4) As we shall see soon, the <u>free particle propagator</u> $\underline{\underline{K_0}}$ [or $G_0 = -i\,\Theta K_0$] has a predominant role in Feynman's formulation. So-- as an exercise, and for its later utility -- we derive K_0. We shall do it from a sum, like (A5).

Derivation of free-particle propagator K_0.

$$\rightarrow K_0(x',t';x,t) = \sum_n u_n^*(x)\, u_n(x')\, e^{-\frac{i}{\hbar}E_n(t'-t)},$$

w/ $u_n(x) = (1/\sqrt{2\pi})\, e^{ik_n x}$, for a free particle in an ∞ 1D box†;

where: $k_n = 2\pi n/L$, $n = 0, \pm1, \pm2, \ldots$ ✓ for periodic boundary conditions, and with box length $L \to \infty$;

and: energy $E_n = \hbar\omega_n$, with $\underline{\omega_n = \hbar k_n^2/2m}$ for a free particle. (16)

As the box length $L \to \infty$: $k_n \to k$, a continuous variable; $\Delta k_n = \frac{2\pi}{L} \to dk$, an ∞smal; and the sum $\sum_n \to \int_{-\infty}^{\infty} dk$, an integral over the wavenumbers. So...

$$\rightarrow \underline{\underline{K_0(x',t';x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\; e^{ik(x'-x)}\; e^{-i\omega(t'-t)}}}. \tag{17}$$

NOTE: at $t'=t$, have: $K_0 = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ik(x'-x)}dk = \delta(x'-x)$, so the normalization is correct, according to the general closure relation in Eq.(10).

NOTE: K_0 in (17) is a free-particle wavepacket: $K_0 = \int_{-\infty}^{\infty}\varphi(k)\, e^{i(kX-\omega T)}dk$, w/ $X = (x'-x)$, $T = (t'-t)$, $\omega = \hbar k^2/2m$, and $\varphi(k) = 1/2\pi$. The momentum spectrum $\varphi(k)$ is flat because we are localizing K_0 in space.

To evaluate the integral in (17), put in $\omega = \hbar k^2/2m$, so that...

$$K_0 = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-qk^2 + iXk}\, dk \leftarrow q = i\hbar T/2m, \text{ w/ } T = t'-t,\ X = x'-x;$$

or// $\underline{\underline{K_0 = \frac{1}{2\pi}\cdot\sqrt{\frac{\pi}{q}}\; e^{-X^2/4q}}}$ ✓ tabulated [e.g. G&R # (3.323.2)] (use convergence factor $\mathrm{Re}\, q \to 0+$) (18)

So the free-particle propagator is...

$$\boxed{\begin{aligned} K_0(x',t';x,t) &= \left[\frac{m}{2\pi i\hbar}/(t'-t)\right]^{1/2} \exp\left\{\frac{im}{2\hbar}|x'-x|^2/(t'-t)\right\}, \text{ in 1D;} \\ K_0(\mathbf{r}',t';\mathbf{r},t) &= \left[\frac{m}{2\pi i\hbar}/(t'-t)\right]^{3/2} \exp\left\{\frac{im}{2\hbar}|\mathbf{r}'-\mathbf{r}|^2/(t'-t)\right\}, \text{ in 3D.}\end{aligned}} \tag{19}$$

---

† We are using "delta-fcn normalization" for the free particle wavefcns $u_n(x)$:

ORTHOGONALITY: $\int_\infty u_n^*(x)\, u_\ell(x)\, dx = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{-i(k_n-k_\ell)x}dx = \delta(k_n - k_\ell)$;

COMPLETENESS: $\int_\infty u_n^*(x')\, u_n(x)\, dk_n = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{-ik_n(x'-x)}dk_n = \delta(x'-x)$.

$\boxed{\text{REMARKS}}$ on free-particle propagator $K_0(x',t';x,t)$ of Eq. (19).

$\boxed{1}$ As noted above, K_0 is a free-particle wavepacket, with completely unspecified momentum, which represents the propagation of a particle -- initially perfectly well-localized $[K_0(t'=t) = \delta(x'-x)]$ -- from (x,t) to (x',t'). The motion is diffusive, as $|K_0| \propto 1/\sqrt{t'}$, in 1D, when $t' \to \infty$. At the same time, per Eq. (8), we can interpret K_0 as the probability amplitude for the free propagation $(x,t) \to (x',t')$ of a "disturbance" originating at (x,t).

