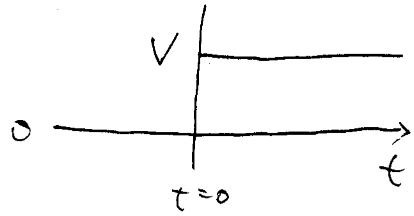
Quantum Mechanics – II

May 17, 2010

$\boxed{\text{Fermi Golden Rule}}$

Conside the perturbation



The lowest order term in the transition amplitude for $i \neq f$ is

$$\frac{-i}{\hbar}\int_0^t dt' \langle f | V_I | i \rangle = \frac{-i}{\hbar}\int_0^t dt' \langle f | e^{\frac{iH_0 t'}{\hbar}} V e^{\frac{-iH_0 t'}{\hbar}} | i \rangle$$

$$= \frac{-i}{\hbar}\int_0^t dt' e^{\frac{-i(E_i - E_f)t'}{\hbar}} \langle f \underbrace{| V | i \rangle}_{\text{III } V_{fi}}$$

$$= \frac{e^{\frac{-i(E_i-E_f)t}{\hbar}} - 1}{E_i - E_f} V_{fi}$$

Denoting $\Delta E = E_i - E_f$, then the amplitude is

$$\mathcal{A} = \frac{e^{-i\frac{\Delta E t}{\hbar}} - 1}{\Delta E} V_{fi} = e^{-\frac{i\Delta E t}{2\hbar}} \frac{\left(e^{-i\frac{\Delta E t}{2\hbar}} - e^{+i\frac{\Delta E t}{2\hbar}}\right)}{\Delta E} V_{fi} = \frac{-2i}{\Delta E} e^{\frac{-i\Delta E t}{2\hbar}} \sin\frac{\Delta E t}{2\hbar}$$

$$\Rightarrow P(i \to f, t) = |\mathcal{A}|^2 = 4 \frac{\sin^2 \frac{\Delta E t}{2\hbar}}{(\Delta E)^2} |V_{fi}|^2$$

- The probability is more and more peaked at $\Delta E = 0$ as the time goes on. (see the plots)
- The range in ΔE in size decreases as $\Delta E \sim \frac{\hbar}{t}$

$\Rightarrow$ the so called "Energy – Time Uncertainty" principle.

But this is not as fundamental as the X–P uncertainty principle

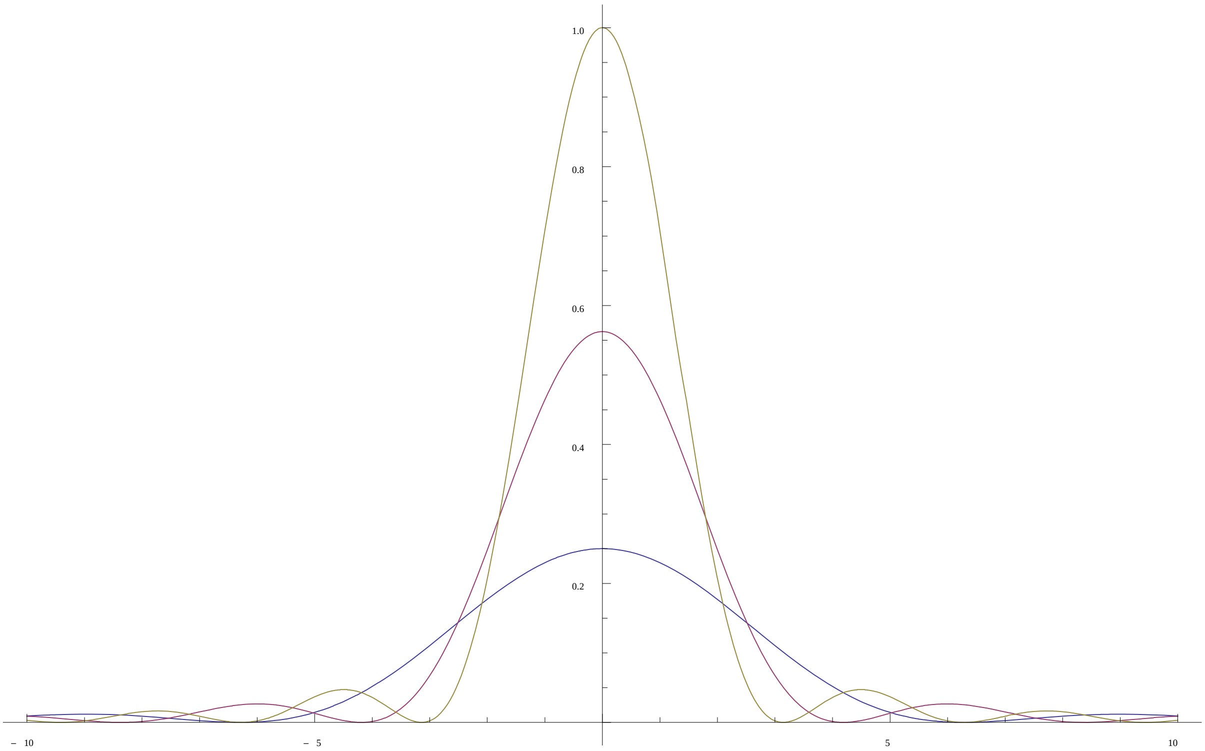
t is not even an operator in QM!

