e.g. of an explicit path $\int$ ___

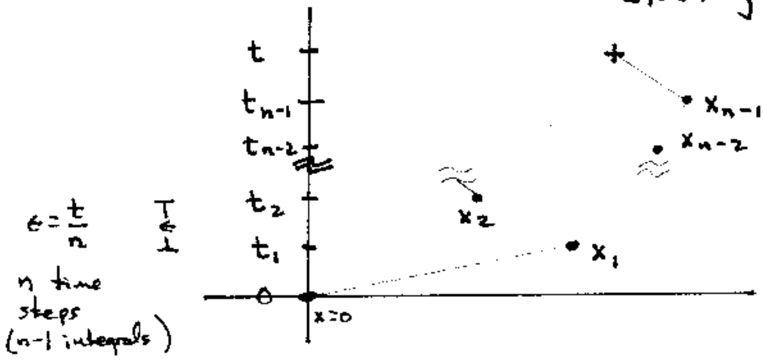
Since path $\int$s are an infinite number of linked integrals that contain all information about a given quantum problem, it's not surprising that not many can be carried out.

The two standard solvable cases are free particle $(V=0)$ and SHO $(V=\frac{1}{2}kx^2)$ problems. Both lead to nested Gaussian integrals, so it's not surprising they can be solved.

Our e.g. : free particle in 1D

$$H = \frac{1}{2m}p^2 = \frac{m\dot{x}^2}{2}$$

find $A(0,0 \to x,t)$. [Result is x and t translation invariant so starting from the origin is sufficiently general.]

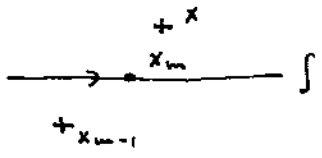


$$A = \int \mathcal{D}x\, e^{iS/\hbar} = \prod_{i=1}^{m=n-1} \eta \int dx_i\, \underbrace{e^{\frac{im}{2\epsilon\hbar}(x_{i+1}-x_i)^2}}_{e^f}$$

$$f = \frac{im}{2\epsilon\hbar}\left\{(x_2-x_1)^2 + (x_3-x_2)^2 + (x_4-x_3)^2 + \dots + (x_m - x_{m-1})^2 + (x-x_m)^2\right\}$$

Let's do the last dx_m integral first

$$f = \underbrace{\frac{im}{2\epsilon\hbar}\left\{(x_2-x_1)^2 + \dots + (x_{m-1}+x_{m-2})^2\right\}}_{f_0 \text{ (indep of } x_m)} + \underbrace{\frac{im}{2\epsilon\hbar}\left\{2x_m^2 - 2(x_{m-1}+x)x_m + x_{m-1}^2 + x^2\right\}}_{f_1}$$



completing the square,

$$\mathcal{I} = \eta \int dx_m\, e^{f} = e^{f_0} \eta \int dx_m \exp\left[\frac{im}{\epsilon\hbar} \left\{ (x_m - x_m^{(0)})^2 + \frac{1}{4}(x_{m-1} - x)^2 \right\} \right]$$

where $x_m^{(0)} = \frac{1}{2}(x + x_{m-1})$

(sensible: this says the "stationary phase point" is midway between the next & prev coords.)

$$\mathcal{I} = e^{f_0}\, e^{\frac{im}{\epsilon\hbar}\cdot\frac{1}{4}(x_{m-1}-x)^2} \cdot \underbrace{\eta \int_{-\infty}^{\infty} dx_m\, e^{\frac{im}{\epsilon\hbar}(x_m - x_m^{(0)})^2}}_{\frac{1}{\sqrt{2}}} \qquad \left[\eta \int_{-\infty}^{\infty} dy\, e^{\frac{im}{2\epsilon\hbar}y^2} \equiv 1 \right]$$

So doing the final integral $\int dx_m$ has simply changed f to

watch this x^2 coeff!

$$f = \frac{im}{2\epsilon\hbar} \left\{ (x_2 - x_1)^2 + \ldots + (x_{m-1} - x_{m-2})^2 + \frac{1}{2}(x_{m-1} - x)^2 \right\}$$

$$= \underbrace{\frac{im}{2\epsilon\hbar} \left\{ (x_2-x_1)^2 + (x_3-x_2)^2 + \ldots + (x_{m-2}-x_{m-3})^2 \right\}}_{\text{new } f_0} + \underbrace{\frac{im}{2\epsilon\hbar} \left\{ (x_{m-1}-x_{m-2})^2 + \frac{1}{2}(x_{m-1}-x)^2 \right\}}_{\text{new } f_1}$$

and multiplied by $\frac{1}{\sqrt{2}}$.

