\frac{d}{dt}|\psi_I\rangle = \left[-\underset{\sim}{U}_s^{0\dagger}\underset{\sim}{H}_s^0\underset{\sim}{U}_s^0 + \underset{\sim}{U}_s^{0\dagger}(\cancel{\underset{\sim}{H}_s^0} + \underset{\sim}{H}_s^1(t))\underset{\sim}{U}_s^0\right]|\psi_I\rangle$$

$$i\hbar\frac{d}{dt}|\psi_I\rangle = \Big(\underbrace{\underset{\sim}{U}_s^{0\dagger}\underset{\sim}{H}_s^1(t)\underset{\sim}{U}_s^0}_{\equiv \underset{\sim}{H}_I^1(t)}\Big)|\psi_I\rangle$$

$$\boxed{i\hbar\frac{d}{dt}|\psi_I\rangle = \underset{\sim}{H}_I^1(t)|\psi_I\rangle}$$

Schrödinger-like equation

Solutions

(A) $\underset{\sim}{H}'_I(t)$ constant in time $\Rightarrow$ eigenvalue situation.

(B) $\underset{\sim}{H}'_I(t)$ not constant in time, but commutes with itself always: $[\underset{\sim}{H}'_I(t_1), \underset{\sim}{H}'_I(t_2)] = 0$ for all t_1, t_2

$\rightarrow$ diagonalize, then integrate.

(C) $[\underset{\sim}{H}'_I(t_1), \underset{\sim}{H}'_I(t_2)] \neq 0$ (quite common)

$$\Rightarrow \underset{\sim}{U}_I(t, t_0) = \underset{\sim}{1} - \frac{i}{\hbar}\int_{t_0}^{t} \underset{\sim}{H}'_I(t')\underset{\sim}{U}_I(t', t_0)\,dt'$$

solves

(a) $|\psi_I(t)\rangle = \underset{\sim}{U}_I(t, t_0)|\psi_I(t_0)\rangle$

$$i\hbar\frac{d}{dt}|\psi_I(t)\rangle = \underset{\sim}{H}'_I(t)|\psi_I(t)\rangle = \underset{\sim}{H}'_I(t)\underset{\sim}{U}(t, t_0)|\psi_I(t_0)\rangle$$

$$= i\hbar\frac{d}{dt}\underset{\sim}{U}_I(t, t_0)|\psi_I(t_0)\rangle + i\hbar\underset{\sim}{U}_I\underbrace{\frac{d|\psi_I(t_0)\rangle}{dt}}_{0}$$

$$i\hbar\frac{d\underset{\sim}{U}_I}{dt} = \underset{\sim}{H}'_I(t)\underset{\sim}{U}_I$$

(b) $\Rightarrow$ differentiate, multiply by $i\hbar$

$$i\hbar\frac{d\underset{\sim}{U}_I(t, t_0)}{dt} = \underset{\sim}{H}'_I(t)\underset{\sim}{U}_I(t, t_0)$$

The equation $\Rightarrow$ is terrific for iterative solution. The result looks like an exponential!

First guess: $\underset{\sim}{U}_I^0(t,t_0) = \underset{\sim}{1}$ $\left(\begin{matrix}\text{true as}\\ \underset{\sim}{H}_I'(t')\to 0\end{matrix}\right)$.

Plug back into the integral equation:

$$\underset{\sim}{U}_I^1(t,t_0) = \underset{\sim}{1} - \frac{i}{\hbar}\int_{t_0}^{t} \underset{\sim}{H}_I'(t')\,\underset{\sim}{U}_I^0(t',t_0)\,dt'$$

$$\underset{\sim}{U}_I^1(t,t_0) = \underset{\sim}{1} - \frac{i}{\hbar}\int_{t_0}^{t} \underset{\sim}{H}_I'(t')\,dt' \qquad \underline{\text{first}}\text{ order}$$

Plug back into the integral equation:

$$\underset{\sim}{U}_I^2(t,t_0) = \underset{\sim}{1} - \frac{i}{\hbar}\int_{t_0}^{t} \underset{\sim}{H}_I'(t')\left(\underset{\sim}{1} - \frac{i}{\hbar}\int_{t_0}^{t'} \underset{\sim}{H}_I'(t'')\,dt''\right)dt'$$

$$= \underset{\sim}{1} - \frac{i}{\hbar}\int_{t_0}^{t} \underset{\sim}{H}_I'(t')\,dt' + \left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^{t}\int_{t_0}^{t'} \underset{\sim}{H}_I'(t')\,\underset{\sim}{H}_I'(t'')\,dt'\,dt''$$

finally,

$$U_I(t,t_0) = \underset{\sim}{1} - \frac{i}{\hbar}\int_{t_0}^{t} \underset{\sim}{H}_I'(t')\,dt' + \left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^{t}\int_{t_0}^{t'} \underset{\sim}{H}_I'(t')\,\underset{\sim}{H}_I'(t'')\,dt'\,dt''$$

$$+ \left(\frac{-i}{\hbar}\right)^3 \int_{t_0}^{t}\int_{t_0}^{t'}\int_{t_0}^{t''} \underbrace{\underset{\sim}{H}_I'(t')\,\underset{\sim}{H}_I'(t'')\,\underset{\sim}{H}_I'(t''')}\,dt'\,dt''\,dt''' + \ldots$$

note: order important since no guarantee $[\underset{\sim}{H}_I'(t_1), \underset{\sim}{H}_I'(t_2)] = 0$