LECTURE 1 & 2 — 17/2/2011, 22/2/2011

Path integrals

Consider a ~~[illegible]~~ particle in one dimension. In QM its position & momentum operator are denoted $\hat{x}, \hat{p}$ with $[\hat{x}, \hat{p}] = i\hbar$.

Let the Hamiltonian of the system be $H(\hat{x}, \hat{p})$. A basic quantity in QM is the amplitude for a particle at position x_i at time t_i to be found at x_f at time t_f. Clearly this amplitude will depend on its time evolution, governed by the Hamiltonian.

If we start at time t' in the state $|x'\rangle$ satisfying ~~[illegible]~~

$\hat{x}|x'\rangle = x'|x'\rangle$ then after a time $t''-t'$ we are in the state

$$e^{-i\frac{H}{\hbar}(t''-t')}|x'\rangle$$

The amplitude for a measurement of this state to result in a position x'' is

$$\langle x''|e^{-i\frac{H}{\hbar}(t''-t')}|x'\rangle.$$

In QM we calculate this using operator methods, expanding the exponential etc.
Here we describe a new way of calculating it, which leads to the same result, but provides a new insight into QM: the path integral.
~~Th~~ Given the state $|x\rangle$ we can evolve it using the Hamiltonian:

$$|x, t\rangle = e^{i\frac{H}{\hbar}t}\,|x\rangle$$

While the usual Schrodinger picture position operator $\hat{x}$ gives ~~the~~ $\hat{x}\,|x\rangle = x\,|x\rangle$, the state $|x, t\rangle$ is no longer an eigenstate of $\hat{x}$.

Now consider $\langle x'', t'' \,|\, x', t'\rangle$

$$= \langle x''|\, e^{-i\frac{H}{\hbar}t''}\, e^{i\frac{H}{\hbar}t'}\,|x'\rangle$$

$$= \langle x''|\, e^{-i\frac{H}{\hbar}(t''-t')}\,|x'\rangle$$

This is precisely the quantity we want to calculate.

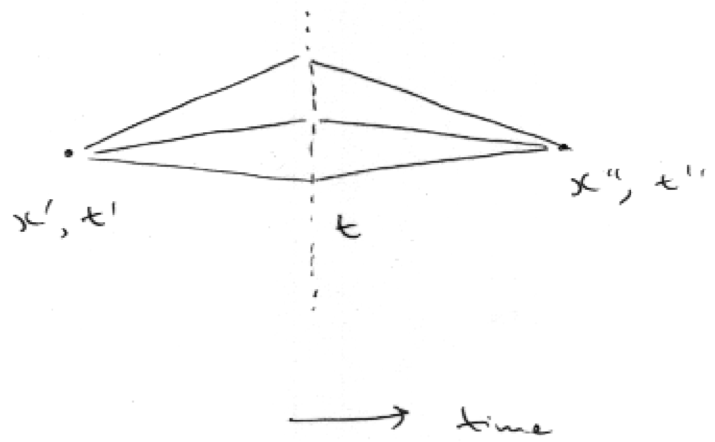
the propagation amplitude, also called "propagator" or "propagation kernel" has the following property:

$$\langle x'', t'' | x', t' \rangle =$$

$$\int dx \, \langle x'', t'' | x, t \rangle \langle x, t | x', t' \rangle$$

where t is any time between t' and t''.

This tells us something rather profound. While in classical physics the propagation from x' to x'' is along the classical path, in quantum mechanics one can treat it as a superposition of quantum propagations to an intermediate point.



By making the number of intermediate points very large, we can convert this to a superposition of paths in space.

So, let us calculate this by inserting a complete set of states

$$\int dx_i \, |x_i, t_i\rangle\langle x_i, t_i|$$

at N equally spaced points $t_1 \cdots t_{N-1}$ between t' and t''. We denote $t' = t_0$ and $t'' = t_N$. Thus,

$$t_{m+1} - t_m = \epsilon, \qquad N\epsilon = t'' - t' .$$

Now $\langle x'', t'' | x', t'\rangle = \langle x'', t_N | x', t_0\rangle$

$$= \int dx_1 \cdots dx_{N-1} \langle x'', t_N | x_{N-1}, t_{N-1}\rangle\langle x_{N-1}, t_{N-1}| \cdots\rangle$$
$$\cdots \langle x_1, t_1 | x', t_0\rangle$$

Now focus on one of the factors:

$$\langle x_{m+1}, t_{m+1} | x_m, t_m\rangle =$$
$$\langle x_{m+1}| e^{-\frac{iH}{\hbar}\epsilon} |x_m\rangle$$

Insert now a complete set of momentum eigenstates $|p\rangle$ (satisfying $\int dp \, |p\rangle\langle p| = \mathbb{1}$).

