Chapter 8: The Path Integral Formulation of Quantum Mechanics

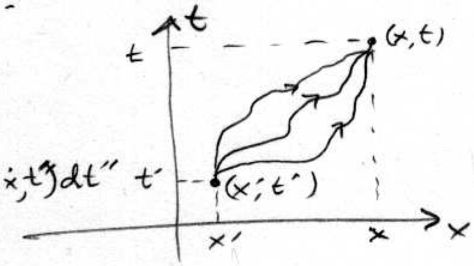
Developed by Dirac and Feynman

A very powerful method which lies at the root of most modern numerical approaches to solve quantum systems non-perturbatively.

8.1. The recipe

To find the propagator $\mathcal{U}(x,t;x',t')$:

(1) Draw all paths in the $x-t$ plane connecting the events (x',t') and (x,t).



(2) Find the classical action $S[x(t)] = \int_{t'}^{t} L(x,\dot{x},t'')dt''$ for each path $x(t)$.

(3) $$\mathcal{U}(x,t;x',t') = A \sum_{\text{all paths}} e^{iS[x(t)]/\hbar}$$

A: normalization factor

→ get quantum mechanical time evolution from classical action!!

8.2. Analysis

There are a number of amazing aspects to this recipe:

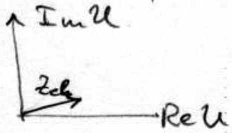
(i) all paths, not only the classically allowed one, contribute to the QM propagator

(ii) each path, even the most dramatically classically forbidden ones (with huge action) get a weight of the <u>same</u> absolute magnitude ($e^{iS/\hbar}$ has magnitude 1)!

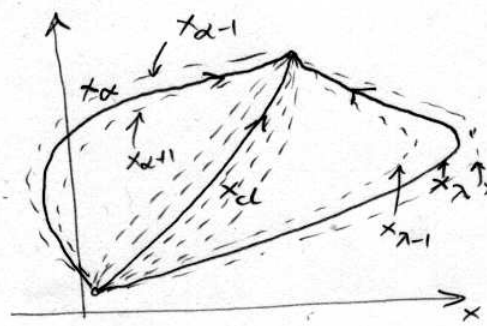
So how does the classical path arise as the only allowed one in some limit of that formula?

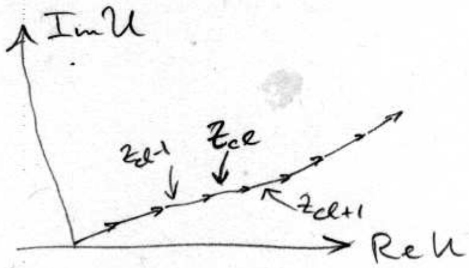
To get some feeling for how the path integral formula works, let us consider only a sum over a few discrete paths (like those shown in the sketch), instead of trying to "integrate over all paths":

Each path contributes to $\mathcal{U}$ a complex number of unit magnitude, which we can represent as a unit vector in the complex $\mathcal{U}$ plane. The classical path minimizes S and contributes $z_{cl} = e^{iS_{cl}/\hbar}$:

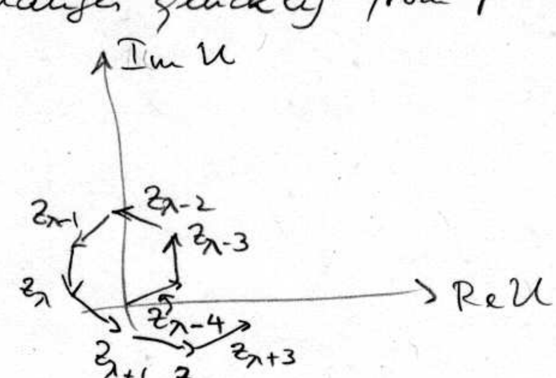


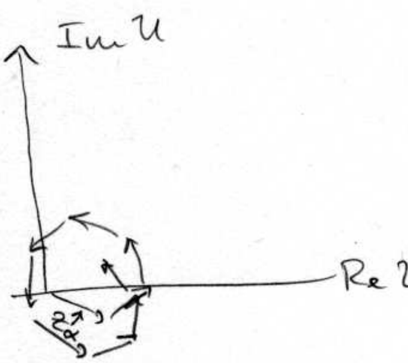
All paths that are close to the classical path have z-values close to z_{cl}, so they add vectors pointing roughly in the same direction:





Paths x_α and x_λ have very large action, and the action changes quickly from path to path:





So these arrows tend to circle around zero, largely cancelling each other and not getting you very far from zero.

