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THE PROPAGATION OF A PARTICLE IN THE ONE-DIMENSIONAL INFINITE SQUARE-WELL BY USING THE PATH INTEGRAL FORMALISM

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Abstract

Path integral was invented by Feynman as an alternative formulation of quantum mechanics. Feynman formulation of quantum mechanics using the so called path integral is arguably the most elegant. The path formulation of quantum field theory represents the transition amplitude (corresponding to the classical correlation function) as a weighted sum of all possible histories of the system from the initial to the final state. In this work, the full propagation for the propagation of a particle in the one dimensional infinite square well by using the path integral formalism will be obtained by using Feynman's path integral approach. Visualization of key results is implemented by Mathematica.

Keywords: Feynman path integral, Propagator, Kernel

Introduction

The path integral formalism, which was invented by the US physicist Richard Feynman, is a tool for calculating such quantum mechanical probabilities. Feynman's recipe, applied to a particle travelling from A to B. The resulting sum tells us the probability of detecting the particle that started out at A at the location B at the specified time. Physicists called such a sum over all possibilities a path integral or sum over histories. In quantum mechanics and quantum field theory, the propagator is a function that specifies the probability amplitude for a particle to travel from one place to another in a given period of time, to travel with a certain energy and momentum. The propagator can be written as a sum over all possible paths between the initial and final points.

Path integral provided a unified view of quantum mechanics, field theory and statistical physics and is nowadays an irreplaceable tool in theoretical physics. Feynman showed that Dirac's quantum action was, for most cases of interest, simply equal to the classical action, appropriately discretized. This means that the classical action is the phase acquired by quantum evolution between two fixed endpoints. Amplitude computed according to Feynman principles will also obey the Schrodinger equation for the Hamiltonian corresponding to the given action. Since the relation between Feynman's formulation and classical mechanics is very close, the path integral formalism often has the important advantage of providing a much more intuitive approach.

Theoretical background

The Time-Evolution Operator

The time evolution from time t_0 to t of a quantum mechanical state is described by a linear operator $\widehat{U}(t, t_0)$. Thus a ket at time t that started out at t_0 being the ket is

$$\left|\alpha(t)\right\rangle = \widehat{U}(t, t_0)\left|a\right\rangle \tag{1}$$

The time evolution operator $\widehat{U}(t, t_0)$, which also is known as a propagator, satisfies three important properties:

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(1) The time evolution operator should do nothing when $t = t_0$

$$\lim_{t\to t_0} \hat{U}(t, t_0) = 1 \tag{2}$$

(2) The propagator should preserve the normalization of state kets. That is, if $|\alpha\rangle$ is normalized at t_0 it should also be normalized at later time t. This leads to the requirement $\langle\alpha|\alpha\rangle = \langle\alpha(t)|\alpha(t)\rangle$

$$= \left\langle\alpha\middle|\hat{U}^\dagger(t, t_0)\hat{U}(t, t_0)\middle|\alpha\right\rangle \tag{3}$$

Which implies $\hat{U}^\dagger(t, t_0)\hat{U}(t, t_0) = 0$ (or)

$$\hat{U}^\dagger(t, t_0) = \hat{U}^{-1}(t, t_0) \tag{4}$$

(3) The propagator should satisfy the composition property

$$\hat{U}(t_2, t_0) = \hat{U}(t_2, t_1)\hat{U}(t_1, t_0) \tag{5}$$

Which means that in order to evolve a state from t_0 to t_2 we might as well first evolve the state from t_0 to t_1 and then evolve the state from so obtained from t_1 to t_2.

Formally, we can evolve a wave function forward in time by applying time-evolution operator.

