Discontinuous changes in $\mathcal{H}$.

14) SUDDEN APPROXIMATION (Davydov, ¶92).

1. The antithesis of the adiabatic approximation, where we assume the Hamiltonian changes "slowly" on the energy/time scales of the QM system (i.e. $|\Delta\mathcal{H}/\Delta t| \ll |\Delta E/\tau|$, ΔE = transition energy & τ = natural period), is the "sudden approximation", where we assume just the opposite. Thus, consider a system where the Hamiltonian $\mathcal{H}$ changes "rapidly" at time $t=0$, i.e. ¶

$$\rightarrow \mathcal{H}(t) = \begin{cases} \mathcal{H}_1, \text{ for } t<0 \leftarrow \text{w/ known eigenstates}: \mathcal{H}_1\phi_n = E_n\phi_n; \\ \mathcal{H}_2, \text{ for } t>0 \leftarrow \text{w/ known eigenstates}: \mathcal{H}_2\theta_\mu = W_\mu\theta_\mu. \end{cases} \tag{54}$$

The $\mathcal{H}_1 \rightarrow \mathcal{H}_2$ switch at $t=0$ occurs in a time interval δt that is short compared to the natural periods of the $\mathcal{H}_1$ system ($\delta t \ll |\hbar/E_n|$). Otherwise $\mathcal{H}_1$ & $\mathcal{H}_2$ are <u>independent</u> of time, and the $\{E_n, \phi_n\}$ and $\{W_\mu, \theta_\mu\}$ are just stationary states -- albeit of <u>different</u> $\mathcal{H}$'s -- which are orthonormal [$\langle\phi_n|\phi_k\rangle = \delta_{nk}$, $\langle\theta_\mu|\theta_\kappa\rangle = \delta_{\mu\kappa}$, etc.].

<u>The problem at hand is this</u>: if the system is initially in an eigenstate m of $\mathcal{H}_1$ at $t<0$, what is the probability of finding state κ of $\mathcal{H}_2$ at $t>0$?

2. We can solve $\mathcal{H}\psi = i\hbar\,\partial\psi/\partial t$ by means of the expansions...

$$\rightarrow \psi(x,t) = \begin{cases} \sum_n a_n\phi_n(x)\, e^{-i(E_n/\hbar)t}, & \text{for } t<0; \\ \sum_\mu b_\mu\theta_\mu(x)\, e^{-i(W_\mu/\hbar)t}, & \text{for } t>0. \end{cases} \tag{55}$$

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¶ An example of a rapid change $\mathcal{H}_1 \rightarrow \mathcal{H}_2$ is that of an atom where the nucleus -- initially of charge Ze -- undergoes <u>beta-decay</u>, so that $Z \rightarrow Z+1$. The electron ejected from the nucleus leaves the atom in a time short compared to the orbital period of the bound e's, so we have $\mathcal{H}(Z) \rightarrow \mathcal{H}(Z+1)$ "suddenly". The present calculation can answer questions like "will we find excited states in the ion after β-decay?"

Transition Probability for a single-step discontinuity in $\mathcal{H}$.

In the expansions of Eq. (55), the $\{a_n\}$ and $\{b_\mu\}$ are independent of time, since $\mathcal{H}_1$ and $\mathcal{H}_2$ are t-independent by assumption. The problem is solved if we can find the $\{b_\mu\}$ in terms of the $\{a_n\}$.