So the result for $\mathcal{U}$ from the total sum is mostly due to the coherent addition from the paths close to x_{cl} whereas the classically forbidden paths interfere destructively and don't contribute to $\mathcal{U}$.

So how far must we deviate from x_{cl} before destructive interference sets in? Roughly, we can expect that coherence is lost once $(S - S_{cl})/\hbar \sim O(\pi)$; so for a path to contribute, its action must be within $\hbar\pi$ of the action of the classical path.

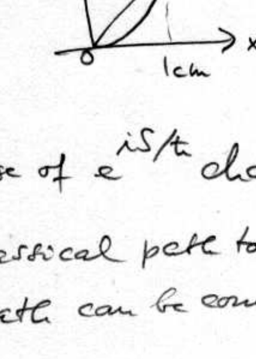
For a classical macroscopic particle $S_{cl} \sim 1\,\text{erg sec} \simeq 10^{27}\hbar$; so for the paths not to interfere destructively, the actual path cannot deviate from the classical path by much more than 1 part in 10^{27} — this is a very tight constraint. For a single electron, on the other hand, the path can deviate quite a bit from its classical path.

Consider a free particle with classical path

$$x_{cl} = vt \qquad v = 1\,\frac{\text{cm}}{\text{sec}}$$

Consider the path

$$x = at^2 \qquad \text{with } a = 1\,\frac{\text{cm}}{\text{sec}^2}$$



Both go through $(0,0)$ and $(1\text{sec}, 1\text{cm})$.

- For $m = 1g$, $\delta S = 1.6 \times 10^{26}\hbar$ (so the phase of $e^{iS/\hbar}$ changes by 1.6×10^{26} rad) when we change from the classical path to the nonclassical path $x \sim t^2$. → non-classical path can be completely neglected.
- For an electron with $m \sim 10^{-27} g$, $\delta S \sim \frac{\hbar}{6}$, so the phase changes by 0.16 rad $\ll \pi$ → assuming that electron moves along classical path leads to conflict with experiment.

8.3 Propagator for a free particle in a simple approximation

Let us simply ignore all non-classical paths; assume that for all paths close to the classical path $S \approx S_{cl}$ (since S is stationary around the classical path):

$$\mathcal{U}(t) = A' \, e^{iS_{cl}/\hbar}$$

(A' "counts" the number of paths that are sufficiently close to the classical path)

(So all paths in the "coherent" range are counted with $e^{iS_{cl}/\hbar}$, all others are counted with weight zero.)

The classical path is $\quad x_{cl}(t'') = x' + \underbrace{\frac{x-x'}{t-t'}}_{v\,=\,\text{const.}}(t''-t')$

$\Rightarrow \mathcal{L} = \frac{m}{2}v^2 = \text{constant in } t''$

$$\Rightarrow \quad S_{cl} = \int_{t'}^{t} dt''\,\mathcal{L} = \frac{m}{2}\frac{(x-x')^2}{t-t'}\,.$$

$$\Rightarrow \quad \boxed{\mathcal{U}(x,t;x',t') = A' \, e^{\frac{im(x-x')^2}{2\hbar(t-t')}}}$$

To find A', require that for $t-t' \to 0$, $\mathcal{U} \to \delta(x-x') = \lim_{\Delta \to 0}\frac{1}{\sqrt{\pi\Delta^2}}e^{-\frac{(x-x')^2}{2\Delta^2}}$

(this works even if Δ is imaginary).

