Feynman's Path Integral in Quantum Mechanics

www.maths.tcd.ie/~fionn/notes/pathintegral/

Canonical Quantisation

The mathematical method of quantisation moves one from a classical theory to a quantum theory. There are several ways to do this. One possible prescription is canonical quantisation, which is in some ways advantageous due to its similarity to the axiomatic quantisation of discrete systems.

Consider a classical field $\varphi(\mathbf{x}, t)$ with conjugate momentum

$$\pi(\mathbf{x}, t) = \frac{\partial \mathscr{L}}{\partial(\partial_0 \varphi)}.$$

In quantum field theory, fields are promoted to operators. This is a natural extension in the same vein as position is an operator in quantum mechanics, as fields are simply a promotion of position from classical mechanics. We then impose the canonical commutation relations

$$\left[\varphi(\mathbf{x}, t), \varphi(\mathbf{y}, t)\right] = \left[\pi(\mathbf{x}, t), \pi(\mathbf{y}, t)\right] = 0; \tag{1}$$

$$\left[\varphi(\mathbf{x}, t), \pi(\mathbf{y}, t)\right] = i\delta^{(3)}(\mathbf{x} - \mathbf{y}). \tag{2}$$

Equation 1 preserves causality, while equation 2 is analogous to $[Q_i, P_j] = i\delta_{ij}$.

This approach retains the Hamiltonian form of the classical theory, but it is not without its inadequacies. For example, in equations 1 & 2, space and time are on a different footing. We lose manifest Lorentz symmetry at the expense of viewing our theory through a Hamiltonian lens.

Feynman's Path Integral Formalism

An alternative to canonical quantisation is the path integral, introduced in the mid–20$^{\text{th}}$ century by Richard Feynman.

The path integral uses the Lagrangian formalism, so differential symmetries of the theory are explicit. There are also similarities with statistical mechanics, allowing quantum field theories to draw from the sophisticated technologies of this well-established branch of mathematical physics. This formalism is symmetric in space and time and thus has a moral advantage over canonical quantisation, as it more directly lends itself to a relativistic theory.

Roughly speaking, for some integration measure $\mathscr{D}q$, the path integral describes a propagator $\langle\psi_1|\psi_2\rangle$ as

$$\langle\psi_1|\psi_2\rangle = \int \mathscr{D}q\, e^{\frac{i}{\hbar}S}, \qquad S = \int \mathrm{d}t\, L,$$

where S is the action of the theory. For $S \gg \hbar$, we recover the classical path.

Intuitively, this approach involves a "sum over histories" of the trajectories of the particle we wish to study. It can be thought of as a logical extension of the famous two–slit experiment to an n–slit experiment. Instead of travelling through two slits simultaneously, the particle travels through n distinct paths simultaneously. As $n \to \infty$, there is a contribution of an infinite number of trajectories. This is known as "Feynman's screen".

We wish to evaluate the amplitude for a particle to evolve from an initial position and time q', t' to a final position and time q'', t''.

In the Schrödinger picture, we would write this as

$$\langle q''|\, e^{-iH(t''-t')}\, |q'\rangle$$

where $e^{-iH(t''-t')}$ is the unitary time translation operator from time t' to time t'', H is the Hamiltonian and $|q'\rangle, |q''\rangle$ are eigenstates of the position operator Q.

An equivalent formulation can be made in the Heisenberg picture, in which the time dependence of the system is encoded in the operators. In this picture,

$$Q(t) = e^{iHt} Q e^{-iHt}.$$

As $|q,t\rangle = e^{iHt}|q\rangle$,

$$\begin{aligned} Q(t)\,|q,t\rangle &= e^{iHt} Q e^{-iHt} e^{iHt}\,|q\rangle \\ &= q\,|q,t\rangle. \end{aligned}$$

Then the transition amplitude we so desire can be expressed as

$$\langle q''|\, e^{-iH(t''-t')}\, |q'\rangle = \langle q'', t''|q', t'\rangle\,. \tag{3}$$