For time-independent Hamiltonian, $|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$, where time-evolution operator ("the propagator"):

$$\hat{U}(t) = e^{-i\Delta Ht/\hbar} \tag{6}$$

Follows from time-independent Schrodinger equation,

$$\hat{H}|\psi\rangle = i\hbar\partial_t|\psi\rangle \tag{7}$$

By inserting the resolution of identity, $I = \sum_i |i\rangle\langle i|$,

Where $|i\rangle$ are eigenstates of $\hat{H}$ with eigenvalue E_i ,

$$|\psi(t)\rangle = e^{-i\Delta Ht/\hbar}\sum_i|i\rangle\langle i|\,\psi(0)\rangle = \sum_i|i\rangle\langle i|\,\psi(0)\rangle e^{-i\Delta E_i t/\hbar} \tag{8}$$

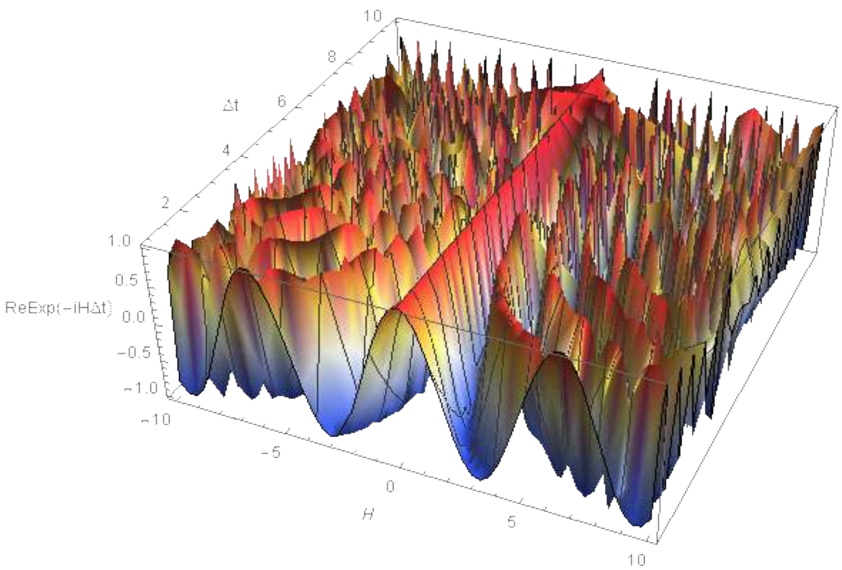

Figure 1. Real part Exp(-iHΔt) in term of H and Δt

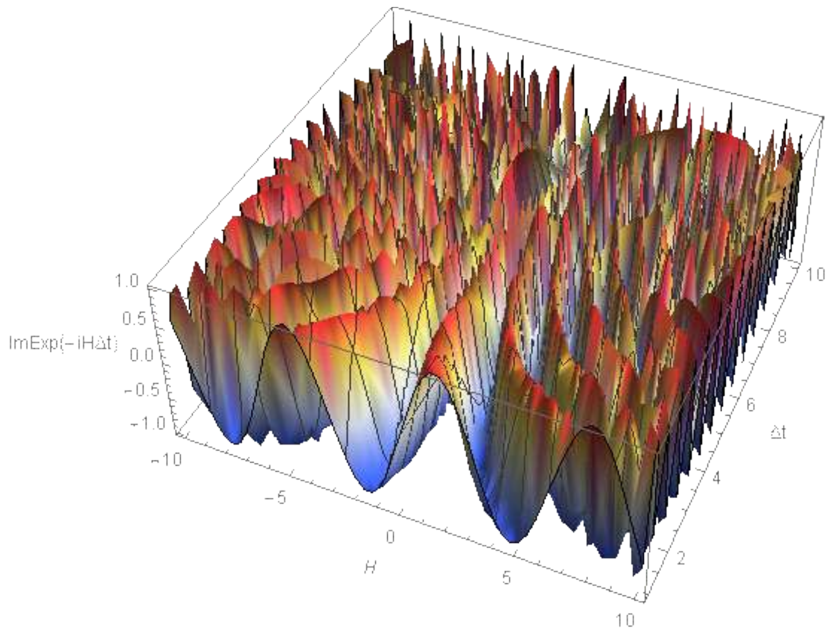

Figure 2. Imaginary part Exp(-iHΔt) in term of H and Δt

Definition of the Propagator

Mathematical form of the propagator. The summation carried out between all the arrows in the initial wavfunction and each single detection event approximates the integral in which the propagator function K is usually employed for a continuous wavefunction,

$$\psi(xb, tb) = \int K(b, a)\, \psi(xb, tb) dxa \tag{9}$$

Here the label 'a' refers to a point in the initial wavefunction, while the label 'b' applies to a point on a later wavefunction. The free-particle propagator K has specific expression.

