Chapter 11 - Quantum Dynamics (Time Dependent Perturbation Theory)

Chapter 7 was about how to get a good approximation to the solution when a "simple" Hamiltonian has a slight change which does not depend on time. This chapter shows how to get an approximate solution when the small change has time dependence.

Start by remembering the time dependent Sch. Eq.

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = H\,\Psi(x,t)$$

We will start by looking at the case where $H = H^{(0)} + H^{(1)}$ where $H^{(0)}$ is time independent and $H^{(1)}$ is time dependent.
The notation in the book sucks so will use a more precise notation.

If $H^{(1)} = 0$, $\quad H^{(0)}|\psi_n^{(0)}\rangle = |\psi_n^{(0)}\rangle E_n^{(0)} \quad$ with $\langle \psi_n^{(0)} | \psi_{n'}^{(0)} \rangle = \delta_{nn'}$

The full time dependent wave function has the form

$$|\Psi(t)\rangle = |\psi_1^{(0)}\rangle e^{-iE_1^{(0)}t/\hbar} C_1 + |\psi_2^{(0)}\rangle e^{-iE_2^{(0)}t/\hbar} C_2 + \dots$$

$$= \sum_{n=1}^{\infty} |\psi_n^{(0)}\rangle e^{-iE_n^{(0)}t/\hbar} C_n$$

Show that each term is separately a solution of the time dependent Sch. Eq.
Show movies

You obtain the coefficients C_n by dotting into $|\Psi(0)\rangle$

$$C_n = \langle \psi_n^{(0)} | \Psi(0) \rangle$$

Suppose you have two wave functions $|\Psi_a(t)\rangle$ and $|\Psi_b(t)\rangle$
Show $\langle \Psi_b(t) | \Psi_a(t) \rangle = \langle \Psi_b(0) | \Psi_a(0) \rangle$ if H is time independent.

$$|\Psi_a(t)\rangle = |\psi_1^{(0)}\rangle e^{-iE_1^{(0)}t/\hbar} C_{1,a} + |\psi_2^{(0)}\rangle e^{-iE_2^{(0)}t/\hbar} C_{2,a} + \dots$$

Just do it!!

$$\langle\Psi_b(t)|\Psi_a(t)\rangle = \sum_{m,n}\left(C_{m,b}\, e^{-iE_m^{(0)}t/\hbar}\right)^* \langle\psi_m^{(0)}|\psi_n^{(0)}\rangle e^{-iE_n^{(0)}t/\hbar} C_{n,a}$$

$$= \sum_{m,n} C_{m,b}^* \; e^{i(E_m^{(0)}-E_n^{(0)})t/\hbar} C_{n,a} \langle\psi_m^{(0)}|\psi_n^{(0)}\rangle$$

$$= \sum_n C_{n,b}^* C_{n,a} = \langle\Psi_b(0)|\Psi_a(0)\rangle$$

This property holds even when the Hamiltonian is time dependent.

$$-i\hbar\frac{\partial}{\partial t}\langle\Psi(t)| = \langle\Psi(t)|H^\dagger$$

$$\frac{\partial}{\partial t}\left[\langle\Psi_b(t)|\Psi_a(t)\rangle\right] = \frac{\partial\langle\Psi_b(t)|}{\partial t}|\Psi_a(t)\rangle + \langle\Psi_b(t)|\frac{\partial|\Psi_a(t)\rangle}{\partial t}$$

$$= \langle\Psi_b(t)|\frac{i}{\hbar}H^\dagger|\Psi_a(t)\rangle + \langle\Psi_b(t)|-\frac{i}{\hbar}H|\Psi_a(t)\rangle$$

$$= 0$$

Since the time derivative is zero, the value must be constant: $\langle\Psi_b(t)|\Psi_a(t)\rangle = \langle\Psi_b(0)|\Psi_a(0)\rangle$

Note this also shows norm conservation: $\langle\Psi_a(t)|\Psi_a(t)\rangle = \langle\Psi_a(0)|\Psi_a(0)\rangle$

If we have a time independent Hamiltonian, then the most general time dependent wave function can be treated using superposition.

Another exactly solvable case is due to II Rabi.

$$|\Psi(t)\rangle = \tilde{C}_1(t)|\psi_1\rangle + \tilde{C}_2(t)|\psi_2\rangle$$

$$H = \begin{pmatrix} E_1 & \frac{\hbar\Omega}{2}e^{i\omega t} \\ \frac{\hbar\Omega}{2}e^{-i\omega t} & E_2 \end{pmatrix}$$

Two states that are coupled by oscillating interaction

To find the equation for the C_1, C_2 plug into the Sch. Eq.

$$\langle \psi_1 | i\hbar \tfrac{\partial}{\partial t} | \Psi(t)\rangle = i\hbar \dot{\tilde{C}}_1 = \langle \psi_1|H|\Psi(t)\rangle = E_1 \tilde{C}_1 + \frac{\hbar\Omega}{2} e^{i\omega t}\tilde{C}_2$$
$$\langle \psi_2 | i\hbar \tfrac{\partial}{\partial t} | \Psi(t)\rangle = i\hbar \dot{\tilde{C}}_2 = \langle \psi_2|H|\Psi(t)\rangle = E_2 \tilde{C}_2 + \frac{\hbar\Omega}{2} e^{-i\omega t}\tilde{C}_1$$

