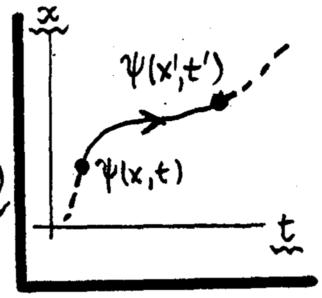
Evolution of Ψ in Schrödinger picture.

An Integral Formulation of QM*

We now discuss an alternate approach to QM, first formulated by Feynman, and used with great success in QED (quantum electrodynamics) and scattering theory (so-called S-matrix theory). In this approach, all interactions which form the wavefcn $\Psi(x,t)$ at a given space-time point (x,t) can be viewed as "scattering" events. We shall formulate Feynman's approach more for its cultural than practical value -- i.e. we won't do many problems, but we want to see how the theory works conceptually.

1) The central problem in QM is answering the question:

[[Given an initial QM state $\Psi(x,t)$, what is $\Psi(x',t')$ at some later time $t'>t$ and new position $x'\neq x$?]] (1)



An answer is provided by solving Schrödinger's Eqtn...

$$\rightarrow i\hbar\frac{\partial}{\partial t'}\Psi(x',t') = \mathcal{H}(x',p';t')\Psi(x',t') \quad \text{w/ boundary/initial condition } \underline{\Psi = \Psi(x,t) \text{ @ } x'=x \text{ \& } t'=t.} \tag{2}$$

We solve this diff^l eqtn for $\Psi(x',t')$, then jump from (x',t') to (x,t) to adjust parameters at the initial point so that $\Psi(x'=x, t'=t) = \Psi(x,t)$. This procedure implicitly assumes continuity in Ψ between distinct space-time points (x,t) & (x',t'), but it does not dwell on the questions: how does $\Psi(x',t')$ evolve from $\Psi(x,t)$? what information is contained in $\Psi(x,t)\rightarrow\Psi(x',t')$?

In fact, in the Schrödinger picture, the evolution $\Psi(x,t)\rightarrow\Psi(x',t')$ is not even relevant -- Ψ is just an auxiliary fcn... once we get it, we immediately destroy the information it contains by integrating over it to generate expectation values.

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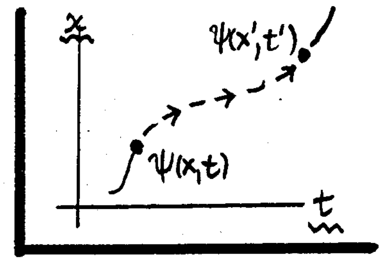
* Related material can be found in Davydov Ch. XIV and Sakurai Ch. 7, on scattering theory. Sakurai treats Feynman's formulation in his Sec. 2.5.

Evolution of ψ in Feynman picture.

But ψ is still a (probability) wave, and the evolution $\psi(x,t)\to\psi(x',t')$ must reflect the interactions which form/distort ψ during $(x,t)\to(x',t')$. If we concentrate on the evolution of ψ, rather than the (instantaneous) interaction $\mathcal{H}$ which produces it [as in Eq. (2)], we can restate the central problem of QM as:



$$\left[\!\left[\text{How does the } \psi\text{-wave propagate from } (x,t) \text{ to } (x',t'), \text{ with interactions present?}\right]\!\right] \quad (3)$$

We know the answer for propagation of a free-particle ψ: $\psi(x,t)$ diffuses to $\psi(x'\neq x, t'>t)$ in accordance with the Uncertainty Principle.¶ We shall now generalize this notion, for a "diffusion" modified by nonzero interactions.

