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

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(Dated: November 24, 2014)

I explore the Feynman path integral and its origins. Equivalency of the Feynman path integral approach to the Schrödinger picture was also examined. The free particle and the harmonic oscillator were solved using the Feynman approach to demonstrate the equivalence. It was found that the solutions to the free particle and harmonic oscillator yielded classical quantities like momentum and energy. The path integral was found to be unambiguous in 2-dimensional space-time (or $\mathbb{R}^2$), while the Schrödinger equation struggled with another dimension. It was also shown that although the mathematical computation of path integrals are difficult, the path integral approach was more intuitive when understanding quantum-mechanical laws.

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. One can retrieve classical mechanics, which is a special case of quantum mechanics, back when $\hbar \to 0$. This is called the semi-classical limit. In the 1940's, Richard Feynman proposed an alternative method for constructing a quantum theory known as the Feynman path integral. He discovered that the Schrödinger equation could be solved by an "averaging of paths". 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 intuitive and more easily generalisable in 2-dimensional space-time [8]. 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 $q_1 = x$. One wishes to find the classical path $x(t)$ for which $\mathcal{S}$ is an extremum. The process of picking out a particular path $x(t)$ out of all the possible paths is the principle of least action.

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

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 famous time-dependent Schrödinger's equation [Eq. 3] is also derived from the Lagrangian. The derivation of Schrödinger's equation has been left out because of brevity, but is shown in [10].

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

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 $\gamma(r)$.

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As one can see by the two components, radial and angular, Schrödinger's equation gets very messy and hard to work with very quickly as $\mathbb{R}^n$ increases. An alternative, and a more insightful, approach to solving quantum mechanical systems is Feynman's formulation of quantum mechanics. More importantly, the Lagrangian is directly related to the path integral by the action. To further demonstrate the equivalency of the path integral formulation with Schrödinger's equation, Schrödinger's equation can be derived from the path integral. 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. An advantage of the path integral is that it is perfectly well-defined in 2-dimensional space-time [8]. However, while the Schrödinger equation is solved by finding the energy eigenvalues, computation of path integrals are more tricky mathematically.

III. FEYNMAN'S PATH INTEGRAL

In the double slit experiment, the event of a fermion- more specifically an electron with low velocity- going from a source to a destination has one amplitude while passing through one of the two slits and has another amplitude for passing through the other slit. The total amplitude of this event is then the superposition or sum of the two amplitudes from the two respective slits. More generally, the amplitude of any event is the sum of the amplitudes for the various alternative ways that the event can occur [7]; these " various ways" can be thought of as possible paths. The double-slit experiment is analogous to the scenario of summing up the contributions to the amplitude in the path integral; however, the path integral is more general. One can think of the path integral as the infinite-slit experiment [3].

Recall earlier that, in classical mechanics, finding the contribution of a particular path $x(t)$ involves the principle of least action. However, in quantum mechanics, there exists not a single particular path of least action that contributes to the total amplitude $K(b,a)$; but rather, all the possible paths have a contribution. Note that $K(b,a)$ is the total amplitude to go from x_a to x_b. The contributions of all the paths are of equal magnitude, but they do not add to $K(b,a)$ at the same time. There exists an phase difference; all the possible trajectories contribute at different phases. It follows that the phase of the contribution of a single possible path is proportional to $\mathcal{S}$ and is given by:

$$\phi[x(t)] = \text{ constant } e^{i\,\mathcal{S}[x(t)]/\hbar} \tag{6}$$

The relationship between the Lagrangian and the path integral manifests here. The phase is proportional to the action, and the action is dependent on the functional Lagrangian. Therefore, the path integral depends on the Lagrangian as well. The total amplitude is the sum of all the contributions from every possible path, so it is given by the sum:

$$K(b,a) = \sum_{\text{paths from a to b}} \phi[x(t)] \tag{7}$$

This is where is gets a little tricky; one may initially want to take limit so that the quantised sum turns into a Riemann integral like students have done in calculus. But for the sake of argument and demonstration, one would get the following.

$$\begin{aligned} K(b,a) &= \int \dots \int \int \phi[x(t)] \mathrm{d}x_1 \mathrm{d}x_2 \dots \mathrm{d}x_{N-1} \\ &= \lim_{\epsilon \to 0} \frac{1}{A} \int \dots \int \int e^{i\,\mathcal{S}[b,a]/\hbar} \frac{\mathrm{d}x_1}{A} \frac{\mathrm{d}x_2}{A} \dots \frac{\mathrm{d}x_{N-1}}{A} \end{aligned} \tag{8}$$

ϵ is the width of the time step, $\phi[x(t)]$ is expanded, and A is a normalising factor. However, as one can see, this normalising factor is often found ad hoc. In other words, there is not a way to define it in general and can only be defined for a specific situation or Lagrangian. $\mathcal{S}[b,a]$ is simply the integral of the Lagrangian with t_a and t_b as lower and upper bounds respectively. One can think of $\mathcal{S}[b,a]$ is the line integral taken over a path passing through points x_i with straight sections between.