Can reduce to time independent equations using

$$\tilde{C}_1 = e^{i\omega t/2} e^{i\bar{E}t/\hbar} C_1 \qquad \tilde{C}_2 = e^{-i\omega t/2} e^{i\bar{E}t/\hbar} C_2 \qquad \bar{E} = \tfrac{1}{2}(E_1+E_2)$$

$$i\dot{C}_1 = \left(\frac{E_1-\bar{E}}{\hbar} + \frac{\omega}{2}\right)C_1 + \frac{\Omega}{2}C_2 = \frac{1}{2}(\omega-\omega_{21})C_1 + \frac{\Omega}{2}C_2$$
$$i\dot{C}_2 = \left(\frac{E_2-\bar{E}}{\hbar} - \frac{\omega}{2}\right)C_2 + \frac{\Omega}{2}C_1 = \frac{1}{2}(\omega_{21}-\omega)C_2 + \frac{\Omega}{2}C_1$$

This is like trying to drive the transition from 1 to 2 using ω.

$\omega = \omega_{21} + \delta$ $\qquad$ δ = detuning in radians/sec

$$i\dot{C}_1 = \frac{\delta}{2}C_1 + \frac{\Omega}{2}C_2 \qquad i\dot{C}_2 = -\frac{\delta}{2}C_2 + \frac{\Omega}{2}C_1$$

$$i\frac{d}{dt}\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \begin{pmatrix} \delta/2 & \Omega/2 \\ \Omega/2 & -\delta/2 \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \left[\frac{\Omega}{2}\sigma_x + \frac{\delta}{2}\sigma_z\right]\begin{pmatrix} C_1 \\ C_2 \end{pmatrix}$$

Can solve as an eigenvalue problem or... take derivative again

$$\ddot{C}_1 = -i\frac{\delta}{2}\dot{C}_1 - i\frac{\Omega}{2}\dot{C}_2 = -\frac{\delta}{2}\left(\frac{\delta}{2}C_1 + \frac{\Omega}{2}C_2\right) - \frac{\Omega}{2}\left(-\frac{\delta}{2}C_2 + \frac{\Omega}{2}C_1\right) = -\left[\frac{\delta^2}{4} + \frac{\Omega^2}{4}\right]C_1$$
$$\ddot{C}_2 = \qquad = -\left[\frac{\delta^2}{4} + \frac{\Omega^2}{4}\right]C_2$$

To make the notation compact, define $\bar{\Omega} = \sqrt{\Omega^2+\delta^2}$

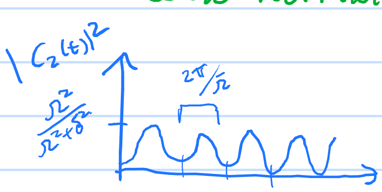
Satisfy the initial conditions $\dot{C}_1(0) = -i\frac{\delta}{2}C_1(0) - i\frac{\Omega}{2}C_2(0)$ etc

$$\left.\begin{aligned} C_1(t) &= C_1(0)\cos\left(\tfrac{1}{2}\bar{\Omega}t\right) - i\,\frac{\delta C_1(0) + \Omega C_2(0)}{\bar{\Omega}}\sin\left(\tfrac{1}{2}\bar{\Omega}t\right) \\ C_2(t) &= C_2(0)\cos\left(\tfrac{1}{2}\bar{\Omega}t\right) - i\,\frac{\Omega C_1(0) - \delta C_2(0)}{\bar{\Omega}}\sin\left(\tfrac{1}{2}\bar{\Omega}t\right) \end{aligned}\right\}\ \text{Most general case}$$

Start 100% in 1 $\quad C_1(t) = \cos\left(\tfrac{1}{2}\bar{\Omega}t\right) - i\frac{\delta}{\bar{\Omega}}\sin\left(\tfrac{1}{2}\bar{\Omega}t\right) \qquad C_2(t) = -i\frac{\Omega}{\bar{\Omega}}\sin\left(\tfrac{1}{2}\bar{\Omega}t\right)$

〃 〃 2 $\quad C_1(t) = -i\frac{\Omega}{\bar{\Omega}}\sin\left(\tfrac{1}{2}\bar{\Omega}t\right) \qquad C_2(t) = \cos\left(\tfrac{1}{2}\bar{\Omega}t\right) + i\frac{\delta}{\bar{\Omega}}\sin\left(\tfrac{1}{2}\bar{\Omega}t\right)$

Check normalization $\quad |C_1(t)|^2 + |C_2(t)|^2 = \underbrace{\cos^2\left(\tfrac{1}{2}\bar{\Omega}t\right) + \frac{\delta^2}{\bar{\Omega}^2}\sin^2\left(\tfrac{1}{2}\bar{\Omega}t\right) + \frac{\Omega^2}{\bar{\Omega}^2}\sin^2\left(\tfrac{1}{2}\bar{\Omega}t\right)}_{=1}$



Screed about book on stimulated emission

Now investigate the case where the time dependence is a perturbation. The book's notation is awkward. So will use notation similar to that in Chap 7.