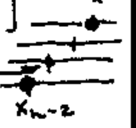
Now we repeat the exercise & do the <u>next</u> time slice integral, $\int dx_{m-1}$. This is

$$\mathcal{I} = \frac{1}{\sqrt{2}} e^{f_0}\, \eta \int_{-\infty}^{\infty} dx_{m-1} \underbrace{\exp\left[\frac{im}{2\epsilon\hbar} \left\{ \frac{3}{2} x_{m-1}^2 - (2x_{m-2} + x)x_{m-1} + x_{m-2}^2 + \frac{1}{2}x^2 \right\} \right]}$$

again complete the square,

$$= \exp\left[\frac{3im}{4\epsilon\hbar} \left\{ (x_{m-1} - x_{m-1}^{(0)})^2 + \frac{2}{9}(x_{m-2} - x)^2 \right\} \right]$$

where $x_{m-1}^{(0)} = \frac{2}{3}x_{m-2} + \frac{1}{3}x$



$$= \frac{1}{\sqrt{2}} e^{f_0}\, e^{\frac{im}{\epsilon\hbar}\cdot\frac{1}{6}(x_{m-2}-x)^2} \underbrace{\eta \int_{-\infty}^{\infty} dx_{m-1}\, e^{\frac{im}{2\epsilon\hbar}\cdot\frac{3}{2}\cdot(x_{m-1}-x_{m-1}^{(0)})^2}}_{\sqrt{\frac{2}{3}}}$$

so after $\eta\int dx_m\, \eta\int dx_{m-1}\, e^{iS/\hbar}$ we have

$$\frac{1}{\cancel{\sqrt{2}}}\cdot\sqrt{\frac{\cancel{2}}{3}}\cdot e^{f}$$

(2 integrals done)

new x^2 coeff.

$$f = \frac{im}{2\epsilon\hbar}\left\{(x_2-x_1)^2+\ldots+(x_{m-4}-x_{m-3})^2+(x_{m-2}-x_{m-3})^2+\frac{1}{3}(x_{m-2}-x)^2\right\}$$

(2 integrals done)

If we iterate this and carry out the remaining $m-2$ integrals, we finally obtain

$$A = \underbrace{\frac{1}{\sqrt{n}}}_{\sqrt{\frac{1}{\cancel{2}}}\sqrt{\frac{\cancel{2}}{\cancel{3}}}\sqrt{\frac{\cancel{3}}{\cancel{4}}}\cdots\sqrt{\frac{\cancel{n-1}}{n}}}\cdot e^{\frac{im}{2\epsilon\hbar}\frac{1}{n}x^2}$$

(m=n-1 integrals done)

(m=n-1 integrals done)

Since $t = n\epsilon$ this is

$$\underline{A[0,0\to x,t]} = \underline{\frac{1}{\sqrt{n}}\, e^{\frac{imx^2}{2\hbar t}}}$$

Although this is the correct result for the path $\int$, it is normally multiplied by an additional factor of η when we write it as a kernel and use it to propagate a wavefunction,

$$\psi(x,t) = \eta\int dx_i\; A[x_i,0\to x,t]\,\psi(x_i,0) \equiv \int dx_i\; K[x_i,0\to x,t]\,\psi(x_i,0)$$

$$\therefore\ K[x_i,0\to x,t] = \eta A[\;] = \sqrt{\frac{m}{2\pi i\epsilon\hbar}}\,\frac{1}{\sqrt{n}}\, e^{\frac{im(x-x_i)^2}{2\hbar t}}$$

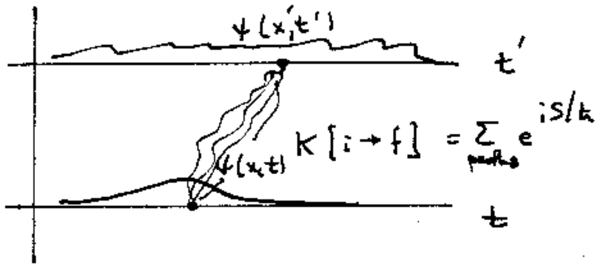
$$= \underline{\left[\frac{m}{2\pi i\hbar t}\right]^{1/2} e^{\,i\frac{m(x-x_i)^2}{2\hbar t}}}$$

<u>This</u> is the Kernel of the free Schrödinger equation. [= response to local source]