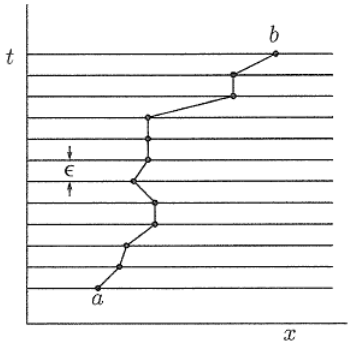

FIG. 1. The path is initially "picked out" by its x coordinate at a lot of specified times separated by ϵ. Then the sum of the paths is an integral over all these specified coordinates [7].

The particular way we defined the subset of all the paths between a and b may not be the best as some mathematical problems arise. Suppose the Lagrangian is variant of $\ddot{\mathrm{x}}$, the acceleration of x, one can see that the velocity would have discontinuities at some points (x_i, t_i). Subsequently, this would mean that the acceleration is not defined at those points (x_i, t_i). However, we need not define a new sum since our current one suffices as the sum over all paths. [Eq. 8] is written in a more manageable form [Eq. 9].

$$K(b,a) = \int_a^b \mathcal{D}\, x(t) e^{i\,\mathcal{S}[b,a]/\hbar} \tag{9}$$

$\mathcal{D}$ is the identifying notation- dependent on the action- for every possible path. In other words, $\mathcal{D}$ can be thought of as a more general $\mathrm{d}x$. $K(b,a)$ is sometimes called the kernel or propagator to go from a to b. The path integral is sometimes written in Bra-ket notation as shown below, but [Eq. 10] will not be used again in the paper.

$$\langle x_f, t_f | x_i, t_i \rangle = \int \mathcal{D}\, x(t) e^{i\,\mathcal{S}[x(t)]/\hbar} \tag{10}$$

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 $x(t_f) = x_f$. Or, in the notation I have used this entire paper, $x_f = x_b$, $x_i = x_a$, $t_f = t_b$, and $t_i = t_a$. The path integral can also be rewritten in terms of the energy eigenvalues and eigenstates [Eq. 11] if the Hamiltonian is invariant of time [3].

$$K(b,a) = \sum_n e^{-iE_n(t_b - t_a)/\hbar} \psi_n^*(x_b)\psi_n(x_a) \tag{11}$$

It follows that, this integral for $K(b,a)$ adds up all the possible paths connecting x_i with x_f. One notes that as $\hbar \to 0$, $e^{i\,\mathcal{S}/\hbar}$ starts to oscillate as the argument diverges to ∞. Another condition is if the action is very large relative to $\hbar$. As the phase factor $\phi[x(t)]$ rapidly oscillates, most of the paths are cancelled out. This is because of the small $\hbar$ limit; neighbouring paths will have slightly varying actions at different phases- thus constructively interfering. The path that does survive makes the action stationary or $\delta\,\mathcal{S} = 0$. This is the classical trajectory; it has the biggest contribution in the small $\hbar$ limit. The kernel in this classical limit, where F is a smooth function and $\mathcal{S}_{cl}$ is the classical action, is given by:

$$K(b,a) = F e^{i\,\mathcal{S}_{cl}/\hbar} \tag{12}$$

In [Fig. 2], one can visualise the integral over multiple *possible* paths. A more detailed diagram, with a specified number of paths, was done in python in [Fig. 6].

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. For example, a classical particle cannot escape a potential barrier, but a quantum particle can tunnel through.

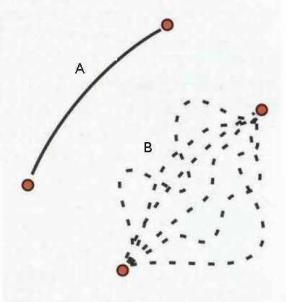

FIG. 2. Case A includes only the classical trajectory while case B includes all possible paths.

We can also generalise the path integral in the case of two events. The action becomes

$$\mathcal{S}[b,a] = \mathcal{S}[b,c] + \mathcal{S}[c,a] \tag{13}$$

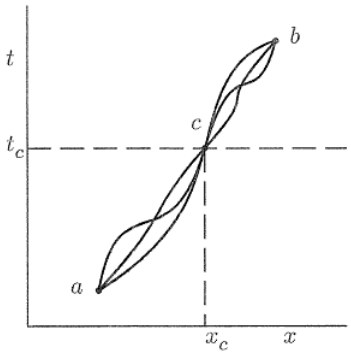

FIG. 3. The amplitude or kernel for $a \to c \to b$ is the product of the two amplitudes [7].