$\boxed{2}$ Although we got the free-particle propagator K_0 fairly easily, it is extremely difficult to get K in the general case -- either by solving the point source eqtn [Eq. (15)], or by evaluating the sum-over-states [Eq. (A5)]*. The point-source eqtn is actually more complicated than the Schrödinger eqtn itself, and the sum-over-states requires that the Schrödinger problem already be solved for the eigenfcns $u_n(x)$ & eigenenergies E_n. Is this progress?

$\boxed{3}$ Even though you can't get K explicitly for most Hamiltonians $\mathcal{H}$, we shall now show that all you really need to do the QM is to know the free-particle propagator K_0 -- which we already have in Eq. (19). In fact, the general Schrödinger problem: $\mathcal{H}\psi = i\hbar\frac{\partial\psi}{\partial t}$, can be solved for ψ (in a perturbation-type series) entirely in terms of the free-particle propagator K_0 (or $G_0 = -i\,\theta\,K_0$) and free-particle wavefcns: $\psi_0(x,t) = (1/\sqrt{2\pi})\,e^{i(kx-\omega t)}$. This was Feynman's insight.

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5) Begin the program in remark $\boxed{3}$ above by defining a more compact notation:

$$\left.\begin{array}{l}\text{Let } (\xi) \text{ represent the space-time point } (x,t), \text{ i.e.: } \psi(\xi) = \psi(x,t), \text{ in 1D.}\\ \text{In 3D: } (\xi) \leftrightarrow (\mathbf{r},t). \text{ And } dx \to d^3x \text{ (3 space cds).}\\ \text{Later, we will use: } d\xi = dx\,dt \text{ (in 1D), or } d\xi = d^3x\,dt \text{ (in 3D).}\end{array}\right\} \quad (20)$$

---

* The only easy solutions for K are those for a free particle, particle in a cnst external field, and SHO. The SHO solution is done by Merzbacher "QM" (2nd ed.), p. 164.

Interactions of a "free" particle with an external coupling V.

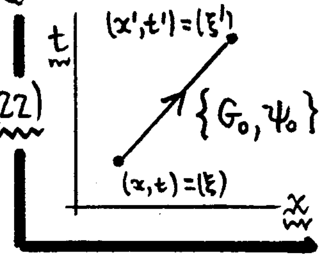
Our integral formulation for ψ [Eqs. (12) & (15)] may then be stated as:

$$\left[\begin{array}{l}\psi(\xi') = i\int G(\xi',\xi)\,\psi(\xi)\,dx, \text{ for } t'>t; \\ \text{w/ } \left(i\hbar\frac{\partial}{\partial t'} - \mathcal{H}'\right) G(\xi',\xi) = \hbar\,\delta(\xi'-\xi) \quad \text{on RHS, symbolically: } \delta(\xi'-\xi) = \delta(x'-x)\,\delta(t'-t).\end{array}\right] \quad (21)$$

We adopt the following piece-by-piece picture of how the particle represented by ψ undergoes an "interaction" (i.e. a coupling to some external potential V), while enroute from space-time point $\xi=(x,t)$ to point $\xi'=(x',t'>t)$.

① Suppose particle propagates $\xi \to \xi'$ as a completely free particle.

$$\xrightarrow{\text{so}} \underline{\underline{\psi_0(\xi') = i\int dx\, G_0(\xi',\xi)\,\psi_0(\xi)}} \quad \begin{cases} G_0 = \text{free-particle propagator, Eq. (19);} \\ \psi_0 = \frac{1}{\sqrt{2\pi}}e^{i(kx-\omega t)} \text{ free-particle wavefcn.} \end{cases} \quad (22)$$



The motion is tracked by the space-time diagram as sketched.

② Suppose free propagation $\xi \to \xi_1\,(t_1>t)$, with an interaction V for a short time Δt_1 at ξ_1, followed by free propagation $\xi_1 \to \xi'\,(t'>t_1)$. Now have perturb$^{\underline{n}}$:

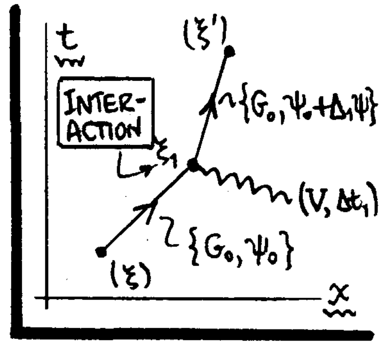
$\underline{\psi_0 \to \psi_0 + \Delta_1\psi}$, at ξ_1 w/ $\Delta_1\psi$ due to particle "scattering" by V at ξ_1.

