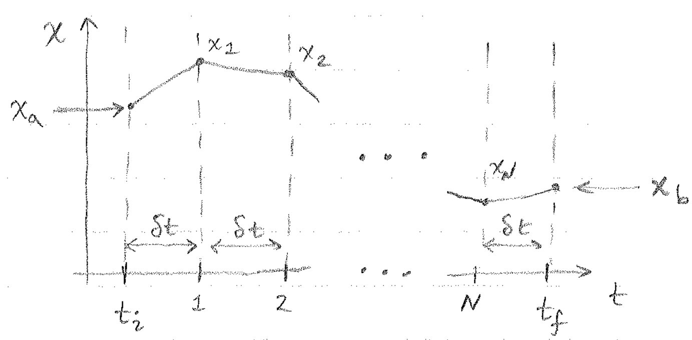
Feynman's Path Integral Formulation of Quantum Mechanics

Consider a 1D one-particle quantum mechanical system governed by the Hamiltonian, $\hat{H}$. The amplitude, $A_{x_a \to x_b}$, for that particle initially $(t = t_i)$ at position $x = x_a$ to be found, at a later time, $(t = t_f)$ at position $x = x_b$ is:

$$A_{x_a \to x_b} = \langle x_b | e^{-\frac{i}{\hbar}\hat{H}(t_f - t_i)} | x_a \rangle \qquad \underline{\text{Quantum Mechanical Kernel}}$$

split $\Delta t = t_f - t_i$ into N intervals

$$= \langle x_b | e^{-\frac{i}{\hbar}\hat{H}\delta t} e^{-\frac{i}{\hbar}\hat{H}\delta t} \cdots e^{-\frac{i}{\hbar}\hat{H}\delta t} | x_a \rangle$$



Insert $\mathbb{1} = \int dx_1 |x_1\rangle\langle x_1|$ between last pair of $e^{-\frac{i}{\hbar}\hat{H}\delta t}$'s.

" $\mathbb{1} = \int dx_2 |x_2\rangle\langle x_2|$ " 2^{nd} to last " " $e^{-\frac{i}{\hbar}\hat{H}\delta t}$'s.

$\vdots$

Insert $\mathbb{1} = \int dx_N |x_N\rangle\langle x_N|$ between first pair of $e^{-\frac{i}{\hbar}\hat{H}\delta t}$'s.

so that

$$A_{x_a \to x_b} = \langle x_b | e^{-\frac{i}{\hbar}\hat{H}\delta t} \int dx_N |x_N\rangle\langle x_N| e^{-\frac{i}{\hbar}\hat{H}\delta t} \cdots e^{-\frac{i}{\hbar}\hat{H}\delta t} \int dx_2 |x_2\rangle\langle x_2| e^{-\frac{i}{\hbar}\hat{H}\delta t}$$
$$\int dx_1 |x_1\rangle\langle x_1| e^{-\frac{i}{\hbar}\hat{H}\delta t} |x_a\rangle$$

Collect integrals, and bring to front.

$$= \int \left(\prod_{i=1}^{N} dx_i \right) \langle x_b | e^{-\frac{i}{\hbar}\hat{H}\delta t} \cdots |x_i\rangle \underbrace{\langle x_i | e^{-\frac{i}{\hbar}\hat{H}\delta t} | x_{i-1}\rangle}_{\text{consider a typical bracket (next pg)}} \langle x_{i-1}| \cdots e^{-\frac{i}{\hbar}\hat{H}\delta t} | x_a \rangle$$

to be contrasted with just N spatial integratio

The amplitude is now a large string $\underline{(N+1)}$ of bra-ket factors of the form $\langle x_i | e^{-\frac{i}{\hbar}\hat{H}\,\delta t} | x_{i-1}\rangle$. Consider one such factor.