The paths are sliced into finite number of segments between time interval δt;, each of which has two end points $\{x(t)\}$. Each path are assigned an action (L) corresponding to the position function $x(t)$. The corresponding probability amplitude for each path is given by

$$A(x) = e^{iS(x)/\hbar} \tag{10}$$

The Action Integral

In physics, action is an attribute of the dynamics of a physical system from which the equations of motion of the system can be derived through the principle of stationary action. Action is a mathematical functional which takes the trajectory, also called path or history, of the system as its argument and has a real number as its result. Generally, the action takes different values for different paths.

Action is a part of an alternative approach to finding such equations of motion. The action is typically represented as an integral over time; take along the path of the system between the initial time and the final time of the development of the system:

$$S = \int_{t_1}^{t_2} L dt \tag{11}$$

Where the integrand L is called the Lagrangian. For the action integral to be well-defined, the trajectory has to be bounded in time and space.

Action has the dimensions of [energy]. [time], and its SI unit is joule-second, which is identical to the unit of angular momentum.

In classical mechanics, the input function is the evolution $q(t)$ of the system between two times t_1 and t_2, where q represents the generalized coordinates. The action $S[q(t)\,]$ is defined as the integral of the Lagrangian L for an input evolution between the two times:

$$S[q(t)\,] = \int_{t_1}^{t_2} L[q(t), \dot{q}(t), t\,]dt \qquad (12)$$

Where the endpoints of the evolution are fixed and defined as $q_1 = q(t_1)$ and $q_2 = q(t_2)$.

The action principle can be extended to obtain the equations of motion for fields, such as the electromagnetic field and gravitational field. The trajectory (path in space time) of a body in a gravitational field can be found using the action principle.

The equation of motion between two times t_1 and t_2 should minimize the action integral

$$S = \int_{t_1}^{t_2} L\big(\dot{q}(t), q(t)\big)\, dt \qquad (13)$$

Assuming that $q(t_1)$ and $q(t_2)$ are fixed, then the function $q(t)$ between t_1 and t_2 should minimized S, the action. Taking the first variation of equation (13),

$$\delta S = \delta \int_{t_1}^{t_2} L(\dot{q}, q)dt = \int_{t_1}^{t_2} L(\dot{q} + \delta\dot{q}, q + \delta q)dt - \int_{t_1}^{t_2} L(\dot{q}, q)dt$$

$$= \int_{t_1}^{t_2} \delta L(\dot{q}, q)dt$$

$$= \int_{t_1}^{t_2} \left(\delta\dot{q}\frac{\partial L}{\partial \dot{q}} + \delta q \frac{\partial L}{\partial q}\right) dt = 0 \qquad (14)$$

In order to take variation into the integrand, we have to assume that $\delta L(\dot{q}, q)$ is taken with constant time.

At constant time, $\dot{q}$ and q are independent variables. Using integration arts on the first term,

$$\delta S = \delta q \frac{\partial L}{\partial \dot{q}}\Big|_{t_1}^{t_2} - \int_{t_1}^{t_2} \delta q \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) dt + \int_{t_1}^{t_2} \delta q \frac{\partial L}{\partial q} dt$$

$$= \int_{t_1}^{t_2} \delta q \left[-\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) + \frac{\partial L}{\partial q}\right] dt = 0 \qquad (15)$$

The first term vanishes because $\delta q(t_1) = \delta q(t_2) = 0$ because $q(t_1)$ and $q(t_2)$ are fixed.

Since $\delta q(t)$ is arbitrary between t_1 and t_2 we must have-

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q} = 0 \qquad (16)$$

The above equation is called the Lagrange equation, from which the equation of motion of a particle can be derived. The derivative of the Lagrangian with respect to the velocity $\dot{q}$ is the momentum

$$p = \frac{\partial L}{\partial \dot{q}} \qquad (17)$$

The derivative of the Lagrangian with respect to the coordinate q is the force. Hence,

$$F = \frac{\partial L}{\partial q} \qquad (18)$$

The above equation of motion is then

$$\dot{p} = F \qquad (19)$$

The solution of the equations of motion for a given initial condition is known as a trajectory of the system.

