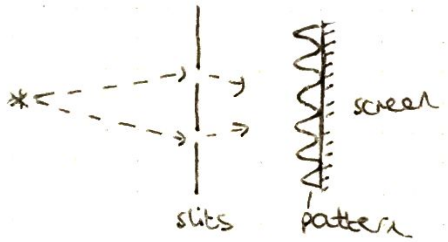
Path Integral Approach to Quantum Mechanics

We saw how using Hamilton's principle in classical mechanics made many problems easier to solve. Feynman developed a similar approach to Quantum Mechanics, which is what this chapter will focus on.

Consider the double slit experiment:



In a classical description the particle goes through only one slit. But in our new description, we will say the particle travels ALL possible paths.

Proposal for Quantum Mechanical Amplitude

Since there is an observed interference pattern, we know that our description will have to contain cancelling and reinforcing phases.

The probability amplitude for a particle to travel from point A to point B is given by:

$$K(B, A) = \text{constant} \times \sum_{\substack{\text{all} \\ \text{paths}}} e^{iS[\text{path}]/\hbar}$$

The probability for a particle to travel from A to B is given by:

$$P(B, A) = |K(B, A)|^2$$

$K(B, A)$ is often called the Quantum Mechanical Kernel.

This approach initially looks a little weird. Every possible path contributes equally up to a phase. What happens in the classical limit?

The Classical Limit

Let's consider a particle with momentum p incident on a hole of radius r. The particle has a de Broglie wavelength $\lambda = \frac{h}{p}$. We know we will only see quantum effects if $\lambda \gtrsim r$. This is why there are no quantum effects if a cricket ball is thrown out of a window. Because h is so small!

So if we take $h \to 0$, we would never see any quantum effects and the theory is now completely classical. Since $\Delta p \, \Delta x \geq \hbar$ (uncertainty principal), if $h \to 0$ then we can know with complete precision both p and x.

If we have a collection of paths:

Even if ΔS is very small, i.e each path is very close to its neighbour, since $h \to 0$ we can say $\Delta S \gg \hbar$

So in the kernel $K(B,A) = \text{constant} \times \sum e^{iS[\text{path}]/\hbar}$, each path will have a <u>very</u> different phase. So each path doesn't give an equal contribution.

The phase points out a direction in the complex plane, so if the phases are random, the sum over all the paths will be <u>0</u>. The only time this isn't true is if we find some paths for which <u>$\Delta S < \hbar$</u>. This is only true around a minimum of S. Thus, in the classical limit, we reproduce Hamilton's principle!

In Quantum theory, the classical trajectory is "smeared" since a particle is equally likely to travel on a neighbouring path provided $\Delta S \leq \hbar$

Wave Functions

Let's see if we can get the wave functions we are used to with this new approach.

We said that we can get the probability that the particle moves from point A to B using the kernel:

$$P(A \to B) = |K(B, A)|^2$$

if the particle was at point A at a time t_A, then it had a wavefunction such that

$$|\psi(t_A)|^2 = \delta(x - x_A) \quad \text{taking point A to be at } (x_A, t_A)$$

and at point $B = (x_B, t_B)$:

$$|\psi(t_B)|^2 = \delta(x - x_B)^2$$

so, provided $t_B > t_A$, $\underline{\psi(x_B, t_B) = K(B, A)}$

If we want the particle to go from point A to point B through another point C:

$$K(B, A, \text{via } C) = \sum_{A \to C} e^{iS_{AC}/\hbar} \cdot \sum_{C \to B} e^{iS_{CB}/\hbar}$$

Note the dot, not add

since $S_{path} = S_{AC} + S_{CB} = \int_0^{t_1} L\,dt + \int_{t_1}^{t_2} L\,dt$

so $K(B, A, \text{via } C) = \text{constant } K(C, A)\, K(B, C)$

if we want to know what $K(B, A)$ is if we allow for every possible path, we simply need to allow C to vary over all possible positions.

We therefore construct the integral:

$$K(B,A) = \text{constant} \int_{-\infty}^{\infty} K(C,A)\, K(B,C)\, dx_c$$

just as we wrote $K(B,A) = \psi(x_B, t_B)$ previously, we can do the same with $K(C,A) = \psi(x_c, t_c)$ so:

$$\psi(x_B, t_B) = \text{constant} \int_{-\infty}^{\infty} \psi(x_c, t_c)\, K(B,C)\, dx_c$$

We have thus derived an expression for the evolution of any wavefunction at some time into the wavefunction at some other time.

We have shown this evolution is controlled by the kernel.

Deriving the Schrödinger Equation

Let's see if we can derive the Schrödinger equation from the path integral expression for the evolution of a wavefunction.

