4.10. Feynman's Path Integral Formulation of Quantum Mechanics Revisited

As we have found earlier, Feynman was able to represent the time evolution of a quantum mechanical system by means of a kernel or Green function which was written as the sum over all possible paths in configuration space each weighted by $\exp(\frac{i}{\hbar}\text{Action})$ for the path. That is the wavefunction at time t and position $\vec{r}$, $\psi(\vec{r},t)$ for the system was related to $\psi(\vec{r}_0,t_0)$ the wavefunction at earlier time t_0 and all other positions $\vec{r}_0$ by the Green function equation

$$\psi(\vec{r},t) = \int d^3r_0\, K(\vec{r},t;\vec{r}_0,t_0)\,\psi(\vec{r}_0,t_0)$$

with the kernel given as the sum over energy eigenstates as

$$K(\vec{r},t;\vec{r}_0,t_0) = \Theta(t-t_0)\sum_n \psi_n^*(\vec{r}_0)\,\psi_n(\vec{r})\,e^{-i\frac{E_n(t-t_0)}{\hbar}}.$$

With repeated application of this formula for smaller and smaller time slices, Feynman was able to represent K as an integral of a new type

$$K(\vec{r},t;\vec{r}_0,t_0) = \int_{\vec{r}(t_0)=\vec{r}_0}^{\vec{r}(t)=\vec{r}} [dp][dx]\, e^{+\frac{i}{\hbar}\int_{t_0}^{t} dt\,[\vec{p}\cdot\dot{\vec{r}} - H(\vec{r},\vec{p})]}$$

with $H(\vec{r},\vec{p})$ the classical Hamiltonian, for instance

$$H(\vec{r},\vec{p}) = \frac{\vec{p}^{\,2}}{2m} + V(\vec{r}) .$$

The Gaussian momentum integrals can be performed in such a case to obtain an integral over all paths

$$K(\vec{r},t;\vec{r}_0,t_0) = \int_{\vec{r}(t_0)=\vec{r}_0}^{\vec{r}(t)=\vec{r}} [dr]\, e^{+\frac{i}{\hbar}\int_{t_0}^{t} dt\, L(\vec{r}(t),\dot{\vec{r}}(t))}$$

where L is the classical Lagrangian

$$L(\vec{r}(t),\dot{\vec{r}}(t)) = \frac{1}{2} m \dot{\vec{r}}(t)^2 - V(\vec{r}(t)) .$$

$$= \vec{p}\cdot\dot{\vec{r}} - H(\vec{r},\vec{p}) .$$

Since the wavefunction $\psi(\vec{r},t)$ is simply the inner product

$$\psi(\vec{r},t) = \langle \vec{r} | \psi(t) \rangle$$ we

as well can re-formulate the dynamical laws of quantum mechanics (Postulate 4) to be that of Feynman in our abstract approach.

For simplicity we work in one-dimension with the position operator denoted by $Q\ (=X)$ and its eigenstates $|q\rangle$ with eigenvalues q; $Q|q\rangle = q|q\rangle$.

In the Schrödinger picture formulation of quantum mechanics the states depend on time while the operators are time independent; thus $|\Psi(t)\rangle_s$ obey the Schrödinger equation

$$i\hbar \frac{d}{dt}|\Psi(t)\rangle_s = H(Q,P)|\Psi(t)\rangle_s$$

and, for instance, $\frac{d}{dt} Q_s = 0$. In the coordinate basis, $Q_s|q\rangle = q|q\rangle$, the vectors $|q\rangle$ are time independent eigenvectors of Q_s, normalized so that

$$\langle q'|q\rangle = \delta(q'-q) \quad \text{and}$$

complete

$$\int_{-\infty}^{+\infty} dq\, |q\rangle\langle q| = 1 .$$

The solution to Schrödinger's equation is simply

$$|\psi(t)\rangle_S = e^{-\frac{iHt}{\hbar}} |\psi(0)\rangle_S .$$

The initial Schrödinger state $|\psi(0)\rangle_S$ is time independent and provides the bridge to the Heisenberg picture formulation of quantum mechanics. The Heisenberg state $|\psi\rangle_H$ is simply

$$|\psi\rangle_H \equiv |\psi(0)\rangle_S = e^{+\frac{i}{\hbar}Ht} |\psi(t)\rangle_S .$$