The Propagation of a Particle in the One-Dimensional Infinite Square-Well by Using the Path Integral Formalism

$$S = \int_{t1}^{t2} dt[L(\dot{\bar{x}}) + \frac{\partial L}{\partial \dot{x}}|_{\dot{\bar{x}}}\,\dot{y} + \frac{1}{2}\frac{\partial^2 L}{\partial \dot{x}\partial \dot{x}}|_{\dot{\bar{x}}}\,\dot{y}^2] \tag{20}$$

$$S = S_{cl} + \frac{m}{2}\int_{t1}^{t2} dt\,\dot{y}^2 \tag{21}$$

And thus, for the kernel:

$$K(x_2, t_2; x_1, t_1) = e^{\frac{iS_{cl}[\bar{x}]}{\hbar}} \int_{y(t_1)=0}^{y(t_2)=0}[dy(t)]\exp\,[\frac{i}{\hbar}\int_{t1}^{t2} dt\,\frac{m}{2}\dot{y}^2 \tag{22}$$

The classical action for a free particle,

$$S_{cl} = \frac{m}{2}\frac{(x_2-x_1)^2}{t_2-t_1} \tag{23}$$

Eqn:(22) thus yields for the kernel:

$$K(x_2, t_2; x_1, t_1) = \exp\left[\frac{i}{\hbar}\frac{m}{2}\frac{(x_2-x_1)^2}{t_2-t_1}\right] \int_{y(t_1)=0}^{y(t_2)=0}[dy(t)]\exp\,[\frac{i}{\hbar}\int_{t1}^{t2} dt\,\frac{m}{2}\dot{y}^2(t) \tag{24}$$

the value of the path integral is only a function of the time difference, i.e.,

$$A(t_2 - t_1) = \int_0^0[dy(t)]\exp\,[\frac{i}{\hbar}\int_{t1}^{t2} dt\,\frac{m}{2}\dot{y}^2 \tag{25}$$

$$K(x_2, t_2; x_1, t_1) = A(t_2 - t_1)\exp\left[\frac{i}{\hbar}\frac{m}{2}\frac{(x_2-x_1)^2}{t_2-t_1}\right] \tag{26}$$

for t_1=t_2($\equiv t$):

$$A(t) = e^{-\frac{i\pi}{4}}\sqrt{-\frac{m}{2\pi\hbar t}} = \sqrt{\frac{m}{2\pi i\hbar t}} \quad , \quad \left(\frac{1}{\sqrt{i}} = e^{-\frac{i\pi}{4}}\right) \tag{27}$$

the phase in such a manner that

$$K(x_2, t; x_1, 0) = \sqrt{\frac{m}{2\pi i\hbar t}}\exp\left[\frac{i}{\hbar}\frac{m}{2}\frac{(x_2-x_1)^2}{t}\right] \tag{28}$$

