Principle of least action and Feynman path integral formulation

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Abstract: In this paper, we presents the Feynman's path integral formulation and its classical analogy to the least action principle. Feynman's path integral is an alternate to the Schrodinger's formulation to quantum mechanics. We also show the equivalence of both these formulations of quantum mechanics.

1. Introduction

While the Schrodinger's formulation of quantum mechanics is analogous to Hamiltonian mechanics, the Feynman path integral formulation in analogous to Lagrangian mechanics. Therefore, we must first revisit the Least Action Principle in Lagrangian Mechanics.

1.1. Principle of least action

In Lagrangian mechanics, we define a quantity called the "action" which is given by the time integral of the Lagrangian :

$$S = \int L dt$$

The least action principle says that a particle will follow a path in space and time for which the action will be minimized. Therefore, to figure out the trajectory of the particle, we must set the derivative of the action to zero: To take the derivative of the action, we use calculus of variations:

$$\delta S = 0$$

$$S = \int L(x, \dot{x}) dt$$

$$\delta S = \int dt \left(\frac{\partial L}{\partial x} \delta x + \frac{\partial L}{\partial \dot{x}} \delta \dot{x} \right)$$

$$\delta S = \int dt \left(\frac{\partial L}{\partial x} \delta x - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \delta x \right) + \left. \frac{\partial L}{\partial \dot{x}} \delta x \right|_{endpoints}$$

$$\text{But, } \left. \frac{\partial L}{\partial \dot{x}} \delta x \right|_{endpoints} = 0$$

$$\therefore \delta S = \int dt \left(\frac{\partial L}{\partial x} \delta x - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \delta x \right) = 0$$

$$\text{But } \delta x \neq 0$$

$$\therefore \frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} = 0$$

This equation gives the trajectory which satisfies the least action principle.

1.2. Historical Remarks and Motivation

In 1933, Dirac observed that action plays no role in quantum mechanics known at that time. He then speculated that the propagator in quantum mechanics could be $exp(\frac{iS}{\hbar})$ where S is the action evaluated along the path.
In 1948, Feynman derived the path integral formulation of quantum mechanics based on Dirac's idea. Feynman defined the propagator to be the sum over all possible paths between the initial and final points, and the contribution of each path will be $exp(\frac{iS}{\hbar})$.
A natural question that arises is, "Why do we need a new formulation?". Feynman himself answered this question in his original paper in which he proposed path integral formulation:

The formulation is mathematically equivalent to the more usual formulations. There are, therefore, no fundamentally new results. However, there is a pleasure in recognizing old things from a new point of view. Also, there are problems for which the new point of view offers a distinct advantage. In addition, there is always the hope that the new point of view will inspire an idea for the modification of present theories, a modification necessary to encompass present experiments. - R. P. Feynman, Space-time approach to non-relativistic quantum mechanics, 1948

1.3. The Fundamental Question in Quantum Mechanics

The fundamental question that we want to answer in quantum mechanics is, given an initial state of a particle $|\Psi(0)\rangle$, and the potential in which the particle resides, how do calculate the time evolution of the state, $|\Psi(t)\rangle$.
The Schrodinger Picture gives a well-established solution tho this question:

$$|\psi(t)\rangle = \sum_{n=0}^{n=\infty} \exp\left[-iE_n t/\hbar\right] \langle n|\psi\left(t_0\right)\rangle |n\rangle$$

where $|n\rangle$ is the eigenspectrum of the Hamiltonian.
But, in the path integral formulation, we directly find the propagator which relates the present state of the particle with all future states.

2. Calculations

We know now, that by finding the propagator we have, in principle, answered the fundamental question in quantum mechanics.

2.1. Deriving the Propagator

Let the propagator be $K\left(x', x, t\right)$. We define this propagator as:

$$K\left(x', x, t\right) \equiv \left\langle x' \left| e^{-\frac{i}{\hbar}Ht} \right| x \right\rangle$$

By definition, the propagator acts on the initial state of the particle to give the final state. So the propagator acting on the initial state would give us the time evolved state.

$$\therefore \Psi\left(x', t\right) = \left\langle x' \left| e^{-\frac{i}{\hbar}Ht} \right| \psi(0) \right\rangle$$

We know that, $\displaystyle\int dx\, |x\rangle\langle x| = 1$
We can use this relation to change the basis. So we get,

$$\Psi\left(x', t\right) = \int dx \left\langle x' \left| e^{-\frac{i}{\hbar}Ht} \right| x \right\rangle \langle x|\psi(0)\rangle$$

But we also know that, $\left\langle x' \left| e^{-\frac{i}{\hbar}Ht} \right| x \right\rangle$ is just the propagator $K(x', x, t)$. Therefore, on substituting, we get,

$$\Psi(x', t) = \int dx K(x', x, t) \psi(x, t = 0)$$

The above equation says that, by knowing the propagator, we can find the wavefunction at any future instant. Therefore, knowing the propagator solves our fundamental question in quantum mechanics. Knowing the propagator is also equivalent to knowing the complete solution of the Schrodinger equation which is proven rigorously in Section 2.2.