$H(t) = H^{(0)} + \lambda H^{(1)}(t)$ $\qquad$ $|\Psi(t)\rangle = |\Psi^{(0)}(t)\rangle + \lambda |\Psi^{(1)}(t)\rangle + \dots$

Plug into the time dependent Schrodinger Eq.

$$i\hbar \frac{\partial}{\partial t}|\Psi^{(0)}(t)\rangle + \lambda i\hbar \frac{\partial}{\partial t}|\Psi^{(1)}(t)\rangle + \dots = H^{(0)}|\Psi^{(0)}(t)\rangle + \lambda H^{(0)}|\Psi^{(1)}(t)\rangle + \dots$$
$$+ \lambda H^{(1)}|\Psi^{(0)}(t)\rangle + \lambda^2 H^{(1)}|\Psi^{(1)}(t)\rangle + \dots$$

This is 1 equation with an infinite number of unknowns. How to solve? Arbitrarily decide to have the sum of superscripts add to the same number.

$$i\hbar \frac{\partial}{\partial t}|\Psi^{(0)}(t)\rangle = H^{(0)}|\Psi^{(0)}(t)\rangle \qquad O(\lambda^0)$$
$$i\hbar \frac{\partial}{\partial t}|\Psi^{(1)}(t)\rangle = H^{(0)}|\Psi^{(1)}(t)\rangle + H^{(1)}|\Psi^{(0)}(t)\rangle \qquad O(\lambda^1)$$
$$i\hbar \frac{\partial}{\partial t}|\Psi^{(2)}(t)\rangle = H^{(0)}|\Psi^{(2)}(t)\rangle + H^{(1)}|\Psi^{(1)}(t)\rangle \quad \text{etc} \quad O(\lambda^2)$$

Time dependent perturbation theory is about how to solve this sequence of equations in particular cases.

$H^{(0)}$ = time independent and $H^{(1)}(t) = 0$ for $t < t_0$

$$|\Psi^{(0)}(t)\rangle = \sum_n e^{-iE_n^{(0)}t/\hbar}|\psi_n^{(0)}\rangle C_n^{(0)}$$
$$|\Psi^{(1)}(t)\rangle = \sum_n e^{-iE_n^{(0)}t/\hbar}|\psi_n^{(0)}\rangle C_n^{(1)}(t) \qquad \text{notice } t \text{ dependence in } C_n^{(1)}$$
$$|\Psi^{(2)}(t)\rangle = \sum_n e^{-iE_n^{(0)}t/\hbar}|\psi_n^{(0)}\rangle C_n^{(2)}(t) \qquad \text{" " " } C_n^{(2)}$$

$$i\hbar \frac{\partial |\Psi^{(a)}(t)\rangle}{\partial t} = \sum_n \left(E_n^{(0)} C_n^{(a)}(t) + i\hbar \dot{C}_n^{(a)}\right) e^{-iE_n^{(0)}t/\hbar}|\psi_n^{(0)}\rangle = H^{(0)}|\Psi^{(a)}\rangle + H^{(1)}|\Psi^{(a-1)}\rangle$$

$$= \sum_n E_n^{(0)} C_n^{(a)}(t) e^{-iE_n^{(0)}t/\hbar}|\psi_n^{(0)}\rangle + \sum_n e^{-iE_n^{(0)}t/\hbar} H^{(1)}(t)|\psi_n^{(0)}\rangle C_n^{(a-1)}(t)$$

Project onto $\langle\psi_m^{(0)}|$ and multiply by $e^{iE_m^{(0)}t/\hbar}$

$$i\hbar \dot{C}_m^{(a)} = \sum_n e^{-i(E_n^{(0)}-E_m^{(0)})t/\hbar} \langle \psi_m^{(0)} | H^{(1)}(t) | \psi_n^{(0)} \rangle C^{(a-1)}(t) = \sum_n e^{i\omega_{mn}t} H_{mn}^{(1)}(t)\, C_n^{(a-1)}(t)$$

$$H_{mn}^{(1)}(t) = \langle \psi_m^{(0)} | H^{(1)}(t) | \psi_n^{(0)} \rangle$$

$$\omega_{mn} = (E_m^{(0)} - E_n^{(0)})/\hbar$$

Use the fact that $C^{(a)} = 0$ for $a \geq 1$ for $t < t_0$

$$C_m^{(a)}(t) = \frac{1}{i\hbar} \sum_n \int_{t_0}^{t} e^{i\omega_{mn}t'} H_{mn}^{(1)}(t')\, C_n^{(a-1)}(t')\, dt'$$

The corrections arise simply from doing integrals over time and knowing matrix elements H_{mn}.

Compare to book notation (Sec 11.1.2)
When the book has (for example) $C_a^{(2)}(t)$, this is what I mean by $C_a^{(0)}(t) + C_a^{(1)}(t) + C_a^{(2)}(t)$. The book's notation is <u>not</u> standard.