Then

$$\langle x_{m+1}, t_{m+1} | x_m, t_m\rangle =$$
$$\int dp_m \langle x_{m+1} | p_m\rangle\langle p_m | e^{-\frac{iH}{\hbar}\epsilon} |x_m\rangle$$

Now notice that we can evaluate

$$\langle p_m | H(\hat{p},\hat{x}) | x_m \rangle$$

but only if all $\hat{p}$'s are on the left and all $\hat{x}$'s on the right. In this case we have:

$$\langle p_m | H(\hat{p},\hat{x}) | x_m \rangle = H(p_m, x_m) \langle p_m | x_m \rangle$$

However, for higher powers this fails:

$$\langle p_m | H(\hat{p},\hat{x}) H(\hat{p},\hat{x}) | x_m \rangle \neq H(p_m, q_m)^2 \langle p_m | q_m \rangle$$

Notice that this problem first arises at order ϵ^2. Therefore we can say that

$$\langle p_m | e^{-i \frac{H(\hat{p},\hat{x})}{\hbar}\epsilon} | x_m \rangle = e^{-\frac{i}{\hbar} H(p_m, x_m)\epsilon + O(\epsilon^2)} \langle p_m | x_m \rangle$$

We will see that terms in the exponent of $O(\epsilon^2)$ and higher will not matter.

Now since $\langle p | x \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar} p x}$, we have:

$$\langle x_{m+1}, t_{m+1} | x_m, t_m \rangle =$$

$$\int \frac{dp_m}{2\pi\hbar}\, e^{-\frac{i}{\hbar}\left(H(p_m, x_m)\epsilon - p_m x_{m+1} + p_m x_m + O(\epsilon^2)\right)}$$

$$= \int \frac{dp_m}{2\pi\hbar}\, e^{-\frac{i}{\hbar}\left[H(p_m, x_m)\epsilon - p_m (x_{m+1} - x_m)\right] + O(\epsilon^2)}$$

Now our original expression becomes:

$$\int dx_1 \cdots dx_{N-1} \, \frac{dp_0}{2\pi\hbar} \cdots \frac{dp_{N-1}}{2\pi\hbar} \, e^{-\frac{i}{\hbar}\sum_{m=0}^{N-1}\left[H(p_m, x_m)\epsilon - p_m(x_{m+1} - x_m) + O(\epsilon^2)\right]}$$

Now take the limit $\epsilon \to 0$, $N \to \infty$ such that $N\epsilon = t'' - t'$ is fixed. In this limit,

$$\sum_{m=0}^{N-1} H(p_m, x_m)\epsilon \quad \longrightarrow \quad \int_{t'}^{t''} H(p(t), x(t))\, dt$$

$$\sum_{m=0}^{N-1} p_m(x_{m+1} - x_m) \quad \longrightarrow \quad \int_{t'}^{t''} p(t)\, \dot{x}(t)\, dt$$

~~Re-naming: think $t' \to 0$, fixed $t'' \to T$~~

Thus we have

$$\int \prod_t dx(t) \frac{dp(t)}{2\pi\hbar} \, e^{+\frac{i}{\hbar}\int_{t'}^{t''} dt\,(p\dot{x} - H)}$$

and the terms of order ϵ^2 have gone away. The expression under the integral is the Hamiltonian action:

$$S = \int dt\,(p\dot{x} - H(p, x))$$

However this is not (yet) the Lagrangian action, as both $x(t)$, $p(t)$ are independent integration variables. If we use the stationary phase approximation for the p-integral then we get:

$$\frac{\partial}{\partial p}(p\dot{x} - H) = 0 \quad \Rightarrow \quad \dot{x} = \frac{\partial H}{\partial p}$$

With this, $p\dot{x} - H = p\frac{\partial H}{\partial p} - H$ is a Legendre transform and defines the Lagrangian $L(x, \dot{x})$. Then

$$\langle x'', t'' | x', t' \rangle = \int [dx]\, e^{\frac{i}{\hbar}\int_{t'}^{t''} L(x,\dot{x})\, dt}$$

and $\int L\, dt$ is the usual action.

The measure $[dx]$ is hard to define rigorously. We can formally write $[dx] = \prod_t dx(t)$. There can also be normalisation factors in $[dx]$, for example when we do

$$\int [dp]\, e^{\frac{i}{\hbar}\int (p\dot{q} - \frac{1}{2m}p^2 - V(q))}$$

then we get a Gaussian integral:

$$\prod_t dp(t)\, e^{\frac{i}{\hbar}(p\dot{q} - \frac{1}{2m}p^2)(t)}$$

which brings down factors of $\sqrt{\frac{2\pi m\hbar}{i\epsilon}}$ and puts $e^{-\frac{i}{\hbar}(\frac{1}{2}\dot{q}^2)}$ in the exponent which gives the Lagrangian.

