

Chapter 11 Time Dependent Perturbation Theory Summary

Time Dependent Perturbation Theory:

Step 1: Write the Hamiltonian in this form:

$$H(t) = H_0 + H'(t); \quad H_0|\psi_n\rangle = E_n|\psi_n\rangle$$

Step 2: Expand your wavefunction in a stationary complete basis, while factoring time dependence from H_0 :

$$|\Psi(t)\rangle = \sum_n C_n(t) e^{-iE_n t/\hbar} |\psi_n\rangle$$

Step 3: Solve time dependent Schrodinger equation in that basis:

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H(t) |\Psi(t)\rangle$$

Step 4: To calculate the probability of transition to a certain state from state n to state k :

$$P_{nk}(t) = |\langle\psi_k|\Psi(t)\rangle|^2 = |C_k(t)|^2$$

$$C_k(t) - C_k(t_0) = -\frac{i}{\hbar} \int_{t_0}^t \langle\psi_k|H'(t')|\psi_n\rangle e^{i\omega_{kn}t'} C_n(t') dt'$$

Step 5: Now we approximate by taking first order perturbation in $H'(t)$:

$$C_k(t) \approx C_k(t)^{(0)} + C_k(t)^{(1)} + C_k(t)^{(2)} + \dots$$

$$P_{nk}(t) = |C_k(t)^{(1)}|^2 = \frac{1}{\hbar^2} \left| \int_{t_0}^t e^{i\omega_{kn}t'} \langle\psi_k|H'(t')|\psi_n\rangle dt' \right|^2$$

Step 6: In **1-D**, write the perturbation Hamiltonian as product of two functions:

$$\langle\psi_k|H'(t)|\psi_n\rangle = \langle\psi_k|F(x)f(t)|\psi_n\rangle = f(t)\langle\psi_k|F(x)|\psi_n\rangle$$

Step 7: Now you need to take care of two components, the integral and the expectation value of $F(x)$:

$$\frac{1}{\hbar^2} \left| \int_{t_0}^t e^{i\omega_{kn}t'} \langle\psi_k|H'(t')|\psi_n\rangle dt' \right|^2 = \frac{1}{\hbar^2} |\langle\psi_k|F(x)|\psi_n\rangle|^2 \left| \int_{t_0}^t e^{i\omega_{kn}t'} f(t') dt' \right|^2$$

Now, we will see different examples of $F(x)$ & $f(t)$

1 $F(x)$

The objective in the following examples is to calculate this part of the probability $P_{nk}(t)$:

$$|\langle \psi_k | F(x) | \psi_n \rangle|^2$$

1.1 $F(x) = x$; Harmonic Oscillator

$$x = \sqrt{\frac{\hbar}{2m\omega}} (a^\dagger + a)$$

Knowing: $a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$ and $a |n\rangle = \sqrt{n} |n-1\rangle$:

$$\begin{aligned} \langle \psi_k | F(x) | \psi_n \rangle &= \sqrt{\frac{\hbar}{2m\omega}} \langle k | a^\dagger + a | n \rangle = \sqrt{\frac{\hbar}{2m\omega}} \left[\sqrt{n} \langle k | n-1 \rangle + \sqrt{n+1} \langle k | n+1 \rangle \right] \\ &= \sqrt{\frac{\hbar}{2m\omega}} \left[\sqrt{n} \delta_{k,n-1} + \sqrt{n+1} \delta_{k,n+1} \right] \\ |\langle \psi_k | F(x) | \psi_n \rangle|^2 &= \frac{\hbar}{2m\omega} [n \delta_{k,n-1} + (n+1) \delta_{k,n+1}] \end{aligned}$$

1.2 $F(x) = x^2$; Harmonic Oscillator

$$\begin{aligned} \langle \psi_k | F(x) | \psi_n \rangle &= \frac{\hbar}{2m\omega} \langle k | a^\dagger a^\dagger + a a^\dagger + a^\dagger a + a a | n \rangle \\ &= \frac{\hbar}{2m\omega} \left[\sqrt{n} \sqrt{n-1} \langle k | n-2 \rangle + \sqrt{n+1} \sqrt{n+2} \langle k | n+2 \rangle + \sqrt{n+1} \sqrt{n+1} \langle k | n \rangle + \sqrt{n} \sqrt{n} \langle k | n \rangle \right] \\ &= \frac{\hbar}{2m\omega} \left[\sqrt{n} \sqrt{n-1} \delta_{k,n-2} + \sqrt{n+1} \sqrt{n+2} \delta_{k,n+2} + (2n+1) \delta_{k,n} \right] \\ |\langle \psi_k | F(x) | \psi_n \rangle|^2 &= \left(\frac{\hbar}{2m\omega} \right)^2 [n(n-1) \delta_{k,n-2} + (n+1)(n+2) \delta_{k,n+2} + (2n+1)^2 \delta_{k,n}] \end{aligned}$$