... calculate $\Delta_1\psi$ from Schrödinger Eqtn, w/ $\mathcal{H} = \mathcal{H}_0(\text{free}) + V$, at ξ_1 ...

$$\left[i\hbar\frac{\partial}{\partial t_1} - \mathcal{H}_0(\xi_1)\right]\psi(\xi_1) = V(\xi_1)\,\psi(\xi_1) \leftarrow \text{plug in } \psi(\xi_1) = \psi_0(\xi_1) + \Delta_1\psi(\xi_1)$$

$$\text{or/ } i\hbar\frac{\partial}{\partial t_1}\Delta_1\psi(\xi_1) = V(\xi_1)\,\psi_0(\xi_1) + \left[\mathcal{H}_0 + \cancel{V}\right]\Delta_1\psi \quad \text{negligible}$$

$$\text{so/ } \underline{\underline{\Delta_1\psi(\xi_1) = -\frac{i}{\hbar}\left[V(\xi_1)\,\Delta t_1\right]\psi_0(\xi_1)}}, \text{ to } \mathcal{O}(V). \quad (23)$$



Now $\Delta_1\psi$ propagates freely from ξ_1 to ξ', so we write...

$$\rightarrow \underline{\underline{\Delta_1\psi(\xi') = i\int dx_1\, G_0(\xi',\xi_1)\,\Delta_1\psi(\xi_1) = \int dx_1\, G_0(\xi',\xi_1)\left[\Omega(\xi_1)\,\Delta t_1\right]\psi_0(\xi_1)}}. \quad (24)$$

We have defined the interaction in freq. units: $\underline{\Omega(\xi) = \frac{1}{\hbar}V(\xi)}$, to eliminate a factor of $\hbar$. Now, put in: $\psi_0(\xi_1) = i\int dx\, G(\xi_1,\xi)\,\psi_0(\xi)$, i.e. free propagation

First-order interaction as a scattering event.

from ξ to ξ_1, to get the perturbation $\Delta_1\psi$ at terminus as...

$$\rightarrow \Delta_1\psi(\xi') = i\int dx \int dx_1\, \Delta t_1\, G_0(\xi',\xi_1)\,\Omega(\xi_1)\,G_0(\xi_1,\xi)\,\psi_0(\xi). \tag{25}$$

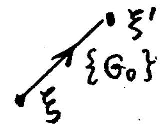
The total wave disturbance @ ξ', after the interaction Ω at ξ_1, is then:

$$\rightarrow \psi(\xi') = \psi_0(\xi') + \Delta_1\psi(\xi')$$

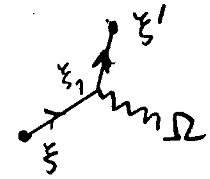
$$= i\int dx\,[\underbrace{G_0(\xi',\xi)}_{1} + \underbrace{\int dx_1\,\Delta t_1\, G_0(\xi',\xi_1)\,\Omega(\xi_1)\,G_0(\xi_1,\xi)}_{2}]\,\psi_0(\xi). \tag{26}$$

Interpret...

① = free propagation: $\xi\rightarrow\xi'$. Gives $\psi_0(\xi')$, Eq. (22);



② = free propagation: $\xi\rightarrow\xi_1$, then interaction for Δt_1 @ ξ_1, followed by free propagation: $\xi_1\rightarrow\xi'$. Gives $\Delta_1\psi(\xi')$, Eq. (25)



NOTE: we can write $\psi(\xi')$ of (26), after one (brief) interaction, as...

$$\left.\begin{aligned} &\rightarrow \psi(\xi') = i\int dx\, G(\xi',\xi)\,\psi_0(\xi),\\ &\text{w/}\ G(\xi',\xi) = G_0(\xi',\xi) + \int dx_1\,\Delta t_1\, G_0(\xi',\xi_1)\,\Omega(\xi_1)\,G_0(\xi_1,\xi). \end{aligned}\right\} \tag{27}$$

The major thing to notice here is that we have completely described the interaction (coupling Ω for Δt_1 @ ξ_1) by means of just the free-particle propagator G_0 and free-particle wave fcns ψ_0, at least to $\mathcal{O}(\Omega)$.

