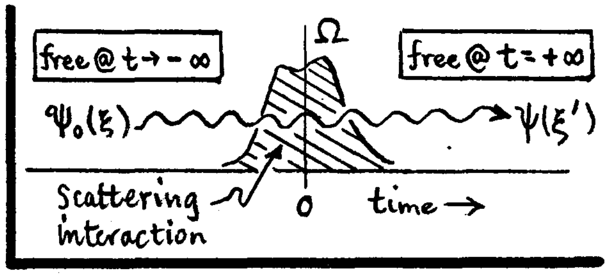
APPLICATION: Feynman Formulation $\leftrightarrow$ S-Matrix Theory.

6) The Feynman formulation of QM by path integrals has a direct relation to actual scattering problems, as we now show. It leads to what is called "S-matrix theory" (the S stands for "scattering"), which we now outline. S-matrix theory has been widely used in actual scattering analysis, as well as general interaction analysis.

$\rightarrow$ Start from: $\psi(\xi') = i\int dx\, G(\xi',\xi)\,\psi_0(\xi)$ $\surd$ w/ $t \to -\infty$ (distant past), $t' \to +\infty$ (distant future). (36)



The fact that $\psi = \psi_0(\xi)$ [free particle] at $t \to -\infty$ means the interaction $\Omega = 0$ there. If the interaction is bounded in time, then $\Omega \to 0$ again as $t \to +\infty$, and so $\psi(\xi')$ must also be free. Let:

$\psi_0(\xi) = (1/\sqrt{2\pi})\exp[i(k_\alpha x - \omega_\alpha t)] = \phi_\alpha(\xi)$ $\surd$ incoming plane wave @ $t = -\infty$; momentum $\hbar k_\alpha$, energy $\hbar\omega_\alpha$, and: $\omega_\alpha = \hbar k_\alpha^2/2m$ for free particle. (37)

So $\psi_\alpha(\xi') = i\int dx\, G(\xi',\xi)\,\phi_\alpha(\xi)$, for scattering: $\phi_\alpha(@\, t=-\infty) \to \psi_\alpha(@\, t=+\infty)$.

But since $\psi_\alpha(\xi')$ becomes free as $t' \to +\infty$, it can at most be a superposition of free particle states ϕ, i.e.

$\rightarrow$ $\psi_\alpha(\xi') = \sum_\beta S_{\beta\alpha}\,\phi_\beta(\xi')$, as $t' \to +\infty$;

w/ $\underline{\underline{S_{\beta\alpha} = \int dx'\, \phi_\beta^*(\xi')\,\psi_\alpha(\xi')}}$ $\surd$ $S_{\beta\alpha}$ is an element of the "scattering matrix" or S-matrix: $\underset{\sim}{S} = (S_{\beta\alpha})$. (38)

&// $|S_{\beta\alpha}|^2$ = probability that scattered state $\psi_\alpha(\xi')$ contains planewave $\phi_\beta(\xi')$, i.e. the prob. of a free-free scattering $\phi_\alpha(\xi) \to \phi_\beta(\xi')$.

Put the expression for $\psi_\alpha(\xi')$ from Eq. (37) into the definition of $S_{\beta\alpha}$, so...

$$\boxed{S_{\beta\alpha} = i\int dx' \int dx\, \phi_\beta^*(\xi')\,G(\xi',\xi)\,\phi_\alpha(\xi)}$$

$\surd$ for $t \to (-)\infty$, $t' \to +\infty$, such that scattering Ω vanishes. (39)

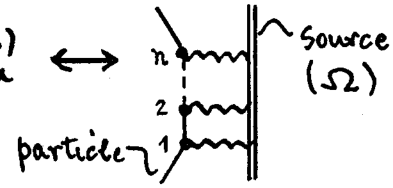
In this form, it is clear that $|S_{\beta\alpha}|^2$ really does measure $\phi_\alpha\left[\begin{smallmatrix}\text{free at}\\ t\to-\infty\end{smallmatrix}\right] \to \phi_\beta\left[\begin{smallmatrix}\text{free at}\\ t\to+\infty\end{smallmatrix}\right]$.