$$\Rightarrow \quad A' = \sqrt{\frac{m}{2\pi i\hbar(t-t')}}$$

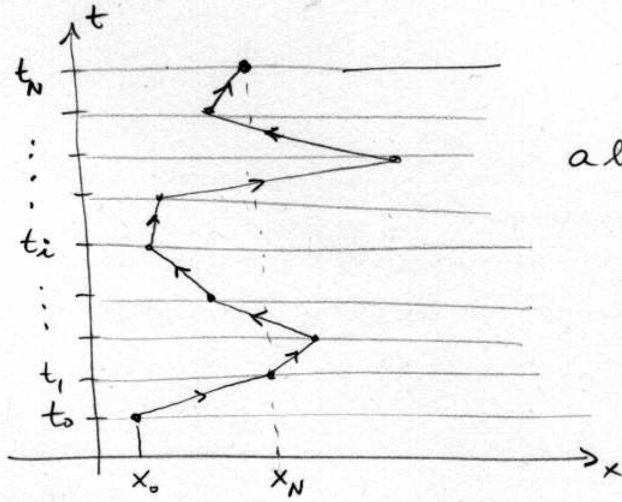
and

$$\boxed{\mathcal{U}(x,t;x',0) = \sqrt{\frac{m}{2\pi i\hbar t}}\; e^{\frac{im(x-x')^2}{2\hbar t}}}$$

This is the exact answer! We got it by just considering the classical action!

This works, however, only for $V(x,\dot{x}) = a + bx + cx^2 + d\dot{x} + ex\dot{x}$; in all these cases $\mathcal{U}(t) = A(t)\,e^{iS_{cl}/\hbar}(t)$. But in general we can't get $A(t)$ from requiring $\mathcal{U}(x,0;x') = \delta(x-x')$ since $A(t)$ can depend on a arbitrary dimensionless function that has $f \to 1$ as $t \to 0$. Here $f = 1$, since you can't construct a nontrivial $f(t)$ using just m, $\hbar$, and t.

8.4. Evaluation of the path integral for a free particle



a highly non-classical path

(since $\mathcal{L}$ does not depend on the acceleration, the sharp changes in velocity don't matter when computing the action)

Consider $\mathcal{U}(x_N, t_N; x_0, t_0)$. We have to perform the path integral

$$\int_{x_0}^{x_N} e^{iS[x(t)]/\hbar}\, \mathcal{D}[x(t)]$$

where $\int_{x_0}^{x_N} \mathcal{D}[x(t)]$ symbolises a sum over all paths $x(t)$ that get me from x_0 at t_0 to x_N at t_N. Let's look at the particle's position at an intermediate time t_i. Summing over all paths means that at all t_i we have to integrate over all positions x_i (from $-\infty$ to $+\infty$) that the particle might have at t_i.

Let us subdivide $T = t_N - t_0$ into a large number of tiny intervals $\Delta t = \frac{T}{N}$ $(N \to \infty)$ and approximate the actual path by short straight lines within those interval (see figure).

Then, for a given path $x(t) = \left(x_0(t_0), x_1(t_1), x_2(t_2), \dots x_i(t_i), \dots, x_N(t_N)\right)$,

We can replace

$$S = \int_{t_0}^{t_N} \mathcal{L}(t)\,dt = \int_{t_0}^{t_N} \frac{m}{2}\dot{x}^2(t)\,dt \longrightarrow \sum_{i=0}^{N-1} \frac{m}{2}\left(\frac{x_{i+1}-x_i}{\Delta t}\right)^2 \Delta t$$

The propagator thus becomes

$$\mathcal{U}(x_N, t_N; x_0, t_0) = \int_{x_0}^{x_N} e^{iS[x(t)]/\hbar}\, \mathcal{D}[x(t)]$$

$$= \lim_{\substack{N\to\infty \\ \Delta t = \frac{t_N - t_0}{N} \to 0}} A \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \dots \int_{-\infty}^{\infty} dx_{N-1}\, e^{\frac{i}{\hbar}\frac{m}{2}\sum_{i=0}^{N-1}\frac{(x_{i+1}-x)^2}{\Delta t}}$$

A must be chosen such that at the end we get the correct dimension for $\mathcal{U}$.