Since $e^{+\frac{i}{\hbar}Ht}$ is unitary we have

$${}_S\langle\psi(t)|Q_S|\phi(t)\rangle_S = {}_H\langle\psi| e^{+\frac{iHt}{\hbar}} Q_S e^{-\frac{i}{\hbar}Ht} |\phi\rangle_H$$

$$\equiv {}_H\langle\psi| Q_H(t) |\phi\rangle_H ,$$

The Heisenberg picture operators depend on time

$$Q_H(t) = e^{+\frac{i}{\hbar}Ht} \underbrace{Q_S}_{=Q_H(0)} e^{-\frac{i}{\hbar}Ht} .$$

The eigenstates of the position operator $Q_H(t)$ at time t are given in terms of the moving coordinate vectors

$$|q,t\rangle \equiv e^{+\frac{i}{\hbar}Ht}|q\rangle .$$

Hence

$$Q_H(t)|q,t\rangle = e^{+\frac{i}{\hbar}Ht} Q_S e^{-\frac{i}{\hbar}Ht} e^{+\frac{i}{\hbar}Ht}|q\rangle$$

$$= e^{+\frac{i}{\hbar}Ht} \underbrace{Q_S|q\rangle}_{=q|q\rangle}$$

$$= q\, e^{+\frac{i}{\hbar}Ht}|q\rangle$$

$$= q|q,t\rangle .$$

$|q,t\rangle$ is a Heisenberg picture state; t is just a label for the moving axes.

Similarly the normalization of the states $|q,t\rangle$ is

$$\langle q',t|q,t\rangle = \langle q'|q\rangle = \delta(q'-q)$$

and Completeness becomes

$$e^{\frac{i}{\hbar}Ht}\left[1 = \int_{-\infty}^{+\infty} dq\,|q\rangle\langle q|\right]e^{-\frac{i}{\hbar}Ht}$$

$$\Rightarrow \quad 1 = \int_{-\infty}^{+\infty} dq\,|q,t\rangle\langle q,t|$$

(i.e. ${}_S\langle\psi(t)|\phi(t)\rangle_S = {}_H\langle\psi|\phi\rangle_H$

$$= \int dq\,{}_S\langle\psi(t)|q\rangle\langle q|\phi(t)\rangle_S$$

$$= \int dq\,{}_H\langle\psi|e^{\frac{iHt}{\hbar}}|q\rangle\langle q|e^{-\frac{iHt}{\hbar}}|\phi\rangle_H$$

$$= \int dq\,{}_H\langle\psi|q,t\rangle\langle q,t|\phi\rangle_H$$

$$\Rightarrow \int dq\,|q,t\rangle\langle q,t| = 1.\;)$$

The kernel or Green function defined by

$$K(q,t;q_0,t_0) \equiv \langle q,t|q_0,t_0\rangle$$

controls the time evolution of the states, all dynamics is contained in K.

$$\begin{aligned}\psi(q,t) &= \langle q|\psi(t)\rangle_S \\ &= \langle q,t|\psi\rangle_H \\ &= \int dq_0 \langle q,t|q_0,t_0\rangle \underbrace{\langle q_0,t_0|\psi\rangle_H}_{=\langle q_0|\psi(t_0)\rangle_S} \\ &= \int dq_0 \langle q,t|q_0,t_0\rangle \psi(q_0,t_0)\end{aligned}$$

$$\boxed{\psi(q,t) = \int dq_0\, K(q,t;q_0,t_0)\, \psi(q_0,t_0)}$$

Note for $t \to t_0$ $\quad K(q,t;q_0,t) = \langle q t|q_0,t\rangle = \delta(q_0-q)$

by the normalization of the $|q,t\rangle$ states.

Also
$$K(q,t;q_0 t_0) = \langle q,t|q_0,t_0\rangle$$
$$= \langle q|e^{-\frac{i}{\hbar}H(t-t_0)}|q_0\rangle$$
$$= \langle q|\,U(t,t_0)\,|q_0\rangle$$
The Kernel is the $\{|q\rangle\}$ basis matrix elements of the time evolution operator U. For early times $t_0 \to -\infty$ U relates the in-coming states to the late time $t \to +\infty$ out-going states, it is the scattering operator $S = U(t_0, -\infty)$, and K is just its position matrix elements.