Now for $S_{\beta\alpha}$ in (39), we have perturbation series for G in (35), i.e. $G = G_0 + \int G_0\Omega G_0 + \iint G_0\Omega G_0\Omega G_0 + \ldots$. Using this, we can write $S_{\beta\alpha}$ as a series..

Scattering Problem via S-Matrix. Born Approximation.

$$\left[\!\left[\; S_{\beta\alpha} = i\int dx' \int dx\, \phi_\beta^*(\xi')\left\{ G_0 + \int G_0 \Omega G_0 + \iint G_0 \Omega G_0 \Omega G_0 + \cdots \right\}\phi_\alpha(\xi), \right.\right.$$

$$= S_{\beta\alpha}^{(0)} + S_{\beta\alpha}^{(1)} + S_{\beta\alpha}^{(2)} + \cdots \quad \text{w/}\quad S_{\beta\alpha}^{(n)} \longleftrightarrow \qquad (40)$$



The successive terms are:

$$S_{\beta\alpha}^{(0)} = i\int dx' \int dx\, \phi_\beta^*(\xi')\, G_0(\xi',\xi)\,\phi_\alpha(\xi) = \int dx'\, \phi_\beta^*(\xi') \underbrace{\left[i\int dx\, G_0(\xi',\xi)\phi_\alpha(\xi)\right]}_{=\phi_\alpha(\xi'),\ \text{by def}^{\underline{n}}}$$

So//

$$\rightarrow \underline{\underline{S_{\beta\alpha}^{(0)} = \int dx'\, \phi_\beta^*(\xi')\,\phi_\alpha(\xi')}} = \begin{cases} \delta_{\beta\alpha},\ \text{no interaction } (0^{\underline{th}} \text{ order}) \\ \text{OR } \delta(k_\beta - k_\alpha),\ \infty \text{ box norm}^{\underline{3}}\text{n}. \end{cases} \qquad (41)$$

and//

$$S_{\beta\alpha}^{(1)} = i\int dx' \int dx\, \phi_\beta^*(\xi')\left[\int d\xi_1\, G_0(\xi',\xi_1)\,\Omega(\xi_1)\, G_0(\xi_1,\xi)\right]\phi_\alpha(\xi)$$

$$= -i\int d\xi_1 \underbrace{\left[i\int dx'\, \phi_\beta^*(\xi')\, G_0(\xi',\xi_1)\right]}_{\phi_\beta^*(\xi_1),\ \text{see prob. \#16}} \Omega(\xi_1) \underbrace{\left[i\int dx\, G_0(\xi_1,\xi)\,\phi_\alpha(\xi)\right]}_{=\phi_\alpha(\xi_1),\ \text{by def}^{\underline{n}}}$$

$$\rightarrow \underline{\underline{S_{\beta\alpha}^{(1)} = -i\int d\xi_1\, \phi_\beta^*(\xi_1)\,\Omega(\xi_1)\,\phi_\alpha(\xi_1)}} \qquad (42)$$

this 1st order amplitude is called the Born Approx$^{\underline{n}}$ to the scattering.

Similarly, we can show...

$$S_{\beta\alpha}^{(2)} = -i\int d\xi_2 \int d\xi_1\, \phi_\beta^*(\xi_2)\left[\Omega(\xi_2)\, G_0(\xi_2,\xi_1)\,\Omega(\xi_1)\right]\phi_\alpha(\xi_1),$$

$$\vdots$$

$$\underline{\underline{S_{\beta\alpha}^{(n)} = -i\int d\xi_n \cdots \int d\xi_1\, \phi_\beta^*(\xi_n)\underbrace{\left[\Omega(\xi_n)\, G_0 \cdots \Omega \cdots G_0\, \Omega(\xi_1)\right]}_{n \text{ factors of } \Omega \text{ (i.e. exchange of } n \text{ quanta)}}\phi_\alpha(\xi_1)}}. \qquad (43)$$

The final state (scattered) wavefcn of Eq. (38) is then...

$$\psi_\alpha(\xi') = \sum_\beta \left[S_{\beta\alpha}^{(0)} + S_{\beta\alpha}^{(1)} + S_{\alpha\beta}^{(2)} + \cdots \right]\phi_\beta(\xi')$$

1st Born Approxn.

$$= \phi_\alpha(\xi') - i\sum_\beta \left[\int d\xi_1\, \phi_\beta^*(\xi_1)\,\Omega(\xi_1)\,\phi_\alpha(\xi_1)\right]\phi_\beta(\xi') - \mathcal{O}(\Omega^2), \qquad (44)$$

The scattering is thus described in terms of planewave (free-particle) states $\phi_\nu(\xi')$ plus integrals of those states over the interaction. See Davydov, Sec. 118.

