Notes on Quantum Mechanics using Lagrangian approach

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A brief introduction to contact transformations due to Dirac and path integral formulation of quantum mechanics with example.

In my beginning is my end - T.S.Eliot, Four Quartets

Contents

1 Introduction

A new approach to quantum theory was developed by Feynman in 1941. His motivation was to look for a formulation which would be in analogy with the Lagrangian approach of classical mechanics. Feynman's theory was based on the conjecture that the transition amplitude

$$\langle x', t + \Delta t | x, t\rangle = w \exp\left(\frac{i}{\hbar}\int_t^{t+\Delta t} L(x, \dot{x})dt\right)$$

where L is the langragian, Δt is assumed to be infinitesimally small and the weight factor w is assumed to be independent of the potential. The expression above is also known as the short time propagator.

Feynman was initially unsuccessful in finding a suitable way of incorporting the action integral in quantum mechanics i.e to retrieve the conventional quantum mechanics starting with action. One of the visiting professor at Princeton told him that there is a paper by Dirac where Lagrangian does come into Quantum Mechanics. Feynman was excited, and searched for the paper the next day.

As it turned out, the basic foundation of path integral formalism was developed over the next few days where Feynman built up on Dirac's idea and derived all the results one by one.

1.1 Functional Calculus - Basic Ideas

The concept of a functional and its calculus is important in the path integral formalism. The prime reason being that mostly we deal with the 'action' and it is also a functional.

A functional takes a function as an argument, as does a function of a function, and assigns it to a number. But they are not the same thing. Whereas, function of a function just looks at the value of the argument function, a functional looks at the entire behaviour of the argument function. In other words, functional takes as input a function y(x) on a domain – not the value of the function at a specific point x, but all the values of y at all the x's in the domain.

This can be better understood with the following example :

If $f(x) = x^2$ and $g(x) = e^{-x}$, then

$$y = g(f(x)) = e^{-f(x)} = e^{-x^2}$$

is a usual function of a function which takes particular 'x' and gives out a 'y' (i.e number).

The functional $y = g[f(x)]$ (square brackets to make the distinction) would also have a value that depends on f(x), but now it will not depend on a particular 'x' but specified range of 'x' (say from 0 to 1).

$$y = g[f(x)] = \int_0^1 f(x)dx = x^2dx$$

Also, the functional derivative is given by :

$$\frac{\delta F}{\delta \phi} = \lim_{h\to 0}\frac{1}{h}\left(\int g(x)(\phi(x) + h\delta(x-\xi))dx - F[\phi(x)]\right)$$

$$= \lim_{h\to 0} \frac{1}{h} \int g(x) h\delta(x-\xi) dx$$

$$= g(\xi)$$

1.2 Principle of Least Action & Euler- Lagrange Equations

One of the most natural and elegant way of determing the path x(t) is through principle of least action. The action S, is calculated for every path and the path that extremises (minimum) the action is the classical path. It means that $S[x(t)]$ will be unaffected in the first order if the $x(t)$ is changed slightly.

The action is given by,

$$S = \int_{t_a}^{t_b} L(\dot{x}, x, t)$$

$$\delta x(t_a) = \delta x(t_b) = 0$$

$$S[x + \delta x] = \int_{t_a}^{t_b} L(\dot{x} + \delta\dot{x}, x + \delta x, t) dt$$

$$= \int_{t_a}^{t_b} \left(L(\dot{x}, x, t) + \delta\dot{x}\frac{\partial L}{\partial \dot{x}} + \delta x \frac{\partial L}{\partial x} \right) dt$$

$$= S[x] + \int_{t_a}^{t_b} \left(\delta\dot{x}\frac{\partial L}{\partial \dot{x}} + \delta x \frac{\partial L}{\partial x} \right) dt$$

Integrating by parts, we get :

Now since, δx vanishes at the boundaries and we can choose δx arbitrarily along any of the infinite paths, we have

This is the classical Euler-Lagrange equation of the motion.

2 Lagrangian in Quantum Mechanics

Quantum Mechanics was based on the Hamiltonian formulation of classical mechanics. The prime reason appears to be that the canonical coordinate and momenta on which Hamiltonian thoery is based has a quite staright forward quantum analog. Since, there exists an alternate approach in the form of Lagrangian, it is obvious to think about a different formulation in its form. Equations of motion can be carved out using the stationary property of the action (time derivative of the Lagrangian) functional. In contrast, no such method exists for Hamiltonian method. Also, the action is more suited to relativistic invariance unlike the former.