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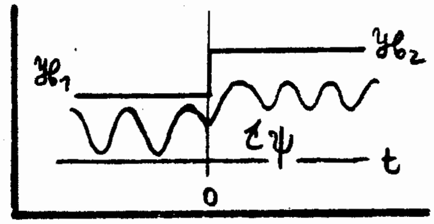
3. In: $\mathcal{H}\psi = i\hbar\,\partial\psi/\partial t$, even when $\mathcal{H}$ changes discontinuously, there's at most a discontinuous change in $\partial\psi/\partial t$, but ψ itself can and must remain continuous. If there were a discontinuity in ψ @ $t=0$, then $|\partial\psi/\partial t| \to \infty$ there, and $\Delta\mathcal{H}$ would have to be infinite. So, during any finite changes $\mathcal{H}_1 \to \mathcal{H}_2 = \mathcal{H}_1 + \Delta\mathcal{H}$, $\psi(t)$ is continuous. For the change $\mathcal{H}_1 \to \mathcal{H}_2$ @ $t=0$ described by the ψ's in Eq. (55), this means



$$\psi(x, t=0+) = \psi(x, t=0-), \text{ or } \boxed{\sum_\mu b_\mu\,\theta_\mu(x) = \sum_n a_n\,\phi_n(x)} \qquad (56)$$

This MASTER EQTN is relatively simple. Operate with $\langle\theta_\kappa|\ \rangle$ to get:

$$\to b_\kappa = \sum_n a_n \langle\theta_\kappa|\phi_n\rangle. \qquad (57)$$

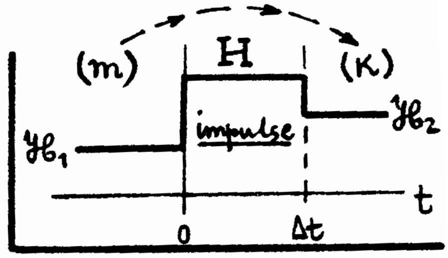
This is a solution to how $\mathcal{H}_1 \to \mathcal{H}_2$ affects the system, in that $|b_\kappa|^2$ gives the probability of finding the eigenstate κ of $\mathcal{H}_2$ (@ $t=0+$) when the initial preparation for $\mathcal{H}_1$ ($t=0-$) is known (i.e. the $\{a_n\}$ are given).

If at $t<0$, the system was in state m, then $a_n = \begin{cases} 1, & n=m \\ 0, & n\neq m \end{cases}$; and (57) reads:

$$\to \boxed{b_\kappa = \langle\theta_\kappa|\phi_m\rangle}, \text{ and } |b_\kappa|^2 = \text{transition prob}^{\underline{y}} \text{ for } m(\text{of } \mathcal{H}_1) \to \kappa(\text{of } \mathcal{H}_2). \qquad (58)$$

We have made no approximations as yet... the identification of the overlap integral b_κ depends only on our assuming: (A) we know the eigenfcns ϕ_m and θ_κ of $\mathcal{H}_1$ and $\mathcal{H}_2$, (B) $\psi(x,t)$ is continuous during $\mathcal{H}_1 \to \mathcal{H}_2$.

Double-step discontinuity in $\mathcal{H}$



4. Now consider a double-step discontinuity in $\mathcal{H}$, as depicted at right. We assume that the Hamiltonian is in 3 pieces...

$$\rightarrow \mathcal{H}(t) = \begin{cases} \mathcal{H}_1, \; t<0 & \longleftarrow \mathcal{H}_1 \phi_n = E_n \phi_n, \text{ known (as above)}, \\ H, \; 0<t<\Delta t & \longleftarrow H \varphi_j = \mathcal{E}_j \varphi_j, \text{ known in principle}, \\ \mathcal{H}_2, \; t>\Delta t & \longleftarrow \mathcal{H}\, \Theta_\mu = W_\mu \Theta_\mu, \text{ known (as above)}. \end{cases} \tag{59}$$

The impulse H here lasts only for a "short" time Δt (learn what "short" means here a bit later) and is meant to model some sudden perturbation which in fact changes the system Hamiltonian from $\mathcal{H}_1$ to $\mathcal{H}_2$ -- e.g. ionization of an atom in a high-speed collision.

If the duration Δt of the impulse H is short enough, we can do the calculation is such a way that we don't actually need to know the eigen-energies & eigenfcns $\{\mathcal{E}_j, \varphi_j\}$ of H; we need only know they exist. As before, we will be interested in calculating the transition amplitude m [initial state of $\mathcal{H}_1$] $\longrightarrow$ K [final state of $\mathcal{H}_2$].