Where c is somewhere between a and b, and $t_a < t_c < t_b$. We can separate and express the action in this way because the Lagrangian depends only on the velocity as the highest order derivative. Substituting $\mathcal{S}[b,a]$ into [Eq. 9] and using the law of exponents, we get the result below.

$$\begin{aligned} K(b,a) &= \int_a^b \mathcal{D}\, x(t) e^{i(\mathcal{S}[b,c]+\mathcal{S}[c,a])/\hbar} \\ &= \int_{-\infty}^{\infty} \int_c^b \mathcal{D}\, x(t) K(c,a) e^{i\,\mathcal{S}[b,c]/\hbar} \mathrm{d}x_c \\ &= \int_{-\infty}^{\infty} K(b,c)K(c,a)\mathrm{d}x_c \end{aligned} \tag{14}$$

From our result above, it is clear that integration must be performed over the variable midpoint x_c as well as the paths between c and b. We can then conclude that amplitudes for events in succession in time multiply.

A. The Free Particle

In $\mathbb{R}^1$, the Lagrangian for the free particle is simply $\mathcal{L} = m\dot{x}^2/2$. The kernel or propagator of the free particle to go from a to b, denoted $K_0(b,a)$, is shown below.

$$K_0(b,a) = \int \mathcal{D}\,x(t) e^{i\int m\dot{x}^2/2\mathrm{d}t/\hbar} \tag{15}$$

We want first to find the classical path, the path that makes $\delta\,\mathcal{S} = 0$, x_c. It is shown below [3].

$$x_c(t) = x_a + \frac{x_b - x_a}{t_b - t_a}(t - t_a) \tag{16}$$

Recall earlier the concept of quantum fluctuation, which is the temporary change in the energy in a point in space. What this means mathematically is that our $x(t)$ can be rewritten in terms of the classical trajectory.

$$x(t) = x_c(t) + \delta x(t) \tag{17}$$

It is noted that $\delta x(t) \to 0$ at the initial and final time boundaries. With previous knowledge of the free particle solution in quantum mechanics, one knows that the free particle is represented by a Gaussian wave packet. When one thinks of waves, a Fourier series is usually constructed.

$$\delta x(t) = \sum_{n=1}^{\infty} a_n \sin\frac{n\pi}{t_b - t_a}(t - t_a) \tag{18}$$

With the Fourier coefficient a_n and a normalisation constant c, which depends on m and $t_f - t_i$, one can rewrite the path integral as an infinite product.

$$\int \mathcal{D}\,x(t) = c\int \prod_{n=1}^{\infty} \mathrm{d}a_n \tag{19}$$

Differentiating $x(t)$ with respect to t and finding the action, which takes advantage of orthogonality, the action is found below.

$$\mathcal{S} = \frac{m}{2}\frac{(x_b - x_a)^2}{t_b - t_a} + \frac{m}{4}\sum_{n=1}^{\infty}\frac{(n\pi)^2}{t_b - t_a}a_n^2 \tag{20}$$

The first term is the classical action. After doing the integral in [Eq. 19], which I omitted for brevity, the kernel of the free particle is finally shown as:

$$K_0(b,a) = \left(\frac{m}{2\pi i\hbar(t_b - t_a)}\right)^{1/2} \exp\left[\frac{im(x_b - x_a)^2}{2\hbar(t_b - t_a)}\right]$$
$$\text{Where } c'(t) = \sqrt{\frac{m}{2\pi i\hbar t}} \tag{21}$$

The kernel, when found, has some interesting applications. One can find the classical momentum and the classical energy of the particle directly from the kernel. Let us first fix time, so the amplitude varies with distance, to achieve [Eq. 22].

$$K_0(b,a;0,0) = left(\frac{m}{2\pi i\hbar(t}^{1/2}\exp\left[\frac{im(x)^2}{2\hbar(t)}\right]$$

One can see that by varying x by the wavelength λ [Fig. 4], the amplitude's phase $\phi[x(t)]$ increases by a factor of 2π.

