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 $U(x,t;x',t')$:

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

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

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

→ 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 ones, contribute to the QM propagator.

(ii) each path, even the most dramatically classically forbidden ones (with huge action) get a weight of the same absolute magnitude ($e^{i S/\hbar}$ 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 few discrete paths (like those shown in the sketch), instead of trying to "integrate over all paths".

Each path contributes to $U$ a complex number of unit magnitude, which we can represent as a unit vector in the complex $U$ plane. The classical path minimizes $S$ and contributes $\frac{e^{iS}}{\sqrt{2\pi}}$.

All paths that are close to the classical path have $z$-values closest to $z_0$, so they add vectors pointing roughly in the same direction.

Paths $x_x$ and $x_x$ have very large action, and the action changes quickly from path to path.

So these arrows trend to circle around zero, largely canceling each other and not getting you very far from zero.
So the result for \( U \) from the total sum is mostly due to the coherent addition from the paths close to \( x \) whereas the classically forbidden paths interfere destructively and don't contribute to \( U \).

So how far must we deviate from \( x \) at before destructive interference sets in? Roughly, we can expect that coherence is lost once \( (S - S_{ee})/2 \approx 0(1) \); so for a path to contribute, its action must be within \( \frac{1}{2} \) of the action of the classical path.

For a classical macroscopic particle \( S \approx 1 \) erg sec \( \approx 10^{27} \hbar \); 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

\[
\begin{align*}
  x &= vt \\
  v &= \frac{1 \text{ cm}}{\text{sec}}
\end{align*}
\]

Consider the path

\[
  x = at^2 \quad \text{with} \quad a = \frac{1 \text{ cm}}{\text{sec}^2}
\]

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

- For \( m = 1 \) g, \( \Delta S = 1.6 \times 10^{-26} \text{ rad} \) (so the phase of \( e^{iS/\hbar} \) changes by \( 1.6 \times 10^{-26} \) rad) when we change from the classical path to the non-classical path \( x = at^2 \). — non-classical path can be completely neglected.

- For an electron with \( m \approx 10^{-21} \) g, \( \Delta S \approx \frac{\pi}{6} \), so the phase change by \( 0.16 \text{ rad} \approx \pi \) — assuming that electron moves along classical path leads to conflict with experiment.
Let us simply ignore all non-classical paths; assume that for all paths close to the classical path, $S \approx S_c$ (since $S$ is stationary around the classical path).

$$U(t) = A' e^{iS_c / \hbar}$$

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

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

The classical path is

$$x_c(t) = x' + \frac{x - x'}{t - t'}(t - t')$$

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

$$\Rightarrow S_{ce} = \int_{t'}^{t} dt' L = \frac{m}{2} \frac{(x - x')^2}{t - t'}$$

$$\Rightarrow U(x, t; x', t') = A' e^{i \frac{m(x-x')^2}{2\hbar(t-t')}}$$

To find $A'$, require that for $t - t' \to 0$, $U \to \delta(x-x') \frac{1}{2\pi \hbar} e^{i \frac{(x-x')^2}{2\hbar}}$ (this works even if $\Delta$ is imaginary).

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

and

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

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

This works however only for $V(x) = a + bx + cx^2 + dx + ex^3$; in all these cases $U(t) = A(t) e^{iS_c / \hbar}$. But in general we can't get $A(t)$ from requiring $U(x, 0; x') = \delta(x-x')$ since $A(t)$ can depend on $x$.
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 \( m, t, \) and \( t \).

8.4. Evaluation of the path integral for a free particle

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

\[
\int_{x_0}^{x_N} e^{i S[x(t)]/\hbar} \mathcal{D}[x(t)]
\]

where \( \int_{x_0}^{x_N} \mathcal{D}[x(t)] \) symbolizes 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 intervals (see figure).
Then, for a given path \( x(t) = (x_0(t_0), x_1(t_1), x_2(t_2), \ldots, x_N(t_N)) \),
we can replace
\[
S = \int_{t_0}^{t_N} x(t) \, dt = \int_{t_0}^{t_N} \frac{m}{2} \dot{x}^2(t) \, dt \rightarrow \sum_{i=0}^{N-1} \frac{m}{2} \left( \frac{x_{i+1} - x_i}{\Delta t} \right)^2 \Delta t
\]
The propagator thus becomes
\[
U(x_N, t_N; x_0, t_0) = \int_{x_0}^{x_N} e^{i S[x(t)]/\hbar} \, D[x(t)]
\]
\[
= \lim_{N \to \infty} A \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} e^{i m \sum_{i=0}^{N-1} \left( \frac{x_{i+1} - x_i}{\Delta t} \right)^2 / 2 \Delta t}
\]
A must be chosen such that at the end we get the correct dimension for \( U \).