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5. As before, we will impose ψ continuous @ $t=0$ and $t=\Delta t$. The ψ's are:

$$\longrightarrow \psi(x,t) = \begin{cases} \sum_n a_n \phi_n(x) \exp\left(-\frac{i}{\hbar} E_n t\right), & \text{for } t<0; \\ \sum_j c_j \varphi_j(x) \exp\left(-\frac{i}{\hbar} \mathcal{E}_j t\right), & 0<t<\Delta t; \\ \sum_\mu b_\mu \Theta_\mu(x) \exp\left(-\frac{i}{\hbar} W_\mu t\right), & t>\Delta t. \end{cases}$$

The $\{a_n\}$, $\{c_j\}$ & $\{b_\mu\}$ are all constants. The E_n & ϕ_n and W_μ & Θ_μ are known; $\{a_n\}$ usu. given. (60)

Continuity in ψ demands:

$$@\; t=0 \;:\; \sum_n a_n \phi_n = \sum_j c_j \varphi_j\;; \tag{61a}$$

$$@\; t=\Delta t \;:\; \sum_j c_j \varphi_j e^{-\frac{i}{\hbar}\mathcal{E}_j \Delta t} = \sum_\mu b_\mu \Theta_\mu e^{-\frac{i}{\hbar} W_\mu \Delta t}. \tag{61b}$$

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Double-step discontinuity: solution for b_K's.

∴ We want to solve Eqs. (61) for the b_K's; they can be projected out of Eq. (61b) by operating through by $\langle\theta_K|\ \rangle$. Then...

$$\rightarrow b_K = \sum_j c_j \langle\theta_K|\varphi_j\rangle e^{-\frac{i}{\hbar}(\mathcal{E}_j - W_K)\Delta t}. \tag{62}$$

The c_j's can be eliminated by means of Eq (61a): $c_j = \sum_n a_n \langle\varphi_j|\phi_n\rangle$, by an obvious operation. Plug this into Eq. (62) to get, exactly:

$$\rightarrow b_K = \sum_n a_n \left\{ \sum_j \langle\theta_K|\varphi_j\rangle e^{-\frac{i}{\hbar}(\mathcal{E}_j - W_K)\Delta t} \langle\varphi_j|\phi_n\rangle \right\}, \tag{63}$$

after rearranging terms. For simplicity, choose $a_n = \delta_{nm}$, as before, so that the initial state of the system is the eigenstate m of $\mathcal{H}_1$. Then...

$$\boxed{b_K = \langle\theta_K| \left[\sum_j |\varphi_j\rangle e^{-\frac{i}{\hbar}(\mathcal{E}_j - W_K)\Delta t} \langle\varphi_j| \right] |\phi_m\rangle}. \tag{64}$$

This expression is still exact; we've made no approx^{n}s. It is the counterpart of the (simpler) single-step transition amplitude $b_K = \langle\theta_K|\phi_m\rangle$ in Eq. (58). But now we have the effects of the impulse sandwiched in.

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7. In (64), we want to get rid of the impulse descriptors $\{\mathcal{E}_j, \varphi_j\}$; this saves us actually solving $\mathcal{I}\varphi_j = \mathcal{E}_j\varphi_j$ (in addition to $\mathcal{H}_1\phi_n = E_n\phi_n$ & $\mathcal{H}_2\theta_\mu = W_\mu\theta_\mu$). We can do this for "short" impulses by the following approximation...