To compute this in Feynman's scheme, we divide the time interval into $N+1$ equal steps of duration ε,

$$t'' - t' = (N+1)\varepsilon.$$

By completion,

$$\int_{-\infty}^{\infty} \mathrm{d}q\, |q\rangle\langle q| = \mathbb{1}, \qquad \int_{-\infty}^{\infty} \mathrm{d}p\, |p\rangle\langle p| = \mathbb{1},$$

so we can insert a complete set of eigenstates into equation 3. For position eigenstates $\{|q\rangle\}$, this gives

$$\langle q'', t''|q', t'\rangle = \int_{-\infty}^{\infty} \prod_{j=1}^{N} \mathrm{d}q_j \, \langle q''| e^{-iH\varepsilon} |q_N\rangle\langle q_N| e^{-iH\varepsilon} |q_{N-1}\rangle \cdots \langle q_1| e^{-iH\varepsilon} |q'\rangle.$$

Due to the $e^{-iH\varepsilon}$ term, we must make explicit the form of our Hamiltonian. Take

$$H(P,Q) = \frac{P^2}{2m} + V(Q), \qquad [Q,P] = i. \tag{4}$$

To evaluate the exponential, we first need to exponentiate non-Abelian operators. To do this, we use the Baker–Campbell–Hausdorff (BCH) formula:

$$\exp\big(\lambda\,(A+B)\big) = \exp(\lambda A)\exp(\lambda B)\exp\left(\tfrac{\lambda^2}{2}[A,B]\right)\cdots$$

where $[A,B] \neq 0$ necessarily. Thus, for small ε we can express $e^{-iH\varepsilon}$ as

$$\exp(-iH\varepsilon) \approx \exp\left(-i\tfrac{P^2}{2m}\varepsilon\right)\exp\big(-iV(Q)\varepsilon\big)$$

by neglecting $\mathcal{O}(\varepsilon^2)$ terms. This approximation is valid as we will be taking the limit $\varepsilon \to 0$ later.

Instead of using position eigenstates $\{|q\rangle\}$, we can insert a complete set of momenta $\{|p\rangle\}$. For a small time translation ε between q_1 and q_2, this can now be expressed as

$$\begin{aligned}
\langle q_2| e^{-iH\varepsilon} |q_1\rangle &= \langle q_2| e^{-i\frac{P^2}{2m}\varepsilon} e^{-iV(Q)\varepsilon} |q_1\rangle \\
&= \int \mathrm{d}p_1 \, \langle q_2| e^{-i\frac{P^2}{2m}\varepsilon} |p_1\rangle\langle p_1| e^{-iV(Q)\varepsilon} |q_1\rangle \\
&= \int \mathrm{d}p_1 \, e^{-i\frac{\varepsilon}{2m}p_1^2} e^{-iV(q_1)\varepsilon} \langle q_2|p_1\rangle\langle p_1|q_1\rangle
\end{aligned}$$

and noting that we have plane wave solutions $\langle q_j|p_i\rangle = \frac{1}{\sqrt{2\pi}} e^{ip_iq_j}$,

$$\begin{aligned}
&= \frac{1}{2\pi}\int \mathrm{d}p_1 \, e^{-i\frac{p_1^2}{2m}\varepsilon} e^{-iV(q_1)\varepsilon} e^{ip_1(q_2-q_1)} \\
&= \frac{1}{2\pi}\int \mathrm{d}p_1 \, e^{-iH(p_1,q_1)\varepsilon} e^{ip_1(q_2-q_1)}.
\end{aligned}$$

For $q_0 \equiv q'$, $q_{N+1} \equiv q''$,

$$\langle q'', t''|q', t'\rangle = \frac{1}{2\pi}\int \prod_{j,k=0}^{N} \mathrm{d}q_k \, \mathrm{d}p_j \, e^{ip_j(q_{j+1}-q_j)} e^{-iH(p_j,q_j)\varepsilon}.$$

Defining the integration measure

$$\mathscr{D}p \equiv \prod_{j=0}^{N} \mathrm{d}p_j, \qquad \mathscr{D}q \equiv \prod_{k=0}^{N} \mathrm{d}q_k$$

and taking the formal limit as $\varepsilon \to 0, N \to \infty$, we arrive at

$$\left\langle q'', t'' \middle| q', t' \right\rangle \xrightarrow[N\to\infty]{\varepsilon\to 0} \int \mathscr{D}p\mathscr{D}q \exp\left[i \int_{t'}^{t''} \mathrm{d}t \big(p(t)\dot{q}(t) - H(p,q) \big) \right].$$

In order to interpret this, we need a result from the Riemann–Lebesgue lemma.