(Energy is not conserved when you turn on the perturbation)

In[1]:= Prob[{e_, t_}] := Sin[e * t / 2]^2 / e^2

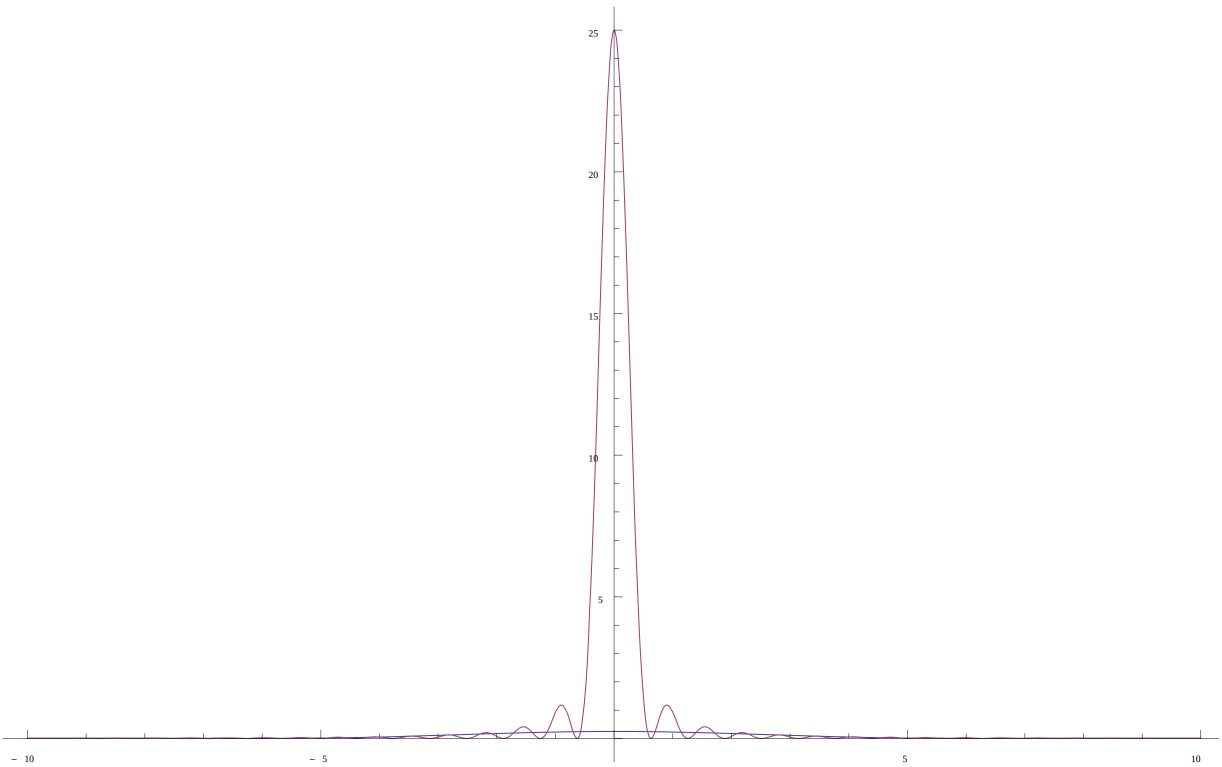
In[7]:= Plot[{Prob[{x, 1.0}], Prob[{x, 1.5}], Prob[{x, 2.0}]}, {x, -10, 10}, PlotRange → All]

Out[7]=



In[9]:= Plot[{Prob[{x, 1.0}], Prob[{x, 10.0}]}, {x, -10, 10}, PlotRange → All]

Out[9]=



* We are often interested in the behavior when t is large.
* Rate of the transition (the probability per unit time)

