# Chapter 20

# Lagrangian Formulation of Quantum Mechanics

## 20.1 Dirac's Transformation Theory Approach

Quantum mechanics as formulated by Heisenberg and Schrödinger, from different approaches and found to be equivalent, is based on the Hamiltonian formalism of classical mechanics. In 1933 Dirac gave a Lagrangian formulation of quantum mechanics, which is based on the Hamilton's principal function. He noted that in classical mechanics the dynamical variables $q$ and $p$ at a time $t_o$ are connected to the these variables at any other time by a contact (canonical) transformation generated by the "action function" $S$ which is the time integral of the Lagrangian taken between these two times: Usually a contact transformation consists of

$$q, p \longrightarrow Q_i(q,p), P_i(q,p),$$

where

$$P = -\frac{\partial S}{\partial Q} \quad , \quad p = \frac{\partial S}{\partial q}, \tag{20.1}$$

with

$$S = S(q, Q).$$

If one takes $q = q(t), p = p(t), Q = q(t_o), P = p(t_o)$ then (20.1) has the form

$$p(t_o) = -\frac{\partial S}{\partial q(t_o)} \quad , \quad p(t) = \frac{\partial S}{\partial q(t)},$$

with

$$S = \int_{t_o}^{t} dt' L(t'). \tag{20.2}$$

which is Hamilton's first principal function and $L(t)$ is the Lagrangian. The main hurdle in going over to quantum mechanics is that Lagrange equation involves partial derivations of the Lagrangian with respect to co-ordinates and velocities which can be done in terms of commutators with the Hamiltonian and one is back to square one, i.e., the Hamiltonian theory. Dirac has overcome this problem through what has come to be known as "transformation theory" in which the key element is the transformation function $< q|Q >$ which connects the representation in which $q$ is diagonal with the one in which $Q$ is diagonal. In general, an operator $\alpha$ can have matrix elements like $< q|\alpha|Q >$ which can be related to both $< q|\alpha|q' >$ and $< Q|\alpha|Q' >$ with the aid of the transformation function

$$< q|\alpha|Q > = \int < q|\alpha|q' > dq' < q'|Q > = \int < q|Q' > dQ' < Q'|\alpha|Q > . \tag{20.3}$$

If we put $\alpha = q$ we get from the above equation

$$< q'|q|Q' > = q' < q'|Q' > . \tag{20.4}$$

Similarly if we put $\alpha = p$ we get

$$< q'|p|Q' > = -i\hbar \frac{\partial}{\partial q'} < q'|Q' > . \tag{20.5}$$

Following the same procedure we get with $\alpha = Q$ and $\alpha = P$

$$< q'|Q|Q' > = Q' < q'|Q' >, \tag{20.6}$$

$$< q'|P|Q' > = i\hbar \frac{\partial}{\partial Q'} < q'|Q' > . \tag{20.7}$$

If we take

$$< q'|Q' >= exp\left[iU\frac{q'Q'}{\hbar}\right], \tag{20.8}$$

and use it in (20.5) and (20.7) we get

$$< q'|p|Q' > = \frac{\partial U(q'Q')}{\partial q'} < q'|Q' >, \tag{20.9}$$

$$< q|P|Q > = -\frac{\partial U(q', Q')}{\partial Q'} < q'|Q' > . \tag{20.10}$$

Comparing (20.9) and (20.10) with (20.5) and (20.7)

$$p = \frac{\partial U}{\partial q} \quad , \quad P = -\frac{\partial U}{\partial Q}.$$

These are quantum analog of classical contact transformation, $U$ being analogue of classical action $S$. We now set $q = q(t)$ and $Q = q(t_o)$ in (20.8) for quantum mechanics as was done in the classical case. It is clear that

$$< q(t)|q(t_o) > \quad \underrightarrow{\text{corresponds to}} \quad \exp\left[\frac{i}{\hbar}\int_{t_o}^{t} dtL(t)\right]. \tag{20.11}$$

It we take $t = t_o + dt$, then we have

$$< q(t+dt)|q(t) > \quad \underrightarrow{\text{corresponds to}} \quad exp\left[\frac{i}{h}L\ dt\right]. \tag{20.12}$$

This suggests that the Lagrangian should be taken as a function of $q(t)$ and $q(t+dt)$ rather than $q(t)$ and $\dot{q}(t)$.