Theorem (Riemann–Lebesgue lemma): Let $f : \mathbb{R} \supseteq I \to \mathbb{C}$ be a measurable function. If $f \in L^1$, then

$$\lim_{z\to\pm\infty} \int_I \mathrm{d}x\, f(x) e^{izx} = 0,$$

i.e. rapidly oscillating functions integrate to zero.

We therefore desire the longest wavelengths in our phase, as it is those which will contribute the most to the integral. This provides a natural and fundamental quantum mechanical motivation for Hamilton's principle of least action. Extremising the phase,

$$\frac{\partial}{\partial p}(p\dot{q} - H) = 0 \quad \Rightarrow \quad \dot{q} = \frac{\partial H}{\partial p} \quad \Rightarrow \quad p = p(\dot{q})$$

and

$$\frac{\partial}{\partial p} i \int \mathrm{d}t (p\dot{q} - H) = 0 \quad \Rightarrow \quad i \int \mathrm{d}t \frac{\partial}{\partial p}(p\dot{q} - H) = 0.$$

We can thus remove the $\mathscr{D}p$ measure, and

$$\begin{aligned} \left\langle q'', t'' \middle| q', t' \right\rangle &= \int \mathscr{D}q \exp\left[i \int_{t'}^{t''} \mathrm{d}t\, (p\dot{q} - H) \right] \\ &= \int \mathscr{D}q \exp\left[i \int_{t'}^{t''} \mathrm{d}t\, L(q, \dot{q}) \right] \\ &= \int \mathscr{D}q\, e^{iS} = Z \end{aligned} \tag{5}$$

by Legendre transformation. Equation 5 is the path integral.

The Green function in quantum mechanics is given by

$$G_{1,2,\ldots,n}(t_1, t_2, \ldots, t_n) = \langle 0 | \, T Q_1(t_1) Q_2(t_2) \cdots Q_n(t_n) \, | 0 \rangle,$$

where T is the time ordering operator and $|0\rangle$ is the vacuum state. The path integral allows us to write this as

$$\begin{aligned}\langle 0|\, T Q_1(t_1) Q_2(t_2)\cdots Q_n(t_n)\,|0\rangle &= \frac{\int \mathscr{D}q\, q_1(t_1) q_2(t_2)\cdots q_n(t_n) e^{iS}}{\int \mathscr{D}q\, e^{iS}} \\ &= \frac{1}{Z}\int \mathscr{D}q\, q_1(t_1) q_2(t_2)\cdots q_n(t_n) e^{iS}.\end{aligned}$$

In general, we will assume that our operators $\varphi(x_i)$ are time ordered ($t_1 > t_2 > \cdots > t_n$) and omit the T operator from the Green function.

The Wick Rotation

In anticipation of the lattice, we will re-express the path integral in imaginary time. This is done by rotating time through $\frac{\pi}{2}$ in the complex plane $\mathbb{C}$.

$$t \to -i\tau, \qquad x^0 \to -ix^4.$$

Under a Wick rotation, the Minkowski invariant line element

$$\mathrm{d}s^2 = \mathrm{d}t^2 - \mathrm{d}x^2 - \mathrm{d}y^2 - \mathrm{d}z^2$$

becomes

$$\mathrm{d}s^2 = -\mathrm{d}x^2 - \mathrm{d}y^2 - \mathrm{d}z^2 - \mathrm{d}\tau^2.$$

In other words, it gains a Euclidean signature. When Minkowski spacetime is rotated in this way, we end up in Euclidean spacetime: $M^{1,3} \to \mathbb{R}^4$. This naturally affects differential operators. The d'Alembertian operator becomes

$$\Box = \sum_{\mu=1}^{4} \partial_\mu \partial_\mu = \partial_\mu \partial_\mu,$$

the Laplacian $\triangle$ in four dimensions.