Let us first rescale our x-variable: $y_i = x_i\sqrt{\frac{m}{2\hbar\Delta t}}$.

We now want to work out

$$\lim_{N\to\infty} A' \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{\infty} dy_2 \dots \int_{-\infty}^{\infty} dy_{N-1}\, e^{-\sum_{k=0}^{N-1}\frac{(y_{k+1}-y_k)^2}{i}}$$

with $A' = A\left(\frac{2\hbar\Delta t}{m}\right)^{\frac{N-1}{2}}$

Let us first do the y_1-integral. The terms in the sum involving y_1 are:

$$\int_{-\infty}^{\infty} dy_1\, e^{-\frac{1}{i}\left[(y_2-y_1)^2 + (y_1-y_0)^2\right]} = \sqrt{\frac{i\pi}{2}}\, e^{-(y_2-y_0)^2/2i}$$

Next the y_2-integral:

$$\int_{-\infty}^{\infty} dy_2\, e^{-\frac{1}{i}(y_3-y_2)^2}\, e^{-\frac{1}{2i}(y_2-y_0)^2} = \dots = \sqrt{\frac{(i\pi)^2}{3}}\, e^{-(y_3-y_0)^2/3i}$$

Keeping going we get for the integral over all y_i

$$\sqrt{\frac{(i\pi)^{N-1}}{N}}\, e^{-\frac{(y_N-y_0)^2}{iN}} = \sqrt{\frac{(i\pi)^{N-1}}{N}}\, e^{\frac{i}{\hbar}\frac{m}{2}\frac{(x_N-x_0)^2}{t_N-t_0}}$$

and thus

$$\mathcal{U}(x_N,t_N;x_0,t_0) = A\left(\frac{2\pi i\hbar\Delta t}{m}\right)^{N/2}\sqrt{\frac{m}{2\pi i\hbar \underbrace{N\Delta t}_{t_N-t}}}\, e^{\frac{i}{\hbar}\frac{m}{2}\frac{(x_N-x_0)^2}{t_N-t_0}}$$

To get the right answer we must set

$$A = \left(\frac{2\pi i\hbar\Delta t}{m}\right)^{-N/2} = B^{-N} \qquad B = \sqrt{\frac{2\pi i\hbar\Delta t}{m}}$$

Conventionally one associates one factor $\frac{1}{B}$ with each of the $N-1$ integration and the last $1/B$ with the overall process:

$$\int \mathcal{D}[x(t)] = \lim_{\substack{\Delta t\to 0\\ N\to\infty}} \frac{1}{B}\int_{-\infty}^{\infty}\frac{dx_1}{B}\int_{-\infty}^{\infty}\frac{dx_2}{B}\cdots\int_{-\infty}^{\infty}\frac{dx_{N-1}}{B}$$

where $B = \sqrt{\frac{2\pi i\hbar\Delta t}{m}}$

This <u>defines</u> the path integral, and reproduces the correctly normalized result from the QM postulates. The same normalization must now be used for all other cases where the particle is not free.

8.5. Equivalence to the Schrödinger equation

The Schrödinger equation tells us that, for $\Delta t \to 0$,

$$|\psi(\Delta t)\rangle - |\psi(0)\rangle = -\frac{i\Delta t}{\hbar}\hat{H}\,|\psi(0)\rangle$$

In the $\hat{X}$-basis this becomes, to first order in Δt,

$$\psi(x,\Delta t) - \psi(x,0) = -\frac{i\Delta t}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,0)\right)\psi(x,0)$$

Let us compare this with the path integral result,

$$\psi(x,\Delta t) = \int_{-\infty}^{\infty} dx' \;\; \mathcal{U}(x,\Delta t; x',0)\,\psi(x',0)$$

with

$$\mathcal{U}(x,\Delta t; x',0) = \sqrt{\frac{m}{2\pi i\hbar\Delta t}}\;\; e^{\frac{i}{\hbar}\left(\frac{m}{2}\frac{(x-x')^2}{\Delta t} - \Delta t\cdot V\left(\frac{x+x'}{2},0\right)\right)}.$$