Now, let $|n\rangle$and$|n'\rangle$ be energy eigenstates. Since, the spectrum of energy is discrete, we know that,

$$\sum_n |n\rangle\langle n| = 1 \text{ and } \sum_{n'} |n'\rangle\langle n'| = 1$$

Therefore, by using the above relations,

$$K(x', x, t) = \sum_{n', n} \langle x'|n'\rangle \left\langle n' \left| e^{-\frac{i}{n}Ht} \right| n \right\rangle \langle n|x\rangle$$

But, $\left\langle n' \left| e^{-\frac{i}{n}Ht} \right| n \right\rangle = e^{\frac{-i}{\hbar}Ht} \langle n'|n\rangle \quad = e^{-\frac{i}{\hbar}Ht}\delta_{nn'}$

Because of the $\delta_{nn'}$ term the summation over n, n' reduces to just a summation over n, and we replace n' by n.

$$K(x', x, t) = \sum_n e^{-\frac{i}{\hbar}E_n t} \langle x'|n\rangle \langle n|x\rangle$$

Now, $\langle x'|n\rangle = \psi_n^\dagger(x')$, the complex conjugate of the n-th wavefunction in the x' basis.
And, $\langle n|x\rangle = \psi_n(x)$

$$\therefore K(x', x, t) = \sum_n e^{-\frac{i}{n}E_n t} \psi_n^\dagger(x') \psi_n(x)$$

This is called the "spectral representation" of the propagator.

Now, we slice the time t into N parts, i.e. we write $t = \left(\frac{t}{N}\right) N$

$$\therefore K(x', x, t) = \left\langle x' \left| \left(e^{-\frac{i}{\hbar}H\left(\frac{t}{N}\right)}\right)^N \right| x \right\rangle$$

$$\therefore K(x', x, t) = \left\langle x' \left| \left(e^{-\frac{i}{\hbar}H\left(\frac{t}{N}\right)}\right) \cdot \left(e^{-\frac{i}{\hbar}H\left(\frac{t}{N}\right)}\right) \cdots \left(e^{-\frac{i}{\hbar}H\left(\frac{t}{N}\right)}\right) \right| x \right\rangle$$

We now use the fact that, $\int dx\,|x_1\rangle\langle x_1| = 1;\ \int dx\,|x_2\rangle\langle x_2| = 1;\ \cdots\ \int dx\,|x_{N-1}\rangle\langle x_{N-1}| = 1$

$$= \iint \ldots \int dx_{N-1} \cdots dx_1 \left\langle x' \left| e^{-\frac{i}{\hbar}H\frac{t}{N}} \right| x_{n-1} \right\rangle \left\langle x_{N-1} \left| e^{-\frac{i}{\hbar}H\frac{t}{N}} \right| x_{N-2} \right\rangle \cdots \left\langle x_1 \left| e^{-\frac{i}{\hbar}H\frac{t}{N}} \right| x \right\rangle$$

We now want to insert momentum states into our expression for the propagator because they will help us eliminate all operators from the expression which is what we intent to do.

$$= \int dx_{N-1} \cdots dx_1 \int dp_{N-1} \cdots dp_0 \, \langle x'|p_{N-1}\rangle \left\langle p_{n-1} \left| e^{-\frac{i}{\hbar}H\left(\frac{1}{N}\right)} \right| x_{n-1} \right\rangle \langle x_{n-1}|p_{n-2}\rangle \ldots$$

The reason we are doing this, is that the Hamiltonian is in terms of the position and momentum, therefore by acting the Hamiltonian on the eigenstates of position and momentum we will be get rid of all operators and be left with just numbers!
We also know that, $\langle x|p\rangle = \dfrac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}px}$ and $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$

$$= \int dx_{N-1} \cdots dx_1 \int dp_{N-1} \cdots dp_0 \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}P_{N-1}x'} \left\langle p_{N-1} \left| e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\frac{t}{N}} e^{-\frac{i}{\hbar}v(\hat{x})\frac{t}{N}} \right| x_{N-1} \right\rangle \langle x_{N-1}|p_{N-2}\rangle \cdots$$

$$\text{Now, } \left(e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\frac{t}{N}}\right) \text{ will act on } \langle p_{N-1}|, \text{ and } \left(e^{-\frac{i}{\hbar}v(\hat{x})\frac{t}{N}}\right) \text{ will act on } |x_{N-1}\rangle$$

