An Introduction to the Path Integral Approach to Quantum Mechanics

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In 1948 Richard Feynman reformulated quantum mechanics using a sum-over-all paths approach. In this derivation he obtained a completely different way of looking at quantum mechanics that demonstrates the close relationship between the classical action and the evolution of the wavefunction. In this paper I will give a short overview of the propagator and how it can be used to describe the system. Then I will discuss the results of the Feynman path integral formulation and its equivalence to the Schrödinger equation. Finally I will explain how this method can be used to solve a specific potential and discuss applications to more advanced topics.

HISTORY AND INTRODUCTION

Werner Heisenberg, Max Born, and Pascual Jordan originally developed matrix mechanics in 1925 and a year later Erwin Schrödinger came up with the differential equation wave function approach. That same year, Paul Dirac demonstrated that matrix mechanics is equivalent to the wave function approach. These remained the standard approaches to quantum mechanics until 1948 when Richard Feynman developed the path integral formulation based off investigations by Eugene Wigner[1]. Feynman's formulation of quantum mechanics determines how the wavefunction evolves in time by finding a propagator which describes how the system evolves in time and which is independent of the initial wavefunction. Feynman's key insight was to recognize the fact that this propagator is directly related to the sum of all possible paths a particle can take between two points.

OVERVIEW

The Feynman path integral formulation depends upon finding the propagator for a given system. The propagator is a function that is independent of the initial conditions and describes how a system evolves in time. In quantum mechanics the propagator is as follows

$$U(t) = \sum |\psi_n\rangle\langle\psi_n| e^{-iEt/\hbar} \tag{1}$$

where we can write the wavefunction in the different eigenstates evaluated in whatever basis happens to be convenient. To obtain this result we recall the following equation which describes how the wavefunction evolves in time.

$$|\Psi(t)\rangle = U(t)|\Psi(0)\rangle$$

All this says is that given some initial wavefunction at some time t_0, chosen arbitrarily to be zero, the propagator, U(t), determines how the wavefunction evolves in time. Analysis of this equation can lead us to the Schrödinger Equation[2]. Now we will show how to derive equation (1) following Shankar[3]. We first start with the Schrödinger equation

$$i\hbar \frac{d}{dt}|\Psi(t)\rangle = H|\Psi(t)\rangle$$

From this we can obtain the time independent Schrödinger equation as $H|\psi_n\rangle = E_n|\psi_n\rangle$. We now use an important property of Schrödinger equation in that we can expand the original wavefunction out in terms of the eigenkets $|\psi_n\rangle$; $|\Psi(t)\rangle = \sum a_n(t)|\psi_n\rangle$ where $a_n(t) = a_n(0)\exp(-iEt/\hbar)$ are obtained from the separation of variables and $a_0(0) = \langle\psi_n|\Psi(0)\rangle$. Now substituting back into the expansion for $|\Psi(t)\rangle$ we obtain

$$\begin{aligned} |\Psi(t)\rangle &= \sum |\psi_n\rangle\langle\psi_n|\Psi(0)\rangle e^{-iEt/\hbar} \\ &= \sum |\psi_n\rangle\langle\psi_n| e^{-iEt/\hbar}|\Psi(0)\rangle \\ &= U(t)|\Psi(0)\rangle \end{aligned}$$

and hence we are able to obtain the expression for the propagator. We can now completely describe the system since this propagator is independent of the initial position of the wavefunction and can describe how the wavefunction evolves in time. We also note that this is entirely equivalent to another form of the propagator which we write as $U(t) = e^{-iHt/\hbar}$ and the curious reader may consult [2] to find a different derivation of (1). We also note that this derivation assumes discrete and non-degenerate energy levels but if we have a continuous spectrum, such as the free particle, we replace the sum with an integration over $|\psi_n\rangle$. If we have degeneracies we have to double sum over the degeneracies.