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2) An answer to the propagation question in (3) above begins by exploiting the expansion postulate of QM as follows. Assume stationary states n, i.e.

$$\left\{\begin{array}{ll} \mathcal{H}' u_n(x') = E_n u_n(x') & \leftarrow \text{QM system with stationary states } n; \\ \text{So}/\!/ \; \psi(x',t') = \sum_n c_n u_n(x') e^{-\frac{i}{\hbar}E_n(t'-t)}, & \Big\} \text{ most general wave} \\ \quad \text{with: } c_n = \int u_n^*(x)\psi(x,t)\,dx\,. & \quad \text{packet for the system.} \end{array}\right\} \quad (4)$$

Put the expansion coefficients c_n back into $\psi(x',t')$, so that...

$$\rightarrow \psi(x',t') = \sum_n \left\{\int u_n^*(x)\psi(x,t)\,dx\right\} u_n(x')\, e^{-\frac{i}{\hbar}E_n(t'-t)}$$

$$= \int\left[\sum_n u_n^*(x)\, u_n(x')\, e^{-\frac{i}{\hbar}E_n(t'-t)}\right]\psi(x,t)\,dx\,;$$

NOTE: ψ satisfies: $\mathcal{H}'\psi = i\hbar\frac{\partial\psi}{\partial t'}$

or//

$$\boxed{\begin{array}{l} \psi(x',t') = \int K(x',t';x,t)\,\psi(x,t)\,dx, \\ \text{w/}\; K(x',t';x,t) = \sum_n u_n^*(x)\,u_n(x')\,e^{-\frac{i}{\hbar}E_n(t'-t)}, \text{ for } t'>t. \end{array}} \quad (5)$$

¶ Sakurai "Modern QM", p. 112; Schiff "QM" (3rd ed.), p. 301; Merzbacher "QM" (2nd ed.), Secs. 2.2–2.4; etc. See also Eq. (19) below.

REMARKS on Eq.(5): $\psi(x',t') = \int K(x',t';x,t)\,\psi(x,t)\,dx$.

1. We have converted Schrödinger's diff'l eqtn: $\mathcal{H}\psi = i\hbar\,\partial\psi/\partial t$ to a linear homogeneous integral eqtn for ψ -- this does not solve the problem, it just recasts it. The fcn $K(x',t';x,t)$ is called the Schrödinger "kernel fcn"; K evidently plays a crucial role in relating $\psi(x,t)$ to $\psi(x',t')$.

2. Since the Schrodinger Eqtn is linear and first-order-in time, then Eq.(5) is the most general expression for $\psi(x',t')$ in terms of $\psi(x,t)$. **NOTE**: superposition holds.

3. Eq.(5) resembles a vector eqtn. If we think of ψ as a vector with components $\psi(x,t)$ labelled by the continuous index x, then--symbolically:

$$\left.\begin{array}{l}
\psi \leftrightarrow \text{vector, with an } \infty \,\#\text{ components}:\ \psi_x(t) = \psi(x,t);\\
\text{So}\ \ \text{Eq.(5)} \Rightarrow \psi_{x'}(t') = \sum_x \mathcal{K}_{x'x}(t',t)\,\psi_x(t),\ \text{or}\ \ \psi' = \underset{\sim}{\mathcal{K}}\,\psi;\\
\text{and}\ \ \underset{\sim}{\mathcal{K}} \text{ is an } \infty\text{-dimensional "matrix", which rotates } \psi \text{ to } \psi'.\\
\text{This "rotation" preserves length}: \sum_x |\psi_x|^2 = \sum_{x'} |\psi_{x'}|^2\ \checkmark \text{ Cons}^{\text{n}}\text{ of probability}
\end{array}\right\}(6)$$

Now rotations are continuous, so here we pick up the idea that K transforms ψ into ψ' in a continuous fashion. We can think of K as consisting of a very large number of successive ∞smal "rotations" $(x,t) \to (x+dx,\, t+dt)$, and we can assert: <u>K propagates ψ from (x,t) to (x',t') continuously</u>.