For the Hamiltonian given by equation 4,

$$S = \int \mathrm{d}t\, \left[\frac{1}{2m}\left(\frac{\mathrm{d}q}{\mathrm{d}t}\right)^2 - V\right], \quad S_E = \int \mathrm{d}\tau\, \left[\frac{1}{2m}\left(\frac{\mathrm{d}q}{\mathrm{d}\tau}\right)^2 + V\right]$$

where S_E is the Minkowski action rotated into Euclidean space. Thus,

$$iS \to -S_E. \tag{6}$$

Wick rotating our path integral of equation 5, we get the expression

$$Z = \int \mathscr{D}q\, e^{iS} \to Z_E = \int \mathscr{D}q\, e^{-S_E}$$

In this form, we may deduce the principle of least action without the allusion to harmonic analysis, as it is obvious that the smallest values of S will contribute the most to Z. Thus $\delta S = 0$ recovers the equations of motion in the classical limit. We have restricted our Hamiltonian to the form of equation 4, however operation 6 ($iS \to -S_E$) remains valid for Lagrangians which are not quadratic in velocities (such as those appearing in fermionic systems).

The Path Integral for Quantum Field Theory

So far, we have developed the path integral only within the context of discrete systems, i.e. quantum mechanics. This leaves a lot to be desired—specifically, we desire a field theoretic path integral.

To translate into a system with infinite degrees of freedom, we make the following substitutions:

$$q^i(t) \to \varphi(\mathbf{x}, t), \qquad Q^i(t) \to \varphi(\mathbf{x}, t),$$

$$\mathscr{D}q \to \mathscr{D}\varphi = \prod_x \mathrm{d}\varphi(x).$$

This allows us to express a scalar field in terms of the path integral,

$$Z = \int \mathscr{D}\varphi\, e^{iS}. \tag{7}$$

Then, the Green function for some points in spacetime $x_1, x_2, \ldots, x_n$ is

$$\begin{aligned} G(x_1, x_2, \ldots, x_n) &= \langle 0|\, T\varphi(x_1)\varphi(x_2)\cdots\varphi(x_n)\,|0\rangle \\ &= \frac{\int \mathscr{D}\varphi\, \varphi(x_1)\varphi(x_2)\cdots\varphi(x_n) e^{iS}}{\int \mathscr{D}\varphi\, e^{iS}} \\ &= \frac{1}{Z}\int \mathscr{D}\varphi\, \varphi(x_1)\varphi(x_2)\cdots\varphi(x_n) e^{iS}. \end{aligned}$$

Notationally, this is often expressed as $\langle \varphi(x_1)\varphi(x_2)\cdots\varphi(x_n)\rangle$. Wick rotating,

$$\langle \varphi(x_1)\varphi(x_2)\cdots\varphi(x_n)\rangle = \frac{1}{Z_E}\int \mathscr{D}\varphi\, \varphi(x_1)\varphi(x_2)\cdots\varphi(x_n) e^{-S_E}$$

where x_i now represent points in Euclidean spacetime.

The Path Integral is Well-Defined on the Lattice

What does the path integral (7) mean? We are integrating over an infinite number of degrees of freedom, which leads us to a modern ultraviolet catastrophe—the integral is not well defined.

In order to force the integral to converge, we could introduce a momentum cut-off. However, for a divergent Feynman integral, such a regularised integral would be strongly dependent on the value of the cut-off. This would be accounted for by renormalising the Green functions such that they converge as the cut-off is lifted, which requires the bare parameters of the theory to be dependent on the cut-off.

A different approach uses the lattice as a regulator of quantum field theory. Discretising spacetime means there are no longer an infinite number of degrees of freedom, so the path integral in lattice spacetime is not divergent. Then the continuum limit is taken to bring us back to reality. This works, as the lattice presents a natural momentum cut-off since, for $x = na$ a point on the lattice, a function $f \in L^2$ has a Fourier transformation

$$f(na) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k\, \tilde{f}(k) e^{ikna}$$

where $\tilde{f}$ is cyclic in momentum, i.e. $\tilde{f}(-\frac{\pi}{a}) = \tilde{f}(\frac{\pi}{a})$. This means the momentum integral is restricted to the $[-\frac{\pi}{a}, \frac{\pi}{a}]$ Brillouin zone and $\tilde{f}(k)$ has a Fourier series representation. This cuts off the momentum at the order of a^{-1}, so the path integral is well defined on the lattice.