tD Pert$^{\underline{b}}$n Theory: Higher Order Terms

11) What we've got in tD Pert$^{\underline{b}}$n Theory so far...

For $\mathcal{H}_0 \to \mathcal{H} = \mathcal{H}_0 + \lambda V(x,t)$, general superposition of states:

$$\psi(x,t) = \sum_k \left[a_k^{(0)} + \lambda a_k^{(1)}(t) + \lambda^2 a_k^{(2)}(t) + \cdots\right] \phi_k(x) e^{i\omega_k t}, \qquad \{\text{Eq. (8)}\}$$

w/ $\{a_k^{(0)}\}$ = cnsts, specifying system initial conditions; $\qquad \{\text{Eq. (10)}\}$

... let $a_k^{(0)} = \delta_{km}$, for system initially in $m^{\underline{th}}$ eigenstate of $\mathcal{H}_0$...

so/

$$i\hbar a_k^{(1)}(t) = \int_{t_0}^{t} V_{km}(\tau) e^{i\omega_{km}\tau} d\tau \; ; \quad (\text{for } \lambda = 1) \qquad \{\text{Eq. (12)}\}$$

and//

$$i\hbar a_k^{(\mu+1)}(t) = \sum_n \int_{t_0}^{t} V_{kn}(\tau) a_n^{(\mu)}(\tau) e^{i\omega_{kn}\tau} d\tau; \quad \mu = 0, 1, 2, \ldots \qquad \{\text{Eq. (11)}\}$$

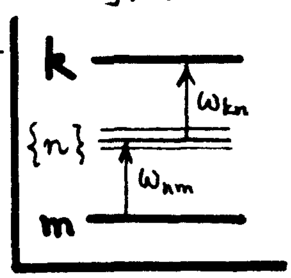
where: $\omega_{kl} = \frac{1}{\hbar}\left[E_k^{(0)} - E_l^{(0)}\right]$, $V_{kl}(\tau) = \int dx\, \phi_k^*(x) V(x,\tau) \phi_l(x)$. $\qquad$ (36)

We have explored the $\mathcal{O}(V)$ term $a_k^{(1)}(t)$; an iteration on μ gives the higher order terms in $\mathcal{O}(V^2)$, etc. in a straightforward but succeedingly more complicated fashion. E.g. for $\mu = 1$, the $\mathcal{O}(V^2)$ correction is...

$$i\hbar a_k^{(2)}(t) = \sum_n \int_{t_0}^{t} d\tau\, V_{kn}(\tau) e^{i\omega_{kn}\tau} \left[a_n^{(1)}(\tau)\right],$$

$$\xrightarrow{\text{or}/} a_k^{(2)}(t) = (1/i\hbar)^2 \sum_n \int_{t_0}^{t} d\tau\, V_{kn}(\tau) e^{i\omega_{kn}\tau} \int_{t_0}^{\tau} d\tau'\, V_{nm}(\tau') e^{i\omega_{nm}\tau'}. \qquad (37)$$

For $\mathcal{O}(V^p)$, $a_k^{(p)}(t)$ will go as $(1/i\hbar)^p \sum_n \sum_{n'} \cdots \times$[p "nested" integrals over $\int_{t_0}^{t} d\tau\, V_{kn'}(\tau) e^{i\omega_{kn'}\tau} \cdots \int_{t_0}^{\tau} d\tau'\, V_{n'n}(\tau') e^{i\omega_{n'n}\tau'} \int_{t_0}^{\tau'} d\tau''\, V_{nm}(\tau'') e^{i\omega_{nm}\tau''}$]. The picture emerges that the transition $m \to k$ can proceed in <u>time-ordered</u> <u>steps</u>, e.g. for (37): $m \to \{n\}$, $\{n\} \to k$, in $\mathcal{O}(V^2)$.



Davydov shows in his ¶ 90 how to "sum" the $a_k^{(p)}(t)$ series. We will confine ourselves to an exercise w/ $a_k^{(2)}(t)$. See Prob. ◯.

Time-Dep$^{\underline{t}}$ Pert$^{\underline{b}}$n Theory when V is not small.

12) The time-dependent perturbation theory developed on pp. tD 1-13 applies when (and is restricted to cases where) $\mathcal{H}_0 \to \mathcal{H} = \mathcal{H}_0 + V(t)$, with V "small" w.r.t. $\mathcal{H}_0$ ... specifically: $|V_{km}| \ll |\hbar\omega_{km}|$, for transitions $m \to k$.

There are two other methods of finding transition amplitudes for $m \to k$ which do not depend on V being "small" w.r.t $\mathcal{H}_0$. Instead, these methods capitalize on special assumptions about how the overall $\mathcal{H}(t)$ changes with t.

I. V(t) is not "small" w.r.t. $\mathcal{H}_0$, but $\mathcal{H}(t) = \mathcal{H}_0 + V(t)$ changes "slowly" w/ t.

"Slowly" means $\Delta\mathcal{H} \ll \hbar\omega_n$ on time scales $\Delta t \sim 1/\omega_n$. One supposes:

$$\to \mathcal{H}_0\phi_n = E_n^{(0)}\phi_n, @\ t = -\infty, \text{ evolves to: } \mathcal{H}(t)\phi_n(t) = E_n(t)\phi_n(t), \tag{38}$$

and that the latter eqtn can be solved at each t. The eigenfcns $\phi_n(t) \to \phi_n(t+\Delta t)$ evolve continuously, and there are few transitions $n \to k$ ... because the Fourier spectrum of V(t) has few high-frequency components to match the required transition freqs ω_{nk}. This method is called the "Adiabatic Approximation".

II. V(t) is not "small" w.r.t. $\mathcal{H}_0$, but $\partial\mathcal{H}/\partial t \to$ large at some t.

An extreme example is if $\mathcal{H}$ jumps from one form, $\mathcal{H}_1$, to another, $\mathcal{H}_2$, @ $t=0$:

$$\left[\begin{array}{llll} \mathcal{H}(t<0) = \mathcal{H}_1, \text{ w/ eigenfcns } & \phi_n & \text{and eigenenergies} & E_n; \\ \mathcal{H}(t>0) = \mathcal{H}_2, \text{ w/ } \quad '' & \Theta_\mu & \quad '' \quad\quad '' & W_\mu. \end{array}\right. \tag{39}$$

The calculation here proceeds on the supposition that even though $\partial\mathcal{H}/\partial t \to$ large, the system overall wavefcn $\Psi(t)$ must be continuous in t. Many transitions will occur (Fourier argument). Method is the "Sudden Approximation".

We shall now develop these alternate methods for tD Perturbation Theory.