# 1 Feynman's path integrals in quantum mechanics

Path integrals is a formulation of quantum mechanics where particles move simultaneously along all possible paths with certain probability amplitude.

## 1.1 Time evolution in Schrödinger's wave-mechanics

The time evolution of a quantum system with Hamiltonian $H$ is described by the time dependent Schrödinger equation,

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi\,, \tag{1}$$

with a formal solution

$$\psi = e^{-\frac{i}{\hbar}Ht}\psi_0\,, \tag{2}$$

where $\psi_0 = \psi|_{t=0}$ and

$$e^{-\frac{i}{\hbar}Ht} \equiv U \tag{3}$$

is the time-evolution operator which propagates the system from time zero to time $t$. The operator can be explicitly calculated if all eigenvalues and eigenvectors of the Hamiltonian $H$ are known.

For example, it can be calculated in the case of a free particle with mass $m$ in one dimension, with the free Hamiltonian

$$H_0 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\,. \tag{4}$$

The matrix elements of the free time-evolution operator $U_0 = e^{-\frac{i}{\hbar}H_0 t}$ are given in momentum space as

$$\langle k'|U_0|k\rangle = \delta_{k'k}e^{-i\frac{\hbar k^2}{2m}t}\,, \tag{5}$$

and in coordinate space as

$$\begin{aligned}\langle x'|U_0|x\rangle &= \int\frac{dk}{2\pi}e^{-i\frac{\hbar k^2}{2m}t}e^{ik(x-x')}\\ &= \sqrt{\frac{m}{2\pi i\hbar t}}e^{\frac{i}{\hbar}\frac{m}{2t}(x'-x)^2}\,.\end{aligned} \tag{6}$$

The latter matrix element is the probability amplitude for the particle to propagate (move) from point $x$ at time zero to $x'$ at time $t$.

## 1.2 Time evolution in path integral formulation

In path integral formulation a particle can propagate from an initial position $x$ to the final position $x'$ simultaneously along all possible paths. The amplitude of the probability for the particle to start at $x$ and end up at $x'$ is given as the "path integral",

$$\langle x'|U|x\rangle = \sum_{p\,\in\,\text{paths}} w(p)\; e^{\frac{i}{\hbar}S(p)}\,, \tag{7}$$

where $w(p)$ is a certain weight factor of path $p$ and

$$S(p) = \int_p L dt \tag{8}$$

is the action integral along the path $p$, and $L$ is the Lagrangian of the particle.

Apparently, when $S \gg \hbar$ only the stationary classical path, $\delta S(p) = 0$, gives a non-vanishing contribution to the path integral, which is the obvious limit of classical physics.

The weight factors $w(p)$ depend upon the class of the paths and cannot be written in a general form. The polygonal paths is the usual class of paths considered in path integral formulations of quantum mechanics.

### 1.2.1 Line segment propagator

Any path can be approximated by a sequence of connected line segments forming a broken line path, also called piecewise linear path, or polygonal path.

The weight factor for the line segment propagator can be found e.g. by considering the motion of a free particle along a straight line and comparing the result with (6).

A free one-dimensional particle with mass $m$, coordinate $x$, and velocity $\dot{x}$ has the Lagrangian

$$L(x,\dot{x}) = \frac{m\dot{x}^2}{2}\,. \tag{9}$$

Assuming the particle moves from $x$ to $x'$ along a straight line with constant velocity $\dot{x} = (x'-x)/t$, the action integral along the path in (7) is given as

$$e^{\frac{i}{\hbar}S} = e^{\frac{i}{\hbar}\frac{m}{2}\left(\frac{x'-x}{t}\right)^2 t} = e^{\frac{i}{\hbar}\frac{m}{2t}(x'-x)^2}\,. \tag{10}$$

The exponent is identical to that of the Schrödinger propagator (6). If now the weight factor is chosen as

$$w = \sqrt{\frac{m}{2\pi i\hbar t}}\,, \tag{11}$$

the line segment propagator for the free particle becomes identical to (6).

