Phys 506 lecture 29: Time dependent perturbation theory

1 Interaction picture review

Our general interaction picture formalism showed

$$|\psi_s(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}_0(t-t_0)}\hat{U}_I\left(t,t_0\right)|\psi_s\left(t_0\right)\rangle$$
$$\hat{U}_I\left(t,t_0\right) = Te^{-\frac{i}{\hbar}\int_{t_0}^{t}\hat{V}_I(t')dt'} = 1-\frac{i}{\hbar}\int_{t_0}^{t}\hat{V}_I\left(t'\right)dt' + \left(\frac{-i}{\hbar}\right)^2\int_{t_0}^{t}dt_1\int_{t_0}^{t}dt_2\,\hat{V}_I(t_1)\hat{V}_I(t_2)+\cdots$$

Then the probability to have a transition from state$|i\rangle$ at t_0 to state $\langle f|$ at time t is

$$P_{f\leftarrow i}(t) = \left|\langle f|e^{\frac{-i}{\hbar}\hat{H}_0(t-t_0)}\hat{U}_I(t,t_0)|i\rangle\right|^2$$

If $\langle f|$ and $|i\rangle$ are eigenstates of $\hat{H}_0$ then $\langle f|e^{-\frac{i}{\hbar}\hat{H}_0(t-t_0)} = e^{-\frac{i}{\hbar}E_f(t-t_0)}\langle f|$ is a phase whose modulus squared $=1$, so

$$\begin{aligned}P_{n\leftarrow m}(t) &= \left|{}_0\langle n|\hat{U}_I\left(t,t_0\right)|m\rangle_0\right|^2\\ &= \left|{}_0\langle n|\left(1-\frac{i}{\hbar}\int_0^t dt'\hat{V}_I(t')+\cdots\right)|m\rangle_0\right|^2\\ &= \left|\delta_{nm}-\frac{i}{\hbar}{}_0\langle n|\int_{t_0}^{t}e^{\frac{i}{\hbar}\hat{H}_0(t-t_0)}\hat{V}\left(t_1\right)e^{-\frac{i}{\hbar}\hat{H}(t_1-t_0)}|m\rangle_0+\cdots\right|^2.\end{aligned}$$

2 Perturbation theory

Define $\omega_{nm} = \left(E_n^0 - E_m^0\right)/\hbar$, then the lowest order approximation, called the first Born approximation is

$$\begin{aligned}P_{n\leftarrow m}(t) &\approx \left|\delta_{nm}-\frac{i}{\hbar}\int_{t_0}^{t}e^{iw_{nm}(t_1-t_0)}{}_0\langle n|\hat{V}(t_1)|m\rangle_0 dt_1\right|^2\\ &= \left|\delta_{nm}-\frac{i}{\hbar}\int_{t_0}^{t}dt_1 e^{iw_{nm}(t_1-t_0)}V_{nm}\left(t_1\right)\right|^2.\end{aligned}$$

So, if $n\neq m$, we have that

$$\boxed{P_{\substack{n\leftarrow m\\ n\neq m}}(t) = \frac{1}{\hbar^2}\left|\int_{t_0}^{t}dt_1 e^{iw_{nm}(t_1-t_0)}V_{nm}\left(t_1\right)\right|^2}$$

3 Harmonic perturbation

When the potential takes the form

$$\hat{V}(t) = e^{i\Omega t}\hat{a}^{\dagger} + e^{-i\Omega t}\hat{a}, \quad \Omega > 0 = \text{ driving frequency and } \hat{a} \text{ is any operator}$$

we have what is called a harmonic perturbation. Assume $a_{nm} = {}_0\langle n|\hat{a}|m\rangle_0 \neq 0$ and $t_0 = 0$, then

$$\begin{aligned}
P_{\substack{n\leftarrow m\\ n\neq m}}(t) &= \frac{1}{\hbar^2}\left|\int_0^t dt_1 e^{iw_{nm}t_1}\left(a_{nm}e^{-i\Omega t_1} + a_{nm}^* e^{i\Omega t_1}\right)\right|^2 \\
&= \frac{1}{\hbar^2}\left|\frac{a_{nm}}{i\left(w_{nm}-\Omega\right)}\left(e^{i(w_{nm}-\Omega)t}-1\right) + \frac{a_{nm}^*}{i\left(w_{nm}+\Omega\right)}\left(e^{i(w_{nm}+\Omega)t}-1\right)\right|^2 \\
&= \frac{1}{\hbar^2}\left\{\frac{|a_{nm}|^2}{\left(w_{nm}-\Omega\right)^2}2\left(1-\cos\left(w_{nm}-\Omega\right)t\right)\right. \\
&\left. + \frac{|a_{nm}|^2}{\left(w_{nm}+\Omega\right)^2}2\left(1-\cos\left(w_{nm}-\Omega\right)t\right) + \text{ cross terms }\right\} \\
&= \frac{4}{\hbar^2}|a_{nm}|^2\left[\frac{\sin^2\left(w_{nm}-\Omega\right)\frac{t}{2}}{\left(w_{nm}-\Omega\right)^2} + \frac{\sin^2(w_{nm}+\Omega)\frac{t}{2}}{\left(w_{nm}+\Omega\right)^2} + \cos\Omega\right].
\end{aligned}$$