Assume $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$.

$$\langle x_i | e^{-\frac{i}{\hbar}\hat{H}\,\delta t} | x_{i-1}\rangle = \langle x_i | e^{-\frac{i}{\hbar}\left(\frac{\hat{p}^2}{2m} + V(\hat{x})\right)\delta t} | x_{i-1}\rangle$$

Apply Baker-Campbell-Hausdorff formula $e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}} e^{[\hat{A},\hat{B}]}$ to split exponential.

$$= \langle x_i | e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\delta t} \, e^{-\frac{i}{\hbar}V(\hat{x})\,\delta t} \, \underbrace{e^{+\frac{1}{2}\frac{1}{2m}[\hat{p}^2, V(\hat{x})]\frac{\delta t^2}{\hbar^2}}}_{\text{Neglect} \sim [1+O(\delta t^2)]|x_{i-1}\rangle} | x_{i-1}\rangle$$

Insert $1 = \int dp\, |p\rangle\langle p|$

(vanishes in continuum limit $\delta t \to 0$)

— Ok if $V(x)$ not too singular (see Trotter's product formula)

$$= \int dp\, \langle x_i | e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\delta t} |p\rangle\langle p| e^{-\frac{i}{\hbar}V(\hat{x})\,\delta t} | x_{i-1}\rangle + O(\delta t^2)$$

$$= \int dp\, \langle x_i | e^{-\frac{i}{\hbar}\frac{p^2}{2m}\delta t} |p\rangle\langle p| e^{-\frac{i}{\hbar}V(x_i)\,\delta t} | x_{i-1}\rangle$$

$$= \int dp\, e^{-\frac{i}{\hbar}\left(\frac{p^2}{2m} + V(x_i)\right)\delta t} \underbrace{\langle x_i | p\rangle}_{\frac{1}{\sqrt{2\pi}} e^{ip.x_i/\hbar}} \underbrace{\langle p | x_{i-1}\rangle}_{\frac{1}{\sqrt{2\pi}} e^{-ip.x_{i-1}/\hbar}}$$

$$= e^{-\frac{i}{\hbar}V(x_i)\delta t} \underbrace{\int \frac{dp}{2\pi}\, e^{\frac{i}{\hbar}\left(-\frac{p^2}{2m}\delta t + p(x_i - x_{i-1})\right)}}_{\text{Evaluate this Gaussian integral (Fresnel's formula)}}$$

$\alpha = \frac{i}{2m}$

$$= e^{-\frac{i}{\hbar}V(x_i)\delta t} \frac{1}{2\pi}\sqrt{\frac{2\pi m \hbar}{i\delta t}}\, \exp\left[i \frac{1}{2} m \frac{(x_i - x_{i-1})^2}{\delta t^2} \right] + O(\delta t^2)$$

Now, plug into original expression for $A_{x_a \to x_b}$: Note the 1 extra momentum integral.

$$A_{x_a \to x_b} = \sqrt{\frac{m}{2\pi i \hbar \delta t}} \prod_{i=1}^{N} \left(\sqrt{\frac{m}{2\pi i \hbar \delta t}} \int dx_i \right) \exp\left[\frac{i}{\hbar} \sum_{i=1}^{N+1} \left(\frac{1}{2} m \frac{(x_i - x_{i-1})^2}{\delta t^2} - V(x_i)\,\delta t \right) \right]$$

correct ✓

with $\left.\begin{aligned} x_{N+1} &\equiv x_b \\ x_0 &\equiv x_a \end{aligned}\right\}$ not to be integrated over.

Apply product to exponent

$$A_{x_a \to x_b} = \sqrt{\frac{m}{2\pi i\hbar\delta t}}^{N+1} \int dx_1 \cdots dx_N \exp\left[\frac{i}{\hbar}\sum_{i=1}^{N+1} \delta t\left(\frac{1}{2}m\frac{(x_i - x_{i-1})^2}{\delta t^2} - V(x_i)\right)\right]$$

Time-sliced action

Take limit $\delta t \to 0$, $N \to \infty$.

$$\sum_i \delta t \to \int dt, \qquad \frac{(x_i - x_{i-1})^2}{\delta t^2} \to \left(\frac{dx}{dt}\right)^2$$

Define $\displaystyle \lim_{N\to\infty} \sqrt{\frac{m}{2\pi i\hbar\delta t}}^{N+1} \int dx_1 \dots dx_N = \int \mathcal{D}x$