As before if we know the energy eigenvectors
$$H|n\rangle = E_n|n\rangle$$
with normalization $\langle m|n\rangle = \delta_{mn}$ and

completeness $\quad \sum_n |n\rangle\langle n| = 1$

we can represent the time evolution as an energy sum

$$\psi(q,t) = \langle q | \psi(t) \rangle_s$$

$$= \sum_n \langle q | n \rangle \langle n | \psi(t) \rangle_s$$

$$= \sum_n \langle q | n \rangle \langle n | e^{-\frac{i}{\hbar} H (t-t_0)} | \psi(t_0) \rangle_s$$

$$= \int dq_0 \sum_n \langle q | n \rangle \underbrace{\langle n | e^{-\frac{i}{\hbar} H(t-t_0)} | q_0 \rangle}_{= e^{-\frac{i}{\hbar} E_n (t-t_0)} \langle n | q_0 \rangle} \langle q_0 | \psi(t_0) \rangle_s$$

$$= \int dq_0 \left[\sum_n \langle q | n \rangle e^{-\frac{i}{\hbar} E_n (t-t_0)} \langle n | q_0 \rangle \right] \psi(q_0, t_0)$$

denoting the energy eigenwavefunctions as

$\psi_n(q) \equiv \langle q | n \rangle$ we have

$$\psi(q,t) = \int dq_0 \left(\sum_n \psi_n(q) e^{-\frac{i}{\hbar} E_n (t-t_0)} \psi_n^*(q_0) \right) \psi(q_0, t_0)$$

Hence the energy representation of the Kernel is

$$K(q,t;q_0,t_0) = \sum_n \psi_n(q)\psi_n^*(q_0)\, e^{-\frac{i}{\hbar}E_n(t-t_0)}$$

as we found earlier. (Note $t \to t_0$

$$K = \sum_n \psi_n(q)\psi_n^*(q_0) = \delta(q_0 - q) \quad \text{by}$$

completeness of the energy eigenstates

$$\langle q | \Big(\sum_n |n\rangle\langle n| = 1\Big) | q_0\rangle$$

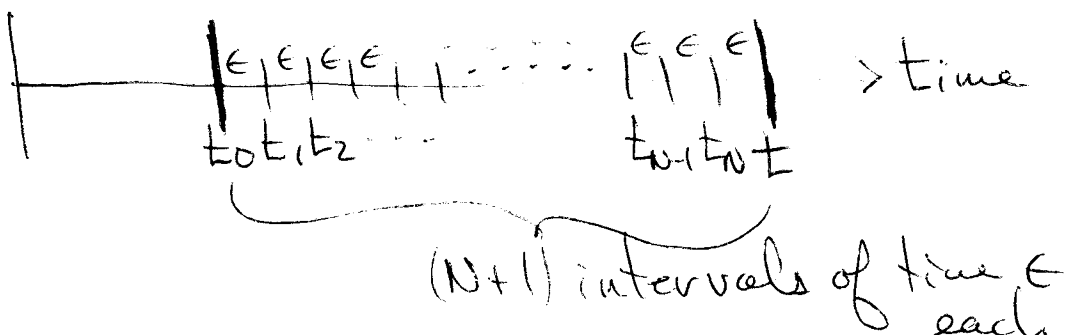
$$\Rightarrow \quad \sum_n \langle q|n\rangle\langle n|q_0\rangle = \langle q|q_0\rangle = \delta(q-q_0)$$

$$= \sum_n \psi_n(q)\psi_n^*(q_0) = \delta(q-q_0).\Big)$$

Of course we could proceed as before to derive the Feynman path integral representation for K from the above energy representation, but let's return to ~~the~~ definition of K as the inner product of position eigenstates at different times and exploit our completeness relation for these states directly,