The correspondence between the left and right hand sides of (20.11) can be examined by breaking up the time interval $(t - t_o)$ into small sections so that

$$B(t,t_o) = e^{\frac{i}{\hbar}\int_{t_o}^{t} dt' L(t')},$$
$$= B(t,t_m)B(t_m,t_{m-1})\cdots B(t_2,t_1)B(t_1,t_o) \tag{20.13}$$
$$< q(t)|q(t_o) > = \int < q(t)|q(t_m) > |dq(t_m) < q(t_m)|q(t_{m-1})dq(t_{m-1}) \cdots < q(t_2)(q(t_1)dq(t_1) < q(t_1)|q(t_o) > \tag{20.14}$$

It will be seen that while (20.13) has no integration, (20.14) has many. However on account of (20.8) each transformation function has the form $e^{iF/\hbar}$ where $F$ is a function of all the $q$'s. Because $\hbar$ is small $F/\hbar$ varies rapidly with $q$'s unless $F$ itself varies little. Thus contribution to integrals come from a very small region where $F$ is stationary with respect to small variations in $q$ and there is no contradiction between (20.13) and (20.14) and the correspondence (20.11) holds and we have what is known as Dirac's "action principle" in quantum mechanics.

The square of the transformation function can be interpreted as probability of $q$ having value $q(t)$ at time $t$ for a state for which an observation of $q$ at an earlier time $t_o$ is certain to give result $q(t_o)$. This is a kind of probability of a *path* is contrast to Hamiltonian quantum mechanics which gives probability of *position.* In order to obtain connection of the Lagrangian approach with the Hamiltonian approach, we note that the Schrödinger wave equation can be written in terms of the transformation function $< x'|x >$ in the integral form as

$$\psi(x', t+\epsilon) = \int dx(x'|x > \psi(x,t). \tag{20.15}$$

This can be verified as follows:

$$< x'|x > = < x'(t')|x(t) >\Big|_{t'=t+\epsilon} = < x'(t)|U(t+\epsilon,t)|x(t) >$$
$$= \exp\left(\frac{i\epsilon}{\hbar}H\right) < x'(t)|x(t) > . \tag{20.16}$$

Substituting (20.16) in (20.15) we get

$$\psi(x', t+\epsilon) = \int dx < x'(t)|x(t) > \exp\left(\frac{i\epsilon H}{\hbar}\right)\psi(x,t). \tag{20.17}$$

Since

$$< x'(t)|x(t) >= \delta(x - x'),$$

and

$$\exp\left(\frac{i\epsilon H}{\hbar}\right)\psi(x,t) = \psi(x, t+\epsilon),$$

equation (20.15) is verified which establishes the desired connection.

## 20.2 Feynman's Path Integral Approach

We have seen in the previous section that in the Lagrangian approach to quantum mechanics, the dynamics is determined by the transformation function $< q(t)|q(t_o) >$ which is interpreted by Dirac as the probability amplitude of the position operator $q$ having a value $q(t)$ at time $t$ for a state for which an observation at an earlier time $t_o$ is certain to give result $q(t_o)$. This is a probability amplitude for a particle path rather than its position which one encounters in Hamiltonian quantum mechanics. Feynman bases his formulation of quantum mechanics on such paths the basic principles of which can be states as:

The probability $P(b,a)$ of a particle moving from a point $a$ to $b$ is given by the square modulus of a complex number $K(b,a)$:

$$P(ba) = |K(b,a)|^2. \tag{20.18}$$

The amplitude of this probability $K(b,a)$ gets contribution from all possible paths from $a$ to $b$

$$K_{ab} = \sum_{\text{path}} k e^{iS/\hbar}. \tag{20.19}$$

The paths contribute equally in magnitude, but with phase determined by the classical action $S$ in units of $\hbar$.

$$S = \int_{\text{path}} dt L(t) \tag{20.20}$$

where $L(t)$ is the classical Lagrangian. The magnitude $k$ is fixed by the formula

$$K(c,a) = \sum_b K(c,b)K(b,a). \tag{20.21}$$

The complex function $K(b,a)$ is actually Dirac's transformation function:

$$K(x(t), x'(t')) =< x(t)|x'(t') >, \tag{20.22}$$

which as per previous section, can be written as

$$< x(t)|x'(t') > \xrightarrow{\text{corresponds to}} \prod_{n=1}^{N} \exp\left[\frac{i}{\hbar} S(x_n t_n, x_{N-1} t_{n-1})\right], \tag{20.23}$$

i.e.,

$$< x_n(t_n)|x_{n-1}(t_{n-1}) > \xrightarrow{\text{corresponds to}} \exp\left[\frac{i}{\hbar} S(x_n t_n, ), x_{N-1}(t_{n-1})\right]. \tag{20.24}$$