Let's start with a particle with the Lagrangian

$L = \frac{1}{2} m \dot{x}^2 - V(x)$ as we had before.

The path integral expression is:

$$\psi(x', t') = A \int_{-\infty}^{\infty} \psi(x, t)\, K(x', t'; x, t)\, dx$$

Let's divide time into infinitesimal time slices and assume the particle travels in a straight line and at constant speed during each slice.

Now let's think about how the particle has evolved at $t+\Delta t$. We will assume that the particle has not travelled very far such that $x = x' + \Delta x$

$$\psi(x', t+\Delta t) = A\int_{-\infty}^{\infty} K(x', t+\Delta t; x, t)\,\psi(x,t)\,dx$$

Since we are assuming the paths are always straight lines:

$$S_{x\to x'} = \int_{t}^{t+\Delta t} L(x,\dot{x})\,dt$$

$$= L\left(\frac{x+\Delta x}{2}, \frac{x'-x}{2}\right)\Delta t$$

we forego the integral since we are working in an infinitesimal interval.

$$= \left[\frac{1}{2}m\left(\frac{x'-x}{\Delta t}\right)^2 - V\left(\frac{x+\Delta x}{2}\right)\right]\Delta t$$

So our kernel is $K(x', t+\Delta t) = Ae^{i\left[\frac{1}{2}m\left(\frac{x'-x}{\Delta t}\right)^2 - V\left(\frac{x+x'}{2}\right)\right]\frac{\Delta t}{\hbar}}$

So the integral is now:

$$\psi(x', t+\Delta t) = A\int_{-\infty}^{\infty} e^{\frac{i\Delta t}{\hbar}\left[\frac{1}{2}m\left(\frac{x'-x}{\Delta t}\right)^2 - V\left(\frac{x+x'}{2}\right)\right]}\,\psi(x,t)\,dx$$

Let's taylor expand all the terms here with small deviation terms:

$$x - x' = \Delta x$$

$$\psi(x', t+\Delta t) = \psi(x', t) + \Delta t\,\frac{\partial\psi(x',t)}{\partial t} + \dots$$

$$\psi(x,t) = \psi(x',t) + \Delta x\,\frac{\partial\psi(x',t)}{\partial x'} + \frac{(\Delta x)^2}{2}\,\frac{\partial^2\psi(x',t)}{\partial x'^2} + \dots$$

$$e^{-\frac{i\Delta t}{\hbar}V\left(\frac{x+x'}{2}\right)} = 1 - \frac{i\Delta t}{\hbar}V(x') + \dots$$

So now we can consider our integral to different order expansions.

To zeroth order:

$$\psi(x',t) = A\int_{-\infty}^{\infty} \exp\left(\frac{i\,m\Delta x^2}{2\hbar\Delta t}\right)\psi(x',t)\,d(\Delta x)$$

note, summing over all x and summing over all Δx are the same!

the V term has gone since to zeroth order it is just 1

$$\Rightarrow \quad \psi(x',t) = A\left(\frac{2\pi i\hbar\Delta t}{m}\right)^{1/2}\psi(x',t)$$

which means $\boxed{A = \left(\frac{2\pi i\hbar\Delta t}{m}\right)^{-1/2}}$

I recommend you compute the integral yourself to make sure you are confident doing it.

Now let's consider 1st order:

$$\Delta t\,\frac{\partial\psi(x',t)}{\partial t} = A\int_{-\infty}^{\infty} e^{\frac{im\Delta x^2}{2\hbar\Delta t}}\left[\frac{-i\Delta t}{\hbar}V(x')\psi(x',t) + \Delta x\frac{\partial\psi(x',t)}{\partial x'} + \frac{(\Delta x)^2}{2}\frac{\partial^2\psi(x',t)}{\partial x'^2}\right]d(\Delta x)$$

Letting odd terms $\to 0$ and computing remaining terms:

$$\Delta t\,\frac{\partial\psi(x',t)}{\partial t} = -i\frac{\Delta t}{\hbar}V(x')\psi(x',t) + \frac{i\hbar\Delta t}{2m}\frac{\partial^2\psi(x',t)}{\partial x'^2}$$

$$\Rightarrow \quad \frac{\partial\psi(x',t)}{\partial t} = \frac{-i}{\hbar}V(x')\psi(x',t) + \frac{i\hbar}{2m}\frac{\partial^2\psi(x',t)}{\partial x'^2}$$

$$\frac{\hbar}{i}\frac{\partial\psi(x',t)}{\partial t} = -V(x')\psi(x',t) + \frac{\hbar^2}{2m}\frac{\partial^2\psi(x',t)}{\partial x'^2}$$

$$\Rightarrow \quad i\hbar\frac{\partial\psi(x',t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x',t)}{\partial x'^2} + V(x')\psi(x',t)$$

This is Schrödinger's equation! Thus, we have derived the equation using path integrals.