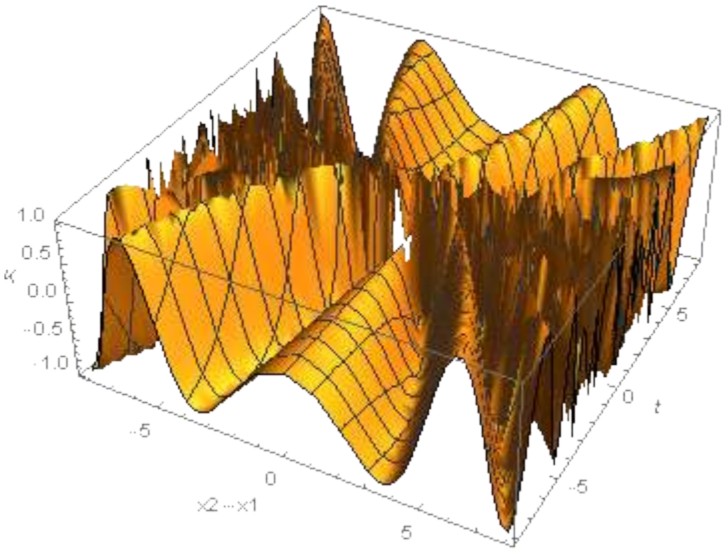

Figure 3. Imaginary part of K

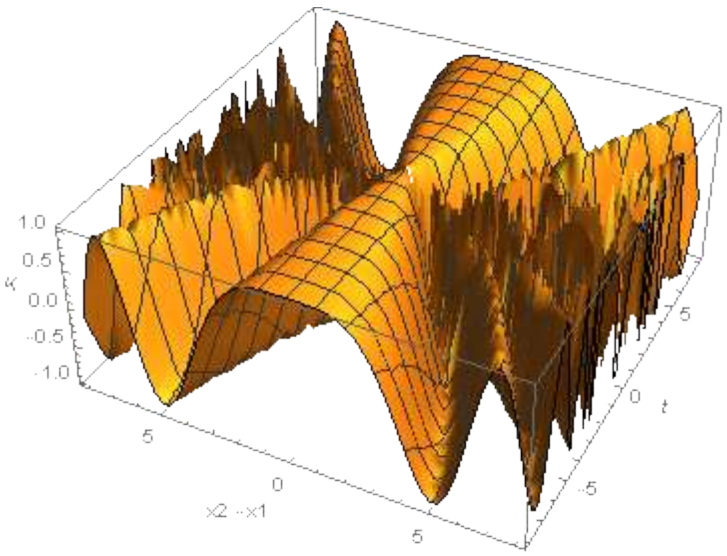

Figure 4. Real part of K

the propagator of the free particle

$$K(x_2,t_2;x_1,t_1) = \sqrt{\frac{m}{2\pi i\hbar(t_2-t_1)}}\exp\left[\frac{i}{\hbar}\frac{m}{2}\frac{(x_2-x_1)^2}{(t_2-t_1)}\right] \tag{29}$$

$$= \sqrt{\frac{m}{2\pi i\hbar(t_2-t_1)}}\,e^{\left(\frac{i}{\hbar}\right)S_{cl}}$$

$$\int_{y(t_1)=0}^{y(t_2)=0}[dy(t)]\exp\left[\frac{i}{\hbar}\int_{t_1}^{t_2}dt\,\frac{m}{2}\dot{y}^2(t)\right] = \left(\frac{m}{2\pi i\hbar(t_2-t_1)}\right)^{\frac{1}{2}} \tag{30}$$

In three dimensions:

$$K(r_2,t_2;r_1,t_1) = \left(\frac{m}{2\pi i\hbar(t_2-t_1)}\right)^{\frac{3}{2}}\exp\left[\frac{i}{\hbar}\frac{m}{2}\frac{(r_2-r_1)^2}{(t_2-t_1)}\right] \tag{31}$$

For future purpose the above boundary condition in mind,

$$\lim_{t\to 0} K(x_2,t;x_1,0) = \delta(x_2-x_1) \tag{32}$$

the Schrodinger wave function for a free particle which was emitted at $x_1 = 0$ at time $t_1 = 0$ and at (x,t) is described by the probability amplitude $\psi(x,t)$,

$$\psi(x,t) = K(x,t;0,0) = \sqrt{\frac{m}{2\pi i\hbar t}}\exp\left[\frac{i}{\hbar}\frac{m}{2}\frac{x^2}{t}\right] \tag{33}$$

$$\psi(x,t) = \sqrt{\frac{m}{2\pi i\hbar t}} \times \exp\left\{\frac{i}{\hbar}\left[\underbrace{m\left(\frac{x_0}{t_0}\right)}_{p_0}x - \underbrace{\frac{m}{2}\left(\frac{{x_0}^2}{{t_0}^2}\right)}_{E_0}t\right]\right\} \tag{34}$$

$$\psi(x,t) \cong \sqrt{\frac{m}{2\pi i\hbar t}} \times \exp\left[\frac{i}{\hbar}(p_0x - E_0t)\right] \tag{35}$$

$$\exp\left[i\left(\frac{2\pi}{\lambda}x - \frac{v}{2\pi}t\right)\right] = \exp\left[\frac{i}{\hbar}(px - Et)\right] \tag{36}$$

$$K(x,t;p,0) \equiv \chi_p, 0(x,t) \int_{x'=-\infty}^{+\infty} dx'\ K(x,t;x',0) \underbrace{\chi_p, 0(x',0)}_{\equiv K(x',0;p,0)} \tag{37}$$

$$(\ K(x,0;p,0) \equiv)\chi_p(x,0) = \frac{1}{\sqrt{2\pi\hbar}} e^{\left(\frac{i}{\hbar}\right)xp} \tag{38}$$

$$\chi_p(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \exp\left[\frac{i}{\hbar}\left(xp - \frac{p^2}{2m}t\right)\right] \tag{39}$$

a particle with momentum p and energy $(p) = \frac{p^2}{2m}$.

