Phys 487 Discussion 12 – Time-Dependent PT with 2-State Systems

Same formula summary as last week : if our Hamiltonian H consists of a time-independent part H_0 with known eigenvalues $E_n^{(0)}$ and eigenstates $|n^{(0)}\rangle$ plus and a much smaller time-*dependent* part H', then we get the following results :

Given • $H(t) = H^{(0)} + H'(t)$, • $\{ E_n^{(0)}, |n^{(0)}\rangle \}$ = the eigen-* of $H^{(0)}$ • initial state $|\psi(t=0)\rangle = |i^{(0)}\rangle$

then $\boxed{|\psi(t)\rangle = \sum_n c_n(t)\, e^{-i\omega_n t} |n^{(0)}\rangle}$ with $\boxed{i\hbar\, \dot{c}_f(t) = \sum_n H'_{fn}\, e^{i\omega_{fn} t} c_n(t)}$

• $\omega_{fn} \equiv \left(E_f^{(0)} - E_n^{(0)}\right)/\hbar$

• $H'_{fn} \equiv \langle f^{(0)} | H' | n^{(0)} \rangle$

& to <u>1st order</u> in $H' \ll H^{(0)}$, $\boxed{c_f(t) \approx \delta_{fi} + \frac{1}{i\hbar}\int_0^t H'_{fi}(t') e^{i\omega_{fi} t'}\, dt'}$

The first box is the solution form, the second box is the <u>exact</u> differential equation it must satisfy, and the third box is the 1st-order perturbative solution. Some names: ω_{fi} is called the **transition frequency** for going from initial state i to final state f, while $c_f(t)$ is the **transition amplitude** for doing the same thing. The **transition probability** that we are usually trying to calculate is

$$\boxed{P_{f\to i} = \left| c_f(t) \right|^2}$$

Problem 1 : Two-State hydrogen atom in electric field *adapted from Griffiths 9.1*

Systems with only two independent states are excellent <u>sandboxes</u> for playing around with time-dependent potentials, e.g. you can write down all the matrix elements of H'_{fn} since there are only four of them.

Let's take a specific case. A hydrogen atom is placed in a time-dependent electric field $\vec{E} = E(t)\hat{z}$.

(a) Calculate all four matrix elements H'_{ij} of the perturbation $H' = eEz$ between the ground state (n = 1) and the quadruply degenerate first excited states (n = 2).

(b) Show that the diagonal elements H'_{ii} of the perturbation are both zero for all five states.

▶ NOTE: There is <u>only one integral</u> to be done here, if you exploit oddness with respect to z; only one of the n = 2 states is "accessible" from the ground state by a perturbation of this form, and therefore the system functions as a two-state configuration — assuming transitions to higher excited states can be ignored.

(c) It is very commonly the case that the diagonal elements H'_{ii} of a time-dependent perturbation are zero. In this case, the exact differential equations

$$i\hbar\, \dot{c}_f(t) = \sum_n H'_{fn}\, e^{i\omega_{fn} t} c_n(t)$$

for the two coefficients $c_a(t)$ and $c_b(t)$ (using Griffiths' notation for two states) reduce to two coupled differential equations without summation signs. Show that the above reduces to these two in the case $H'_{ii} = 0$:

$$\dot{c}_a = \frac{1}{i\hbar} H'_{ab}\, e^{-i\omega_0 t} c_b \quad \text{and} \quad \dot{c}_b = \frac{1}{i\hbar} H'_{ba} e^{i\omega_0 t}\, c_a$$

These are Griffiths' equation 9.13, on which the first part of his chapter 9 are based.

NOTATION CHANGE : We will henceforth stop placing a superscript $^{(0)}$ on the states and energies of the unperturbed system. Reason? We are ALWAYS referring to the states of the unperturbed system in time-dependent PT, so there is no reason to flag it with such notation. As we mentioned in class, the goal of time-dependent PT is quite different from that of time-independent PT.

- t-indep. PT : calculate changes to the eigenenergies & eigenstates of H_0 produced by the perturbation H'
- t-dep. PT : calculate transition probabilities caused by H' between states of the unperturbed system H_0

Problem 2 : Rabi flopping frequency *adapted from Griffiths 9.7*

A rare example of a system that can be solved exactly is the important case of a two-state problem with a sinusoidal oscillating potential. The system is often an atom or a molecule, with two states of particular interest or relevance ; the perturbation usually comes from an incident electromagnetic wave whose frequency ω is tuned to the transition frequency $\omega_{ab} = (E_a - E_b)/\hbar$ between the two states.

Here is a simplified expression for the sinusoidal perturbation $V(\vec{r})\cos(\omega t)$ after it is applied to a system with two states a and b in the case that the driving frequency ω is very close to the transition frequency ω_{ab} : [1]

$$H'_{ba} = \frac{V_{ba}}{2} e^{-i\omega t}, \quad H'_{ab} = \frac{V_{ab}}{2} e^{i\omega t}, \quad H'_{aa} = H'_{bb} = 0 \quad \text{with} \quad V_{ab} \equiv \langle \psi_a | V | \psi_b \rangle .$$

(a) Solve the two coupled equations you obtained in problem 1(c) using the initial conditions $c_a(0) = 1$ and $c_b(0) = 0$ (i.e. the system starts in state a at time $t = 0$). Express your results for $c_a(t)$ and $c_b(t)$ in terms of

$\omega_r \equiv \frac{1}{2}\sqrt{(\omega - \omega_{ab})^2 + (|V_{ab}|/\hbar)^2}$, called the **Rabi flopping frequency.** Answers in footnote[2].

(b) Determine the transition probability $P_{a\to b}(t)$ and show that it never exceeds 1. Confirm that $|c_a(t)|^2 + |c_b(t)|^2 = 1$ at all times. (What would it mean if that were *not* true? Ask if you're not sure!)

(c) Check that $P_{a\to b}(t)$ reduces to the perturbation theory result

$$P_{a\to b}(t) = |c_b(t)|^2 \approx \frac{|V_{ab}|^2 \sin^2[(\omega_{ab} - \omega)t/2]}{(\omega_{ab} - \omega)^2}$$

when the perturbation is "small", and state precisely what small *means* in this context, as a constraint on V.

(d) At what time does the system first return to its initial state?

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[1] Griffiths §9.1.3 shows how the approximation $\omega \approx \omega_0 \equiv \omega_{ab}$ is applied.

[2] **Q2(a)** results : $c_b(t) = -\frac{i}{2\hbar\omega_r} V_{ba} e^{i(\omega_{ab}-\omega)t/2} \sin(\omega_r t)$, $c_a(t) = e^{i(\omega-\omega_{ab})t/2}\left[\cos(\omega_r t) + i\left(\frac{\omega_{ab}-\omega}{2\omega_r}\right)\sin(\omega_r t)\right]$.