A case that often arises is when $|\Psi^{(0)}(t)\rangle = |\psi_n^{(0)}\rangle e^{-iE_n^{(0)}t/\hbar}$

$$C_m^{(1)}(t) = \frac{1}{i\hbar} \int_{t_0}^{t} e^{i\omega_{mn}t'} H_{mn}^{(1)}(t')\, dt'$$

$$C_\ell^{(2)}(t) = \frac{1}{i\hbar} \sum_m \int_{t_0}^{t} e^{i\omega_{\ell m}t'} H_{\ell m}^{(1)}(t')\, C_m^{(1)}(t')\, dt' = \frac{1}{(i\hbar)^2} \sum_m \int_{t_0}^{t} e^{i\omega_{\ell m}t'} H_{\ell m}^{(1)}(t') \int_{t_0}^{t'} e^{i\omega_{mn}t''} H_{mn}^{(1)}(t'')\, dt''\, dt'$$

etc

This is a matrix element version of what is called the Dyson series. Note the connection to

$$\frac{1}{i\hbar} e^{iH^{(0)}t'/\hbar} H^{(1)} e^{-iH^{(0)}t'/\hbar} \quad \underline{\text{and}} \quad \frac{1}{i\hbar} e^{iH^{(0)}t'/\hbar} H^{(1)}(t') e^{-iH^{(0)}t'/\hbar} \frac{1}{i\hbar} e^{iH^{(0)}t''/\hbar} H^{(1)}(t'') e^{-iH^{(0)}t''/\hbar}$$

Before doing the case sinusoidal perturbations, let's look at the case we did exactly

$$H_{12} = H_{21}^* = \frac{\hbar\Omega}{2} e^{i\omega t} \qquad C_1(0) = 1, \quad C_2(0) = 0$$

$$C_1^{(1)}(t) = \frac{1}{i\hbar} \int_0^t e^{i\omega_{12}t'} \frac{\hbar\Omega}{2} e^{i\omega t'}\, 0\, dt' = 0$$

$$C_2^{(1)}(t) = \frac{1}{i\hbar} \int_0^t e^{i\omega_{21}t'} \frac{\hbar\Omega}{2} e^{-i\omega t'}\, 1\, dt' = \frac{\Omega}{2i} \int_0^t e^{-i\delta t'} dt' = \frac{\Omega}{2i} \frac{e^{-i\delta t} - 1}{-i\delta} = \frac{\Omega}{i\delta} e^{-i\delta t/2} \sin\left(\frac{\delta t}{2}\right)$$

Let's compare

Exact $|C_2|^2 = \frac{\Omega^2}{\Omega^2+\delta^2} \sin^2\left(\frac{\sqrt{\Omega^2+\delta^2}}{2} t\right)$

1st order Pert $|C_2|^2 = \frac{\Omega^2}{\delta^2} \sin^2\left(\frac{\delta}{2} t\right)$

There's good agreement if $\Omega \ll \delta$

This result should be reminiscent of the time independent perturbation theory. Works well when the coupling between states is small compared to energy spacing.

Note there is exact agreement at small t. Do Taylor series!

Although it's tedious, there are interesting features at 2nd order

$$C_2^{(2)}(t) = \frac{1}{i\hbar}\int_0^t e^{i\omega_{21}t'} \frac{\hbar\Omega}{2} e^{-i\omega t'} C_1^{(1)}(t')\,dt' = 0$$

$$C_1^{(2)}(t) = \frac{1}{i\hbar}\int_0^t e^{i\omega_{12}t'} \frac{\hbar\Omega}{2} e^{i\omega t'} \frac{\Omega}{2\delta}\left(e^{-i\delta t'}-1\right)dt'$$

$$= \frac{\Omega^2}{4i\delta}\int_0^t e^{i\delta t'}\left(e^{-i\delta t'}-1\right)dt' = \frac{\Omega^2}{4i\delta}\left[\underbrace{t}_{\text{secular term}} - \underbrace{\frac{e^{i\delta t}-1}{i\delta}}_{\text{oscillating term}}\right]$$

$$[\;] = t - \frac{(1+i\delta t - \frac{\delta^2 t^2}{2} - 1)}{i\delta} = \frac{\delta t^2}{2i} + O(t^3)$$

There's trouble if you let $t \to \infty$. If you stop at finite t, then time dependent perturbation theory always converges if you go to high enough order.

Stimulated emission and absorption of electromagnetic waves. The main effect is from electric dipole transitions. If light has the polarization $\hat{\varepsilon}$, then

$$H = H^{(0)} - q\,E(t)\,\hat{\varepsilon}\cdot\vec{r} \qquad E(t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathcal{E}(\omega)\,e^{-i\omega t}\,d\omega$$

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What is the probability that the system starts in the state a and finishes in the state b?

$$C_b(\infty) = \frac{1}{i\hbar}\int_{-\infty}^{\infty} e^{i\omega_{ba}t}\, E(t)\, dt\ \vec{\mathcal{P}}_{ba}\cdot\hat{\varepsilon} \qquad \vec{\mathcal{P}}_{ba} = -q\langle\psi_b^{(0)}|\vec{r}|\psi_a^{(0)}\rangle$$

$$= \frac{1}{i\hbar}\sqrt{2\pi}\,\mathcal{E}(\omega_{ba})\,\hat{\varepsilon}\cdot\vec{\mathcal{P}}_{ba}$$

From this, the probability to make a transition to state b is

$$P_b = \frac{2\pi}{\hbar^2}|\mathcal{E}(\omega_{ba})|^2\,|\hat{\varepsilon}\cdot\vec{\mathcal{P}}_{ba}|^2$$

What is the condition that this is a good approximation?

$$\Sigma_b P_b \ll 1$$

Before moving on, want to relate the transition probability to other physical properties of the system: light interacting w/ atom.