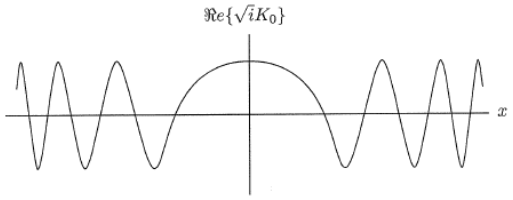

FIG. 4. The plot of the real part of $\sqrt{i}$ times our kernel with varying distance [7].

$$2\pi = \frac{m(x+\lambda)^2}{2\hbar t} - \frac{mx^2}{2\hbar t} = \frac{mx\lambda}{\hbar t} + \frac{m\lambda^2}{2\hbar t} \tag{22}$$

If one takes the condition that $x \gg \lambda$ such that we can neglect the quantity λ^2 with respect to the quantity $x\lambda$, one rearranges for λ.

$$\lambda = \frac{2\pi\hbar}{mxt^{-1}} \tag{23}$$

One can see that the momentum mx/t is in the denominator of λ. Classically, this is a particle which moves to x from the origin in a time t, velocity x/t, and momentum mx/t. Quantum-mechanically, one can rearrange λ for the de Broglie wavelength $\lambda = h/p$ where $h = 2\pi\hbar$ is just the non-reduced Planck constant.

To recover energy, one now fixes the distance and varies the time. Again, one plots $\Re(\sqrt{i}K_0)$ in [Fig. 5].

Similar to before, the amplitude's phase decreases by a factor of 2π when one increases the time by a period T.

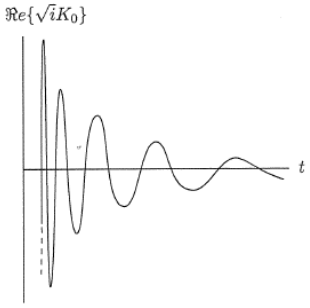

FIG. 5. The plot of the real part of $\sqrt{i}$ times our kernel with varying time [7].

$$2\pi = \frac{mx^2}{2\hbar t} - \frac{mx^2}{2\hbar(t+T)} = \frac{mx^2}{2\hbar t^2}\left(\frac{T}{1+T/t}\right) \tag{24}$$

Using the angular frequency $\omega = 2\pi/T$ and using the condition $t \gg T$ like before, we can rearrange for ω.

$$\omega \approx \frac{m}{2\hbar}\left(\frac{x}{t}\right)^2 \tag{25}$$

$(m/2)(x/t)^2$ is just the classical energy $E = \hbar\omega$ of the free particle. Finally, classical mechanics is recovered from our path integral.

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 $\mathcal{L} = m\dot{x}^2/2 - 1/2m\omega^2x^2$. We need to calculate the path integral below.

$$K(b,a) = \int \mathcal{D}\,x(t) e^{i\int(m\dot{x}^2/2) - 1/2m\omega^2x^2)\mathrm{d}t/\hbar} \tag{26}$$

Our classical path x_c, the path that dominates when $\mathcal{S}[b,a] \gg \hbar$, is shown to be

$$x_c(t) = x_a\frac{\sin[\omega(t_b-a)]}{\sin[\omega(t_b-t_a)]} + x_b\frac{\sin[\omega(t-t_a)]}{\sin[\omega(t_b-t_a)]} \tag{27}$$

The action along the classical trajectory is given by:

$$\mathcal{S}_c[b,a] = \frac{1}{2}m\omega\frac{(x_a^2+x_b^2)\cos\omega(t_b-t_a) - 2x_ax_b}{\sin\omega(t_b-t_a)} \tag{28}$$

Once again, like in the free particle problem, there is quantum fluctuation around the classical path x_c. One can expand $\delta x(t)$ in Fourier series, again, like in the free particle case.

$$\mathcal{S}[b,a] = \mathcal{S}_c + \sum_{n=1}^{\infty}\frac{m}{4}\left(\frac{(n\pi)^2}{t_b-t_a} - \omega^2(t_b-t_a)\right)a_n^2 \tag{29}$$

I skip over the integral due to brevity once again. Like in the free particle case, the path integral is an infinite product of Fresnel integrals over a_n. Although, unlike in the free particle case, our action does not depend only on x, $\dot{x}$, and t. However, once again, classical quantities can be recovered.

$$K(b,a) = e^{i\,\mathcal{S}_c/\hbar}\left[\frac{m}{2\pi i\hbar(t_b-t_a)}\right]^{1/2}\prod_{n=1}^{\infty}\left[1-\left(\frac{\omega(t_b-t_a)}{n\pi}\right)^2\right]^{-1/2} \tag{30}$$

IV. DISCUSSION

A. Future questions

Although the path integral is well defined in $\mathbb{R}^2$, the path integral in 4-dimensional space-time is still an unsolved problem in quantum field theory. As far as potential experiments, one can use the path integral with Picard- Lefschetz theory as a computational method to solve the double-well potential [9]. There has also been attempts to build an extended Feynman path integral. In this paper, we only dealt with non-relativistic particles. The Klein- Gordon equation and the equation for which the wave-function collapses are also derived from the Feynman path integral[9]. The Klein- Gordon equation is a relativistic version of Schrödinger's equation just like the Dirac equation. The ability to derive the Klein-Gordon equation from the path integral suggests some relation between the path integral and relativistic particles.