Path Integral for a free Particle

Let's consider a free particle. We will split the trajectory of the free particle into Δt time slices. In this case, the potential $V = 0$.

We worked out previously $K(B, A) = \sqrt{\frac{M}{2\pi i \hbar \Delta t}}\, e^{\frac{i\Delta t}{\hbar}\left[\frac{1}{2}M\left(\frac{x'-x}{\Delta t}\right)^2 - V\left(\frac{x+x'}{2}\right)\right]}$

so in our free particle case:

$$K(x_1, x_0) = \sqrt{\frac{M}{2\pi i \hbar \Delta t}}\, e^{\frac{iM}{2\hbar}\left[\frac{(x_1 - x_0)^2}{\Delta t}\right]}$$

so if we want $x_0 \to x_1 \to x_2$, as with $A \to C \to B$:

$$K(x_2, x_0) = \frac{M}{2\pi i \hbar \Delta t} \int e^{\frac{iM}{2\hbar}\left[\frac{(x_1 - x_0)^2}{\Delta t} + \frac{(x_2 - x_1)^2}{\Delta t}\right]} dx_1$$

$$= \sqrt{\frac{M}{2\pi i \hbar 2\Delta t}}\, e^{\frac{iM}{2\hbar}\left[\frac{(x_2 - x_0)^2}{2\Delta t}\right]}$$

Note the $2\Delta t$'s

Note that this is the same as for one time slice but with the time doubled and distance lengthened ($x_0 \to x_2$ instead of $x_0 \to x_1$)

if we repeat this for n time slices, i.e $x_0 \to x_1 \to x_2 \to \ldots \to x_n$:

$$K(x_n, x_0) = \sqrt{\frac{M}{2\pi i \hbar n \Delta t}}\, e^{\frac{iM}{2\hbar}\left[\frac{(x_n - x_0)^2}{n\Delta t}\right]}$$

$$= \sqrt{\frac{M}{2\pi i \hbar (t_n - t_0)}}\, e^{\frac{iM}{2\hbar}\left[\frac{(x_n - x_0)^2}{(t_n - t_0)}\right]}$$

Thus, we have found the kernel for a free particle.

But what does this mean?

Interpreting the Free Particle Kernel

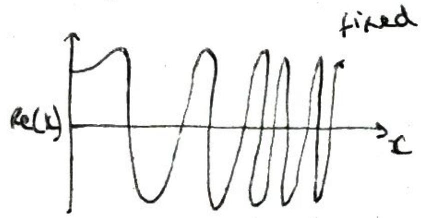
if we set $x_0 = 0$ and $t_0 = 0$ for simplicity, and let $x_n = n$ and $t_n = t$:

$$K(x,t) = \sqrt{\frac{m}{2\pi i \hbar t}}\; e^{\frac{imx^2}{2\hbar t}}$$

we previously stated if the particle started from a dirac delta function at origin (which it has here since $x_0 = 0$), the free particle wavefunction is $\psi(x,t) = K(x,t)$

if we plot the real part of $K(x,t)$:

The wavelength shortens at larger x.



i.e oscillations get closer together

Classically, for a particle to travel a distance x in a time t, $p = m\frac{x}{t}$

In QM, we set the condition $\Delta\text{phase} = 2\pi$ [max phase difference is always 2π]

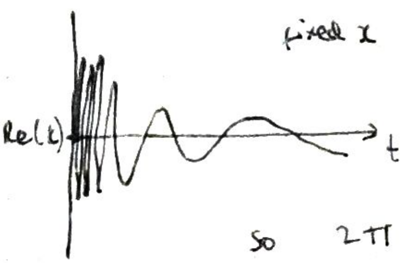
$$= \frac{m(x+\lambda)^2}{2\hbar t} - \frac{mx^2}{2\hbar t}$$

$$\approx \frac{mx\lambda}{\hbar t}$$

so $2\pi = \dfrac{mx\lambda}{\hbar t}$

$$\Rightarrow \lambda = \frac{2\pi\hbar}{mx/t} = \underline{\underline{\frac{h}{p}}}$$ we have extracted de Broglie wavelength

Similarly, if we plot the real part of $K(x,t)$ at fixed x:



again: $\Delta\text{phase} = 2\pi = \dfrac{mx^2}{2\hbar t} - \dfrac{mx^2}{2\hbar(t+T)}$

$$= \frac{mx^2}{2\hbar t}\left(1 - \left(1+\frac{T}{t}\right)^{-1}\right)$$

$$\approx \frac{mx^2}{2\hbar t^2}T$$

so $2\pi = \dfrac{mx^2}{2\hbar t^2}T$

$$\Rightarrow \frac{2\pi}{T} = \omega = \frac{mx^2}{2\hbar t^2} = \frac{1}{2}m\left(\frac{x}{t}\right)^2\frac{1}{\hbar} \Rightarrow \omega = E\frac{1}{\hbar}$$

so $\underline{\underline{E = \hbar\omega}}$ Another known result we found in Quantum Mechanics.