Suppose $E(t) = E_0\, e^{-t^2/\tau^2}\cos(\omega t)$. What does the transition probability look like?

$$\mathcal{E}(\omega_{ba}) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{i\omega_{ba}t}\, E(t)\, dt = \frac{E_0}{\sqrt{2\pi}}\frac{1}{2}\int_{-\infty}^{\infty}\left[e^{i(\omega_{ba}+\omega)t} + e^{i(\omega_{ba}-\omega)t}\right]e^{-t^2/\tau^2}dt$$

$$= \frac{E_0}{\sqrt{2\pi}\,2}\sqrt{\pi}\,\tau\left[e^{-\tau^2(\omega+\omega_{ba})^2/4} + e^{-\tau^2(\omega-\omega_{ba})^2/4}\right]$$

Usually $\tau \gg 2\pi/\omega$,

The probability is very well approximated by:

$$P_b \cong \frac{2\pi}{\hbar^2}\frac{E_0^2\tau^2}{8}|\hat{\varepsilon}\cdot\vec{\mathcal{P}}_{ba}|^2\left[e^{-\tau^2(\omega+\omega_{ba})^2/2} + e^{-\tau^2(\omega-\omega_{ba})^2/2}\right]$$

The energy flux for a constant laser $I = \frac{1}{2}\varepsilon_0 c E_0^2$

$$P_b = \frac{\pi I_{max}\tau^2}{\hbar^2\varepsilon_0 c\, 2}|\hat{\varepsilon}\cdot\vec{\mathcal{P}}_{ba}|^2\left[e^{-\tau^2(\omega+\omega_{ba})^2/2} + e^{-\tau^2(\omega-\omega_{ba})^2/2}\right]$$

A common way that people think about this process is in terms of the rate of excitation.

why?

$$P_b = \int_{-\infty}^{\infty} R_{b\leftarrow a}(t)\,dt = \int_{-\infty}^{\infty} R_{b\leftarrow a}(0)\, e^{-2t^2/\tau^2}dt = R_{b\leftarrow a}(0)\,\tau\sqrt{\frac{\pi}{2}}$$

$$R_{b\leftarrow a}(0) = \sqrt{\frac{\pi}{2}}\frac{I_{max}\tau}{\hbar^2\varepsilon_0 c}|\hat{\varepsilon}\cdot\vec{\mathcal{P}}_{ba}|^2\left[e^{-\tau^2(\omega+\omega_{ba})^2/2} + e^{-\tau^2(\omega-\omega_{ba})^2/2}\right] = \frac{\pi I(\omega_{ba})}{\hbar^2\varepsilon_0 c}|\hat{\varepsilon}\cdot\vec{\mathcal{P}}_{ba}|^2 = \frac{\pi}{\varepsilon_0\hbar^2}|\hat{\varepsilon}\cdot\vec{\mathcal{P}}_{ba}|^2\rho(\omega_{ba})$$

$\rho(\omega)\,d\omega$ is the energy per volume between ω and $\omega + d\omega$

There are interesting "selection rules" for the transition

$[L_z, x] = i\hbar y \qquad [L_z, y] = -i\hbar x \qquad [L_z, z] = 0$

How to show? Just do it.

$[xP_y - yP_x, x] = [xP_y, x] - [yP_x, x] = 0 - y[P_x, x] \stackrel{\checkmark}{=} i\hbar y$

Use this commutator relation to show:

$[L_z, x \pm iy] = \pm\hbar\,(x \pm iy)$

The reason is now we can show the restriction on m in the transition matrix element

$$\langle n'l'm' | [L_z, x \pm iy] | nlm \rangle = \pm\hbar \langle n'l'm' | x \pm iy | nlm \rangle$$
$$= \hbar(m' - m) \langle n'l'm' | x \pm iy | nlm \rangle \quad \text{why??}$$

For $x \pm iy$, $m' = m \pm 1$ are the only nonzero elements

$$\langle n'l'm' | [L_z, z] | nlm \rangle = 0 = \hbar(m'-m) \langle n'l'm' | z | nlm \rangle$$

For z, $m' = m$ are the only nonzero elements

The book goes through the steps to show the only nonzero transitions are for $|l - l'| = 1$

Example problem: When a fast proton goes past an atom it moves (essentially) in a straight line. $\vec{R}_{ion} = (b, 0, vt)$. Calculate the transition probability after the proton is past. Atom at $(0,0,0)$

First find $\vec{E}(t)$ $\qquad \vec{E}(t) = \dfrac{e}{4\pi\varepsilon_0} \dfrac{(-b, 0, -vt)}{(b^2 + v^2t^2)^{3/2}}$

$$C_b(\infty) = \frac{1}{i\hbar} \int_{-\infty}^{\infty} e^{i\omega_{ba}t} [E_x(t)\,\vec{\rho}_{ba} \cdot \hat{x} + E_z(t)\,\vec{\rho}_{ba} \cdot \hat{z}]\,dt$$
$$= \frac{\sqrt{2\pi}}{i\hbar} [\mathcal{E}_x(\omega_{ba})\,\vec{\rho}_{ba} \cdot \hat{x} + \mathcal{E}_z(\omega_{ba})\,\vec{\rho}_{ba} \cdot \hat{z}]$$