B. Wiener Process

A Wiener process, also known as standard Brownian motion, is a stochastic time-continuous process. It resembles the paths that contribute in the path integral. It turns out that a wiener process forms a basis to the path integral. I have simulated one-dimensional wiener processes with a varied number of paths using Python as shown below. I used a population mean $\mu = 0$, a standard deviation $\sigma = 10$, and $n = 200$ endpoints.

The graphs are all plotted in 1-dimensional space-time. The main purpose of the simulation was to show the variance among the possible, randomly generated, paths. It should be noted that numpy's random sampling is actually pseudorandom; although for our purposes, it is random enough.

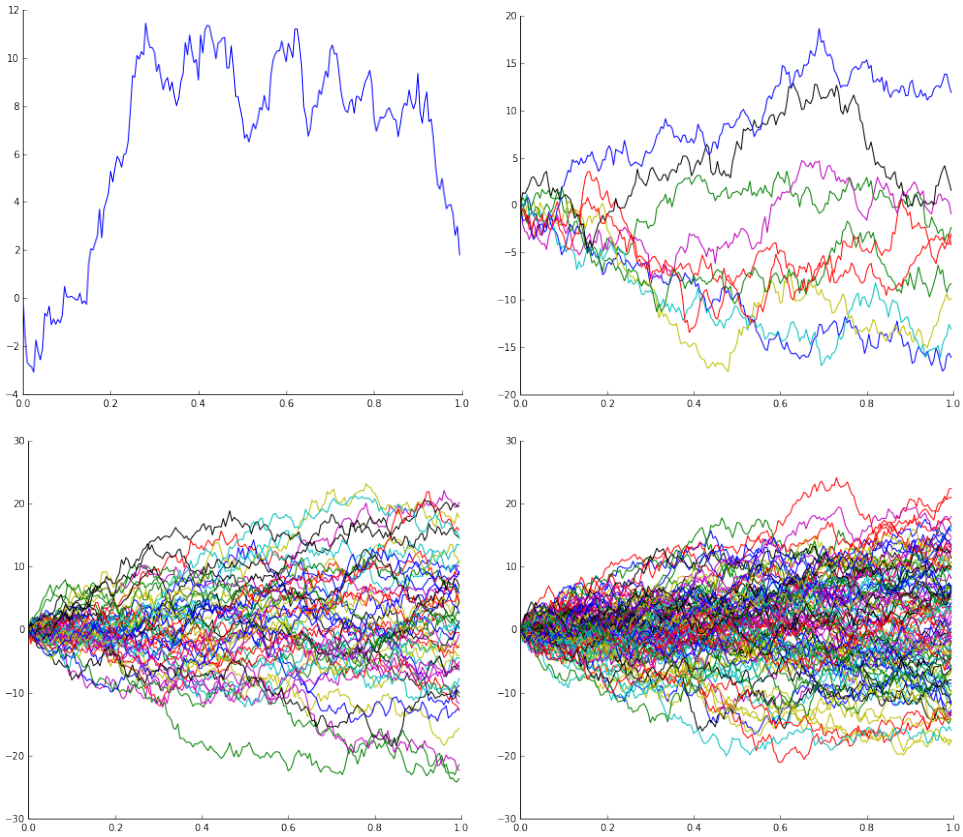

FIG. 6. Wiener processes with 1, 10, 50, and 100 paths respectively. ($\mu = 0$, $\sigma = 10$, $n = 200$)

V. CONCLUSION

While the Schrödinger equation focuses on the evolution of states and operations respectively, the path integral formulation focuses instead on the connection between Lagrangian mechanics and quantum mechanics. The Schrödinger equation and the Feynman path integral can both be derived from the Lagrangian; however, the Lagrangian is a bit messy in 2-dimensional spacetime while the path integral is perfectly well-defined. It is important to note that the calculations, done in this paper, for the free particle and harmonic oscillator were not easy- in any means- to do. I still think the operator approach can be applied to a broader spectrum of problems and has easier calculations. This is why I chose only the free particle and harmonic oscillator as examples in this paper; they were the least mathematically rigorous. However, the concept that the amplitude of an event is a sum of amplitudes for the different ways that the event can occur provides a more intuitive approach to quantum-mechanical laws.

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