7) As a final application of Feynman's formulation, we show that it is equivalent to orthodox time-dependent perturbation theory, including all orders of the perturbation.* This exercise clearly identifies the perturbative nature of the G-fcn expansion in Eq.(34), and pinpoints the dynamics of the orthodox theory.

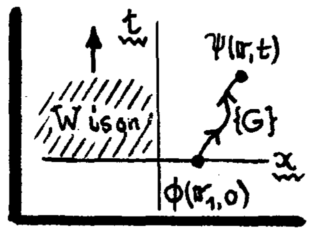
(a) Set $\hbar=1$, and consider a Schrödinger system perturbed by coupling W @ $t>0$:

$$\rightarrow \left(i\frac{\partial}{\partial t}-\mathcal{H}\right)\psi(\mathbf{r},t)=W(\mathbf{r},t)\,\psi(\mathbf{r},t),\ t>0 \quad \begin{cases}\mathcal{H}=\text{reference Hamiltonian}\\ W=\text{perturbation}\begin{cases}0,\ \text{for } t<0;\\ \neq 0,\ \text{for } t>0.\end{cases}\end{cases} \tag{45}$$

$\mathcal{H}=-(1/2m)\nabla^2+V(\mathbf{r})$ is a static Hamiltonian generating eigenfcns $u_n(\mathbf{r})$ and eigenenergies ω_n at $t<0$, via: $\mathcal{H}u_n=\omega_n u_n$. The perturbation W is turned on at $t=0$. We attack the problem of finding $\psi(\mathbf{r},t>0)$ by Feynman's method.

(b) If the initial state of the system is $\phi(\mathbf{r},0)$ [before W], then the state at some later time $t>0$ [after W] is specified, to lowest order in the coupling W, by:

$$\rightarrow \psi(\mathbf{r},t)=\phi(\mathbf{r},t)+\int_0^t dt_1\int_\infty d^3x_1\, G(\mathbf{r},t;\mathbf{r}_1,t_1)\,W(\mathbf{r}_1,t_1)\,\phi(\mathbf{r}_1,t_1);$$



w// G satisfying: $\left(i\frac{\partial}{\partial t}-\mathcal{H}\right)G(\mathbf{r},t;\mathbf{r}_1,t_1)=\delta(\mathbf{r}-\mathbf{r}_1)\,\delta(t-t_1)$,

So//

$$G(\mathbf{r},t;\mathbf{r}_1,t_1)=-i\sum_n u_n^*(\mathbf{r}_1)\,\boxed{u_n(\mathbf{r})\,e^{-i\omega_n(t-t_1)}},\ \text{for } t_1<t. \tag{46}$$

The information on G has been worked out in problem # 11, and ϕ is any solution to the homogeneous problem: $[i(\partial/\partial t)-\mathcal{H}]\,\phi(\mathbf{r},t)=0$. In what follows, G and ϕ play the role of free-particle descriptors -- they are free of any influence of the perturbation $W(\mathbf{r},t)$, although they include the binding interaction $V(\mathbf{r})$.

Upon putting G into the integral, we can write:

$$\rightarrow \psi(\mathbf{r},t)=\phi(\mathbf{r},t)+\sum_n a_{n\phi}^{(1)}(t)\,\boxed{u_n(\mathbf{r})\,e^{-i\omega_n t}},$$

$\leftarrow$ eigenfcns $|n\rangle$ of original system

(next page)

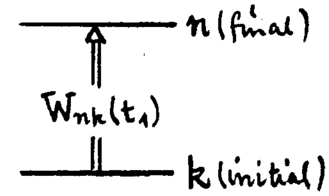
* Davydov derives the results here by orthodox methods in his Sec. 90, then connects them to the S-matrix (and hence Feynman, in reverse order) in his Sec. 101.