Now we have an exponential of operators acting on their eigenstates, So we must first understand what that means

$$\begin{aligned} e^{\hat{A}}|a\rangle &= \left(1 + \hat{A} + \frac{1}{2}\hat{A}A^{\dagger} \ldots\right)|a\rangle \\ &= \left(1 + a + \tfrac{1}{2}a^2 + \ldots\right)|a\rangle \\ &= \mathrm{e}^{a}|a\rangle \end{aligned}$$

Therefore, using the above results:

$$= \int dx_{N-1} \cdots dx_1 \int d_{p_{N-1}} dp_0 \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}p_{N-1}-x'} e^{-\frac{i}{\hbar}\frac{p_{N-1}^2}{2m}\left(\frac{t}{N}\right)} e^{-\frac{i}{\hbar}v(x_{N-1})\left(\frac{t}{N}\right)} \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar}p_{N-1}x_{N-1}} \ldots$$

$$= \int dx_{N-1}dx_1 \int dp_{N-1} \ldots d_{p_0} \frac{1}{2\pi\hbar} e^{\frac{i}{\hbar}p_{N-1}\left(x'-x_{N-1}\right)} e^{-\frac{i}{\hbar}V(x_{N-1})\left(\frac{t}{N}\right)} e^{-\frac{i}{\hbar}\frac{p_{N-1}^2}{2m}\left(\frac{t}{N}\right)} \ldots$$

Now, lets just consider one of the momentum integrals:

$$\int dp_{N-1} \frac{1}{2\pi\hbar} \exp\left(-\frac{i}{\hbar}\frac{p_{N-1}^2}{2m}\left(\frac{t}{N}\right) + \frac{i}{\hbar}P_{N-1}\left(x' - x_{N-1}\right)\right)$$

$$\text{Let } t \equiv -i\tau \quad \text{and } \tfrac{\tau}{N} = \Delta\tau$$

$$= \int_{-\infty}^{\infty} d_{p_{N-1}} \frac{1}{2\pi\hbar} \exp\left(-\frac{i}{\hbar}\frac{p_{N-1}^2}{2m}\left(\frac{t}{N}\right) + \frac{i}{\hbar}P_{N-1}\left(x' - x_{N-1}\right)\right)$$

$$= \int_{-\infty}^{\infty} dp_{N-1} \frac{1}{2\pi\hbar} \exp\left(-\frac{\Delta\tau}{\hbar}\frac{p_{N-1}^2}{2m} + \frac{i}{\hbar}p_{N-1}\left(x' - x_{N-1}\right)\right)$$

$$= \frac{1}{2\pi\hbar} \exp\left(\frac{-m}{2\hbar}\frac{\left(x' - x_{N-1}\right)^2}{\Delta\tau}\right)\sqrt{\frac{2m\hbar}{\Delta\tau}} \underbrace{\int due^{-u^2}}_{\sqrt{\pi}}$$

$$\text{Where, } u = \sqrt{\frac{\Delta\tau}{2m\hbar}}\left(p_{N-1} - \frac{im}{\Delta\tau}\left(x' - x_{N-1}\right)\right)$$
$$\therefore du = \sqrt{\tfrac{\Delta\tau}{2m\hbar}}dp_{N-1}$$

$$\text{So, } \int dp_{N-1} \frac{1}{2\pi\hbar} \exp\left(-\frac{i}{\hbar}\frac{p_{N-1}^2}{2m}\left(\frac{t}{N}\right) + \frac{i}{\hbar}P_{N-1}\left(x' - x_{N-1}\right)\right) =$$
$$\frac{m}{\sqrt{2\pi\hbar\Delta\tau}} \exp\left(-\frac{m}{2\hbar}\frac{\left(x' - \frac{x_{N-1}}{\Delta\tau}\right)^2}{\Delta\tau}\right)$$

We repeat this N times and substitute it back into our equation for the propagator.

$$K(x', x, t) = \int dx_{N-1} \cdots x_1 \left(\frac{m}{2\pi\hbar\Delta\tau}\right)^{N/2} \exp\left(\frac{-m}{2\hbar}\frac{\left(x' - x_{N-1}\right)^2}{\Delta\tau} - \frac{\Delta\tau}{\hbar}V\left(x_{N-1}\right)\right)\cdots$$