The only trick is to figure out the Fourier transform. From Abramowitz + Stegun

$$K_1(z) = \frac{\Gamma(3/2)\,2z}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{\cos(t)}{(t^2+z^2)^{3/2}}\,dt = \frac{\Gamma(3/2)\,z}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{e^{it}}{(t^2+z^2)^{3/2}}\,dt$$

$$\mathcal{E}_x(\omega_{ba}) = \frac{1}{\sqrt{2\pi}}\left(\frac{-be}{4\pi\varepsilon_0}\right) \int_{-\infty}^{\infty} \frac{e^{i\omega_{ba}t}}{(b^2+v^2t^2)^{3/2}}\,dt \qquad s = \omega_{ba} t \qquad dt = \frac{1}{\omega_{ba}}\,ds$$

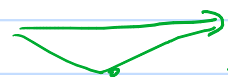
$$= \frac{1}{\sqrt{2\pi}}\left(\frac{-be}{4\pi\varepsilon_0}\right)\frac{1}{\omega_{ba}} \int_{-\infty}^{\infty} \frac{e^{is}}{\left(b^2+\frac{v^2}{\omega_{ba}^2}s^2\right)^{3/2}}\,ds$$

$$= \frac{1}{\sqrt{2\pi}}\left(\frac{-be}{4\pi\varepsilon_0}\right)\frac{\omega_{ba}^2}{v^3} \int_{-\infty}^{\infty} \frac{e^{is}}{\left(b^2\frac{\omega_{ba}^2}{v^2}+s^2\right)^{3/2}}\,ds = \frac{1}{\sqrt{2\pi}}\left(-\frac{be}{4\pi\varepsilon_0}\right)\frac{\omega_{ba}^2}{v^3}\,\frac{\sqrt{\pi}}{\Gamma(3/2)}\,\frac{v}{b\omega_{ba}}\,K_1\!\left(\frac{b\omega_{ba}}{v}\right)$$

$$\mathcal{E}_z(\omega_{ba}) = \frac{1}{\sqrt{2\pi}}\left(-\frac{ve}{4\pi\varepsilon_0}\right) \int_{-\infty}^{\infty} \frac{t\,e^{i\omega_{ba}t}}{(b^2+v^2t^2)^{3/2}}\,dt = \frac{v}{ib}\,\frac{\partial}{\partial\omega_{ba}}\,\mathcal{E}_x(\omega_{ba})$$

For large z $\quad K_1(z) \sim \sqrt{\frac{\pi}{2z}}\, e^{-z}\left(1 + \frac{3}{8z} - \frac{15}{128z^2} \cdots\right)$ asymptotic series

When is the probability small? $\frac{b\omega_{ba}}{v} \gg 1$



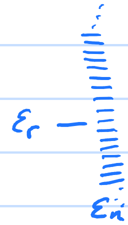
large angle during one period $2\pi/\omega_{ba}$

The book doesn't cover the golden rule, but is very important. Why does atom emit a photon when it starts in an excited state?? The following are essentially the same process:
$Na(3p) \to Na(3s) + hf$ (photon emission), $n \to p + e^- + \bar{\nu}_e$ (beta decay), ${}^{238}_{92}U \to {}^{234}_{90}Th + \alpha$ (alpha emission), $He(2s^2) \to He^+(1s) + \varepsilon s$ (electron emission), ...

In all of these processes, the initial system decays into the other with the survival probability decreasing exponentially with time. The only difference is in the decay rate (or inversely the lifetime) and the type of particles in the final state. The products have a Lorentzian distribution of total energy.

A single state is at the same energy as a continuum of states. Identify the continuum in each of the examples.
Make a simple model that consists of a single state ψ_r (initial state), a discretized continuum of states ψ_n ($n = \ldots -2, -1, 0, 1, 2 \ldots$) The state ψ_r can interact with the ψ_n and vice versa, the ψ_n don't interact with each other, the energy of ψ_r is ε_r, the energy of ψ_n is $\varepsilon_n = n\Delta\varepsilon$, and the coupling bet een ψ_r and ψ_n is $\langle\psi_r|H|\psi_n\rangle = \lambda\sqrt{\Delta\varepsilon}\,\exp[-\alpha(\varepsilon_n-\varepsilon_r)^2]$
where α is much smaller than $1/\Delta\varepsilon^2$ (will take the limit $\alpha \to 0$)

Students should have a visualization of model



If the system starts in ψ_r, population goes into quasi cont. comes back on time scale $t \sim 2\pi/\Delta\varepsilon$

Schrodinger's equation

$$|\Psi(t)\rangle = |\psi_r\rangle a_r + \dots |\psi_{-2}\rangle a_{-2} + |\psi_{-1}\rangle a_{-1} + |\psi_0\rangle a_0 + \dots$$

$$\langle\psi_r| i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = i\hbar \dot{a}_r = \varepsilon_r a_r + \lambda\sqrt{\Delta\varepsilon} \sum_{n=-\infty}^{\infty} e^{-\alpha(\varepsilon_r-\varepsilon_n)^2} a_n$$

$$\langle\psi_n| i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = i\hbar \dot{a}_n = \varepsilon_n a_n + \lambda^*\sqrt{\Delta\varepsilon}\, e^{-\alpha(\varepsilon_r-\varepsilon_n)^2} a_r$$

Make the transformation to get rid of fast dependence due to the diagonal energy terms.