The first term is large if $\omega_{mn} > 0$ and $\omega_{nm} \approx \Omega$, while the second term is large if $\omega_{nm} < 0$ and $\omega_{nm} \approx -\Omega$. Both conditions are called resonance.

$$w_{nm} \to \Omega \qquad E_n = E_m + \hbar\Omega \qquad \text{stimulated absorption}$$

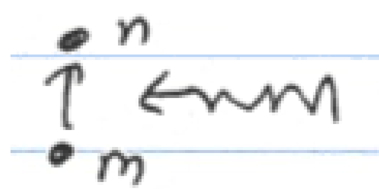

Figure 1: Figure displaying how a photon of energy ω_{nm} can be absorbed and excite from the lower state m to the upper state n. This is called stimulated absorption.

$$-w_{nm} \to \Omega \qquad E_n = E_m - \hbar\Omega \qquad \text{stimulated emission}$$

Accuracy: expect first Born to be accurate for $P_{n\leftarrow m} \ll 1$. The worst case is on resonance where $P_{n\leftarrow m} \sim ct^2$, which is larger than 1 for long enough time.

In general probabilities oscillate with time (recall cyclotron resonance problem)

The problem with first order perturbation theory is it neglects depletion and return

depletion: expect probability of $P_{n\leftarrow m}$ to decrease when most m's are gone

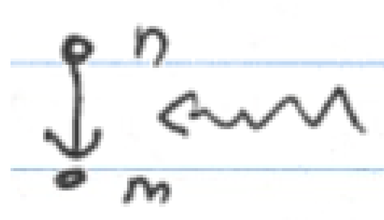

Figure 2: Figure displaying how a photon of energy $-\omega_{nm}$ can stimulate an emission from the upper state n to the lower state m. This is called stimulated emission.

return: after n's populated, they re-emit back to m.

Both processes are higher order effects.

Example: photo-ionization of Hydrogen - when a photon knocks an electron out of H, little chance it will return back. In this case, neglecting return is OK.

4 Example of perturbation theory for an exactly solvable problem

Compare to the solvable example of last lecture.

Recall we showed

$$|\psi_s(t)\rangle = e^{i\omega t(\hat{a}^\dagger \hat{a}+\frac{1}{2})}\exp\left[-\frac{c}{\hbar(\Omega+\omega)}(e^{i(\omega+\Omega)t}-1)\hat{a}^\dagger + \frac{c}{\hbar(\Omega+\omega)}(e^{i(\omega+\Omega)t}-1)\hat{a}\right]$$
$$* \, e^{i\frac{c^2}{\hbar^2(\Omega+\omega)^2}[(\omega+\Omega)t-\sin(\omega+\Omega)t]}|\psi_s(0)\rangle$$

for $\hat{H} = \underbrace{\hbar\omega(\hat{a}+\hat{a}+\frac{1}{2})}_{\hat{H}_0} + \underbrace{ce^{i\Omega t}\hat{a}^\dagger + ce^{-i\Omega t}\hat{a}}_{\hat{V}} \qquad c \in \mathbb{R}.$

Consider the following operator identity:

$$e^{\tau(\hat{A}+\hat{B})}e^{-\tau\hat{B}}e^{-\tau\hat{A}} = f(\tau) \quad \text{with } [\hat{A},\hat{B}] = \text{ number}$$
$$e^{\tau(\hat{A}+B)}(\hat{A}+\hat{B})e^{-\tau\hat{B}}e^{-\tau A} - e^{\tau(A+B)}\hat{B}e^{-\tau\hat{B}}e^{-\tau\hat{A}} - e^{\tau(\hat{A}+\hat{B})}e^{-\tau\hat{B}}\hat{A}e^{-\tau\hat{A}}$$
$$= \frac{df(\tau)}{d\tau}$$
$$e^{\tau(\hat{A}+\hat{B})}\left[\hat{A}, e^{-\tau\hat{B}}\right]e^{-\tau\hat{A}} = \frac{df(\tau)}{d\tau}$$

$$\text{But } [\hat{A}, e^{-\tau\hat{B}}] = \sum_{n=0}^{\infty}\frac{(-\tau)^n}{n!}[\hat{A},\hat{B}^n] = \sum_{n=0}^{\infty}\frac{(-\tau)^n}{n!}[\hat{A},\hat{B}]\hat{B}^{n-1}n \text{ when } [\hat{A},\hat{B}] = \text{number}$$
$$= -\tau[\hat{A},\hat{B}]e^{-\tau\hat{B}}$$

