From Lagrange to Feynman: Path Integral Formulation for the Harmonic Oscillator and the Free Particle

Eric Yeung*

Department of Physical Sciences, University of Toronto, Toronto M1C 1A4, Canada

(Dated: October 29, 2014)

It will be shown that Feynman's path integral formulation is not only equivalent to Schrödinger's equation, but more easily generalisable in $\mathbb{R}^n$.

* eric.yeung@mail.utoronto.ca

I. INTRODUCTION

In classical and quantum mechanics, one often wishes to find the position and momentum of a particle or system. Erwin Schrödinger formulated a partial differential equation which describes quantum states of time-variant physical systems with the help of wave-functions. Newton's second law is its classical equivalent when either $\hbar \to 0$ or $m \to \infty$. In the 1940's, Richard Feynman proposed an alternative method for constructing a quantum field theory known as the Feynman path integral. In this paper, I shall show that both Schrödinger's equation and Feynman's path integral are equivalent, and that Feynman's approach is more easily generalisable in $\mathbb{R}^n$. I will also demonstrate the path integral approach by utilising it to solve the free particle and the harmonic oscillator. For the sake of simplicity, I only deal with non-relativistic, linear, and up to $\mathbb{R}^2$ systems henceforth.

II. LAGRANGIAN FORMALISM AND SCHRÖDINGER'S EQUATION

I begin with the action $\mathcal{S}$ and the functional $\mathcal{L}$, for one generalised coordinate $q_1 = x$.

$$\mathcal{S} = \int_{t_1}^{t_2} \mathcal{L}[x, \dot{x}; t]\, \mathrm{d}t \tag{1}$$

Where the Lagrangian is simply $\mathcal{L} = T - U$ where T and U are the kinetic and potential energies respectively; it also satisfies the Euler-Lagrange equation

$$\frac{\partial \mathcal{L}}{\partial x} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{x}}\right) = 0 \tag{2}$$

The Lagrangian proves to be a more formal and powerful approach than Newton's formalism. The Schrödinger equation is solved by finding the energy eigenvalues, while the Lagrangian is solved by the Euler-Lagrange equation. The famous time-independent Schrödinger's equation [Eq. 3] is also derived from the Lagrangian.

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + V\right)\Psi = i\hbar\frac{\partial \Psi}{\partial t} \tag{3}$$

The derivation, coincidentally done by Feynman, begins with the

And finally we arrive at [Eq. 3] again as expected.

To make the limitations of the Schrödinger equation more explicit, let us consider a case of the infinite circular well. The infinite circular well is a two dimensional system. The symmetry of the circular well allows us to separate the wave-function into two spacial components such that $\Psi(r,\theta) = \gamma(r)\xi(\theta)$ where we deal with polar coordinates trivially. Because the the wave function is separable, one can treat the infinite circular well as two, not necessarily independent,one dimensional problems. Expressing the Laplacian ∇^2 in terms of r and θ, and with help from the Dirichlet boundary condition $V(x) = 0$, we obtain our Schrödinger equation in $\mathbb{R}^2$ [6].

$$-\frac{\hbar}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}\right)\Psi(r,\theta) = E\Psi(r,\theta) \tag{4}$$

Substituting the separable wave function $\Psi(r,\theta) = \gamma(r)\xi(\theta)$, one arrives at [Eq. 5] where $k = \frac{\sqrt{2mE}}{\hbar}$ and μ is a separation constant similar to E.

$$\frac{d^2\gamma(r)}{dr^2} + \frac{1}{r}\frac{d\gamma(r)}{r} - \frac{\mu^2}{r^2}\gamma(r) = -k^2\gamma(r) \tag{5}$$

The above is only the radial component of the Schrödinger equation because there contains only $\gamma(r)$. The angular component would resemble the following:

$$\frac{d^2\xi(\theta)}{d\theta^2} - \frac{\mu^2}{r^2}\xi(\theta) = -k^2\xi(\theta) \tag{6}$$

As one can see by the two components, Schrödinger's equation gets very messy and hard to work with very quickly as $\mathbb{R}^n$ increases. Before we continue, the path integral can also be derived from the Schrödinger equation and vice versa. But since this paper is a connection to PHYC54, we will only look at the derivations from the Lagrangian or the Hamiltonian.