$$a_g(t) = c_g(t) e^{-i\varepsilon_g t/\hbar}$$

$$i\hbar \dot{c}_r = \lambda\sqrt{\Delta\varepsilon} \sum_{n=-\infty}^{\infty} e^{-\alpha(\varepsilon_r-\varepsilon_n)^2} e^{-i(\varepsilon_n-\varepsilon_r)t/\hbar} c_n(t)$$
$$i\hbar \dot{c}_n = \lambda^*\sqrt{\Delta\varepsilon}\, e^{-\alpha(\varepsilon_r-\varepsilon_n)^2} e^{i(\varepsilon_n-\varepsilon_r)t/\hbar} c_r(t)$$

Use the initial conditions $c_r(0)=1$ $\quad c_n(0)=0$

$$c_n(t) = -i\frac{\lambda^*}{\hbar}\sqrt{\Delta\varepsilon}\, e^{-\alpha(\varepsilon_r-\varepsilon_n)^2} \int_0^t e^{i(\varepsilon_n-\varepsilon_r)t'/\hbar} c_r(t')\,dt'$$

Substitute into the $\dot{c}_r$ equation

$$\dot{c}_r(t) = -\frac{|\lambda|^2}{\hbar^2}\Delta\varepsilon \sum_{n=-\infty}^{\infty} e^{-2\alpha(\varepsilon_n-\varepsilon_r)^2} \int_0^t e^{i(\varepsilon_n-\varepsilon_r)(t'-t)/\hbar} c_r(t')\,dt'$$

There are no approximations to this point. We are interested in the times $t \ll 2\pi/\Delta\varepsilon$ so the discrete approximation of the continuum is not apparent.

The order of the sum and the integral is not relevant so do the sum first

$$\Delta\varepsilon \sum_{n=-\infty}^{\infty} e^{-2\alpha(\varepsilon_n-\varepsilon_r)^2} e^{i(\varepsilon_n-\varepsilon_r)(t'-t)/\hbar} \cong \int e^{-2\alpha(\varepsilon-\varepsilon_r)^2} e^{i(\varepsilon-\varepsilon_r)(t'-t)/\hbar} d\varepsilon$$
$$= \sqrt{\frac{\pi}{2\alpha}}\, e^{-(t'-t)^2/8\alpha\hbar^2}$$

$$\dot{c}_r(t) = -\frac{|\lambda|^2}{\hbar^2}\sqrt{\frac{\pi}{2\alpha}} \int_0^t e^{-\frac{(t'-t)^2}{8\hbar^2\alpha}} c_r(t')\,dt'$$

What is the effect of $\alpha \to$ tiny???

Can pull the $C_0(t')$ out of the integral. Why??

$$\dot{C}_r(t) = -\frac{|\lambda|^2}{\hbar^2}\sqrt{\frac{\pi}{2\alpha}}\int_0^t e^{-\frac{(t-t')^2}{8\hbar^2\alpha}}dt'\, C_r(t) = -\frac{|\lambda|^2}{\hbar^2}\sqrt{\frac{\pi}{2\alpha}}\;\frac{1}{2}\sqrt{\pi 8\hbar^2\alpha}\; C_r(t)$$

$$= -\Gamma/2\, C_r(t) \qquad \text{where} \qquad \Gamma = \frac{2\pi|\lambda|^2}{\hbar}$$

This equation is straightforward to solve $C_r(t) = e^{-\frac{\Gamma}{2}t}$

Substitute this into the equation for $C_n(t)$

$$C_n(t) = -i\frac{\lambda^*}{\hbar}\sqrt{\Delta\varepsilon}\; e^{-\alpha(\varepsilon_r-\varepsilon_n)^2}\int_0^t e^{(-\frac{\Gamma}{2}+i(\varepsilon-\varepsilon_r)/\hbar)t'}dt'$$

$$= -i\frac{\lambda^*}{\hbar}\sqrt{\Delta\varepsilon}\;\frac{1}{-\Gamma/2+i(\varepsilon_n-\varepsilon_0)/\hbar}\left[e^{(-\Gamma/2+i(\varepsilon_n-\varepsilon_r)/\hbar)t}-1\right]$$

In the limit $t\to\infty$ the first term in [ ] goes to 0

$$C_n(\infty) = \frac{\lambda^*\sqrt{\Delta\varepsilon}}{(\varepsilon_n-\varepsilon_r)+i\frac{\Gamma\hbar}{2}}$$

This gives the Lorentzian energy distribution of final states!!

$$P(\varepsilon) = \frac{|\lambda|^2}{(\varepsilon-\varepsilon_r)^2+(\frac{\Gamma\hbar}{2})^2} = \frac{\hbar\Gamma/2\pi}{(\varepsilon-\varepsilon_r)^2+(\Gamma\hbar/2)^2}$$

Note: this gives conservation of norm $\sum_n |C_n|^2 = \int P(\varepsilon)d\varepsilon = \frac{\pi}{(\frac{\Gamma\hbar}{2})}\hbar\Gamma/2\pi = 1$

We can connect this to the usual treatment. "Fermi's Golden Rule" gives the decay rate as

$$\Gamma_{FGR} = \frac{2\pi}{\hbar}|\langle f|H|i\rangle|^2\,\rho \leftarrow \text{density of states}$$