$$\text{so } \frac{df(\tau)}{d\tau} = \tau[\hat{B},\hat{A}]f(\tau) \Rightarrow f(\tau) = e^{\frac{\tau^2}{2}[\hat{B},\hat{A}]}, \qquad \text{let } \tau = 1$$
$$\text{or } e^{\hat{A}+\hat{B}} = e^{\frac{1}{2}[\hat{B},\hat{A}]}e^{A}e^{B}$$

$$\text{apply to } \hat{A} = \frac{-c}{\hbar(\omega+\Omega)}\left(e^{i(\omega+\Omega)t}-1\right)a^\dagger$$
$$\hat{B} = \frac{c}{\hbar(\omega+\Omega)}\left(e^{-i(\omega+\Omega)t}-1\right)\hat{a}$$
$$[\hat{B},\hat{A}] = \frac{-c^2}{\hbar^2(\omega+\Omega)^2}2(1-\cos(\omega+\Omega)t).$$

Thus, if we start in the ground state, we find

$$\begin{aligned}P_{m\leftarrow 0}(t) &= \Big|{}_0\langle m|e^{i\omega t(\hat{a}^\dagger\hat{a}+\frac{1}{2})}e^{-\frac{c}{\hbar(\omega+\Omega)}\left(e^{i(\omega+\Omega)t}-1\right)a^\dagger}\; e^{\frac{c}{\hbar(\omega+\Omega)}\left(e^{-i(\omega+\Omega)t}-1\right)\hat{a}}|0\rangle_0 \\ &\times\; e^{-\frac{c^2}{\hbar^2(\omega+\Omega)^2}(1-\cos(\omega+\Omega)t)}e^{i\frac{c^2}{\hbar^2(\omega+\Omega)^2}((\omega+\Omega)t-\sin(\omega+\Omega)t)}\Big|^2 \\ &= e^{-\frac{2c^2}{\hbar^2(\omega+\Omega)^2}(1-\cos(\omega+\Omega)t)}\left|{}_0\langle m|e^{-\frac{c}{\hbar(\omega+\Omega)}\left(e^{i(\omega+\Omega)ta^2t}-1\right)\hat{a}^\dagger}|0\rangle_0\right|^2.\end{aligned}$$

But, ${}_0\langle m| = {}_0\langle 0|\frac{(\hat{a})^m}{\sqrt{m!}}$ and $e^{-\frac{c}{\hbar(\omega+\Omega}\left(e^{i(\omega+\Omega)t}-1\right)\hat{a}^\dagger} = \sum_{n=0}^{\infty}\left(-\frac{c}{\hbar(\omega\Omega)}(e^{i(\omega+\Omega)t}-1)\right)^n\frac{1}{n!}(\hat{a}^\dagger)^n$. We need $n=m$ and $\langle 0|\,(\hat{a})^m\left(\hat{a}^\dagger\right)^m|0\rangle = m!$, so

$$P_{m\leftarrow 0}(t) = e^{-\frac{2c^2}{\hbar^2(\omega+\Omega)^2}(1-\cos(\omega+\Omega)t)}\left[\frac{c^2}{\hbar^2(\omega+\Omega)^2}2(1-\cos(\omega+\Omega)t)\right]^m\frac{1}{m!}$$

$$\boxed{P_{m\leftarrow 0}(t) = \frac{1}{m!}\left(\frac{2c^2}{\hbar^2(\omega+\Omega)^2}\right)^m(1-\cos(\omega+\Omega)t)^m e^{-\frac{2c^2}{\hbar^2(\omega+r)^2}(1-\cos(\omega+\Omega)t)}}$$

This is the exact solution.

One can directly check that

$$\begin{aligned}&\sum_{m=0}^{\infty}\frac{1}{m!}\left(\frac{2c^2}{\hbar^2(\omega+\Omega)^2}\right)^m(1-\cos(\omega+\Omega)t)^m e^{-\frac{2c^2}{\hbar^2(\omega+\Omega)^2}(1-\cos(\omega+\Omega)t)} \\ &= \exp\left[\frac{2c^2}{\hbar^2(\omega+\Omega)^2}(1-\cos(\omega+\Omega)t) - \frac{2c^2}{\hbar^2(\omega+n)^2}(1-\cos(\omega+\Omega)t)\right] \\ &= 1 \text{ as it must.}\end{aligned}$$

Compare to the harmonic calculation

$$\begin{aligned}&\langle m|c\hat{a}^\dagger|0\rangle = 0 \text{ unless } m=1 \\ &\langle m|\hat{a}^\dagger|0\rangle = c\delta_{m1} \quad \text{and} \quad \omega_{10}=\omega \\ &P_{1\leftarrow 0}(t) \cong \frac{4c^2}{\hbar^2}\frac{\sin^2(\omega+\Omega)t\frac{1}{2}}{(\omega+\Omega)^2},\end{aligned}$$

which agrees with the above form for $m=1$ to lowest order in c^2 when we note that

$$1-\cos(\omega+\Omega)t = 2\sin^2[(\omega+\Omega)t/2].$$