In three dimensions:

$$\chi_p(x,t) = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}} \exp\left[\frac{i}{\hbar} r.p - \frac{i}{\hbar}\frac{p^2}{2m}t\right] \tag{40}$$

So for the free propagator in momentum,

$$K(p_2,t;p_1,0) = \ \delta(p_2 - p_1) \exp\left[-\frac{i}{\hbar}\frac{{p_1}^2}{2m}\right] t \tag{41}$$

With this form for K we can, conversely, return to real space:

$$K(x_2,t;x_1,0)$$
$$= \int \frac{dp}{2\pi\hbar} e^{\left(\frac{i}{\hbar}\right)(x_2-x_1)p} \exp\left[-\frac{i}{\hbar}\frac{p^2}{2m}t\right] \tag{42}$$

$$K_L(x_f,t_f;x_i,t_i) = \sqrt{\frac{m}{2\pi i\hbar(t_f-t_i)}}\left\{\exp\left[\frac{i}{\hbar}\frac{m}{2}\frac{(x_f-x_i)^2}{(t_f-t_i)}\right] - \exp\left[\frac{i}{\hbar}\frac{m}{2}\frac{(-x_f-x_i)^2}{(t_f-t_i)}\right]\right\}$$
$$= K(x_f,t_f;x_i,t_i) - K(-x_f,t_f;x_i,t_i) \tag{43}$$

$$K_L(x_f,t_f;x_i,t_i) = \sum_{r=-\infty}^{+\infty}(-1)^r\ K(x_r,t_f;x_i,t_i) \tag{44}$$

And obtain for propagator,

$$K_L(x_f,t_f;x_i,t_i) = \frac{i}{L}\sum_{n=-\infty}^{+\infty} \exp\left[-\frac{i}{\hbar}E_n(t_f-t_i)\right] \times\ \exp[-ik_n x_i] sin(k_n x_f) \tag{45}$$

The appearance of the δ-function implies energy and momentum quantization:

$$E_n = \frac{1}{2m}\frac{\pi^2\hbar^2}{L^2}n^2 \quad , \qquad k_n = \frac{\pi n}{L} \tag{46}$$

So final result reads $(t_f > t_i)$,

$$K_L(x_f,t_f;x_i,t_i) = \frac{2}{L}\sum_{n=1}^{\infty} \exp\left[-\frac{i}{\hbar}E_n(t_f-t_i)\right]\ sin(k_n x_i)\ sin(k_n x_f) \tag{47}$$