One of the main advantages of the path integral formalism is that it enables one to discuss trajectories for the motion of particle in quantum mechanics and thus makes it resemble classical mechanics more. Dirac for the first time discussed about the Lagrangian in Quantum Mechanics in the paper [8] [9] . He argued that the propagator is analogous to $\exp(iS/\hbar)$. The main motivation was not to take the ideas of the classical Lagrangian theory, not the equations.

The motivation to go ahead with this approach is that the classical equation of motion comes out in a very simple way. If you take the limit $h \to 0$, the weight factor $\exp(iS/\hbar)$ oscillates very rapidly. Therefore, we expect that the main contribution to the path integral comes from paths that make the action stationary. This is nothing but the derivation of EL equation from the classical action. Therefore, the classical trajectory dominates the path integral in the small h limit. Secondly, we know what path the particle has chosen, even when we know the initial and final positions. This is a natural generalization of the two-slit experiment. Even if we know where the particle originates from and where it hit on the screen, we know which slit the particle came from. As it is discussed in [1], we can consider drilling infinite holes in the screen and we have to consider the contribution from all paths i.e the particle can come from any hole as it desires. The effectiveness of the path integral can also be clearly seen in how effectively it can calculate partition functions in statistical mechanics.

2.1 Contact Transformations & Transition Kernel

One of the most important ideas that can be directly lifted from classical mechanics was that of Contact Transformations (also called Canonical Transformations & Symplectomorphism). A transformation $(q,p) \mapsto (Q(q,p,t), P(q,p,t))$ is called a contact trnaformation if it preserves the Poisson bracket which is given by :

$$\{f,g\} = \frac{\partial f}{\partial x^i}\frac{\partial g}{\partial p_i} - \frac{\partial g}{\partial x^i}\frac{\partial f}{\partial p_i} = -\{g,f\}$$

Let there be some K that satisfies :

$$\dot{Q}^i = \frac{\partial K}{\partial P_i}; \dot{P}_i = \frac{\partial K}{\partial Q^i}$$

$$K(Q,P,t) = H(q,p,t) + \dot{F}(q,p,Q,P,t) \tag{1}$$

$$\delta \int_{t_i}^{t_f} \left(p_i \dot{q}^i - H(q,p,t)\right) dt = \delta \int_{t_i}^{t_f} \left(P_i \dot{Q}^i - K(Q,P,t)\right) dt$$

Out of the four generating functions , we have $F_1(q,Q,t)$.

$$\dot{F}_1(q,Q,t) = \frac{\partial F_1}{\partial q^i}\dot{q}^i + \frac{\partial F_1}{\partial Q^i}\dot{Q}^i + \frac{\partial F_1}{\partial t}$$

which upon substitution in (1) gives :

$$p_i = \frac{\partial F_1}{\partial q_i}; P_i = -\frac{\partial F_1}{\partial Q_i}$$

Now, F_1 can be identified with S and we can write with loss of generality,

$$p_r = \frac{\partial S}{\partial q_r}; P_r = -\frac{\partial S}{\partial Q_r}$$

$$\langle q^{'}|\alpha|Q^{'}\rangle = \int \langle q^{'}|\alpha|q^{''}\rangle dq^{''}\langle q^{''}|Q^{'}\rangle = \int \langle q^{'}|Q^{''}\rangle dQ^{''}\langle Q^{''}|\alpha|Q^{'}\rangle$$

$$\langle q'|q_r|Q'\rangle = q'_r\langle q'|Q'\rangle$$

$$\langle q'|p_r|Q'\rangle = -i\hbar\frac{\partial}{\partial q'_r}\langle q'|Q'\rangle \tag{2}$$

$$\langle q'|Q_r|Q'\rangle = Q'_r\langle q'|Q'\rangle$$

$$\langle q'|P_r|Q'\rangle = i\hbar\frac{\partial}{\partial Q'_r}\langle q'|Q'\rangle$$

$$\langle q'|f(q)g(Q)|Q'\rangle = \int\int \langle q'|f(q)|q''\rangle dq''\langle q''|Q''\rangle dQ''\langle Q''|g(Q)|Q'\rangle$$

$$= f(q')g(Q')\langle q'|Q']\rangle$$

$$\langle q'|\sum_k f_k(q)g_k(Q)|Q'\rangle = \sum_k f_k(q')g_k(Q')\langle q'|Q'\rangle$$

$$\langle q'|\alpha(qQ)|Q'\rangle = \alpha(q'Q')\langle q'|Q'\rangle$$

This is a remarkable equation as it gives the relation between $\alpha(qQ)$ which is a function of operators and $\alpha(q'Q')$ which is function of numerical variables.