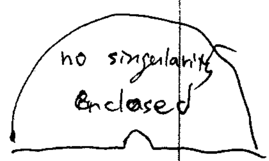
$$\Gamma(i\to f) = \lim_{t\to\infty} \frac{P(i\to f, t)}{t} = \lim_{t\to\infty} 4\, \frac{\sin^2 \frac{\Delta E t}{2\hbar}}{t\,(\Delta E)^2} |V_{fi}|^2$$

$$\boxed{\Gamma(i\to f) = \frac{2\pi}{\hbar}\,\delta(E_f - E_i)\,|V_{fi}|^2}$$ (Fermi's Golden rule)

To see it, we caculate its area

$$\frac{4}{t}\int_{-\infty}^{\infty} d(\Delta E)\, \frac{\sin^2\frac{\Delta E t}{2\hbar}}{(\Delta E)^2} \overset{x=\frac{\Delta E t}{2\hbar}}{=} \frac{4}{t}\int_{-\infty}^{\infty}\left(\frac{2\hbar}{t}\right)dx \left(\frac{t}{2\hbar}\right)^2 \frac{\sin^2 x}{x^2}$$

$$= \frac{2}{\hbar}\underbrace{\int_{-\infty}^{\infty} dx\, \frac{\sin^2 x}{x^2}}_{\pi}$$



Lets go to the next order

$$\langle f| \left(\frac{-i}{\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt''\, V_I(t')\, V_I(t'')\, |i\rangle$$

$$= \sum_m \left(\frac{-i}{\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt'' \langle f| V_I(t') |m\rangle\langle m| V_I(t'')|i\rangle$$

$$= \sum_m \left(\frac{-i}{\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt''\, e^{\frac{i(E_f-E_m)t'}{\hbar}} V_{fm}\, e^{\frac{i(E_m-E_i)t''}{\hbar}} V_{mi}$$

$$= \sum_m \frac{V_{fm}V_{mi}}{E_m - E_i}\left[\frac{e^{\frac{it}{\hbar}(E_f-E_i)} - 1}{E_f - E_i} - \frac{e^{\frac{it}{\hbar}(E_f-E_m)} - 1}{E_f - E_m}\right]$$

The first term has the same large t behavior as in the 1st order perturbation when $\Delta E \to 0$, But the 2nd term doesn't grow (except $E_m = E_i$, which we will deal later)

$$\Rightarrow \Gamma(i\to f, t) = \frac{2\pi}{\hbar}\,\delta(E_i - E_f)\left| V_{fi} + \sum_m \frac{V_{fm}V_{mi}}{E_i - E_m}\right|^2$$

Harmonic Perturbation

$$V(t) = 2\hat{V}_0 \cos\omega t$$

First order perturbation.

$$\left(\frac{-i}{\hbar}\right)\int_0^t dt' \langle f | V_I(t') | i \rangle = \left(\frac{-i}{\hbar}\right)\int_0^t dt' \langle f | e^{\frac{iH_0 t'}{\hbar}} 2\hat{V}_0 \cos\omega t' e^{-\frac{iH_0 t'}{\hbar}} | i \rangle$$

$$= \frac{-i}{\hbar}\int_0^t dt' e^{\frac{-i(E_i - E_f)t'}{\hbar}} (e^{i\omega t'} + e^{-i\omega t'}) \langle f | \hat{V}_0 | i \rangle$$

$$= \langle f | \hat{V}_0 | i \rangle \left[\underbrace{\frac{e^{\frac{-i}{\hbar}t(E_i - E_f - \omega\hbar)} - 1}{E_i - E_f - \omega\hbar}}_{e^{i\omega t} \text{ emitting a quanta } \hbar\omega} + \underbrace{\frac{e^{\frac{-i}{\hbar}t(E_i - E_f + \hbar\omega)} - 1}{E_i - E_f + \hbar\omega}}_{e^{-i\omega t} \text{ absorbing a quanta } \hbar\omega} \right]$$

$e^{i\omega t}$ emitting a quanta $\hbar\omega$ / $e^{-i\omega t}$ absorbing a quanta $\hbar\omega$

Similarly, we have

$$\Gamma(i \to f) = \frac{2\pi}{\hbar}\left[\delta(E_i - E_f - \omega\hbar) + \delta(E_i - E_f + \omega\hbar)\right] |V_{fi}|^2$$

☆ There is no time translation inv. but a discrete time translation inv. $t \to t + \frac{2\pi}{\omega}$ (just like $x \to x + a$ in a periodic lattice with lattice spacing a, which conserves the momentum modulo $\frac{2\pi\hbar}{a}$), the energy is conserved modulo $\hbar\omega$

☆ 2nd perturbation : $E_f = E_i \pm 2\hbar\omega$, E_i .