Hence a calculation using the path integral is usually normalised at the end so that normalisation factors drop out.

$$\sqrt{\frac{2\pi m\hbar}{i\epsilon}} \times \frac{1}{2\pi\hbar} \rightarrow \sqrt{\frac{m}{2\pi i\hbar\epsilon}}$$

Thus: $\prod_{i=1}^{N-1}\left(\sqrt{\frac{m}{2\pi i\hbar\epsilon}}\, dx_i\right)$

The path integral makes the classical limit rather explicit. As $\hbar \to 0$, the stationary phase approximation becomes better and we have
$$\frac{\delta S[x]}{\delta x(t)} \equiv \frac{\delta S}{\delta x} - \frac{d}{dt}\frac{\delta S}{\delta \dot{x}} = 0$$
which is the Euler-Lagrange equation.

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The form of the path integral is of an integral over a <u>measure</u> e^{iS}. (It reminds of the Boltzmann weight $e^{-\beta H}$ common in statistical mechanics).

In fact we can show that inserting $x(t)$ in the functional integral is equivalent to computing the matrix element of the Heisenberg-rep operator
$$\hat{x}(t) = e^{i\frac{H}{\hbar}t}\,\hat{x}\,e^{-i\frac{H}{\hbar}t}$$
namely $\langle x'', t'' | \hat{x}(t) | x', t' \rangle$.

To show this, note that
$$\int [dx]\, e^{iS}\, x(t) = \int dx\, \langle x'', t'' | x, t \rangle\, x(t) \langle x, t | x', t' \rangle$$

This is easy to understand if we recall the representation of the LHS as many integrals over x at intermediate times. The integral over x at the fixed time t is simply treated separately.

Now $\langle x'', t'' | x, t \rangle x(t) = \langle x'', t'' | \hat{x}(t) | x, t \rangle$

and we can do the dx integral to get

$$\langle x'', t'' | \hat{x}(t) | x', t' \rangle$$

For two insertions of $x(t)$, things are more complicated. Suppose we insert $x(t_1)$ and $x(t_2)$:

$$\int [dx] \, e^{iS} x(t_1) x(t_2).$$

Now if $t_1 > t_2$ then this becomes:

$$\langle x'', t'' | \hat{x}(t_1) \hat{x}(t_2) | x', t' \rangle$$

but if $t_2 > t_1$ then it is:

$$\langle x'', t'' | \hat{x}(t_2) \hat{x}(t_1) | x', t' \rangle$$

which is a different quantity!

$$\hat{x}(t_1) \hat{x}(t_2) = e^{\frac{i}{\hbar} H t_1} \hat{x} \, e^{\frac{i}{\hbar} H (t_2 - t_1)} \hat{x} \, e^{-\frac{i}{\hbar} H t_2}$$

while

$$\hat{x}(t_2) \hat{x}(t_1) = e^{\frac{i}{\hbar} H t_2} \hat{x} \, e^{\frac{i}{\hbar} H (t_1 - t_2)} \hat{x} \, e^{-\frac{i}{\hbar} H t_1}$$

We can collect the two answers into one by defining

$$T(\hat{x}(t_1) \hat{x}(t_2)) = \theta(t_1 - t_2) \hat{x}(t_1) \hat{x}(t_2) + \theta(t_2 - t_1) \hat{x}(t_2) \hat{x}(t_1)$$

Then:

$$\int [dx] \, e^{iS} x(t_1) x(t_2) = \langle x'', t'' | T(\hat{x}(t_1) \hat{x}(t_2)) | x', t' \rangle$$

The time-ordered product plays a fundamental role in quantum field theory.

Let us now calculate $\langle x'', t'' | x', t' \rangle$ for a free particle using both operator quantum mechanics and path integrals. The Hamiltonian is:

$$H = \frac{\hat{p}^2}{2m}$$

In the operator formalism, we have:

$$\langle x'', t'' | x', t' \rangle = \langle x'' | e^{-\frac{i}{\hbar} \frac{\hat{p}^2}{2m} (t''-t')} | x' \rangle$$

This is conveniently evaluated by inserting a complete set of momentum eigenstates.

$$RHS = \int dp \, \langle x'' | e^{-\frac{i}{\hbar} \frac{\hat{p}^2}{2m} (t''-t')} | p \rangle \langle p | x' \rangle$$

$$= \int dp \, e^{-\frac{i}{\hbar} \frac{p^2}{2m} (t''-t')} \underbrace{\langle x'' | p \rangle \langle p | x' \rangle}_{\frac{e^{ip(x''-x')/\hbar}}{2\pi\hbar}}$$

$$= \int \frac{dp}{2\pi\hbar} e^{-\frac{i}{\hbar} \frac{p^2}{2m} (t''-t')} e^{ip(x''-x')/\hbar}$$

This is a Gaussian integral. To be sure it is convergent, add a factor $e^{-\epsilon p^2}$ and take $\epsilon \to 0$ at the end. (This ϵ is not related to the infintesimal time intervals!)