Feynman put forth the point that if the time interval $(t_n - t_{n-1}) = n \in\rightarrow 0$, the path becomes a straight line. In this case $n \propto \frac{1}{\epsilon}$ but $t_N = t$ is finite. He therefore put the equality

$$< x_n(t_n)|x_{n-1}(t_{n-1}) > \lim_{\substack{\epsilon\to 0\\ N\to\infty}} \frac{1}{A} \exp\left[\frac{i}{\hbar}(x_n(t_n, ), x_{n-1}(t_{n-1}))\right], \tag{20.25}$$

in place Diracs relation (20.24). The constant $A$ occuring in this equation depends on the Lagrangian. From this, Feynman obtained

$$\begin{aligned} < x(t), x'(t') > &= \lim_{\substack{\epsilon\to 0\\ N\to\infty}} \int dx_1 \int dx_2 \cdots \int dx_N \prod_{n=1}^{N} < x_n(t_n)|x_{n-1}(t_{n-1}) >, \\ &= \lim_{\substack{\epsilon\to 0\\ N\to\infty}} \int_{\frac{dx_1}{A}} \int \frac{dx_2}{A} \cdots \int \frac{dx_N}{A} \exp\left[\frac{i}{\hbar} S(x_n(t_n, ), x_{n-1}(t_{n-1}))\right], \end{aligned} \tag{20.26}$$

where

$$S(x_n(t_n), x_{n-1}(t_{n-1})) = \int_{t_{n-1}}^{t_n} dt' L(x'(t', dotx'(\dot{t}')). \tag{20.27}$$

Equation (20.26) can be written in shorthand as

$$< x(t)|x'(t') >= \int_{x'(t')}^{x(t)} D(x(t)) \exp \frac{i}{\hbar} S(x(t), x'(t')). \tag{20.28}$$

Feynman's formula (20.26) for Dirac's transformation function can be considered as a sum of action over space-time paths. Dirac had considered such splitting of the path as can be seen from the presentation in the previous section but his final formula was a correspondence, not an equality.

In Feynman's formalism, the transformation function is taken as the wave function:

$$< x(t)|x'(t') >= \psi(x, t), \tag{20.29}$$

although it is the probability amplitude for a particle coming from $x'(t')$ to be $x(t)$ and as such it has more information than what one would obtain from $\psi(x, t)$. With the definition (20.28), eqn. (20.21) would become

$$\psi(x, t) = \int dx'' < x(t)|x''(t'') > \psi(x'', t'') \tag{20.30}$$

Physically it tells us that the amplitude $\psi(x(t))$ for the particle to arrive at $x(t)$ is the sum (integral) over all possible values $x''(t'')$ to arrive at $x''(t'')$ is $\psi(x''t'')$ multiplied by the transformation function $< x(t)|x''(t'') >$

## 20.3 Dirac-Feynman Action Principle

Combining (20.25) and (20.30) of the foregoing section we get

$$\psi(x_{n+1}, t + \epsilon) = \int \frac{dx_n}{A} \exp\left[\frac{i}{\hbar} S(x_{n+1}, x_n)\right] \psi(x_n, t), \tag{20.31}$$

which is known as "Feynman equation" for the wave function. It tells that if the amplitude of the wave $\psi$ is known on a given surface consisting of all $x_n$ at a given time $t$, its value at a nearby point at a time $(t+\epsilon)$ is sum of contributions from all points on the surface at time $t$. Each contribution is delayed by an amount proportional to the action it would require to get from the surface to the point along the path of least action of classical mechanics. In this sense it is an action principle which can be named as, Dirac-Feynman action principle. It can also be called the Huygen's principles for matter waves as Feynman puts it. He also notes that Kirchofs' corrections to Huygen's principle are not needed since one has first order derivative in time.

## 20.4 Equivalence of Feynman and Schrödinger Equations

The first step in establishing the equivalence is to determine the normalization constant $A$ occurring in the Feynman equation (20.31). This is most easily done for a particle moving moving in one dimension under the action of a force for which

$$S(x_{n+1}, x_n) = \frac{m\epsilon}{2}\left(\frac{x_{n+1} - x_n}{\epsilon}\right)^2 - \epsilon V(x_{n+1}), \tag{20.32}$$

which on substitution in (20.31) gives

$$\psi(x_{n+1}, t+\epsilon) = \int \frac{dx_n}{A} \exp\left[\frac{i\epsilon}{\hbar}\left\{\frac{m}{2}\left(\frac{x_{n+1} - x_n}{\epsilon}\right)^2 - V(x_{n+1})\right\}\right], \tag{20.33}$$

In terms of

$$x = x_{n+1} \qquad \xi = x_{n+1} - x_n,$$

equation (20.33) has the form

$$\psi(x, t+\epsilon) = \int \frac{d\xi}{A} \exp\left[\frac{i\epsilon}{\hbar}\left(\frac{m\xi^2}{2\epsilon} - \epsilon V(x)\right)\right] \psi(x - \xi, t). \tag{20.34}$$