Eigenmode expansions of Kernels

The path integral describes the time evolution of a wavefunction,

$$\psi(x',t') = \int dx \;\; K[x,t \to x',t'] \, \psi(x,t)$$



which implies that it has an especially simple representation in energy eigenfunctions,

$$K[x,t \to x',t'] = \underbrace{\sum_n}_{\text{all energy eigenfunctions}} \psi_n(x',t') \, \psi_n^*(x,t) = \sum_n \psi_n(x')\psi_n^*(x) e^{i\omega_n(t-t')}$$

$$\omega_n \equiv E_n/\hbar$$

to see this, suppose we are initially in an energy eigenstate $\psi_m(x,t)$

$$= \psi_m(x) \, e^{-i\omega_m t} \qquad \omega_m \to E_m/\hbar$$

At a later time t' this is

$$\psi(x',t') = \int dx \, K[x,t \to x',t'] \;\; \psi_m(x) \, e^{-i\omega_m t}$$

$$= \sum_n \psi_n(x') \, e^{i\omega_n(t-t')} \; e^{-i\omega_m t} \underbrace{\int dx \, \psi_n^*(x) \, \psi_m(x)}_{\delta_{mn}}$$

$$= \psi_m(x') \, e^{-i\omega_m t'} \quad \checkmark$$

So, this implies correctly that an energy eigenstate evolves into itself.

It also implies that the kernel contains all energy eigenstate wavefunctions, which may be extracted from the $K[0,0 \to x,t]$ (for example) by Fourier transforming with respect to time:

$$K[0,0\to x,t] = \sum_n \psi_n(x)\psi_n^*(0)\, e^{i\omega_n t}$$

$$\int dt\, K[0,0\to x,t]\, e^{-i\omega t} = \sum_n 2\pi\delta(\omega-\omega_n)\,\psi_n(x)\psi_n^*(0)$$

may want to choose the initial point $\neq 0$, if this vanishes.

x_f - dependence gives $\psi_n(x)$

F.T. is singular iff $\omega=\omega_n$ (energy of an eigenmode)

As an example, let's try to build up our free particle Kernel from all the energy eigenmodes.

$$K[0,0\to x,t] = \sum_n \psi_n(x)\psi_n^*(0)\, e^{-i\omega_n t}$$

these are plane waves, and the $\sum_{\text{modes}} \to \int_{-\infty}^{\infty} dk$ (to an overall constant),

some new norm

$$K = c\int_{-\infty}^{\infty} dk\, e^{ikx - i\frac{E_k}{\hbar}t} = c\int_{-\infty}^{\infty} dk\, e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)}$$

this is another stationary phase integral. Completing the square, we find

$$K = c\int_{-\infty}^{\infty} dk\, e^{-i\frac{\hbar t}{2m}\left[\left(k-\frac{mx}{\hbar t}\right)^2 - \frac{m^2x^2}{\hbar^2t^2}\right]}$$

$$= c\cdot \underbrace{\sqrt{\frac{2m\,\pi}{i\hbar t}}}_{\text{“}\sqrt{\frac{\pi}{a}}\text{”}}\cdot e^{+\frac{im}{2\hbar}\frac{x^2}{t}}$$

This is exactly the result of our path $\int$, if the overall norm is $c=\frac{1}{2\pi}$.

Thus you could pull off the plane wave solution e^{ikx} from the Fourier transform

$$\int_{-\infty}^{\infty} dt\, e^{-i\omega t} \cdot \sqrt{\frac{m}{2\pi i \epsilon t}}\, e^{+\frac{im}{2\hbar}\frac{x^2}{t}} \quad \propto \quad e^{i\underbrace{\sqrt{\frac{2m\omega}{\hbar}}}_{k}x}$$

but this is not exactly a well-known integral!

Implications of $e^{iS/\hbar}$ for wfns: "p_{op}"

Conventional 'operator' QM is often defined by introducing canonical commutation relations between coordinates and momenta,

$$[q_i, p_j] = i\hbar\,\delta_{ij}$$

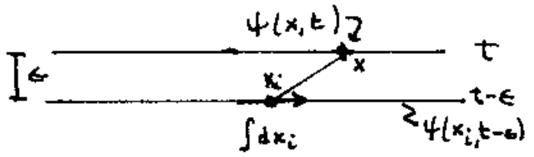
and if the wavefunction is defined in a q with diagonal coordinate basis, e.g. $\psi(x)$, momentum then can be reprecanted by an operator,

$$p_{op} = -i\hbar \frac{\partial}{\partial x} \quad .$$

How does this follow in path integrals, which describes QM without operators, purely in terms of trajectories $\{x(t)\}$ and classical actions?

Using time slices to define path $\int$s, we wrote the evolution equation for a wavefunction $\psi(x,t)$ in a single time slice as

$$\psi(x,t) = \eta \int_{-\infty}^{\infty} dx_i\, e^{iS/\hbar}\, \psi(x_i, t-\epsilon)$$



$$S = \int_{t_i}^{t_f} \left[\tfrac{1}{2} m\dot{x}^2 - V(x)\right] dt = \underbrace{\frac{m(x-x_i)^2}{2\,\epsilon^2}}_{m\dot{x}^2} \cdot \epsilon - V(x_i)\cdot\epsilon$$

Note v or $p = mv$ are only defined by two (or more) time slices:

$$v = \frac{x - x_i}{\epsilon}$$

is the obvious choice.