$K(q,t;q_0,t_0) \equiv \langle q,t|q_0,t_0\rangle$. Let's divide the time interval (t_0,t) into $(N+1)$ short intervals ϵ

$$t > t_N > t_{N-1} > \cdots > t_1 > t_0$$



At each time t_i, $i=1 \ldots N$, we insert 1 as a sum over the complete set of states $\{|q,t_i\rangle\}$

$$\langle q,t|q_0,t_0\rangle = \int \left(\prod_{i=1}^{N} dq_i\right) \langle q,t|q_N,t_N\rangle\langle q_N t_N|q_{N-1},t_{N-1}\rangle$$

$$\cdots \langle q_2 t_2|q_1,t_1\rangle\langle q_1,t_1|q_0,t_0\rangle$$

As previously for small time intervals ϵ we can evaluate the Kernel

$$\langle q_{i+1}, t_{i+1} | q_i, t_i \rangle = \langle q_{i+1} | e^{-\frac{i}{\hbar} H (t_{i+1} - t_i)} | q_i \rangle$$

$$= \langle q_{i+1} | e^{-\frac{i}{\hbar} H \epsilon} | q_i \rangle$$

$$= \langle q_{i+1} | (1 - \tfrac{i}{\hbar} H \epsilon) | q_i \rangle + O(\epsilon^2).$$

The Hamiltonian has the form

$$H = H(P, Q) = \frac{1}{2m} P^2 + V(Q)$$

so that

$$\langle q_{i+1} | H | q_i \rangle = \frac{1}{2m} \langle q_{i+1} | P^2 | q_i \rangle + \langle q_{i+1} | V(Q) | q_i \rangle$$

$$= \frac{1}{2m} \langle q_{i+1} | P^2 | q_i \rangle + V(q_i) \delta(q_{i+1} - q_i).$$

In order to evaluate the P^2 term, consider a complete set of momentum eigenstates $|p\rangle$

$$P|p\rangle = p|p\rangle \quad \text{with}$$

continuum normalization $\langle p' | p \rangle = \delta(p' - p) \, (2\pi\hbar)$

and completeness $\displaystyle\int_{-\infty}^{+\infty} \frac{dp}{(2\pi\hbar)} |p\rangle\langle p| = 1.$

The momentum operator has the matrix elements

$$\langle q|P = \frac{\hbar}{i}\frac{\partial}{\partial q}\langle q| \quad ; \quad \text{that is}$$

$$\langle q|\underbrace{P|p\rangle}_{=p|p\rangle} = \frac{\hbar}{i}\frac{\partial}{\partial q}\langle q|p\rangle$$

$\Rightarrow$ The differential equation

$$p\langle q|p\rangle = \frac{\hbar}{i}\frac{\partial}{\partial q}\langle q|p\rangle$$

$$\Rightarrow \quad \langle q|p\rangle = N e^{\frac{i}{\hbar}pq} \quad \text{as we know.}$$

Since we have normalization

$$\langle p'|p\rangle = (2\pi\hbar)\delta(p'-p) = \int dq \langle p'|q\rangle\langle q|p\rangle$$

$$= \int dq\, N^2 e^{\frac{i}{\hbar}(p-p')q}$$

$$= \hbar N^2 \int \frac{dq}{\hbar} e^{\frac{i}{\hbar}(p-p')q} = \hbar N^2 (2\pi)\delta(p-p')$$

$$\Rightarrow N = 1.$$

Hence

$$\langle q_{i+1}|P^2|q_i\rangle = \int_{-\infty}^{+\infty}\frac{dp}{(2\pi\hbar)}\langle q_{i+1}|p\rangle\langle p|P^2|q_i\rangle$$

$$= \int\frac{dp}{(2\pi\hbar)}\,p^2 e^{\frac{i}{\hbar}p(q_{i+1}-q_i)}$$

and

$$\langle q_{i+1}|H|q_i\rangle = \int_{-\infty}^{+\infty}\frac{dp_i}{(2\pi\hbar)}\left[\frac{p_i^2}{2m}+V\left(\frac{q_{i+1}+q_i}{2}\right)\right]e^{\frac{i}{\hbar}p_i(q_{i+1}-q_i)}$$

where $\delta(q_{i+1}-q_i) = \int_{-\infty}^{+\infty}\frac{dp_i}{(2\pi\hbar)}\,e^{\frac{i}{\hbar}p_i(q_{i+1}-q_i)}$