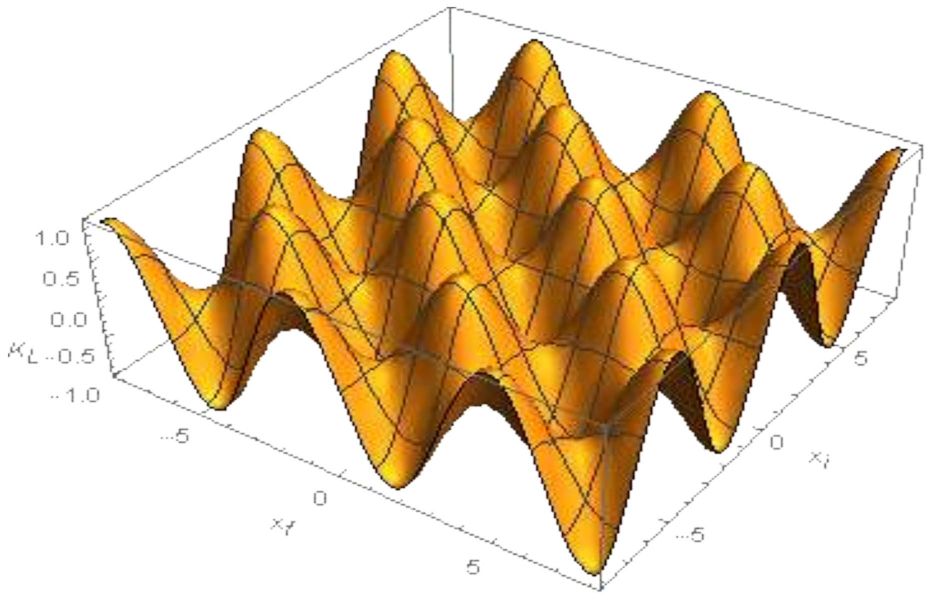

Figure 5. 3D visualization figure of K_L with x_i and x_f

Results and Discussion

From the some basic properties of the kernel, the retarded propagator satisfies

$$\left\lfloor i\eta\partial_{if} - \hat{H}\left(x_f, p_f = (\eta/i)\partial_{xf}, t_f\right)\right\rfloor K_r\left(x_f, x_i; t_f - t_i\right) = i\eta\delta\left(t_f - t_i\right)\delta\left(x_f - x_i\right)$$

Thus the retarded propagator is a Green's function for the Schrodinger equation.

For time-evolution operator the generator expression for a time-dependent Hamiltonian involves the time-ordered exponential is $U\left(t_f, t_i\right) = T\left(e^{-(i/\eta)\int_{t_i}^{t_f} dt'\hat{H}(t')}\right)$

The another key property of the time-evolution operator is

$$U\left(t_f, t_i\right) = U\left(t_f, t\right)U\left(t, t_i\right) \; t_i < t < t_f \, .$$

The evolution from time t_i to t_f is the same as evolution from t_i to t, following by evolution from t to t_f.

The action is functional because it takes a function as argument and returns a number. Particles always follow a path of least action. By varying (minimizing the variance of) the action, the path actually followed by a particle can be determined. There are an infinite number of paths connecting the two fixed points. This means that there are an infinite number of paths for the particle to follow between these two points. The actual path that the particle follows is the path of least action. The path of least action represents a minimum.

The principle of least action gives rise to the Euler-Lagrange equations. Hence the Lagrangian satisfies the Euler-Lagrange equation independently for each coordinate. The probability amplitude for the evolution of the system from the initial state $\left|q_0\right\rangle$ to the final state $\left|q_N\right\rangle$ is proportional to a weighted sum over all classical paths kinematically allowed, where each path is weighted with iS (with S being the classical action corresponding to the path). The larger is N, the number of intermediate steps, the better is the approximation of the classical action with the discrete sum of equation.

From the knowledge of the solution of the Schrodinger equation for a generic non-relativistic system, the wave function $\psi(\vec{q},t)$ is equivalent to the knowledge of the Green function of the Schrodinger equation with a particle initial condition.

According to Feynman's formulation of quantum mechanics, the particle explores all possible paths between fixed initial and final events. The action along these many paths plays a fundamental role.

It can be seen that from the path integral formalism, the propagator in the constant field is

$$K(x_2,t_2;x_1,t_1)=\left[2\pi i k(x_2)k(x_1)\int_{x_1}^{x_2}\frac{dx}{k(x)^3}\right]^{-\frac{1}{2}}\times\exp\left[i\int_{x_1}^{x_2}dx k(x)-\frac{i}{\eta}E_{cl}(t_2-t_1)\right]$$

Conclusion

In this paper the path integral expression for the propagator in quantum mechanics, especially the free particle and particle in the one-dimensional infinite potential well were derived. From the calculations, it can be clarified that all path contributes in a sense the quantum particle takes all paths and the amplitudes for each path add according to the usual quantum mechanical rule for combining amplitudes. By this path integral formalism, the propagator can be written as a sum over all possible paths between the initial and final points. Each path contributes $\exp\left[\frac{is}{\hbar}\right]$ to the propagator. In this work, it can be seen that path integral formalism are vividly described and important physical interpretations concerning the free particle have been given. The time evolution of the state is visualized in terms of Hamiltonian (H) and the time (Δt). It gives us the nature of shaply attenuated wave patterns. 3D visualization of K_L with x_i and x_f shows the sinusoidal wave patterns. Real and imaginary parts of kernel K is visualized in terms of space $(x_{2-}x_1)$ and time t. It shows the random wave patterns.

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