

Phys 487 Discussion 9 – Time-Dependent Perturbation Theory

From today's class : Consider a system with Hamiltonian $H(t) = H^{(0)} + H'(t)$, where $\{ E_n^{(0)}, |n^{(0)}\rangle \}$ are the known eigen-values/states of the “unperturbed” time-independent part $H^{(0)}$. We can express any time-dependent state $|\Psi(t)\rangle$ of this system as a superposition of the unperturbed states $|n^{(0)}\rangle$ with amplitudes $c_n(t)$:

$$\boxed{|\Psi(t)\rangle = \sum_n c_n(t) e^{-i\omega_n t} |n^{(0)}\rangle} \quad \text{where} \quad \boxed{i\hbar \dot{c}_f(t) = \sum_n H'_{fn} e^{i\omega_{fn} t} c_n(t)} \quad \begin{aligned} &\bullet \omega_{fn} \equiv (E_f^{(0)} - E_n^{(0)}) / \hbar \\ &\bullet H'_{fn} \equiv \langle f^{(0)} | H' | n^{(0)} \rangle \end{aligned}$$

If H' is *very small* compared to H_0 , we can obtain an approximate solution for the amplitudes $c_n(t)$ by expanding them in powers of this smallness \rightarrow this is **time-dependent perturbation theory**. We find

$$\boxed{c_f(t) \approx \delta_{fi} + \frac{1}{i\hbar} \int_{t_0}^t dt' H'_{fi}(t') e^{i\omega_{fi} t'}} \quad \text{at 1st order in } H' \ll H_0, \text{ given the initial state } |\Psi(t_0)\rangle = |i^{(0)}\rangle.$$

ω_{fi} is called the **transition frequency** for going from initial state i (at time t_0) to final state f (at time t); $c_f(t)$ is called the **transition amplitude** for this $i \rightarrow f$ transition. The **transition probability** that we are usually trying to calculate is, as usual, the magnitude² of the corresponding amplitude :

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

Problem 1 : 1D SHO TM in a decaying electric field

Checkpoints & Comment ¹

Consider a one-dimensional harmonic oscillator that is in the ground state $|0\rangle$ of the unperturbed Hamiltonian at $t = -\infty$. NOTE: Since ALL the eigenstates $|n\rangle$ that we're going to talk about are eigenstates of the unperturbed Hamiltonian, we can suppress the ⁽⁰⁾ subscript without confusion! The following perturbation is applied between $t = -\infty$ and $+\infty$:

$$H'(t) = -qEx e^{-t^2/\tau^2}$$

where q is the particle's charge and E is a constant electric field. What is the probability that the oscillator is in the state $|n\rangle$ at $t = \infty$? If you are disturbed that the sum of your non-zero probabilities is > 1 , see the footnote!

¹ Q1 : $P_{0 \rightarrow 0} = |c_0(\infty)|^2 = 1 \dots P_{0 \rightarrow 1} = |c_1(\infty)|^2 = q^2 E^2 \tau^2 \pi / (2m\omega\hbar) \exp(-\omega^2 \tau^2 / 2) \dots P_{0 \rightarrow n} = |c_n(\infty)|^2 = 0$ for $n > 1$

NOTE : Are you disturbed by $P_{0 \rightarrow 0} + P_{0 \rightarrow 1} > 1$? $P_{0 \rightarrow 0} = 1$ would seem to imply that all other transition probabilities must be 0! First, it is most excellent that you are disturbed! To resolve this issue, you must take into account that our formula for the transition amplitudes $c_f(t)$ is only accurate to first order in the small parameter ϵ that we placed in front of H' in our derivation. In this problem, H' has an “ E ” in it, and that looks like ϵ , so just treat E as the parameter of explicit smallness. The amplitudes we obtained are

$$c_0(t) = 1 + \text{order}(E^2) \quad \text{and} \quad c_{n>1}(t) = E \cdot \text{stuff} + \text{order}(E^2)$$