Let us first rescale our \( x \)-variable: \( y_i = x_i \sqrt{m \Delta t} \).

We now want to work out
\[
\lim_{N \to \infty} A' \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} e^{-\sum_{k=0}^{N-1} \frac{(y_{k+1} - y_k)^2}{2i}}
\]
with \( A' = A \left( \frac{2\pi \Delta t}{m} \right)^{N/2} \).

Let us first do the \( y_1 \)-integral. The terms in the sum involving \( y_1 \) are:
\[
\int_{-\infty}^{\infty} e^{-\frac{i}{2} \left( (y_2 - y_1)^2 + (y_1 - y_0)^2 \right)} \, dy_1 = \sqrt{\frac{i \pi}{2}} \, e^{-\frac{(y_2 - y_0)^2}{2i}}
\]
Next the \( y_2 \)-integral:
\[
\int_{-\infty}^{\infty} e^{-\frac{i}{2} \left( (y_3 - y_2)^2 + (y_2 - y_0)^2 \right)} \, dy_2 = \sqrt{\frac{(i \pi)^2}{3}} \, e^{-\frac{(y_3 - y_0)^2}{3i}}
\]
Keeping going we get for the integral over all \( y \):
\[
\sqrt{\frac{(ix)^{N-1}}{N}} \ e^{-\frac{(y_N-y_S)^2}{2N}} = \sqrt{\frac{(ix)^{N-1}}{N}} \ e^{\frac{i}{\hbar} \frac{m}{2} \frac{(y_N-y_S)^2}{t_N-t_0}}
\]

and thus:
\[
U(x_N, t_N; x_0, t_0) = A \left(\frac{2\pi i t \Delta t}{m}\right)^{N/2} \sqrt{\frac{m}{2\pi i t \Delta t}} e^{\frac{i}{\hbar} \frac{m}{2} \frac{(x_N-x_0)^2}{t_N-t_0}}
\]

To get the right answer we must set
\[
A = \left(\frac{2\pi i t \Delta t}{m}\right)^{-N/2} = B^{-N}, \quad B = \sqrt{\frac{2\pi i t \Delta t}{m}}
\]

Conventionally one associates one factor \( 1/B \) with each of the \( N-1 \) integration and the last \( 1/B \) with the overall process:
\[
\int S[x(t)] = \lim_{\Delta t \to 0} \lim_{N \to \infty} \frac{1}{B} \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \cdots \int_{-\infty}^{\infty} dx_{N-1}
\]

where
\[
B = \sqrt{\frac{2\pi i t \Delta t}{m}}
\]

This defines the path integral, and reproduce the correctly normalized result from the QM postulate. The same normalization must now be used for all other cases where the particle is not free.
The Schrödinger equation tells us that, for $\Delta t \to 0$,

$$\langle \Psi(\Delta t) \rangle - \langle \Psi(0) \rangle = -\frac{i\Delta t}{\hbar} \hat{H} \langle \Psi(0) \rangle$$

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

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

Let us compare this with the path integral result,

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

with

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

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

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

So we need to do the integral

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

Since $\Delta t$ is infinitesimal and this small, the first term oscillate 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 0).

The region of coherence is \( \frac{m}{2\pi \Delta t} (x - x')^2 \leq \pi \)
or \[ \left| \gamma \right| = \left| x - x' \right| \leq \sqrt{\frac{2\pi \Delta t}{m}}. \]

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

\[
\Psi(x, \Delta t) = \sqrt{\frac{m}{2\pi i \Delta t}} \int_{-\infty}^{\infty} dy \, e^{\frac{i m}{2 \Delta t} y^2} e^{-\frac{i \Delta t}{\hbar} V(x + \frac{y}{2}, 0)} \Psi(x + y, 0).
\]

Since \( \gamma \) has to be small by the above argument in order to contribute, we can expand \( V \) and \( \Psi \):

\[
\Psi(x + y, 0) = \Psi(x, 0) + \frac{\partial \Psi}{\partial x}(x) + \frac{1}{2} \Psi''(x) + \ldots
\]

\[
e^{-\frac{i \Delta t}{\hbar} V(x + \frac{y}{2}, 0)} = 1 - \frac{i \Delta t}{\hbar} V(x + \frac{y}{2}, 0) + \ldots
\]

We keep all terms up to order \( \Delta t \sim \gamma^2 \) and dropped all smaller terms than that.