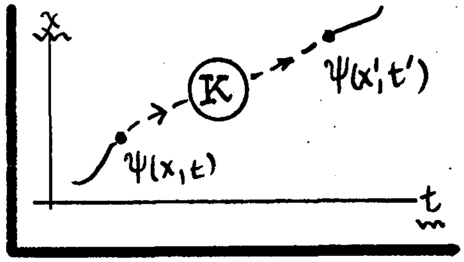
4. Eq.(5) incorporates the basic idea of Huygen's Principle -- that the wave disturbance @ (x',t') results from contributions from all points (x,t)...

$$\left.\begin{array}{ll}
\Delta\psi(x',t') \propto \psi(x,t)\,\Delta x & \\
\text{Say}\ \ \Delta\psi(x',t) = K(x',t';x,t)\,\psi(x,t)\,\Delta x\ \checkmark & \text{K specifies propagation of an elementary wavelet } \Delta\psi \text{ from source at } (x,t) \text{ to pt. } (x',t').\\
\text{So}\ \ \psi(x',t') = \int K(x',t';x,t)\,\psi(x,t)\,dx, & \text{by superposition of all } \Delta\psi\text{'s}.
\end{array}\right\}(7)$$

Remarks on integral form for ψ, and on propagator K.

$\boxed{\text{REMARKS}}$ on: $\psi' = \int K\psi\, dx$, cont'd.

5. If we retain the notion that $\psi(x,t)$ represents a probability amplitude (or wave) for finding a particle at the particular space-time pt. (x,t), then our integral eqtn can be interpreted in the following way...



$$\underbrace{\psi(x',t')}_{④} = \underbrace{\int dx}_{③}\, \underbrace{K(x',t';x,t)}_{②}\, \underbrace{\psi(x,t)}_{①}. \qquad (5)$$

w/ ① probability amplitude for particle to be found at (x,t);

② probability for propagation from (x,t) to (x',t'); then $K\psi$ represents probability amplitude at (x',t') from a particle coming from (x,t);

③ sum over all possible paths $(x,t) \to (x',t')$ [$x = x(t)$ implicitly];

④ probability amplitude for particle to be found at $(x' \neq x,\ t' > t)$. (8)

Evidently, it makes sense to call $K(x',t';x,t)$ a "propagator" [in terms of remarks 3, 4 & 5 above]. And, after Feynman, we call $\int K\psi\, dx$ a "path integral."† Clearly, ψ will not be an "auxiliary fcn" in this formulation of QM.

6. If ψ propagates from (x,t) to (x',t'), then $t' \geq t$, by causality. To respect causality, we must impose $K(x',t';x,t) \equiv 0$ for $t' < t$. Then $\partial K/\partial t$ can be singular at $t = t'$; K is beginning to look like a Green's fcn.

7. Finding the propagator K is the chief dynamical problem in this formulation. But when this is done, we can claim we have a complete solution to the QM, i.e.

$$\left.\begin{array}{l} \psi(x',t') = \int K(x',t';x,t)\,\psi(x,t)\,dx, \text{ and:} \\ K(x',t';x,t) = \sum_n u_n^*(x)\,u_n(x')\,e^{-\frac{i}{\hbar}E_n(t'-t)} \end{array}\right\} \checkmark \text{ equivalent to solving S. Eq.: } \mathcal{H}\psi = i\hbar\,\partial\psi/\partial t. \qquad (9)$$

In both cases, we get ψ everywhere. Now we should study propagators.

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† See R.P. Feynman & A.R. Hibbs "QM & Path Integrals" (McGraw-Hill, 1965).

3) We've noted in remark # 6 above that the propagator $\mathbb{K}$ may be singular. In fact, at $t'=t$, $\mathbb{K}$ becomes...

$$\left[\begin{array}{l} @\ t'=t\ :\ \underline{\underline{\mathbb{K}(x',t;x,t) = \sum_n u_n^*(x)\,u_n(x') = \delta(x-x')}},\ \text{by closure on } \{u_n\}. \\ \text{Interpretation: for } \infty\text{smal time intervals, } (t'-t)\to 0,\ \text{propagation to } x' \text{ is} \\ \text{possible only from an } \infty\text{smal neighborhood of } x,\ \text{i.e. } (x'-x)\to 0 \text{ as } (t'-t)\to 0. \\ \text{Alternatively, at } t'=t, \text{ the particle must be precisely localized at } x'=x. \end{array}\right] \quad (10)$$