where “order” explicitly shows the size of the uncertainties (the unknown terms) from a formula that is good to 1st-order in E only. Square those to see how accurate the corresponding probabilities are. Keeping only the leading error order (of course!), we get

$$P_{0 \rightarrow 0}(t) = [1 + \text{order}(E^2)]^2 \approx 1 + \text{order}(E^2) \quad \text{and} \quad P_{0 \rightarrow n>1}(t) = [E \cdot \text{stuff} + \text{order}(E^2)]^2 \approx E^2 \cdot \text{stuff}^2 + \text{order}(E^3)$$

Thus $P_{0 \rightarrow 0}$ is accurate to first order in E (the leading unknown terms are $\text{order}(E^2)$)

while $P_{0 \rightarrow n>0}$ is accurate to second order in E (the leading unknown terms are $\text{order}(E^3)$)

The total probability that disturbed you was $1 + \text{stuff} \cdot E^2$, which is to be expected since $P_{0 \rightarrow 0}$ is only accurate to order E^1 .

MESSAGE : The formula is actually doing what we want 99.999% of the time, which is to find the probabilities of *changing state*, from an initial state i to some *different* state f . Our 1st-order amplitude formula gets those $i \neq f$ probabilities right to 2nd order. If you really need the probability $P_{i \rightarrow i}$ of staying in the *same* state to 2nd order as well, you must calculate $1 - \sum_{f \neq i} P_{i \rightarrow f}$.

Problem 2 : 1D SHO TM again

Show that if the perturbation is $H'(t) = -\frac{qEx}{1+(t/\tau)^2}$, then $P_{0 \rightarrow 1} \approx \frac{q^2 E^2 \pi^2 \tau^2}{2m\omega\hbar} e^{-2\omega\tau}$.

► Integration hint: substitute $u = \omega t$.

Problem 3 : Hydrogen Atom with decaying electric field

*Hints & Checkpoints*²

A hydrogen atom is in the ground state at $t = -\infty$. An electric field $\vec{E}(t) = \hat{z} E e^{-t^2/\tau^2}$ is applied until $t = +\infty$. Show that the probability that the atom ends up in any of the $n = 2$ states is

$$P_{1 \rightarrow 2} \approx \left(\frac{qE}{\hbar}\right)^2 \left(\frac{2^{15} a_0^2}{3^{10}}\right) \pi \tau^2 e^{-\omega^2 \tau^2 / 2} \quad \text{where } \omega \text{ is the transition frequency } \omega \equiv \frac{E_{2lm} - E_{100}}{\hbar}.$$

Does the answer depend on whether or not we incorporate spin in the picture?

² Q3 Hints : Oooh, in this question we have *several* final states; how many do we have and what are they?

... there are 4 final states: $|nlm\rangle = |200\rangle, |21+1\rangle, |210\rangle, |21-1\rangle$. What are their wavefunctions?

... the hydrogen wavefunctions $\psi_{nlm}(r, \theta, \phi)$ can be constructed from two *separated pieces* found on the 486 formula sheet

... remember separation of variables for central-force problems?

... $\psi_{nlm}(r, \theta, \phi) = R_{nl}(r) Y_{lm}(\theta, \phi) \rightarrow$ go hunting on the 486 formula sheet!

... should you add the transitⁿ amplitudes then square to get total probability, or square the amplitudes first then add probabilities?

... you should add probabilities! If this is not 100% clear, please ask, it is a very important point!

... the matrix elements H'_{fi} will boil down to the form $\langle \psi_{2lm} | z | \psi_{100} \rangle$, how do you express z in spherical coords?

... draw a sketch! (or look in the spherical coordinates section of the 486 formula sheet) $\rightarrow z = r \cos\theta$

... only one matrix element is non-zero, STARE at your integrals looking for zeros before you do any work!

... the only transition with non-zero amplitude is $100 \rightarrow 210$