PATH INTEGRAL PROPAGATOR

As we have just seen above, if we are able to work out the propagator we can completely describe the system at any time. However there is a great difficulty in working out these propagators due to the complicated nature of the summations. Instead we turn to the path integral

method due to Feynman to evaluate these propagators. The actual derivation of the propagator is fairly involved and too long to be derived in this short introduction but can be read in either [3] or [4]. Instead I will discuss the consequences of the path integral formulation. The major result of the derivation is that between two points $(x,t) \rightarrow (x',t')$

$$U(x,t;x',t') = A \sum_{\text{all paths}} e^{iS[x(t)]/\hbar} \tag{2}$$

where A is a normalisation factor and $S[x(t)]$ is the classical action corresponding to each path and is denoted by

$$S = \int \mathcal{L} dt$$

An alternate way to write this formulation to better acknowledge that there are an infinite number of paths is

$$U(x,t;x',t') = \int_x^{x'} e^{iS[x(t)]/\hbar} D[x(t)] \tag{3}$$

where it is implied by the $D[x(t)]$ that we sum over all the paths connecting $(x,t),(x',t')$.

An immediate consequence of this formula is that all paths are equally weighted. Thus a question arises is as to how the classical path is favoured in the classical limit and by what mechanism is the classical path chosen over the other paths if they are equally weighted?

One way to think of the above formula is for each path to represent a vector in the complex plane. Assume, without loss of generality, that each vector is of unit length. Here the action determines the phase of the vector. As we move far away from the classical path there is destructive interference as all the different non-classical paths tend to cancel each other out. As we move towards the classical path the picture changes. We know that Hamilton's principle is

$$\delta S = \delta \int \mathcal{L} dt = 0$$

which serves as the basis for analytical classical mechanics as both the Hamiltonian and Lagrangian formulation follow from it. What it states is that the variation along the classical path is at an extremum. Thus when we start moving towards the particles classical path we start having constructive interference because the variation in the path is zero and hence we are able to regain the classical path. This means that the destructive interference effectively cancels the contribution of all paths that are not near the classical path and constructive interference near the classical path allows us to regain the classical path. Thus despite all being equally weighted the classical path is very important.

Above the term 'moving towards the particles classical path' was used, but what exactly do we mean by 'moving towards'? How far away from the particle's classical path must we go before we encounter destructive interference? Effectively we can make an elementary guess that $S[x_{cl}(t)]/\hbar \approx \pi$ or otherwise if the action is $\pi\hbar$ away from the classical path we have destructive interference. The classical action of a macroscopic particle is on the order of 1 erg sec $\approx 10^{27}\hbar$[3] which is much greater then $\pi\hbar$. In this case we are well beyond the $\pi\hbar$ and hence the classical path completely dominates the sum. However for an electron, which has a very tiny mass, has an approximate action of $\hbar/6$[3] which is well within the $\pi\hbar$ needed and thus we cannot think of the electron moving along it's classical path since many of the non-classical paths contribute to the summation.

EQUIVALENCE TO THE SCHRÖDINGER EQUATION

Feynman has now told us the propagator is equivalent to summing over the action of all the possible paths between two points. But does this give us the correct result as predicted by the Schrödinger equation? To show the equivalence imagine a system evolving from $(x-\xi,t-\epsilon) \rightarrow (x,t)$[5]. We know that the propagator tells us exactly how this system evolves and we can approximate this as a straight line and constant velocity between the two points. Thus we are only summing over a single path

$$\Psi(x,t) \approx A \int_{-\infty}^{\infty} d\xi e^{iS/\hbar} \Psi(x-\xi,t-\epsilon)$$

where A is a normalisation constant and the action is determined by $S = [1/2m(\xi/\epsilon)^2 - V(x)]\epsilon$ which is the action to the first order of epsilon. Now we have that

$$\Psi(x,t) \approx A \int_{-\infty}^{\infty} d\xi e^{\frac{im\xi^2}{2\hbar\epsilon}} e^{-\frac{i}{\hbar}V(x)\epsilon} \Psi(x-\xi,t-\epsilon)$$

with the intention of taking the limit $\epsilon \rightarrow 0$. Now as the we take this limit the first exponential oscillates very rapidly unless the ξ is smaller then the ϵ. Thus if we pick a small neighbourhood about ξ such that it is smaller then ϵ we can expand out terms into Taylor Series about ϵ, ξ and hence

$$\Psi(x,t) \approx A \int_{-\infty}^{\infty} d\xi e^{\frac{im\xi^2}{2\hbar\epsilon}} [\Psi - \frac{\partial\Psi}{\partial t}\epsilon - \frac{i}{\hbar}V\Psi\epsilon + \cdots - \frac{\partial\Psi}{\partial x}\xi + \frac{1}{2}\frac{\partial^2\Psi}{\partial x^2}\xi^2 + \cdots]$$