This last statement implies that $\mathbb{K}$ actually represents the particle (and its localization) in a way similar to ψ itself. But, in turn, this can be true only if $\mathbb{K}$ satisfies the Schrödinger Eqtn. Which it does! For we note that...

$$\mathbb{K}(x',t';x,t) = \sum_n a_n(x,t)\,u_n(x')\,e^{-\frac{i}{\hbar}E_n t'},\quad \text{w/ } a_n(x,t) = u_n^*(x)\,e^{\frac{i}{\hbar}E_n t}$$

... assume $x \neq x'$ & $t < t'$...

$$\xrightarrow{\text{So}} i\hbar\frac{\partial \mathbb{K}}{\partial t'} = \sum_n a_n \underbrace{[E_n u_n(x')]}_{\mathcal{H}' u_n(x')} e^{-\frac{i}{\hbar}E_n t'} = \mathcal{H}'\mathbb{K} \quad \begin{array}{l}\mathbb{K} \text{ satisfies S. Eq.} \\ @\ x\neq x' \ \&\ t<t'.\end{array} \qquad (11)$$

$\Rightarrow$ $\mathbb{K}$ is a wavefcn, similar to ψ itself, that describes the motion <u>of a particle initially well-localized (precisely) @ $x'=x$ & $t'=t$.</u>

The derivation of Eq. (11) excludes $x'=x$ & $t'=t$, where $\mathbb{K}$ can be singular. It is at this initial point that $\mathbb{K}$ differs from the usual ψ-fcn. To see better what happens at (x',t'), start from $\psi(x',t') = \int \mathbb{K}(x',t';x,t)\,\psi(x,t)\,dx$ [i.e. Eq. (5)], and--respecting causality--to ensure $\mathbb{K}\equiv 0$ for $t'<t$, multiply both sides by the unit step fcn $\theta(t'-t)$ $\left\{\begin{array}{l}\theta(\tau)=1, \text{ for } \tau>0 \\ \theta(\tau)=0, \text{ for } \tau<0\end{array}\right.$. Then Eq. (5) is

$$\left[\begin{array}{l} \theta(t'-t)\,\psi(x',t') = i\int G(x',t';x,t)\,\psi(x,t)\,dx, \\ \text{w/ } G(x',t';x,t) = -i\,\theta(t'-t)\,\mathbb{K}(x',t';x,t). \end{array}\right. \qquad (12)$$

Differential Eqtn for the (modified) propagator ; $G = -i\,\theta(t'-t)\,K$.

Now, operate on both sides of Eq. (12) by the Schrödinger operator $\left(i\hbar\frac{\partial}{\partial t'} - \mathcal{H}'\right)$:

$$\rightarrow \left(i\hbar\frac{\partial}{\partial t'} - \mathcal{H}'\right)\theta(t'-t)\,\psi(x',t') = i\left(i\hbar\frac{\partial}{\partial t'} - \mathcal{H}'\right)\int G(x',t';x,t)\,\psi(x,t)\,dx$$

... $\frac{\partial}{\partial t'}\theta\psi = \delta(t'-t)\psi + \theta\frac{\partial\psi}{\partial t'}$. The 2nd term cancels vs. $\theta\mathcal{H}'\psi = i\hbar\theta\frac{\partial\psi}{\partial t'}$ ...

... the operator acts only on primed coordinates and can be taken inside the integral sign ...

so// $\rightarrow i\hbar\,\delta(t'-t)\,\psi(x',t') = i\int\left[\left(i\hbar\frac{\partial}{\partial t'} - \mathcal{H}'\right)G\right]\psi(x,t)\,dx$. (13)

Let the [ ] on the RHS in (13) be : $[\;] = \hbar f(x',x)\,\delta(t'-t)$; the delta fcn in $(t'-t)$ matches the singularity on the LHS. Then (13) reads...