Model: $\langle f|H|i\rangle = \lambda\sqrt{\Delta\varepsilon}$, $\rho = \overset{\text{1 state per }\Delta\varepsilon}{1/\Delta\varepsilon}$, $\Gamma_{FGR} = \frac{2\pi}{\hbar}|\lambda|^2\cancel{\Delta\varepsilon}\frac{1}{\cancel{\Delta\varepsilon}}$ ✓✓✓

Example: A particle has a 2D potential

$$H = P_x^2/2m - \alpha\delta(x) + \frac{P_y^2}{2m} + \frac{1}{2}m\omega_y^2y^2 + \beta xy$$

The last term allows energy to transfer between x+y degrees of freedom. Suppose $\hbar\omega_y >$ binding energy in x. Then the state $\psi_{gs}(x)\psi_{n_y>0}(y)$ will decay into the continuum.

We need to figure out how to deal with the continuum.

$$\psi_r = \psi_{gs}(x)\,\psi_n(y) \qquad \psi_{gs} = \frac{\sqrt{m\alpha}}{\hbar} e^{-m\alpha|x|/\hbar^2} \qquad \mathcal{E}_r = -\frac{m\alpha^2}{2\hbar^2} + (n_y + \tfrac{1}{2})\hbar\omega_y$$

$$K_{gs} = \frac{m\alpha}{\hbar^2}$$

The coupling term, βxy, means $n_y \to n_y - 1$ and $\psi_f(x) = C\sin(kx)$

Why is the x-function $\sin(kx)$ and not even?

Put wall at $|X| = L$ with $L \to$ really big.

$$\psi_n = \sqrt{\frac{2}{2L}} \sin\left(\frac{n_x \pi x}{L}\right) \psi_{n_y-1}(y) \qquad \mathcal{E}_n = \frac{\hbar^2\pi^2 n_x^2}{2mL^2} + (n_y - 1 + \tfrac{1}{2})\hbar\omega_y$$

Figure out which n_x : $\mathcal{E}_n = \mathcal{E}_r \Rightarrow E_{x,1} n_x^2 = -\frac{m\alpha^2}{2\hbar^2} + \hbar\omega_y = -\frac{\hbar^2 K_{gs}^2}{2m} + \hbar\omega_y = \mathcal{E}_x$

Figure out $\Delta\mathcal{E}$: $\Delta\mathcal{E} = \frac{d\mathcal{E}}{dn_x} = 2E_{x,1} n_x = 2E_{x,1}^{1/2}(E_{x,1} n_x^2)^{1/2} = 2\sqrt{E_{x,1}}\sqrt{\mathcal{E}_x}$

Figure out $\langle\psi_r|H|\psi_n\rangle$: $\lambda\sqrt{\Delta\mathcal{E}} = \beta \int_{-\infty}^{\infty} x\,\psi_{gs}(x)\psi_{n_x}(x)\,dx \int_{-\infty}^{\infty} \psi_{n_y}(y)\,y\,\psi_{n_y-1}(y)\,dy$

$$= \beta\, 2\sqrt{K_{gs}} \frac{1}{\sqrt{L}} \int_0^\infty e^{-K_{gs}x} \sin(k_n x)\, x\,dx \sqrt{\frac{\hbar}{2m\omega_y}}\sqrt{n_y}$$

$$\int_0^\infty e^{-Kx}\sin(kx)\,x\,dx = \frac{2Kk}{(K^2+k^2)^2}$$

$$\lambda = \beta\, 2\sqrt{K_{gs}} \frac{1}{\sqrt{L}} \sqrt{\frac{\hbar n_y}{2m\omega_y}} \frac{2K_{gs}k_n}{(K_{gs}^2 + k_n^2)^2} \frac{1}{\sqrt{2}\,E_{x,1}^{1/4}\mathcal{E}_x^{1/4}}$$

$$K_{gs}^2 + k_n^2 = \frac{2m}{\hbar^2}(-\mathcal{E}_{gs} + \mathcal{E}_{n_x}) = \frac{2m}{\hbar^2}\hbar\omega_y = \frac{2m\omega_y}{\hbar}$$

$$\lambda = 2\beta\sqrt{K_{gs}} \frac{1}{\sqrt{L}} \sqrt{\frac{\hbar n_y}{2m\omega_y}} \frac{2\hbar^2 K_{gs}k_n}{4m^2\omega_y^2} \left(\frac{L^2 m}{\pi^2\hbar^2}\right)^{1/4} \frac{1}{2^{1/4}} \frac{1}{\mathcal{E}_x^{1/4}} \qquad \mathcal{E}_x = \mathcal{E}_{gs} + \hbar\omega_y = \frac{\hbar^2 k_n^2}{2m}$$

$$= \beta K_{gs}^{3/2} \frac{\hbar\sqrt{n_y}}{\omega_y^{5/2} m^{1/4}\sqrt{\pi}\,2^{1/4}} \mathcal{E}_x^{1/4}$$

Notice that L has disappeared. As it should!! Why? Fermi RMP

$$\Gamma = 2\pi\frac{\lambda^2}{\hbar} = \sqrt{2}\,\beta^2 K_{gs}^3 \frac{\hbar n_y}{\omega_y^5 m^{1/2}} \mathcal{E}_x^{1/2}$$

Qualitative trends? β^2, n_y, $\mathcal{E}_x^{1/2}$