(no integration over intermediate times, since only 1 time step)

We used $L = T - V$; we took $\int_0^{\Delta t} dt''\, V(x(t''),t'') = \Delta t\, V\left(\frac{x+x'}{2},0\right) + \mathcal{O}((\Delta t)^2)$.

straight line between x and x', evaluated at midpoint

So we need to do the integral

$$\psi(x,\Delta t) = \sqrt{\frac{m}{2\pi i\hbar\Delta t}}\int_{-\infty}^{\infty} dx'\; e^{\frac{i}{\hbar}\frac{m}{2}\frac{(x-x')^2}{\Delta t}}\; e^{-\frac{i}{\hbar}\Delta t\, V\left(\frac{x+x'}{2},0\right)}\;\psi(x',0)$$

Since Δt is infinitesimal and $\hbar$ is small, the first term oscillates extremely rapidly as we move x' along the real axis. When such a rapidly oscillating function multiplies a smooth function like $\psi(x',0)$, the integral vanishes mostly due to the random phase of the exponential. The only substantial contribution comes from the region where the phase is stationary, just as for the path integration. Here the only stationary point is $x = x'$ where the phase is minimal (namely zero).

The region of coherence is $\frac{m}{2\hbar\Delta t}(x-x')^2 \lesssim \pi$

or $|\eta| \equiv |x-x'| \lesssim \sqrt{\frac{2\pi\hbar\Delta t}{m}}$.

With this in mind, let's work on the integral:

$$\psi(x,\Delta t) = \sqrt{\frac{m}{2\pi i\hbar\Delta t}} \int_{-\infty}^{\infty} d\eta \, e^{\frac{i}{\hbar}\frac{m}{2\Delta t}\eta^2} e^{-\frac{i}{\hbar}\Delta t\, V(x+\frac{\eta}{2};0)} \psi(x+\eta,0).$$

Since η has to be small by the above argument in order to contribute, we can expand V and ψ:

$$\psi(x+\eta,0) = \psi(x,0) + \eta\frac{\partial\psi}{\partial x}(x) + \frac{1}{2}\eta^2\frac{\partial^2\psi}{\partial x^2}(x) + \dots$$

$$e^{-\frac{i}{\hbar}\Delta t\, V(x+\frac{\eta}{2};0)} = 1 - \frac{i\Delta t}{\hbar}V(x+\eta/2,0) + \dots = 1 - \frac{i\Delta t}{\hbar}V(x,0) + \dots$$

We kept all term up to order $\Delta t \sim \eta^2$ and dropped all smaller terms than that.

So

$$\psi(x,\Delta t) = \sqrt{\frac{m}{2\pi i\hbar\Delta t}} \int_{-\infty}^{\infty} d\eta \, e^{\frac{im\eta^2}{2\hbar\Delta t}} \Big[\psi(x,0) - \frac{i}{\hbar}\Delta t\, V(x,0)\psi(x,0) + \underbrace{\eta\frac{\partial\psi}{\partial x}}_{\text{vanishes by symmetric integration}} + \frac{\eta^2}{2}\frac{\partial^2\psi}{\partial x^2}\Big]$$

$$= \sqrt{\frac{m}{2\pi i\hbar\Delta t}} \Big[\psi(x,0)\sqrt{\frac{2\pi i\hbar\Delta t}{m}} - \frac{\hbar\Delta t}{2im}\sqrt{\frac{2\pi i\hbar\Delta t}{m}}\frac{\partial^2\psi}{\partial x^2} - \frac{i\Delta t}{\hbar}\sqrt{\frac{2\pi i\hbar\Delta t}{m}} V(x,0)\psi(x,0)\Big]$$

or

$$\psi(x,\Delta t) - \psi(x,0) = -\frac{i\Delta t}{\hbar}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,0)\right]\psi(x,0)$$

which agrees with the prediction from the Schrödinger equation.