$\rightarrow \psi(x',t') = \int f(x',x)\,\psi(x,t)\,dx$, at $t'=t$ ∫ works, because (clearly): $\delta(t'-t)\psi_{t'} = \delta(t'-t)\psi_t$. (14)

If (14) is true for any ψ, then we must have ; $f(x',x) = \delta(x'-x)$. Thus, have:

$$\boxed{\left(i\hbar\frac{\partial}{\partial t'} - \mathcal{H}'\right)G(x',t';x,t) = \hbar\,\delta(x'-x)\,\delta(t'-t)}\,,\quad t'\geq t. \tag{15}$$

This eqtn [rather than Eq. (11)] accounts for the singularities in the propagator, and it shows that G is the point-source solution, or Green's fcn, for the Schrödinger operator : $\left(i\hbar\frac{\partial}{\partial t'} - \mathcal{H}'\right)$. Everywhere but at the initial point $x'=x$, $t'=t$, G is indistinguishable from the Schrödinger wavefcn ψ' which satisfies : $\left(i\hbar\frac{\partial}{\partial t'} - \mathcal{H}'\right)\psi' = 0$. The "point-source" term on the RHS of (15) just specifies the fact that G starts from an initial condition of being perfectly well-localized at $x'=x$ and $t'=t$.

ASIDE General utility of a Green's fcn.

Suppose you want to solve a differential equation of the form...

$\rightarrow \underset{\sim}{L}(\xi')\,\phi(\xi') = \rho(\xi')$ ∫ $\underset{\sim}{L}$ is a linear operator, ρ is a known source fcn; problem is to solve for the (unknown) fcn ϕ. (A1)

An example is Poisson's eqtn in electrostatics : $\nabla^2\phi = -4\pi\rho$. Green's method of solution assumes you can find a solution G to the point-source eqtn:

Utility of a Green's fcn G.

$$\rightarrow \underset{\sim}{L}(\xi')G(\xi',\xi) = \delta(\xi'-\xi). \tag{A2}$$

G is called the Green's fcn for the operator $\underset{\sim}{L}$. Now operate by $\int d\xi\, \rho(\xi) \times$ on both sides of this eqtn...

$$\rightarrow \int d\xi\, \rho(\xi) \times \underset{\sim}{L}(\xi')G(\xi',\xi) = \int d\xi\, \rho(\xi) \times \delta(\xi'-\xi),$$

or//

$$\underset{\sim}{L}(\xi')\underbrace{\left[\int d\xi\, \rho(\xi)\, G(\xi',\xi)\right]}_{\text{identify as } \phi(\xi'),\text{ a particular solution to } \underset{\sim}{L}\phi = \rho.} = \rho(\xi'). \tag{A3}$$

The general solution to (A1) is then:

$$\underline{\underline{\phi(\xi') = \phi_0(\xi') + \int G(\xi',\xi)\,\rho(\xi)\,d\xi}} \quad \begin{cases} \underset{\sim}{L}\phi_0 = 0, & \text{sol}^{\text{n}} \text{ to homog}^{\text{s}} \text{ eqtn;} \\ \underset{\sim}{L}G = \delta, & \text{point-source sol}^{\text{n}}. \end{cases} \tag{A4}$$

By means of G, sol$^{\text{n}}$ of $\underset{\sim}{L}(\xi')\phi(\xi') = \rho(\xi')$, with ρ an <u>arbitrary</u> source fcn, is reduced to solving <u>point-source</u> eqtn $\underset{\sim}{L}(\xi')G(\xi',\xi) = \delta(\xi'-\xi)$.

This procedure can be carried out for the Schrödinger Eqtn in detail -- you will do this as a problem [see ϕ507 prob$^{\text{m}}$ #10], and we will derive the result in a somewhat different way a bit later. For now, however, note that for the Schrödinger Eqtn, you can get the Green's fcn/propagator G either by solving the differential eqtn (15) or by evaluating the sum over states, Eq.(9) & (12):

$$\rightarrow \underline{\underline{G(x',t';x,t) = -i\,\theta(t'-t)\sum_n u_n^*(x)\,u_n(x')\,e^{-\frac{i}{\hbar}E_n(t'-t)}}}. \tag{A5}$$