Hence, the amplitude is:

$$A_{x_b \to x_a} = \int_{x(t_i)=x_a}^{x(t_f)=x_b} \mathcal{D}x \, \exp\left[\frac{i}{\hbar}\underbrace{\int_{t_i}^{t_f} dt\left(\frac{1}{2}m\left(\frac{dx}{dt}\right)^2 - V(x)\right)}_{\text{Identify as the action, } S.}\right]$$

pure "Configuration form"

$$= \int_{x(t_i)=x_a}^{x(t_f)=x_b} \mathcal{D}x \; e^{iS[x]/\hbar}$$

Discussion:

The path integral gives the matrix element of the time-evolution operator:

$$\int \mathcal{D}x \, e^{iS[x]} = \langle x_b | \hat{U}(t_f, t_i) | x_a \rangle \equiv K(x_a, x_b; t_f - t_i)$$

Quantum mechanical kernel.

And since $-i\hbar \frac{\partial}{\partial t}\hat{U}(t) = \hat{H}\hat{U}(t)$ [Equation of motion],
the quantum mechanical kernel satisfies:

$$-i\hbar\frac{\partial}{\partial t} K(x_a, x_b; t) = \hat{H} K(x_a, x_b; t)$$

n.b: the heat kernel is related to the QM via a Wick rotation.

Canonical Form of Functional Integral

Instead of evaluating the Gaussian integral, immediately plug into original expression for $\mathcal{A}_{x_a \to x_b}$:

$$\mathcal{A}_{x_a \to x_b} = \left(\prod_{i=1}^{N} \int dx_i\right)\left(\prod_{i=1}^{N+1} \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar}\right) e^{\frac{i}{\hbar}\sum_{i=1}^{N+1}\left[p_i(x_i - x_{i-1}) - \left(\frac{p_i^2}{2m} + V(x_i)\right)\delta t\right]}$$

One momentum integral for each of the N+1 bracket factor.

Taking the continuum limit, $N \to \infty$, $\delta t \to 0$, the exponent tends to

$$S[p_i, x_i] = \underbrace{\delta t \sum_{i=1}^{N+1}}_{\to \int dt} \left[\underbrace{\frac{(x_i - x_{i-1})}{\delta t}}_{\to \dot{x}(t)} p_i - \underbrace{\left(\frac{p_i^2}{2m} + V(x_i)\right)}_{= H(p,x)} \right]$$

$$\longrightarrow \int_{t_i}^{t_f} dt \left[\dot{x}(t)p(t) - H\big(p(t), x(t)\big) \right]$$ Canonical Action

The integration measure tends to

$$\to \lim_{N\to\infty} \left(\prod_{i=1}^{N} \int dx_i\right)\left(\prod_{i=1}^{N+1} \int \frac{dp_i}{2\pi\hbar}\right) \overset{\text{"abbr. as"}}{\equiv} \int_{x(t_i)=x_a}^{x(t_f)=x_b} \mathcal{D}x \int_{-\infty}^{+\infty} \frac{\mathcal{D}p}{\text{“}2\pi\hbar\text{”}}$$

So, all together: Hamiltonian/canonical form:

$$\boxed{A_{x_a \to x_b} = \int_{x(t_i)=x_a}^{x(t_f)=x_b} \mathcal{D}x \int \frac{\mathcal{D}p}{\text{“}2\pi\hbar\text{”}} e^{\frac{i}{\hbar}\int_{t_a}^{t_b} dt \left[\dot{x}(t)p(t) - H(p(t), x(t))\right]}}$$

If the Hamiltonian is indeed of the form $H = \frac{p^2}{2m} + V(x)$, the Gaussian integration over $\mathcal{D}p$ can be done by completing the square. The result is

from 1 extra $\int dp$.

$$\mathcal{A}_{x_a \to x_b} = \sqrt{\frac{m}{2\pi i\hbar\delta t}} \left(\prod_{i=1}^{N} \sqrt{\frac{m}{2\pi i\hbar\delta t}} \int dx_i\right) e^{\frac{i}{\hbar}\sum_{i=1}^{N+1} \delta t\left(\frac{1}{2}m\frac{(x_i - x_{i-1})^2}{\delta t^2} - V(x_i)\right)}$$

$$\longrightarrow \int \mathcal{D}x \; e^{\frac{i}{\hbar}\int dt\left[\frac{1}{2}m\dot{x}^2 - V(x)\right]}$$