So

\[
\Psi(x, \Delta t) = \sqrt{\frac{m}{2\pi i \Delta t}} \int_{-\infty}^{\infty} dy \, e^{\frac{i m y^2}{2 \Delta t}} \left[ \Psi(x, 0) - \frac{i \Delta t}{\hbar} \frac{\partial}{\partial x} V(x, 0) \Psi(x, 0)
\right.

\[
\left. + \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial \Psi}{\partial x} \frac{y^2}{2} \frac{\partial^2 V}{\partial x^2} \right]
\]

Vanishes by symmetric integration.

\[
= \sqrt{\frac{m}{2\pi i \Delta t}} \left[ \Psi(x, 0) \sqrt{\frac{2\pi i \Delta t}{m}} - \frac{i \Delta t}{2\im} \sqrt{\frac{2\pi i \Delta t}{m}} \frac{\partial^2 V}{\partial x^2} \right. 
\]

\[
- \frac{i \Delta t}{\hbar} \sqrt{\frac{2\pi i \Delta t}{m}} V(x, 0) \Psi(x, 0) \right].
\]
\[
\psi(x, \Delta t) - \psi(x, 0) = -\frac{i\Delta t}{\hbar} \left[ -\frac{1}{2m} \frac{\partial^2}{\partial x^2} + V(x, 0) \right] \psi(x, 0)
\]

which agrees with the prediction from the Schrödinger equation.

8.6 Potential of the form \( V(x, \xi) = a + bx + cx^2 + d\xi + e\xi^2 \)

Let us write each path as

\[
\begin{align*}
X(t) &= X_{ce}(t) + y(t), & y(0) = y(t) = 0 \\
\dot{X}(t) &= \dot{X}_{ce}(t) + \dot{y}(t) \\
X_c &= X(t), & \dot{X}(t) = X_{ce}(t) + y(t) = X_{ce}(t) + y(t) \\
dx_c = dy_c, & \int_0^T dx_c(t) = \int_0^T dy_c(t)
\end{align*}
\]

Hence

\[
W(x, t; x', 0) = \int_0^T \mathcal{L}[x, \dot{x}, 0] dt = \int_0^T \dot{S} [x_{ce}(t) + y(t)] dt
\]

Expand the action around its minimum at \( x(t) = x_{ce}(t) \),

\[
\begin{align*}
S[x_{ce} + y] &= \int_0^t \mathcal{L}(x_{ce} + y, \dot{x}_{ce} + \dot{y}) dt = \int_0^t \mathcal{L}(x_{ce}, \dot{x}_{ce}) + \frac{\partial \mathcal{L}}{\partial x} \bigg|_{x_{ce}} y + \frac{\partial \mathcal{L}}{\partial \dot{x}} \bigg|_{x_{ce}} \dot{y} + \frac{1}{2} \left( \frac{\partial^2 \mathcal{L}}{\partial x^2} \bigg|_{x_{ce}} y^2 + 2 \frac{\partial^2 \mathcal{L}}{\partial x \partial \dot{x}} \bigg|_{x_{ce}} y \dot{y} + \frac{\partial^2 \mathcal{L}}{\partial \dot{x}^2} \bigg|_{x_{ce}} \dot{y}^2 \right)
\end{align*}
\]

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 \( \int \hbar \mathcal{H} \mathcal{S} \). The linear pieces \( \chi \) and \( \rho \) vanish due to the classical equation of motion \( \left[ \frac{d}{dt} \frac{\partial \mathcal{H}}{\partial \chi} - \frac{\partial \mathcal{H}}{\partial \chi} \right] = 0 \).

In the last piece, using the assumed form

\[
\mathcal{L} = T - V = \frac{1}{2} m \dot{x}^2 - a - bx - c x^2 - dx - ex x,
\]

we get

\[
\frac{1}{2} \frac{\partial^2 \mathcal{L}}{\partial x^2} = -c \quad \frac{\partial^2 \mathcal{L}}{\partial x \partial t} = -e \quad \frac{1}{2} \frac{\partial^2 \mathcal{L}}{\partial t^2} = m
\]

Hence

\[
\mathcal{U}(x, t, x', t') = \int \mathcal{D}[y(t')] e^{\frac{i}{\hbar} \int_{t'}^{t} \left( \frac{1}{2} m \dot{y}^2 - cy^2 - ey y \right)} A(t) \quad \text{(*)}
\]

\[
= \int \mathcal{D}[y(t')] e^{\frac{i}{\hbar} \int_{t'}^{t} \left( \frac{1}{2} m \dot{y}^2 - cy^2 - ey y \right)} A(t)
\]

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

Since (*) is independent of \( \mathcal{V} \), the same value \( A(t) \) holds for potentials \( V(x) = a + bx \).

For the harmonic oscillator, \( c = \frac{1}{2} m a^2 \), and we must do the integral

\[
A(t) = \int \mathcal{D}[y(t')] e^{\frac{i}{\hbar} \int_{t'}^{t} \left( \frac{m}{2} (\dot{y}^2 - \omega^2 y^2) \right)}
\]

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)