Substituting back $\Delta\tau = i\Delta t$

$$= \int dx_{N-1} \cdots \cdot dx_1 \left(\frac{mN}{2\pi i\hbar\Delta t}\right)^{N/2} \exp\left(\frac{i\Delta t}{\hbar}\left[\frac{m}{2}\frac{\left(x' - x_{N-1}\right)^2}{\Delta t^2} - V\left(x_{N+1}\right)\right]\right)$$

$$\boxed{K(x', x, t) = \left\langle x' \middle| e^{-\frac{i}{\hbar}Ht} \middle| x \right\rangle = \lim_{N\to\infty} \left(\frac{mN}{2\pi i\hbar\Delta t}\right)^{N/2} \int \prod_{i=1}^{N-1} \exp\left(\frac{i}{\hbar}\Delta t\left[\underbrace{\frac{m\left(x_{i+1} - x_i\right)^2}{2\Delta t^2} - V\left(x_i\right)}_{Lagrangian}\right]\right)}$$

This is the propagator.
This is also written in shart hand notation as :

$$K(x', x, t) = \int Dx(t)e^{\frac{i}{\hbar}S} \text{ where S is the action.}$$

2.2. Equivalence to the Schrodinger Picture

Consider an initial state $|\Psi(x_0, t_0)\rangle$, after some time α, and at some position γ away, the state can be described as follows.

$$|\Psi(x_0, t_0 + \alpha)\rangle = \int_{-\infty}^{\infty} d\gamma |\Psi(x_0 + \gamma, t_0 + \alpha)\rangle K(x_0 + \gamma, \alpha; x_0) \qquad \text{....... equation 1}$$

Particles velocity is $\approx \frac{\gamma}{\alpha}$

And its position is $\approx x + \frac{\gamma}{2}$

So the propagator is,

$$K\left(x_0+\gamma,\alpha;x_0\right)=A(\alpha)\exp\left[\frac{i}{\hbar}\int_0^\alpha dt\left(\frac{m}{2}\dot{x}(t)^2-V(x(t))\right)\right]$$

$$\approx A(\alpha)\exp\left[\frac{i}{\hbar}\left(\frac{m}{2\alpha}\gamma^2-V\left(x_0+\frac{\gamma}{2}\right)\alpha\right)\right]$$

Now we expand the quantities in the propagator expression in a power series of α and γ.

$$\frac{i\alpha}{\hbar}\exp\left[-V\left(x_0+\frac{\gamma}{2}\right)\right]=1-\frac{i\alpha}{\hbar}V\left(x_0+\frac{\gamma}{2}\right)+\ldots$$

$$V\left(x_0+\frac{\gamma}{2}\right)=V\left(x_0\right)+\gamma\frac{d}{d\gamma}V\left(x_0\right)+\ldots$$

We also expand $|\Psi(x_0+\gamma,t_0)\rangle$ around x_0.

$$|\psi\left(x_0+\gamma,t_0\right)\rangle=|\psi\left(x_0,t_0\right)\rangle+\gamma\frac{d\,|\psi\left(x_0,t_0\right)\rangle}{dx}+\frac{1}{2}\gamma^2\frac{d^2\,|\psi\left(x_0,t_0\right)\rangle}{dx^2}+\ldots$$

Substituting these approximations back into equation 1.

$$|\psi\left(x,t_0+\alpha\right)\rangle=A(\alpha)\left[1-\frac{i\alpha}{\hbar}V\left(x_0\right)\right]\int_{-\infty}^{\infty}d\gamma\left[|\psi\rangle+\frac{1}{2}\gamma^2\frac{d^2|\psi\rangle}{dx^2}\right]\exp\left[\frac{i}{\hbar}\frac{m}{2\alpha}\gamma^2\right]$$

Evaluating this Gaussian Integral gives us,

$$|\psi\left(x_0,t_0+\alpha\right)\rangle=A(\alpha)\sqrt{\frac{2\hbar\pi\alpha}{im}}\left[1-\frac{i\alpha}{\hbar}V\left(x_0\right)+\frac{\hbar\alpha}{2mi}\frac{d^2}{dx^2}\right]|\psi\left(x_0,t_0\right)\rangle$$

For small values of α the first term on the right must be equal to $|\psi(x_0,t_0+\alpha)\rangle$,
$\therefore A(\alpha)=\sqrt{\frac{m}{2i\hbar\pi\alpha}}$
We can rearrange the above equation and take limit $\alpha\to 0$, So we have
$\lim_{\alpha\to 0} i\frac{|\psi(x_0,t_0+\alpha)\rangle-|\Psi(x_0,t_0)\rangle}{\hbar\alpha}=i\hbar\frac{d}{dt}\Psi(x,t_0)$

Therefore, we get the Schrodinger equation starting from the path integral formulation.

$$i\hbar\frac{d}{dt}\,|\psi\left(x,t_0\right)\rangle=\left(V\left(x_0\right)-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)|\psi\left(x_0,t_0\right)\rangle$$

Hence the Schrodinger's picture and the path integral formulation are equivalent.