Remark: Square the results of the sum of Kronecker deltas individually, i.e.:

$$|A\delta_{na} + B\delta_{nb} + C\delta_{nc}|^2 = |A|^2 \delta_{na} + |B|^2 \delta_{nb} + |C|^2 \delta_{nc}$$

Remark: Notice how when $F(x) = x$ can give you transitions up to state $|n \pm 1\rangle$, and when $F(x) = x^2$ can give you transitions up to state $|n \pm 2\rangle$.

One can deduce that when $F(x) = x^p$ one can get transitions up to state $|n \pm p\rangle$. This is because p will be the highest power of the creation and annihilation operators terms. i.e., we will have:

$$\begin{aligned} (a^\dagger)^p |n\rangle &= \sqrt{\prod_{i=1}^p (n+i)} |n+p\rangle \\ (a)^p |n\rangle &= \sqrt{\prod_{i=0}^{p-1} (n-i)} |n-p\rangle \end{aligned}$$

2 $f(t)$

The objective in the following examples is to calculate this part of the probability $P_{nk}(t)$:

$$\left| \int_{t_0}^t e^{i\omega_{kn}t'} f(t') dt' \right|^2$$

2.1 $f(t) = e^{-t/\tau}$; $t_0 = 0$; $t = t$

$$\begin{aligned} \int_{t_0}^t e^{i\omega_{kn}t'} f(t') dt' &= \int_0^t e^{i\omega_{kn}t'} e^{-t'/\tau} dt' = \int_0^t e^{-t'/\tau (1-i\tau\omega_{kn})} dt' \\ &= \frac{\tau [1 - e^{-t/\tau (1-i\tau\omega_{kn})}]}{1 - i\tau\omega_{kn}} \\ \left| \int_0^t e^{i\omega_{kn}t'} e^{-t'/\tau} dt' \right|^2 &= \frac{2\tau^2 e^{-\frac{t}{\tau}} (\cosh(\frac{t}{\tau}) - \cosh(it\omega))}{1 + \tau^2\omega^2} \end{aligned}$$

2.2 $f(t) = e^{-t^2/\tau^2}$; $t_0 = 0$; $t = \infty$

$$\int_{t_0}^t e^{i\omega_{kn}t'} f(t') dt' = \int_0^\infty e^{i\omega_{kn}t'} e^{-t'^2/\tau^2} dt' = \int_0^\infty e^{i\omega_{kn}t' - t'^2/\tau^2} dt'$$

Now let's examine the exponent of the exponential carefully:

$$i\omega_{kn}t - t^2/\tau^2 = -\frac{1}{\tau^2} [t^2 - i\omega_{kn}\tau^2 t]$$

Now we will complete the square:

$$\begin{aligned} x^2 - bx &= \left(x - \frac{b}{2}\right)^2 - \left(\frac{b}{2}\right)^2 \\ -\frac{1}{\tau^2} [t^2 - i\omega_{kn}\tau^2 t] &= -\frac{1}{\tau^2} \left[\left(t - \frac{i\omega_{kn}\tau^2}{2}\right)^2 + \left(\frac{\omega_{kn}\tau^2}{2}\right)^2 \right] \end{aligned}$$

Now, we will use u-substitution:

$$u = t - i\omega_{kn}\tau^2/2; \quad du = dt$$

The integral now becomes:

$$\int_0^\infty e^{i\omega_{kn}t' - t'^2/\tau^2} dt' = e^{-\omega_{kn}^2\tau^2/4} \int_0^\infty e^{-u^2/\tau^2} du = \frac{1}{2} e^{-\omega_{kn}^2\tau^2/4} \sqrt{\pi\tau}$$

Remark: When you have ω multiplied by τ , they always have to have the same power in your final result, otherwise you **DID** a mistake.

When you have:

$$[\omega\tau]^n \gg 1 \quad \text{Adiabatic Transition}$$

$$[\omega\tau]^n \ll 1 \quad \text{Abrupt/Sudden Transition}$$