So,

$$\psi(x,t) = \eta \int_{-\infty}^{\infty} dx_i\, e^{\frac{im(x-x_i)^2}{2\epsilon\hbar} - \frac{i\epsilon}{\hbar}V(x_i)}\, \psi(x_i, t-\epsilon)$$

The effect of multiplying the evolving wavefunction by $p = mv$, which is a quantity defined "between" time slices, is

$$p\Big|_{t-\epsilon,t} \cdot \psi(x,t) = \eta \int_{-\infty}^{\infty} dx_i \; \underbrace{m\frac{(x-x_i)}{\epsilon}}_{mv=p} \; e^{\frac{im(x-x_i)^2}{2\epsilon\hbar} - \frac{i\epsilon V(x_i)}{\hbar}} \psi(x_i, t-\epsilon)$$

note $\frac{\partial}{\partial x} e^{\frac{im(x-x_i)^2}{2\epsilon\hbar}} = \frac{im}{\epsilon\hbar}(x-x_i)$, so $-i\hbar\frac{\partial}{\partial x}$ on $\psi(x,t)$ has the effect

$$-i\hbar\frac{\partial}{\partial x}\psi(x,t) = \eta \int_{-\infty}^{\infty} dx_i \underbrace{\left\{(-i\hbar)\cdot\frac{im}{\epsilon\hbar}(x-x_i)\right\}}_{\frac{m(x-x_i)}{\epsilon} = p} e^{i\frac{m(x-x_i)^2}{2\epsilon\hbar} - \frac{i\epsilon}{\hbar}V(x_i)} \psi(x_i, t-\epsilon)$$

$\therefore$ $-i\hbar\frac{\partial}{\partial x}$ applied to a wavefunction $\psi(x,t)$ has the same effect as multiplying the evolving wavefunction by $p = \frac{m\Delta x}{\Delta t}$.

<u>$[q,p]$ comm rels – origin in terms of path $\int$s</u>

Since path $\int$s involve only classical quantities, how can we ever find a result equivalent to non-commuting operators?

The answer is that the product qp is not yet well defined, since q "lives on" one time slice and p is defined on two. We should be careful to distinguish between

$t+\epsilon$
t $\quad p_{i,i+1} = m(x_{i+1}-x_i)/\epsilon$ $\quad x_i$ and

$t+\epsilon$ $\quad x_{i+1}$
t $\quad p_{i,i+1} = m(x_{i+1}-x_i)/\epsilon$

Do these very similar quantities really have an $\mathcal{O}(\epsilon^0)$ difference in their weighted path integrals?

Try inserting their difference in the path integral describing the evolution of a wavefunction

$$(x_i\, p_{i,i+1} - x_{i+1}\, p_{i,i+1}) \cdot \psi(x,t)$$

$$= \eta \int_{-\infty}^{\infty} dx_i \left\{ x_i \frac{m(x-x_i)}{\epsilon} - x \frac{m(x-x_i)}{\epsilon} \right\} e^{\,i m \frac{(x-x_i)^2}{2\epsilon\hbar} - \frac{i\epsilon V(x_i)}{\hbar}}$$

$$\cdot\, \psi(x_i, t-\epsilon)$$

Neglect V (small ϵ) and replace $\psi(x_i, t-\epsilon)$ by $\psi(x,t)$ (small ϵ), and we still have to evaluate

$$\underbrace{\eta \int_{-\infty}^{\infty} dx_i \left(\frac{-m(x-x_i)^2}{\epsilon} \right) \cdot e^{\,i \frac{m(x-x_i)^2}{2\epsilon\hbar}}}_{-\frac{m}{\epsilon} \cdot \frac{i\epsilon\hbar}{m} \,=\, -i\hbar}$$

So, it makes an $\mathcal{O}(\hbar)$ difference whether we write px with x on the "earlier" or "later" time slice.
If we follow the convention that we write the earliest quantity on the right, we conclude that

$$(\underset{x_{i+1}}{x}\,\underset{p_{i,i+1}}{p} - \underset{p_{i,i+1}}{p}\,\underset{x_i}{x}) \cdot \psi(x,t) = +i\hbar \cdot \psi(x,t)$$

or $[x,p] \cdot \psi = +i\hbar \cdot \psi$

Thus, the "canonical commutation relations" of operator QM are equivalent to putting x infinitesimally earlier/later than p in the path integral.

Wow.