Chapter 11 Time Dependent Perturbation Theory Summary

Time Dependent Perturbation Theory:

Step 1: Write the Hamiltonian in this form:

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

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

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

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 $H'(t)$:

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

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

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 $a|n\rangle = \sqrt{n}|n-1\rangle$:

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

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

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

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:

$$\left(a^\dagger\right)^p|n\rangle = \sqrt{\prod_{i=1}^{p}(n+i)}\,|n+p\rangle$$

$$(a)^p|n\rangle = \sqrt{\prod_{i=0}^{p-1}(n-i)}\,|n-p\rangle$$

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

$$\int_{t_0}^{t} e^{i\omega_{kn}t'} f(t')dt' = \int_{0}^{t} e^{i\omega_{kn}t'} e^{-t'/\tau}dt' = \int_{0}^{t} e^{-t'/\tau\,(1-i\tau\omega_{kn})}dt'$$
$$= \frac{1 - e^{-t/\tau\,(1-i\tau\omega_{kn})}}{1 - i\tau\omega_{kn}}$$
$$\left|\int_{0}^{t} e^{i\omega_{kn}t'} e^{-t'/\tau}dt'\right|^2 = \frac{1 - 2e^{-\frac{t}{\tau}}\cos(\omega_{kn}t) + e^{-\frac{2t}{\tau}}}{\tau^2\omega_{kn}^2 + 1}$$

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:

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

Now we will complete the square:

$$x^2 - bx = \left(x - \frac{b}{2}\right)^2 - \left(\frac{b}{2}\right)^2$$

$$-\frac{1}{\tau^2}\left[t^2 - i\omega_{kn}\tau^2 t\right] = -\frac{1}{\tau^2}\left[\left(t - \frac{i\omega_{kn}\tau^2}{2}\right)^2 + \left(\frac{\omega_{kn}\tau^2}{2}\right)^2\right]$$

Now, we will use u-substitution:

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

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:

$$[\omega\tau]^n >> 1 \qquad \text{Adiabatic Transition}$$
$$[\omega\tau]^n << 1 \qquad \text{Abrupt/Sudden Transition}$$