2.3. The Free Particle

Let $x(t)$ describe a trajectory from (x_a,t_a) to (x_b,t_b). We consider many intermediate points as $(x_1,t_1),(x_2,t_2)\cdots(x_{N-1},t_{N-1})$. Also, since V(x)=0, the action between the interval t_i and t_{i+1} is given by,

$$S_i = \int_{t_i}^{t_{i+1}} \frac{m}{2}\dot{x}(t)^2 dt = \frac{m}{2}\left(\frac{x_{i+1}-x_i}{t_{i+1}-t_i}\right)^2 (t_{i+1}-t_i) = \frac{m}{2\Delta t}\left(x_{i+1}-x_i\right)^2$$

We then sum over all the possible paths.

$$\langle \Psi\left(x_N, t_N\right) | \Psi\left(x_0, t_0\right)\rangle = A(t)\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} \exp\left[\frac{i}{\hbar}\frac{m}{2\Delta t}\sum_{i=1}^{N}\left(x_i^2 - x_{i-1}^2\right)\right] dx_1 \cdots dx_{N-1}$$

We now perform the integrations one by one.

Let, $k = \frac{im}{2\hbar\Delta t}$

$$\int_{-\infty}^{\infty} \exp\left[k\left(x_2^2 - x_1^2\right) + k\left(x_1^2 - x_0^2\right)\right] dx_1 =$$

$$\int_{-\infty}^{\infty} \exp\left[2kx_1^2 + kx_1(-2x_2 - 2x_0) + k(x_2^2 + x_0^2)\right] dx_1$$

$$= \frac{\sqrt{\pi}}{\sqrt{2}\sqrt{k}} \exp\left[\frac{k}{2}\left(x_2 - x_0\right)^2\right]$$

We then observe a pattern that after n integrations a factor of $\frac{k}{n+1}(x_N - x_0)^2$ appears in the exponent.

$$K(x_N, t_N; x_0, t_0) = A(t_N - t_0)\exp\left[\frac{k}{N}(x_N - x_0)^2\right]$$

$$K(x, t; x_0) = A(t)\exp\left[\frac{im}{2t\hbar}(x - x_0)^2\right]$$

After Normalizing,

$$K(x, t; x_0) = \sqrt{\frac{m}{2\pi i\hbar t}}\exp\left[\frac{im}{2t\hbar}(x - x_0)^2\right]$$

3. Discussion

The Feynman path integral approach is richer in application, scope and rigor. One can introduce all of quantum theory from this perspective. Path integral formulation naturally leads to an investigation of the Aharanov-Bohm effect, and one can do stationary perturbation theory using Feynman kernels. It has connections to Green Functions and one can demonstrate the use of path integrals in quantum field theory.
We started our formulation of quantum mechanics from the principle that a particle takes no well defined trajectory between two points at which it is observed, we define the transition probability amplitude between two points as a summation over all paths. Then, we connect the contribution to the amplitude from any given path with the corresponding classical action along the path in the manner suggested by Dirac. We have derived the free particle propagator in a way that fully demonstrates the integrate over all possible paths principle. Though our analysis has been brief, and with less emphasis on straightforward rigor than on pragmatism, it is clear that the scope and success of Feynmans method is truly remarkable.

4. Conclusion

The path integral formulation is a description of quantum theory that generalizes the action principle of classical mechanics. It replaces the classical notion of a single, unique classical trajectory for a system with a sum, over an infinity of quantum mechanically possible trajectories to compute amplitude of wavefunction. This formulation has proven crucial to the subsequent development of theoretical physics, because unlike other methods, the path integral allows one to easily change coordinates between very different canonical descriptions of the same quantum system. Another advantage is that it is in practice easier to guess the correct form of the Lagrangian of a theory than the Hamiltonian. One of the biggest advantages of the Path integral formulation is that it can easily be extended to quantum gravity and relativistic cases, as they require just a change in the expression of Lagrangian. All in all, one can say that the Path integral formulation is a much more fundamental and intuitive way to understand and develop Quantum Mechanics with deep reaching consequences, one can use it to solve extremely difficult problems which normally would be difficult to solve with the Schrodinger Approach like extension to Quantum Statistical Mechanics and Quantum Chromodynamics and the entire field of Quantum Field Theory

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