Time-dept. Pert$^{\underline{b}}$n Theory: 1st & 2nd order transitions. $\boxed{\hbar=1}$

w/ $a^{(1)}_{n\phi}(t) = -i\int_0^t dt_1\, e^{i\omega_n t_1}\int d^3x_1\, u_n^*(\mathbf{r}_1)W(\mathbf{r}_1,t_1)\phi(\mathbf{r}_1,t_1)$. (47)

Conventionally, $a^{(1)}_{n\phi}$ is the first (lowest) order amplitude for a transition $\phi\to n$ driven by W. Let us suppose that the initial state of the system is simple, i.e. let ϕ be the k^{th} eigenstate: $\underline{\phi(\mathbf{r},t)=u_k(\mathbf{r})e^{-i\omega_k t}}$. Then Eq.(47) is...

$$\boxed{\begin{aligned}&\psi(\mathbf{r},t)=u_k(\mathbf{r})e^{-i\omega_k t}+\sum_n a^{(1)}_{nk}(t)\,u_n(\mathbf{r})e^{-i\omega_n t};\\ &\text{w/ } a^{(1)}_{nk}(t)=-i\int_0^t dt_1\, W_{nk}(t_1)\,e^{i(\omega_n-\omega_k)t_1},\\ &\text{\& } W_{nk}(t_1)=\int_\infty d^3x_1\, u_n^*(\mathbf{r}_1)W(\mathbf{r}_1,t_1)u_k(\mathbf{r}_1).\end{aligned}}$$



(48)

This result is precisely a statement of 1st order time-dept. pertur$^{\underline{b}}$n theory [Davydov Eq.(90.9); Sakurai Eq.(5.6.17)]. The probability for a transition $k\to n$ in the original system depends on $W_{nk}(t_1)=\langle n|W(\mathbf{r}_1,t_1)|k\rangle$ being nonzero.

(c) The $\sum_n$ add-on to state $|k\rangle$ in Eq.(48) can be interpreted as a "wavelet" $\Delta^{(1)}\psi(\mathbf{r},t)$ generated by an $O(W)$ "scattering" of $|k\rangle$ from the interaction W. In $O(W^2)$, get:

$$\to \Delta^{(2)}\psi(\mathbf{r},t)=\int_0^t dt_1\int_0^{t_1}dt_2\int_\infty d^3x_1\int_\infty d^3x_2\, G(\mathbf{r},t;\mathbf{r}_1,t_1)W(\mathbf{r}_1,t_1)\cdot$$

$$\cdot\, G(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)W(\mathbf{r}_2,t_2)\phi(\mathbf{r}_2,t_2), \qquad (49)$$

where $\underline{t_2<t_1<t}$ is a time-ordering demanded by the def$^{\underline{n}}$ of the G-fcns. Put in G of Eq(46), and put in $\phi(\mathbf{r}_2,t_2)=u_k(\mathbf{r}_2)e^{-i\omega_k t_2}$ as above [initially, have $|k\rangle$]:

$$\to \Delta^{(2)}\psi(\mathbf{r},t)=(-i)^2\sum_{n,m}\boxed{u_n(\mathbf{r})e^{-i\omega_n t}}\int_0^t dt_1\int_0^{t_1}dt_2\int_\infty d^3x_1\int_\infty d^3x_2\,\cdot$$

$$\cdot\left[u_n^*(\mathbf{r}_1)W(\mathbf{r}_1,t_1)u_m(\mathbf{r}_1)e^{i\omega_{nm}t_1}\right]\cdot\left[u_m^*(\mathbf{r}_2)W(\mathbf{r}_2,t_2)u_k(\mathbf{r}_2)e^{i\omega_{mk}t_2}\right],$$

or/

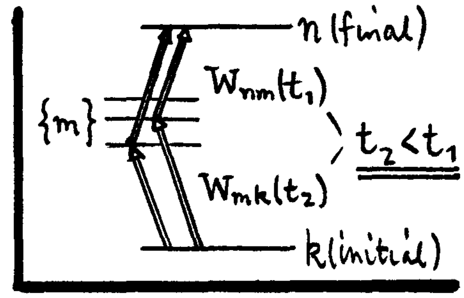
$$\Delta^{(2)}\psi(\mathbf{r},t)=\sum_n a^{(2)}_{nk}(t)\boxed{u_n(\mathbf{r})e^{-i\omega_n t}}, \quad \text{eigenfcns } |n\rangle \text{ of original system}$$