So

$$\langle q_{i+1}|\underbrace{H(P,Q)}_{\substack{\text{quantum}\\ \text{operator}\\ \text{Hamiltonian}}}|q_i\rangle = \int_{-\infty}^{+\infty}\frac{dp_i}{(2\pi\hbar)}\underbrace{H\left(p_i,\frac{q_{i+1}+q_i}{2}\right)}_{\substack{\text{classical}\\ \text{function}\\ \text{Hamiltonian}}}e^{\frac{i}{\hbar}p_i(q_{i+1}-q_i)}$$

and

$$\langle q_{i+1}t_{i+1}|q_i,t_i\rangle$$

$$= \int_{-\infty}^{+\infty}\frac{dp_i}{(2\pi\hbar)}\,e^{\frac{i}{\hbar}p_i(q_{i+1}-q_i)}\,e^{-\frac{i}{\hbar}H\left(p_i,\frac{q_{i+1}+q_i}{2}\right)\epsilon} + O(\epsilon^2)$$

So for each time slice we plug in a similar expression to obtain

$$\boxed{\begin{aligned} \langle q, t | q_0, t_0 \rangle &= \int_{-\infty}^{+\infty} \left(\prod_{i=1}^{N} dq_i\right)\left(\prod_{j=0}^{N} \frac{dp_j}{(2\pi\hbar)}\right) \times \\ &\times e^{\frac{i}{\hbar}\left[\sum_{i=0}^{N} p_i(q_{i+1}-q_i) - \epsilon H(p_i, \frac{1}{2}(q_{i+1}+q_i))\right]} + O(\epsilon^2) \end{aligned}}$$

where we have defined $q = q_{N+1}$ and recall $t - t_0 = (N+1)\epsilon$.

As usual we consider more and more $N \to \infty$ shorter time intervals $\epsilon \to 0$ so that $t - t_0 = (N+1)\epsilon$ is fixed and write this ∞ product of integrals as a Feynman functional integral

$$\langle q, t | q_0, t_0 \rangle = \int_{q_0}^{q} [dq][dp]\, e^{\frac{i}{\hbar}\int_{t_0}^{t} dt\,[p\dot{q} - H(p,q)]}$$

$$\equiv \lim_{\substack{N\to\infty \\ \epsilon\to 0 \\ t-t_0=(N+1)\epsilon}} \int_{-\infty}^{+\infty} dq_1 \cdots dq_N \int_{-\infty}^{+\infty} \frac{dp_0}{2\pi\hbar} \cdots \frac{dp_N}{2\pi\hbar}\, e^{\frac{i}{\hbar}\epsilon\sum_{i=0}^{N}\left[p_i \frac{(q_{i+1}-q_i)}{\epsilon} - H\left(p_i, \frac{q_{i+1}+q_i}{2}\right)\right]}$$

Since $p\dot{q}-H$ looks like the Lagrangian L, we can re-express the functional integral in terms of summing over all classical paths by performing the momentum functional integrals. Since they are Gaussian integrals, we find

$$\cdots \int_{-\infty}^{+\infty} \frac{dp_i}{2\pi\hbar} e^{\frac{i}{\hbar} p_i (q_{i+1}-q_i) - \frac{i}{\hbar}\epsilon \frac{p_i^2}{2m}} \cdots$$

$$= \cdots \frac{1}{\sqrt{\frac{2\pi i \epsilon}{m\hbar}}} e^{\frac{i}{\hbar}\frac{m}{2}\frac{(q_{i+1}-q_i)^2}{\epsilon}} \cdots .$$

This yields

$$\boxed{\begin{aligned} &\langle q, t | q_0, t_0 \rangle \\ &= \lim_{\substack{N\to\infty \\ \epsilon\to 0 \\ t-t_0=(N+1)\epsilon}} \int_{-\infty}^{+\infty} \frac{dq_1}{\sqrt{\frac{2\pi i\epsilon}{m\hbar}}} \cdots \frac{dq_N}{\sqrt{\frac{2\pi i\epsilon}{m\hbar}}} \frac{1}{\sqrt{\frac{2\pi i\epsilon}{m\hbar}}} \times \\ &\qquad \times e^{\frac{i}{\hbar}\sum_{i=0}^{N} \epsilon \left[\frac{m}{2}\left(\frac{(q_{i+1}-q_i)}{\epsilon}\right)^2 - V\left(\frac{q_{i+1}+q_i}{2}\right)\right]} \end{aligned}}$$