Barrier Problems

Using the kernel for a free particle, we can solve problems that involve particle starting from a point source, passing through a barrier and ending up on a screen.

We take

$$K = C(t)\, e^{\frac{imx^2}{2\hbar t}}$$

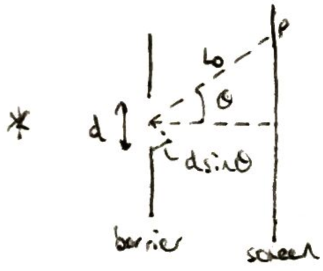
If we assume the source is at infinity, then the distance from source to any point on barrier is the same. So each point on barrier is an equal emitter of particles, so we can sum $e^{iS/\hbar}$ for paths from barrier to screen:

$$K(\text{screen}) = A(t) \int_{\text{barrier}} e^{\frac{imx_{path}^2}{2\hbar t}} f(s)\, ds$$

$A(t)$ is a constant depending on time and $f(s)$ is 0 or 1 depending on if that point on barrier allows particles through. This is useful for diffraction gratings.

Let's do an example with a single slit:

Example - Single Slit



in this case we will assume $d \ll L_0$

The distance between a point on screen and each element of the hole is $L_0 + x\sin\theta$

where $-\frac{d}{2} \le x \le \frac{d}{2}$

so $$K(P,t) = A(t) \int_{-d/2}^{d/2} e^{\frac{im(L_0 + x\sin\theta)^2}{2\hbar t}}\, dx$$

but $L_0 \gg d$ so $$K(P,t) \approx A(t) \int_{-d/2}^{d/2} e^{imL_0^2/2\hbar t}\, e^{i2mL_0 x\sin\theta/2\hbar t}\, dx$$

$$\approx A e^{imL_0^2/2\hbar t} \frac{\hbar t}{imL_0\sin\theta} \left[e^{imL_0 x\sin\theta} \right]_{-d/2}^{d/2}$$

so $K(P,t) \simeq \dfrac{-iA(t)\hbar t e^{imL_0^2/2\hbar t}}{mL_0 \sin\theta} 2\sin\left(\dfrac{mL_0 d\sin\theta}{2\hbar t}\right)$

So the probability of finding the particle at P is:

$$P(x,t) = |K(P,t)|^2 = \frac{|A|^2 \hbar^2 t^2}{m^2 L_0^2 \sin^2\theta} 4\sin^2\left(\frac{mL_0 d\sin\theta}{2\hbar t}\right)$$

$$\simeq \text{constant} \times \frac{\sin^2(\alpha\sin\theta)}{\beta\sin^2\theta}$$

where α and β are constants

Note the minima is when $\dfrac{mL_0 d\sin\theta}{2\hbar t} = n\pi$

$$\Rightarrow d\sin\theta = \frac{2\hbar t}{mL_0} n\pi = n\frac{h}{p} = n\lambda$$

so minima when $\underline{d\sin\theta = n\lambda}$ as we expect.

The Kernel in terms of Wave Functions

In order to switch between Schrödinger equation formalism and path integral formalism, we need an expression for kernel in terms of wave function.

$(*)$

we already know: $\psi(x,t_2) = \displaystyle\int_{-\infty}^{\infty} K(x,t_2;y,t_1)\,\psi(y,t_1)\,dy$

we also know $H\phi_n = E_n\psi_n$ The time independent SE

Using completeness, at time t_1 a wavepacket is:

$$\psi(x,t_1) = \sum_{n=1}^{\infty} c_n\phi_n(x) \quad \text{so} \quad c_n = \int_{-\infty}^{\infty}\phi_n^*(y)\psi(y,t_1)\,dy$$

switch $x \to y$ to show answer does not depend on integration variable

we also know $\psi(x,t_2) = \displaystyle\sum_{n=1}^{\infty} c_n\phi_n(x)e^{-iE_n(t_2-t_1)/\hbar}$ sub this into that

so: $$\psi(x,t_2) = \int_{-\infty}^{\infty}\sum_{n=1}^{\infty}\phi_n(x)e^{-iE_n(t_2-t_1)/\hbar}\,\phi_n^*(y)\,\psi(y,t_1)\,dy$$

compare this to $(*)$ to find:

$$\boxed{K(x,t_2;y,t_1) = \sum_{n=1}^{\infty}\phi_n(x)\phi_n^*(y)e^{-iE_n(t_2-t_1)/\hbar}}$$