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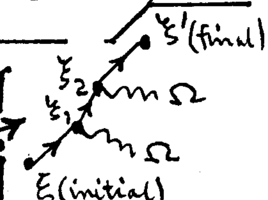
③ Now, account for a second "scattering" by Ω enroute: i.e. Ω acts also for Δt_2 @ ξ_2, w/ $t_2 > t_1$. We need to calculate the dgm



By analogy with $\Delta_1\psi(\xi_1)$ of Eq. (23), there is another wavelet $\Delta_2\psi(\xi_2)$ generated by the scattering at ξ_2. At ξ', $\Delta_2\psi$ contributes

$$\rightarrow \Delta_2\psi(\xi') = \int dx_2\,\Delta t_2\, G_0(\xi',\xi_2)\,\Omega(\xi_2)\,\psi(\xi_2), \tag{28}$$

in analogy with Eq. (24). Note that ψ @ ξ_2 is not free -- it has already been scattered at ξ_1. In fact $\psi(\xi_2)$ looks like Eq. (26), viz...

Second-order interaction as a double scattering event.

$$\rightarrow \psi(\xi_2) = i\int dx\left[G_0(\xi_2,\xi) + \int dx_1\,\Delta t_1\,G_0(\xi_2,\xi_1)\,\Omega(\xi_1)\,G_0(\xi_1,\xi)\right]\psi_0(\xi). \qquad (29)$$

When this is put in Eq. (28), the new wavelet becomes...

$$\rightarrow \Delta_2\psi(\xi') = i\int dx\int dx_2\,\Delta t_2\,G_0(\xi',\xi_2)\,\Omega(\xi_2)\,G_0(\xi_2,\xi)\,\psi_0(\xi) + \qquad (30)$$

$$+\,i\int dx\int dx_2\,\Delta t_2\int dx_1\,\Delta t_1\,G_0(\xi',\xi_2)\,\Omega(\xi_2)\,G_0(\xi_2,\xi_1)\,\Omega(\xi_1)\,G_0(\xi_1,\xi)\,\psi_0(\xi)$$

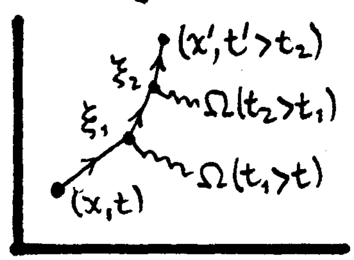
1st term RHS $\leftrightarrow$ scattering of $\psi_0(\xi)$ by Ω at ξ_2,
2nd term RHS $\leftrightarrow$ " " $\Delta_1\psi(\xi_1)$ by Ω at ξ_2.

The total wave which arrives at ξ', after scatterings at ξ_1 and ξ_2, is:

$$\rightarrow \psi(\xi') = \overset{\text{Eq.(22)}}{\psi_0(\xi')} + \overset{\text{Eq.(24)}}{\Delta_1\psi(\xi')} + \overset{\text{Eq.(30)}}{\Delta_2\psi(\xi')}$$

$$= i\int dx\Big[G_0(\xi',\xi) + \sum_{\substack{i=1\\(t<t_i)}}^{2}\int dx_i\,\Delta t_i\,G_0(\xi',\xi_i)\,\Omega(\xi_i)\,G_0(\xi_i,\xi) +$$

$$+\sum_{\substack{j,i=1\\(t<t_i<t_j)}}^{2}\int dx_j\,\Delta t_j\int dx_i\,\Delta t_i\,G_0(\xi',\xi_j)\,\Omega(\xi_j)\,G_0(\xi_j,\xi_i)\,\Omega(\xi_i)\,G_0(\xi_i,\xi)\Big]\psi_0(\xi). \qquad (31)$$



Notice the time-ordering: the scatterings at $\xi_1, \xi_2, \ldots$ take place <u>sequentially</u> @ $t<t_1<t_2<\cdots<t'$. The double scattering result in (31) may be written symbolically as:

$$\left[\begin{array}{l}\psi(\xi') = i\int dx\,G(\xi',\xi)\,\psi_0(\xi),\\[4pt] \text{w/}\;\; G = \underset{\substack{\text{free}\\\text{propagation}}}{G_0} + \underset{\substack{\text{single scattering}\\(\text{at } \xi_1 \text{ or } \xi_2)}}{\sum\int G_0\Omega G_0} + \underset{\substack{\text{double scattering}\\(\text{at } \xi_1 \text{ and } \xi_2)}}{\sum\sum\iint G_0\Omega G_0\Omega G_0}.\end{array}\right\} \qquad (32)$$