As before for $\epsilon = dt$; $\frac{q_{i+1}-q_i}{\epsilon} = \frac{dq}{dt}$

The timeslice sum in the exponent becomes the time integral

$$\sum_{i=0}^{N-1} dt \to \int_{t_0}^{t} dt$$

and

$$\frac{i}{\hbar}\sum_{i=0}^{N-1}\epsilon\left[\frac{m}{2}\left(\frac{q_{i+1}-q_i}{\epsilon}\right)^2 - V\left(\frac{q_i+q_{i+1}}{2}\right)\right]$$

$$\longrightarrow \frac{i}{\hbar}\int_{t_0}^{t} dt'\left[\frac{m}{2}\dot{q}(t')^2 - V(q(t'))\right].$$

This is just the classical action

$$S(q;t,t_0) \equiv \int_{t_0}^{t} dt'\, L(q(t'),\dot{q}(t'))$$

times $\frac{i}{\hbar}$ with classical Lagrangian

$$L(q(t),\dot{q}(t)) = \frac{1}{2}m\dot{q}^2(t) - V(q(t)).$$

Thus we finally obtain the form of the Green function or Kernel in quantum mechanics as a Feynman path integral

$$\langle q,t|q_0,t_0\rangle = \int_{q(t_0)=q_0}^{q(t)=q} [dq]\, e^{\frac{i}{\hbar}S(q;t,t_0)}$$

where $S(q;t,t_0) = \int_{t_0}^{t} dt'\, L(q(t'),\dot{q}(t'))$.

This Feynman path integral is defined as the infinite product of integrals

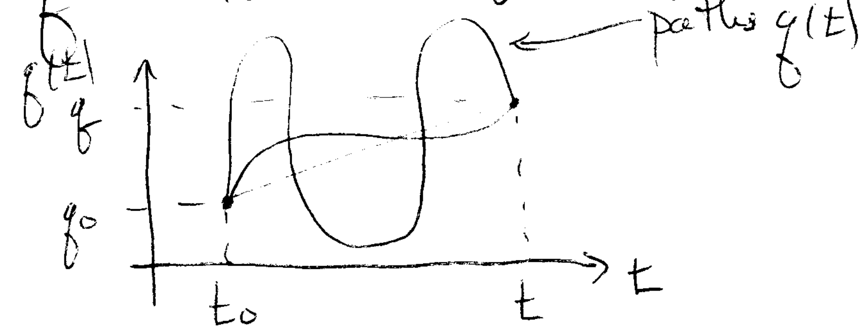
$$\langle q,t|q_0,t_0\rangle \equiv \lim_{\substack{N\to\infty \\ \epsilon\to 0 \\ t-t_0=(N+1)\epsilon}} \sqrt{\frac{m\hbar}{2\pi i\epsilon}} \int_{-\infty}^{+\infty} \frac{dq_1}{\sqrt{\frac{2\pi i\epsilon}{m\hbar}}} \cdots \frac{dq_N}{\sqrt{\frac{2\pi i\epsilon}{m\hbar}}} \times$$

$$\times\, e^{\frac{i}{\hbar}\sum_{i=0}^{N}\epsilon\left[\frac{m}{2}\left(\frac{q_{i+1}-q_i}{\epsilon}\right)^2 - V\left(\frac{q_i+q_{i+1}}{2}\right)\right]}$$

with the boundary conditions $q_{N+1}=q$ at time t and $q_0=q_0$ at time t_0.

Cryptically then, we have that the Green function (Kernel or transformation function as it is sometimes called)

$\langle q,t|q_0,t_0\rangle = K(q,t;q_0,t_0)$ is just a sum over all paths $q(t)$ from q_0 at time t_0 to q at time t



with each path's contribution to the sum weighted by $e^{\frac{i}{\hbar}S}$ where

S is the classical action for such a path. So

$$K(q,t;q_0,t_0) = \sum_{\text{paths}} e^{\frac{i}{\hbar}S} .$$

If $\hbar \to 0$, only one path contributes, the path of stationary phase

$$\frac{\delta S}{\delta q(t)} = \frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = 0 .$$ This

is just the classical Newtonian trajectory which is a solution to the above Euler-Lagrange equation.