In the limit $\epsilon \to 0$ the term $e^{im\xi^2/2\hbar\epsilon}$ oscillates rapidly giving zero contribution to the integral except for small $\xi$. We can therefore expand $\psi(x-\xi,t)$ in a Taylor series in $\xi$ and obtain

$$\psi(x,t+\epsilon) = e^{\frac{-i\epsilon}{\hbar}V(x)} \int \frac{d\xi}{A} \exp\left(\frac{im\xi^2}{2\hbar\epsilon}\right) \times \left[\psi(x,t) - \xi\frac{\partial\psi}{\partial x} + \frac{\xi^2}{2}\frac{\partial^2\psi}{\partial x^2} + \cdots\right]. \tag{20.35}$$

Performing integration, we get

$$\psi(x,t+\epsilon) + \epsilon\frac{\partial\psi(xt)}{\partial t} = \frac{1}{A}e^{-i\epsilon V(x) over \hbar}\left(\frac{2\pi i\hbar}{m}\right)^{1/2} \times \left[\psi(xt) + \frac{i\epsilon\hbar}{2m}\ \frac{\partial^2\psi}{\partial x^2} + \cdots\right]. \tag{20.36}$$

Terms of order $\epsilon$ on both sides of this equation agree if

$$A = \left(\frac{2\pi i\epsilon\hbar}{m}\right)^{1/2} \tag{20.37}$$

Further, taking

$$e^{\frac{-i\epsilon V(x)}{\hbar}} = 1 - \frac{i\epsilon}{\hbar}V(x) \tag{20.38}$$

and substituting (20.39) and (20.40) in (20.38) gives

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\ \frac{\partial^2\psi}{\hbar}V(x) \tag{20.39}$$

which establishes the equivalence between Feynman and Schrödinger equation.

The equivalence can be established by showing that for a free particle moving in one dimension the probability amplitude $K(ab)$ defined in section 20.2 satisfies Schrödinger equation.

For this case

$$L = \frac{1}{2}m\dot{x}^2 \tag{20.40}$$

Writing

$$\dot{x}^2 = \left(\frac{x_n - x_{n+1}}{dt}\right)^2 dt = \frac{1}{\epsilon}(x_n - x_{n+1})^2 \tag{20.41}$$

where $dt = \epsilon$, we have from (20.26)

$$K(a,b) = \lim_{\substack{\epsilon\to 0\\ n\to\infty}} \int \frac{dx_1}{A} \int \frac{dx_2}{A} \cdots \int \frac{dx_{n-1}}{A} \exp\left[\frac{im}{2\epsilon}\sum_{n=1}^{n}(x_n - x_{n-1})^2\right]. \tag{20.42}$$

Substituting $A$ from (20.37) in (20.42) and making use of the identity

$$\int_{-\infty}^{\infty} dx_2 e^{-a(x_1-x_2)^2 - a(x_2-x_3)^2} = \left(\frac{\pi}{a}\right)^{1/2} e^{\frac{-1}{2}(x_1-x_3)^2} \tag{20.43}$$

and carrying out all integrations, the final result comes out to be

$$K(a,b) = \left[\frac{m}{2\pi i\hbar(t_b - t_a)}\right]^{1/2} \exp\left[\frac{im(X_b - X_a)^2}{2(t_b - t_a)}\right], \tag{20.44}$$

which is the Green's function for one-dimensional Schrödinger equation and satisfies the equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_a^2}K(a,b) = i\hbar\frac{\partial}{\partial t_a}K(a,b). \tag{20.45}$$

## 20.5 Concluding Remarks

It is instructive to put the four formulations of quantum mechanics for comparison in the same form as has been done by Feynman.

1. (a) Schrödinger Wave Mechanics :

$$\psi(x, t+\epsilon) = -\frac{i\epsilon H}{\hbar}\psi(x,t) \tag{20.46}$$

2. (b) Heisenberg Quantum Mechanics:

$$x(t+\epsilon) = \exp\left[\frac{i\epsilon H}{\hbar}\right] x(t) \exp\left[-\frac{i\epsilon H}{\hbar}\right] \tag{20.47}$$

3. (c) Dirac's Lagrangian Quantum Mechanics:

$$\psi(x', t+\epsilon) = \int dx < x'|x >_\epsilon \psi(xt) \tag{20.48}$$

4. (d) Feynman Formulation:

$$\psi(x_{k+1}, t+\epsilon) = \int \frac{dx_k}{A} \exp\left[\frac{i}{\hbar} S(x_{k+1}, x_k)\right] \psi(x_k, t) \tag{20.49}$$

In this connection, the following remarks are in order

(a) The wave function $\psi(x', t+\epsilon)$, represents a state in a representation in which $x'$ is diagonal while $\psi(x, t)$ represents, a state in which $x$ is diagonal. Dirac's transformation function $< x'|x >_\epsilon$ relates these two.

(b) Dirac's $< x'|x >_\epsilon$ and Feynman's $\frac{1}{A}\exp[\frac{i}{\hbar}S(x', x)]$ are analogous.

(c) Feynman states in his paper in Reviews of Modern Physics that "Dirac's remarks were starting point of the present development".

## References and Sources

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