$$\text{w/ } a^{(2)}_{nk}(t)=(-i)^2\sum_m\int_0^t dt_1\, W_{nm}(t_1)e^{i\omega_{nm}t_1}\int_0^{t_1}dt_2\, W_{mk}(t_2)e^{i\omega_{mk}t_2}, \qquad (50)$$

where: $\omega_{ij}=\omega_i-\omega_j$, is the Bohr transition frequency for $|j\rangle\to|i\rangle$.

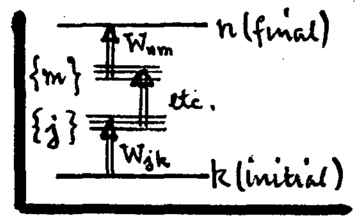
Time-dept. perturb$^{\underline{b}}$n theory: process @ $O(W^\lambda)$. $\boxed{\hbar=1}$

The interpretation of $a_{nk}^{(2)}(t)$ is that it accounts for all possible two-step processes for $|k\rangle\to|n\rangle$, i.e. transitions through "intermediate states" $|m\rangle$ as shown. We have $|k\rangle\to|m\rangle$ @ time t_2, then $|m\rangle\to|n\rangle$ at time t_1. It is easy to see why the time ordering $t_2<t_1$ is necessary -- this is just causality.



(d) The procedure in Eqs. (46)-(50) [of reducing the terms in the G-fcn expansion to the language of time-dept. pert$^{\underline{b}}$n theory] can be extended to $O(W^\lambda)$. Solution is:

$$\rightarrow \psi(\mathbf{r},t) = u_k(\mathbf{r})e^{-i\omega_k t} + \sum_{\lambda=1}^{\infty}\Delta^{(\lambda)}\psi(\mathbf{r},t);$$



w/ $$\Delta^{(\lambda)}\psi(\mathbf{r},t) = \sum_n a_{nk}^{(\lambda)}(t)\,u_n(\mathbf{r})\,e^{-i\omega_n t},$$

&/ $$a_{nk}^{(\lambda)}(t) = (-i)^\lambda \sum_{m,l,\dots,j}\int_0^t dt_1\,W_{nm}(t_1)\,e^{i\omega_{nm}t_1}\int_0^{t_1}dt_2\,W_{ml}(t_2)\,e^{i\omega_{ml}t_2}\cdot\ldots$$

$$\ldots\cdot\int_0^{t_{\lambda-1}}dt_\lambda\,W_{jk}(t_\lambda)\,e^{i\omega_{jk}t_\lambda},$$ w/ causal time-ordering: $\underline{t>t_1>t_2>\ldots>t_\lambda}$. (51)

$a_{nk}^{(\lambda)}$ accounts for all possible λ-step processes for $|k\rangle\to|n\rangle$. The transition goes through $(\lambda-1)$ sets of intermediate states: $k\to\{j\}\to\ldots\to\{l\}\to\{m\}\to n$, while obeying the causal time-ordering noted. A "scattering" occurs at each new state.

(e) Altogether, the final-state wavefunction in Eq. (51) can be written as:

$$\boxed{\begin{aligned}&\psi(\mathbf{r},t) = u_k(\mathbf{r})\,e^{-i\omega_k t} + \sum_n a_{nk}(t)\,u_n(\mathbf{r})\,e^{-i\omega_n t},\\ &\text{w/ } a_{nk}(t) = \sum_{\lambda=1}^{\infty}a_{nk}^{(\lambda)}(t),\ \text{and } a_{nk}^{(\lambda)}(t)\ \text{defined in (51).}\end{aligned}}$$ (52)

This is effectively all of time-dept. pertur$^{\underline{b}}$n theory in QM. Here we have developed it as just a relabeling of Feynman's integral formulation of QM. The Feynman notion of propagation of a state ψ from ξ to ξ' via $G(\xi',\xi)$, i.e. $\psi(\xi') = i\int G(\xi',\xi)\,\psi(\xi)\,dx$, is evidently a fundamental & far-reaching idea!