Generally, if the particle is not free but moves in a potential $V$ with the Lagrangian

$$L(x,\dot{x}) = \frac{m\dot{x}^2}{2} - V(x)\,, \tag{12}$$

the short line propagator can be approximated as

$$we^{\frac{i}{\hbar}S} = \sqrt{\frac{m}{2\pi i\hbar t}}e^{\frac{i}{\hbar}\left(\frac{m}{2t}(x'-x)^2 - V(\frac{x+x'}{2})t\right)}\,. \tag{13}$$

### 1.2.2 Polygonal path formulation

In the polygonal path formulation the time is discretized into $N+1$ equidistant points $t_n = n\Delta t$ where $n = 0 \dots N$ and $\Delta t = t/N$; and the particle is assumed to move from $x = a$ to $x = b$ along a polygon $\{(t_0, a), (t_1, x_1), \dots, (t_N, b)\}$.

Using the obvious composition rule

$$\langle b|U|a\rangle = \int dx \langle b|U|x\rangle\langle x|U|a\rangle \,, \tag{14}$$

the path integral along this polygon can be written as

$$\langle b|U|a\rangle = \tag{15}$$
$$\int dx_1 \sqrt{\frac{m}{2\pi i\hbar\Delta t}} e^{\frac{i}{\hbar}S_1} \int dx_2 \sqrt{\frac{m}{2\pi i\hbar\Delta t}} e^{\frac{i}{\hbar}S_2} \dots$$
$$\int dx_{N-1} \sqrt{\frac{m}{2\pi i\hbar\Delta t}} e^{\frac{i}{\hbar}S_{N-1}} \sqrt{\frac{m}{2\pi i\hbar\Delta t}} e^{\frac{i}{\hbar}S_N}$$

where the short time action is defined using the midpoint rule,

$$S_n = \Delta t L\left(\frac{x_n + x_{n-1}}{2}, \frac{x_n - x_{n-1}}{\Delta t}\right) \tag{16}$$

### 1.2.3 Space discretization

If the space is also discretized into $M$ equidistant points $x_n = x_{\min} + n\Delta x$, where $n = 0 \dots M-1$ and $\Delta x = (x_{\max} - x_{\min})/(M-1)$, the short-time propagator $U(\Delta t)$ becomes a complex matrix with matrix elements

$$\langle x_n|U(\Delta t)|x_{n'}\rangle \equiv U(\Delta t)_{nn'}$$
$$= \sqrt{\frac{m}{2\pi i\hbar\Delta t}}\, e^{\frac{i\Delta t}{\hbar}L\left(\frac{x_n + x_{n'}}{2}, \frac{x_n - x_{n'}}{\Delta t}\right)} \tag{17}$$

and the finite time propagator $U(t)$ becomes a product of short-time propagators,

$$U(t) = \Delta x^{N-1} U(\Delta t)^N. \tag{18}$$

### 1.2.4 Real time propagation and the spectrum of the system

The energy levels can be extracted by a Fourier transform of the trace of the propagator:

$$\mathrm{trace}\big(U(t)\big) = \sum_\nu \langle\nu|e^{-\frac{i}{\hbar}Ht}|\nu\rangle = \sum_\nu e^{-\frac{i}{\hbar}E_\nu t}, \tag{19}$$

where $E_\nu$ and $|\nu\rangle$ are the eigenvalues and eigenfunctions of the system's Hamiltonian,

$$H|\nu\rangle = E_\nu|\nu\rangle \,. \tag{20}$$

### 1.2.5 Imaginary time propagation and eigen-function

Propagation of a random state $|\psi\rangle$ in imaginary time $t = -i\hbar\tau$,

$$U(-i\hbar\tau) = e^{-\tau H} \,. \tag{21}$$

apparently reduces the contributions of excited states and converges to the ground state $|0\rangle$,

$$e^{-\tau H}|\psi\rangle \overset{\tau\to\infty}{\longrightarrow} |0\rangle \,. \tag{22}$$

The trace of the imaginary time propagator is apparently the partition function, with the temperature $T = 1/\tau$,

$$\mathrm{trace}\,(U(-i\hbar\tau)) = \sum_\nu e^{-\tau E_\nu} \,, \tag{23}$$

For small temperatures the system cools down to the ground state $|0\rangle$.