3rd perturbation : $E_f = E_i \pm 3\hbar\omega$, ---

Relationship to the time independent perturbation theory

Consider the case $f = i$

$$\langle \underbrace{i^{(0)}}_{\text{unperturbed state}} | U_I(t) | i^{(0)} \rangle = \langle i^{(0)} | e^{+\frac{iH_0 t}{\hbar}} \underbrace{U(t)}_{\text{full time evolution by } H} | i^{(0)} \rangle = \sum_m \langle i^{(0)} | e^{\frac{iH_0 t}{\hbar}} \underbrace{|m\rangle}_{\text{full eigenstate by } H} \langle m | U(t) | i^{(0)} \rangle$$

$$= e^{\frac{iE_i^{(0)} t}{\hbar}} \sum_m |\langle i^{(0)} | m \rangle|^2 e^{-\frac{iE_m t}{\hbar}} \quad \longrightarrow \text{full eigen energy of } H$$

We separate $m = i$ and $m \neq i$, and denote the WF normalization $\sqrt{Z_i} \equiv \langle i^{(0)} | i \rangle$

$$= Z_i e^{-\frac{i}{\hbar} t (E_i - E_i^{(0)})} + \sum_{m \neq i} |\langle i^{(0)} | m \rangle|^2 e^{-i \frac{(E_m - E_i^{(0)})}{\hbar} t}$$

since $E_i = E_i^{(0)} + \underset{\sim O(V)}{\Delta_i^{(1)}} + \underset{\sim O(V^2)}{\Delta_i^{(2)}} + \cdots$, $\underset{\sim O(V)}{\langle i^{(0)} | m \rangle}$

$$= Z_i \left[1 - \frac{i}{\hbar} (\Delta_i^{(1)} + \Delta_i^{(2)}) t + \frac{1}{2!} \left(\frac{-i}{\hbar}\right)^2 (\Delta_i^{(1)} t)^2 \right]$$

$$+ \sum_{m \neq i} \underbrace{|\langle i^{(0)} | m \rangle|^2}_{} e^{-\frac{i}{\hbar} (E_m^{(0)} - E_i^{(0)}) t} + O(V^3)$$

since $O(V^2)$, we only need unperturbed one

Now from the Dyson series,

$$\langle i^{(0)} | U_I(t) | i^{(0)} \rangle = 1 - \frac{i}{\hbar} \int_0^t \overbrace{\langle i^{(0)} | V | i^{(0)} \rangle}^{V_{ii}} dt'$$

$$+ \left(\frac{-i}{\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt'' \Big[\langle i^{(0)} | V_I(t') | i^{(0)} \rangle \langle i^{(0)} | V_I(t'') | i^{(0)} \rangle$$

$$+ \sum_{m \neq i} \langle i^{(0)} | e^{\frac{iH_0 t'}{\hbar}} V e^{-\frac{iH_0 t'}{\hbar}} | m^{(0)} \rangle \langle m^{(0)} | e^{\frac{iH_0 t''}{\hbar}} V e^{-\frac{iH_0 t''}{\hbar}} | i^{(0)} \rangle \Big]$$

$$\simeq 1 - \frac{i}{\hbar} V_{ii} t + \frac{1}{2} \left(\frac{-i}{\hbar}\right)^2 V_{ii}^2 t^2 + \left(\frac{-i}{\hbar}\right) \sum_{m \neq i} \frac{|V_{im}|^2}{E_i^{(0)} - E_m^{(0)}} t$$

$$- \sum_{m \neq i} \frac{|V_{im}|^2}{(E_i^{(0)} - E_m^{(0)})^2} + \sum_{m \neq i} \frac{|V_{im}|^2}{(E_i^{(0)} - E_m^{(0)})^2} e^{-\frac{i}{\hbar} t (E_m^{(0)} - E_i^{(0)})}$$

By comparing these two expression, we can identify that,

$$\Rightarrow \quad Z_i = 1 - \sum_{m \neq i} \frac{|V_{im}|^2}{(E_i^{(0)} - E_m^{(0)})^2}$$

$$\Delta_i^{(1)} = V_{ii}$$

$$\Delta_i^{(2)} = \sum_{m \neq i} \frac{|V_{im}|^2}{E_i^{(0)} - E_m^{(0)}}$$

also $|i\rangle = |i^{(0)}\rangle + \sum_{m \neq i} \frac{V_{mi}}{E_i^{(0)} - E_m^{(0)}} |m^0\rangle$

$\Rightarrow$ All agree with the time-independent result.