Let us use this result for $\alpha = p_r$ and use :

$$\langle q'|Q'\rangle = e^{\frac{iU}{\hbar}}$$

where U is a function of q' and Q'

$$\langle q'|p_r|Q'\rangle = \frac{\partial U(q'Q')}{\partial q'_r}\langle q'|Q'\rangle$$

using eq. 1 above.

Comparing we get,

$$p_r = \frac{\partial U(qQ)}{\partial q_r} \tag{3}$$

Similarly using $\alpha = P_r$ we get,

$$P_r = -\frac{\partial U(qQ)}{\partial Q_r} \tag{4}$$

Dirac later also conjectured that the transition kernel can relate the initial wave function to the later wave function through the following equation :

$$\psi(x,t) = \int G(x,x_0)\psi(x_0,t_0)dx_0 \qquad where, t > t_0 \tag{5}$$

G is called the Kernel or a 'Propagator'. As discussed above, it was immediately recognised that the kernel was analogous to $exp(iS/\hbar)$.

But, analogous has a tricky meaning and is not explicit enough to establish the relation between different mechanics.

3 Path Integral Approach

Feynman in his nobel lecture said - '*So, I simply put them equal, taking the simplest example . But soon found that I had to put a constant of proportionality A in, suitably adjusted. When I substituted and just calculated things out by Taylor-series expansion, out came the Schrödinger equation. So I turned to Professor Jehle, not really understanding, and said, "Well you see Professor Dirac meant that they were proportional." Professor Jehle's eyes were bugging out – he had taken out a little notebook and was rapidly copying it down from the blackboard and said, "No, no, this is an important discovery.*"

3.1 The Quantum Mechanical Amplitude

In dealing with classical motion, only the path that extremises the action is of importance wheras in quantum mechanics all the paths that connect the starting and end points are of importance. Every possible path to go from 'a' to 'b' contributes to the amplitude. They moreover contributes equally to the amplitude but through different phases. The probability P(b,a) to go from x_a at time t_a to x_b at later time t_b is the absolute square of the amplitude $P(a,b) = |K(b,a)|^2$.

The amplitude $K(b,a)$ is the sum of contribution $\varphi[x(t)]$ from each path.

$$K(b,a) = \sum_{a \to b} \varphi[x(t)]$$

The contribution of a given path has a phase which is proportional to action S.

$$\varphi[x(t)] = A \times \exp\left(\frac{i}{\hbar} S[x(t)]\right)$$

where, A is a constant.

4 Recovering Schrödinger Equation from Path Integral

Schrödinger equation determines infinitesimal change in the wave function. To recover the Schrödinger equation. we have to consider infinitesimal form of the transition amplitude or the path integral.

$$S = \int L dt = L_{average} \epsilon \tag{6}$$

$$S = \frac{1}{2\epsilon} m(x-y)^2 - U\left(\frac{x+y}{2}\right)\epsilon \tag{7}$$

$$G(x,y) = \exp\left(i\frac{(x-y)^2}{2\epsilon\hbar}\right)(1-U)\frac{\epsilon}{\hbar} \tag{8}$$

Let us introduce a new variable, $\zeta = x - y$ and write $\psi(x, t+\epsilon)$ in terms of it.

$$\psi(x,t+\epsilon) \approx \int \exp\left(\frac{im\zeta^2}{2\hbar\epsilon}\right)\left(1 - \frac{i\epsilon}{\hbar}U(x-\frac{\epsilon}{2})\right)\psi(x-\zeta,t)d\zeta \tag{9}$$

Remembering that,

$$\psi(x-\zeta,t) = \psi(x,t) - \zeta\frac{\partial\zeta}{\partial x} + \frac{1}{2}\zeta^2\frac{\partial^2\zeta}{\partial^2 x} + ... \tag{10}$$

We finally get after throwing away the second order terms and letting $\epsilon \to 0$

$$\psi(x,t) = \int exp(\frac{im\zeta^2}{2\hbar\epsilon})\psi(x,t)d\zeta \tag{11}$$