III. FEYNMAN'S PATH INTEGRAL

An alternative, and a more insightful, approach to solving quantum mechanic systems is Feynman's formulation of quantum mechanics. Unlike Schrödinger's equation, in which one has to integrate operators such as the angular momentum operator $\hat{L} = \mathbf{r} \times -i\hbar\nabla$, the path integral is simply over numbers.

$$\langle x_f, t_f | x_i, t_i \rangle = \int \mathcal{D}\, x(t) e^{i\,\mathcal{S}[x(t)]/\hbar} \tag{7}$$

Where x_f, x_i are the initial and final positions; t_f, t_i are the initial and final times respectively. The boundary conditions are almost always $x(t_i) = x_i$ and $x(t_f) = x_f$. Additionally, $\mathcal{S}$ is the action aforementioned and $\mathcal{D}$ is a weight factor- dependent on the action- for each path. This integral adds up all the possible paths connecting x_i with x_f with the some weight $\mathcal{D}$. One notes that as $\hbar \to 0$, $e^{i\,\mathcal{S}/\hbar}$ starts to oscillate as the argument diverges to ∞. As the phase factor rapidly oscillates, most of the paths are cancelled out. The paths that do survive make the action stationary or $\delta\,\mathcal{S} = 0$. This is the classical trajectory; it has the biggest contribution in the small $\hbar$ limit.

In [Fig. 1], one can visualise the integral over multiple *possible* paths.

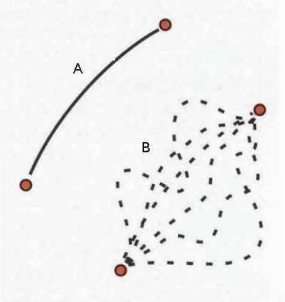

FIG. 1. Case A includes only the classical trajectory while case B includes all possible paths.

Note that one cannot know the path that the particle follows- even with the two conditions x_f, x_i; this is exactly why we integrate, or in other words sum, all the possible paths. This is analogous to the double-slit experiment; however, the path integral is more general. One can think of it as the infinite-slit experiment [3]. As stated earlier, the classical trajectory has the largest contribution to the quantum particle's path if $\hbar$ is small; the particle's trajectory can deviate from the classical one if $\delta\,\mathcal{S} \approx \hbar$ or as $\hbar$ increases. This deviation can also be described by quantum fluctuation which is a temporary change in the energy in a point in space. The ability to deviate from classical paths is what differentiates quantum and classical particles. A classical particle cannot escape a potential barrier, but a

quantum particle can tunnel through.

The derivation of the path integral starts with the classical Lagrangian:

A. The Free Particle

In $\mathbb{R}^1$, the Lagrangian for the free particle is simply $\mathcal{L} = m\dot{x}^2/2$. Our path integral is shown below.

$$\langle x_f, t_f | x_i, t_i \rangle = \int \mathcal{D}\, x(t) e^{i \int m\dot{x}^2/2 \mathrm{d}t/\hbar} \tag{8}$$

We want first to find the classical path x_c. It is shown to be:

$$x_c(t) = x_i + \frac{x_f - x_i}{t_f - t_i}(t - t_i) \tag{9}$$

B. The Harmonic oscillator

As with the free particle, we shall approach the one-dimensional problem. The Lagrangian of the harmonic oscillator in $\mathbb{R}^1$ is $\mathcal{L} = m\dot{x}^2/2 - 1/2m\omega^2 x^2$. We need to calculate the path integral below.

$$\langle x_f, t_f | x_i, t_i \rangle = \int \mathcal{D}\, x(t) e^{i \int (m\dot{x}^2/2) - 1/2m\omega^2 x^2) \mathrm{d}t/\hbar} \tag{10}$$

Our classical path x_c is shown to be:

$$x_c(t) = x_i \frac{\sin[\omega(t_f - t)]}{\sin[\omega(t_f - t_i)]} + x_f \frac{\sin[\omega(t - t_i)]}{\sin[\omega(t_f - t_i)]} \tag{11}$$

IV. DISCUSSION

Although most of this paper has been theoretical, lattice field theory is an application of Feynman's approach that does require computation. All the computation will be done in either Julia or Python.

V. APPENDIX

In this section, we solve the free particle and the harmonic oscillator using the Schrödinger equation. This was left out of the main paper because of brevity.

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