8.6 Potentials of the form $V(x,\dot{x}) = a + bx + cx^2 + d\dot{x} + ex\dot{x}$

Let us write each path as

$$x(t'') = x_{cl}(t'') + y(t''), \quad y(0) = y(t) = 0$$

$$\dot{x}(t'') = \dot{x}_{cl}(t'') + \dot{y}(t'')$$

$$x_i \equiv x(t_i'') = x_{cl}(t_i'') + y(t_i'') \equiv x_{cl}(t_i'') + y_i$$

$$dx_i = dy_i \quad , \quad \int_{x'}^{x} \mathcal{D}[x(t'')] = \int_0^0 \mathcal{D}[y(t'')]$$

Hence

$$U(x,t;x';0) = \int_0^0 \mathcal{D}[y(t'')]\, e^{\frac{i}{\hbar}S[x_{cl}(t'') + y(t'')]}$$

Expand the action around its minimum at $x(t) = x_{cl}(t)$:

$$S[x_{cl}+y] = \int_0^t dt''\, \mathcal{L}(x_{cl}+y, \dot{x}_{cl}+\dot{y}) = \int_0^t dt'' \left[\mathcal{L}(x_{cl},\dot{x}_{cl}) + \left.\frac{\partial \mathcal{L}}{\partial x}\right|_{x_{cl}} y\right.$$

$$\left. + \left.\frac{\partial \mathcal{L}}{\partial \dot{x}}\right|_{x_{cl}} \dot{y} + \frac{1}{2}\left(\left.\frac{\partial^2 \mathcal{L}}{\partial x^2}\right|_{x_{cl}} y^2 + 2\left.\frac{\partial^2 \mathcal{L}}{\partial x_{cl}\,\partial \dot{x}_{cl}}\right|_{x_{cl}} y\dot{y} + \left.\frac{\partial^2 \mathcal{L}}{\partial \dot{x}_{cl}^2}\right|_{x_{cl}} \dot{y}^2\right)\right]$$

Again, higher order terms in $y, \dot{y}$ can be neglected due to the fact that only for small $y, \dot{y}$ the phases don't oscillate rapidly, averaging to zero.

The first term integrates to $S_{cl} \equiv S[x_{cl}]$. The linear pieces $\sim y$ and $\dot{y}$ vanish due to the classical equation of motion $\left[\frac{d}{dt''}\frac{\partial \mathcal{L}}{\partial \dot{x}} - \frac{\partial \mathcal{L}}{\partial x}\right]_{x_{cl}} = 0$.

In the last piece, using the assumed form

$$\mathcal{L} = T - V = \frac{1}{2}m\dot{x}^2 - a - bx - cx^2 - d\dot{x} - ex\dot{x},$$

we get

$$\frac{1}{2}\frac{\partial^2 \mathcal{L}}{\partial x^2} = -c, \quad \frac{\partial^2 \mathcal{L}}{\partial x \partial \dot{x}} = -e, \quad \frac{1}{2}\frac{\partial^2 \mathcal{L}}{\partial \dot{x}^2} = m$$

Hence

$$U(x,t;x',0) = e^{iS_{cl}/\hbar} \underbrace{\int_0^0 \mathcal{D}[y(t'')]\, e^{\frac{i}{\hbar}\int_0^t dt''\left(\frac{1}{2}m\dot{y}^2 - cy^2 - ey\dot{y}\right)}}_{A(t)} \qquad (*)$$

$$= e^{iS_{cl}(t)/\hbar} A(t).$$

For the free particle $c = e = 0$, and we found $A(t) = \sqrt{\frac{m}{2\pi i\hbar t}}$.

Since $(*)$ is independent of a and b, the same value $A(t)$ holds for potentials $V(x) = a + bx$. For the harmonic oscillator, $c = \frac{1}{2}m\omega^2$, and we must do the integral

$$A(t) = \int_0^0 \mathcal{D}[y(t'')]\, e^{i/\hbar \int_0^t dt''\left(\frac{m}{2}(\dot{y}^2 - \omega^2 y^2)\right)}.$$

This integral is not trivial (see Feynman & Hibbs (1965))

It gives the result presented at the bottom of p. 145.

(See also the derivation in H. Kleinert, Path Integrals in Quantum Mechanics, Statistics, ... p. 111–116)