Assume: $\left|\frac{1}{\hbar}(\mathcal{E}_j - W_K)\right|\Delta t \ll 1$, (always true for sufficiently small Δt);

So// $e^{-\frac{i}{\hbar}(\mathcal{E}_j - W_K)\Delta t} = 1 - \frac{i}{\hbar}(\mathcal{E}_j - W_K)\Delta t + \dots$

and// Eq. (64) $\Rightarrow b_K = \langle\theta_K| \left[\sum_j |\varphi_j\rangle \left\{ 1 - \frac{i}{\hbar}(\mathcal{E}_j - W_K)\Delta t + \dots \right\} \langle\varphi_j| \right] |\phi_m\rangle$. (65)

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Sudden Approx^n (small Δt) for $m \to k$ amplitude.

Now, in (65), we use the completeness relation $\sum_j |\varphi_j\rangle\langle\varphi_j| = 1$ to write...

$$b_k \simeq \langle\theta_k|\phi_m\rangle - \frac{i}{\hbar}\Delta t \underbrace{\sum_j \langle\theta_k|(\mathcal{E}_j - W_k)|\varphi_j\rangle\langle\varphi_j|\phi_m\rangle}, \text{ to } \mathcal{O}(\Delta t)$$

$$= \sum_j \langle\theta_k|(H - \mathcal{H}_2)|\varphi_j\rangle\langle\varphi_j|\phi_m\rangle = \langle\theta_k|(H-\mathcal{H}_2)|\phi_m\rangle,$$

so//

$$\boxed{b_k \simeq \langle\theta_k|\phi_m\rangle - \frac{i}{\hbar}\Delta t \langle\theta_k|\Delta H_2|\phi_m\rangle}$$ $m \to k$ transition amplitude, w/ $\Delta H_2 = H - \mathcal{H}_2$. (66)

REMARKS

(a) 1$^{\text{st}}$ term in b_k is previous single-step result for $\mathcal{H}_1 \to \mathcal{H}_2$, Eq. (58). 2$^{\text{nd}}$ term is lowest-order effect of impulse H over duration Δt.

(b) Approxn is valid if $\Delta t \to 0$, as in Eq. (65). Although $\langle\Delta H_2\rangle$ can be "large", it must be true that $\left|\frac{1}{\hbar}\Delta t\langle\Delta H_2\rangle\right| \ll 1$, for (66) to hold.

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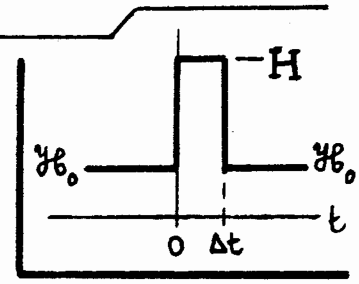
8. Eq. (66) is often used in cases where the initial and final $\mathcal{H}$'s are the same, i.e. $\mathcal{H}_1 = \mathcal{H}_2 = \mathcal{H}_0$. A case would be that of a high-energy non-ionizing collision for an atom. In (66), then the final system eigenfcns θ_k are the same as the initial system eigenfcns ϕ_k, and the ampl. is:



$$\left[\!\left[b_k \simeq \delta_{km} - \frac{i}{\hbar}\Delta t \langle\phi_k|\Delta H|\phi_m\rangle \right]\!\right]$$ $m \to k$ transition amplitude under impulse $\Delta H = H - \mathcal{H}_0$. (67)

The approxn is valid for $|\Delta t\langle\Delta H\rangle| \ll \hbar$. Even though ΔH may be "large", $|b_k|^2$ for $m \to k \neq m$ is still small in the sense of pert^{b}n theory.

NOTE: the final system wavefcn (at $t > \Delta t$) for b_k of (67) is by now...

$$\Psi(x,t) = \sum_k b_k \phi_k(x) e^{-\frac{i}{\hbar}E_k t}, \text{ for } t > \Delta t,$$

$$\simeq \underbrace{\phi_m e^{-\frac{i}{\hbar}E_m t}}_{\text{initial state } m} - \underbrace{\frac{i}{\hbar}\Delta t \sum_{k \neq m} \langle k|\Delta H|m\rangle \phi_k e^{-\frac{i}{\hbar}E_k t}}_{\text{states mixed in by impulse } \Delta H}. \quad (68)$$