Let $A = \frac{i}{m\hbar}(t''-t')$ and $B = \frac{i(x''-x')}{\hbar}$

Then above =

$$\int \frac{dp}{2\pi\hbar}\, e^{-\frac{1}{2}Ap^2 + Bp} = \sqrt{\frac{2\pi}{A}}\, e^{\frac{B^2}{2A}}$$

$$= \frac{1}{2\pi\hbar}\sqrt{\frac{2\pi m\hbar}{i(t''-t')}}\, e^{\frac{im}{2\hbar}\frac{(x''-x')^2}{t''-t'}}$$

$$= \cancel{\sqrt{\frac{-im}{2\pi\hbar(t''-t')}}\, e^{\frac{im}{2\hbar}\frac{(x''-x')^2}{t''-t'}}}$$

$$= \sqrt{\frac{-im}{2\pi\hbar(t''-t')}}\; e^{\frac{im}{2\hbar}\frac{(x''-x')^2}{t''-t'}}$$

Our next task is to reproduce this result using the path integral.

For the ~~path~~ integral, we need to evaluate

$$\int [dx] \, e^{\frac{i}{\hbar} S[x]}$$

with $S = \int_{t'}^{t''} \frac{m}{2} \dot{x}^2 \, dt$

and $x(t') = x'$, $x(t'') = x''$.

Note that we cannot be sure about the normalisation of the answer! This is because we dropped normalisation factors ~~$\sqrt{\ldots}$~~ ~~at each of the~~ $\sqrt{\frac{m}{2\pi i \hbar \epsilon}}$ at each of the integration points. Moreover, we do not want to discretise the path integral all over again to evaluate it, since this amounts to undoing the original steps and going back to operators!

In the spirit of a "sum over paths" a derivation would go as follows.

We want to perform $\int [dx]$ over all paths satisfying $x(t') = x'$, $x(t'') = x''$.

Let us therefore <u>shift variables</u>:

$$x(t) = x_{cl}(t) + \eta(t)$$

where x_{cl} is the <u>classical</u> path from x' to x'', satisfying the eqn of motion $\ddot{x} = 0$ as well as the boundary conditions, and $\eta(t') = \eta(t'') = 0$. Since x_{cl} is a <u>fixed</u> path, we have

$$[dx] = [d\eta]$$

and $\int [dx]\, e^{iS[x]} =$

$$\int [d\eta]\, e^{\frac{i}{\hbar} S_{cl}[x] + \frac{i}{2\hbar} \frac{\delta^2 S}{\delta \eta^2} \eta^2}$$

Here $S_{cl} = \int_{t'}^{t''} \frac{m}{2} \dot{x}_{cl}^2\, dt$ Now $\dot{x}_{cl} = \frac{x'' - x'}{t'' - t'}$

so $S_{cl} = \frac{m}{2} \frac{(x'' - x')^2}{t'' - t'}$

Hence $e^{\frac{i}{\hbar} S_{cl}} = e^{\frac{im}{2\hbar} \frac{(x'' - x')^2}{t'' - t'}}$

and we have already found the main part of the answer!.
The normalization factor must arise from

$$\int [d\eta]\, e^{\frac{im}{2\hbar} \dot{\eta}^2} \quad \text{with } \eta(t') = \eta(t'') = 0.$$

This can formally be written:

$$\int [d\eta]\, e^{-\frac{im}{2\hbar} \eta \partial_t^2 \eta} = \det{}^{-\frac{1}{2}} \left(-\frac{im}{2\pi\hbar} \partial_t^2 \right)$$

This is on the face of it divergent → recurrence of the normalization issue!.

However at least in this case the prefactor can be computed quite easily. If we set $t'' = t'$ then no propagation has occurred

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

Now one of the defining properties of the δ-fn is:

$$\lim_{a \to 0} \frac{1}{\sqrt{\pi}\, a} e^{-\frac{(x'-x'')^2}{a^2}} = \delta(x' - x'')$$

We can use this in present case, where a is imaginary:

$$a^2 = \frac{-2\hbar (t'' - t')}{im} = \frac{2 i \hbar (t'' - t')}{m}$$

So $$\frac{1}{\sqrt{\pi}\, a} = \sqrt{\frac{m}{2\pi i \hbar (t'' - t')}}$$

and this is precisely the desired answer!