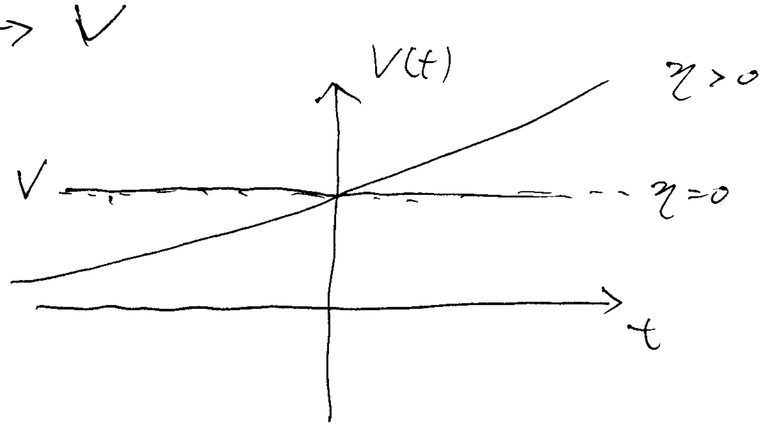
※ Dyson series contains all information we have obtained from the time-independent perturbation theory!!

$\boxed{\text{Energy shift and decay width}}$

One way to deal with the singularity in $\frac{1}{E_i - E_m}$ term is to gradually turn on the perturbation from $t = -\infty$

$V(t) = Ve^{\eta t}$, so when $t \to -\infty$ $V(t) = 0$

At the end of the calculation, we set $\eta \to 0$, such that $V(t) \to V$



One can repeat the previous discussion by replacing

$$V \rightarrow V e^{\eta t} \quad \text{and set } \eta \rightarrow 0 \text{ at the end.}$$

or $$e^{-\frac{i}{\hbar}(E_i - E_f)t} \rightarrow e^{-\frac{i}{\hbar}(E_i - E_f + i\hbar\eta)}$$

In summary, just replace the $\dfrac{1}{E_i - E_f}$ by $\dfrac{1}{E_i - E_f + i\hbar\eta}$

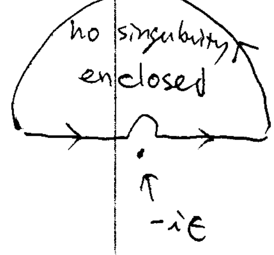
$$\Rightarrow E_i = E_i^{(0)} + V_{ii} + \sum_{m \neq i} \frac{|V_{im}|^2}{E_i^{(0)} - E_m^{(0)} + i\hbar\eta}$$

$$\Rightarrow Z_i = 1 - \sum_{m \neq i} \frac{|V_{im}|^2}{|E_i^{(0)} - E_m^{(0)} + i\hbar\eta|^2}$$ now is a complex number

The physical meaning is more clean compared to Sakurai.

As one knows

$$\lim_{\epsilon \to 0} \frac{1}{x + i\epsilon} = \underbrace{P\left(\frac{1}{x}\right)}_{\text{principle value}} - i\pi\delta(x)$$ can be seen from



(the face value except at the singularity)

Therefore

$$E_i = E_i^{(0)} + V_{ii} + P\left(\sum_{m \neq i} \frac{|V_{mi}|^2}{E_i^{(0)} - E_m^{(0)}}\right) - i\pi \sum_{m \neq i} |V_{mi}|^2 \delta(E_i^{(0)} - E_m^{(0)})$$

The full time evolution of $|i\rangle$ (the full eigenvector) is

$$e^{-\frac{i}{\hbar}E_i t}, \quad |i(t)\rangle = e^{-\frac{i}{\hbar}E_i t}|i(0)\rangle$$

The probability, at $t = t$, the state stays at $|i\rangle$ is.

$$P(i \to i, t) = \cancel{\exp}\,|\langle i(t)|i(0)\rangle|^2$$
$$= \exp\left[-\frac{2\pi}{\hbar} \sum_{m \neq i} |V_{mi}|^2 \delta(E_i^{(0)} - E_m^{(0)})\, t\right]$$

define $\Gamma_i = 2\pi \sum_{m \neq i} |V_{mi}|^2 \, \delta(E_i^{(0)} - E_m^{(0)})$

it is the decay width.

And the mean lift time is

$$\tau_i \equiv \frac{\hbar}{\Gamma_i}$$

- This Prob($i \to i$) descreasing is compensated by the growth in $m \neq i$ states.
- Prob sum is still 1 (conserved).