This can be simplified by using the standard result of a Gaussian Integral and gives :

$$\psi(x,t) = \sqrt{\frac{2\pi i\hbar\epsilon}{m}}\psi(x,t) \tag{12}$$

We have

$$K = \sqrt{\frac{m}{2\pi i\hbar\epsilon}}\exp(\frac{iS}{\hbar}) \tag{13}$$

Plugging Taylor's expansion and writing

$$U\left(x - \frac{\zeta}{2}\right)\epsilon = U(x)\epsilon$$

$$\psi(x,t+\epsilon) \approx A\int \exp\left(\frac{im\zeta^2}{2\hbar\epsilon}\right)\left[1 - \frac{i\epsilon}{\hbar}U(x)\right]\left(\psi(x,t) - \zeta\frac{\partial\psi}{\partial x} + \frac{\zeta^2}{2}\frac{\partial^2\psi}{\partial x^2}\right)d\zeta$$

$$\psi(x,t+\epsilon) \approx \left[1 - \frac{i\epsilon}{\hbar}U(x)\psi(x,t)\right] - \left[A\frac{\partial\psi}{\partial x}\int exp(\frac{im\zeta^2}{2\hbar\epsilon})\zeta d\zeta\right] + \frac{A}{2}\frac{\partial^2\psi}{\partial x^2}\int exp(\frac{im\zeta^2}{2\hbar\epsilon})\zeta^2 d\zeta \tag{14}$$

Now, we see that the second term is an odd integral and it vanishes. The third can be readily evaluated [1]

$$\psi(x,t+\epsilon) = \psi(x,t) - \frac{i}{\hbar}\epsilon U(x)\psi(x,t) + \frac{1}{2}\frac{i\hbar\epsilon}{m}\frac{\partial^2\psi}{\partial x^2} \tag{15}$$

$$\psi(x,t+\epsilon) - \psi(x,t) = \frac{-i}{\hbar}\epsilon U(x)\psi(x,t) + \frac{1}{2}\frac{i\hbar\epsilon}{m}\frac{\partial^2\psi}{\partial x^2} \tag{16}$$

Simplifying we get,

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + U(x)\psi(x,t) \tag{17}$$

This is nothing but the time-dependent Schrödinger Equation. Also, we note that this can be extended to deal with any arbitrary time difference Δt by slicing it into N intervals. [7]

[1]

$$\int x^2\exp(-\xi x^2)dx = \frac{1}{2\xi}\sqrt{\frac{\pi}{\alpha}}$$

4.1 Propagator for Harmonic Oscillator

One of the major applications of the path integral formalism in intial days was to reproduce the results for the quantum harmonic oscillator obtained through the usual Schrödinger equation.

In case of harmonic oscillator, the lagrangian is given by :

$$L(x, \dot{x}) = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2 \tag{18}$$

We have to determine $S[x_{cl}(t)]$, for which, we look for a classical path $x_{cl}(t)$ which obeys $x_{cl}(0) = x_0$ and $x_{cl}(T) = x_f$.
The Euler-Lagrange equation gives us the classical equation of motion as :

$$m\ddot{x_{cl}} + m\omega^2 x_{cl} = 0$$

The general solution can be written as :

$$x_{cl}(t) = A\sin(\omega t) + B\cos(\omega t)$$

The boundary conditions $x_{cl}(0) = x_0$ and $x_{cl}(T) = x_f$ are satisfied for :

$$A = \frac{x_f - x_0\cos(\omega T)}{\sin(\omega T)} \quad ; \quad B = x_0$$

and that gives the classical path as ,

$$x_{cl}(t) = \frac{x_f - x_0\cos(\omega T)}{\sin(\omega T)}\sin(\omega t) + x_0\cos(\omega t) \tag{19}$$

Also, the velocity along the classical path is given by :

$$\dot{x_{cl}}(t) = \omega\left(\frac{x_f - x_0\cos(\omega T)}{\sin(\omega T)}\right)\cos(\omega t) - \omega x_0\sin(\omega t) \tag{20}$$

Using (19) and (20) in (18) and in turn using its time derivative in (13), gives the propagator 'K' for the harmonic oscillator as

$$K(x_f, T; x_0) = \sqrt{\frac{m\omega}{2\pi i\hbar\sin(\omega T)}}\exp\left(\frac{i}{2sin(\omega T)}\left[(x_f^2 + x_0^2)\cos(\omega T) - 2x_f x_0\right]\right)$$

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