Now that we have expanded the terms, the Ψ is independent of ξ and hence all the integrals can easily be performed as they are all Gaussian integrals.

$$\Psi(x,t) \approx A\sqrt{\frac{2\pi i\hbar\epsilon}{m}} \left[\Psi + \left(-\frac{\partial\Psi}{\partial t} - \frac{i}{\hbar}V\Psi + \frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2}\right)\epsilon + \cdots\right]$$

Now to make the terms in the order of ϵ vanish we set $A = (m/2\pi i\hbar\epsilon)^{1/2}$ and hence the terms in front of the ϵ are

$$i\hbar\frac{\partial\Psi}{\partial t} = \frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi \tag{4}$$

which is the time-dependent Schrödinger equation. Thus the Feynman path integral formulation is entirely equivalent to the Schrödinger wave equation.

APPLICATION

To demonstrate the Feynman path integral formulation, we will look at the case of the general potential $V = a + bx + cx^2 + d\dot{x} + ex\dot{x}$, of which the well-known harmonic oscillator is a special case. The evaluation of path integrals of this form can be found in both [4] and [2] and hence I will discuss only the results. It can be found that for the above potential the propagator is

$$U(x,t;x',t') = e^{iS_{cl}/\hbar}A(t) \tag{5}$$

This is a very interesting result because it says that the propagator depends only on the classical path and some function $A(t)$ which has to be determined through other means. Consider the case of the free particle. As we explained above it makes sense that the classical path plays an important role in the evaluation of the path integral and we even reasoned that it dominates the calculation. It turns out that it completely dominates the summation and we can easily work out the propagator for the free particle.

Now consider the harmonic oscillator. Suppose we wanted to write it down in position space in the form (1). We can derive all the wave functions and energy levels and then plug them in to obtain the propagator in position space

$$\begin{aligned} U(x,t;x',t') &= \sum |\psi\rangle\langle\psi| e^{-iEt/\hbar} \\ &= \sum_{n=0}^{\infty} A_n \exp\left(-\frac{m\omega}{2\hbar}x^2\right) H_n(x)\times \\ &\qquad A_n \exp\left(-\frac{m\omega}{2\hbar}x'^2\right) H_n(x') \\ &\qquad \times \exp[-i(n+1/2)\omega(t-t')] \end{aligned}$$

where $H_n(x)$ are the Hermite polynomials[6]. This is a very complicated sum and once evaluated can completely describe the system. Evaluating the sum is no easy task and no attempt to do so will be made here. However if we instead look at the propagator from Feynman's point of view, all we need to do is obtain the classical action of the oscillator and we are within a function $A(t)$ from the sum. The classical action is easily derived as

$$S_{cl} = \frac{m\omega}{2\sin\omega t}[(x_0^2 + x'^2)\cos\omega t - 2x_0x']$$

In this case the function $A(t)$ can be evaluated using Fourier series [4] and works out to be

$$A(t) = \left(\frac{m}{2\pi\hbar it}\right)^{1/2}$$

Thus the propagator for the harmonic oscillator is

$$U = \left(\frac{m}{2\pi\hbar it}\right)^{1/2}\left[\frac{im\omega}{2\hbar\sin\omega t}[(x_0^2 + x'^2)\cos\omega t - 2x_0x']\right] \tag{6}$$

This expression for the propagator can in fact be used to find the energy levels and the wave functions[4] and we are able to completely describe the harmonic oscillator without resorting to solving a complicated PDE but instead the equation of motion for a harmonic oscillator, which is much easier.

CONCLUSION

While this method looks much more complicated, the path integral formulation has a much deeper application in quantum mechanics. One such example is that it allows us to formulate driven quantum harmonic oscillators which play an important role in quantum electrodynamics since we can represent the E-M field as quantum driven harmonic oscillators [4]. Finally the path integral method leads to perturbation calculations through Feynman diagrams and plays an important role in relativistic quantum mechanics alongside the Dirac equation.

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