CHAPTER I

INTRODUCTION : HISTORICAL REVIEW AND FEYNMAN PROPAGATOR

1.1 Introduction and Historical Review

The hydrogen atom is the dynamical system consists of two particles difference in charge, the proton or nucleus with positive charge (+ e) another is the electron with negative charge (-e) moving about the first particle under the influence of attractive Coulomb potential. It was the success of the old quantum theory that could be used to calculate the energy spectrum of the hydrogen atom. Then, the new quantum theory was discovered, first Heisenberg discovered the matrix mechanics, and later, Schroedinger discovered wave mechanics. By using the new quantum theory one can calculate the energy spectrum and the wave functions of the hydrogen atom exactly. Now one of the major topics which comprises vital part of current textbooks on quantum mechanics is the hydrogen atom problem. In 1948, Feynman (1) proposed a new approach to quantum mechanics which provides the propagator or the probability amplitude of a particle as a path integral over all possible histories of the system that is characterized by the Lagrangian. Then the path integral approach has attracted much attention and has proven useful in many areas of physics including statistical mechanics, many body theory, field theory and others. A strange fact is that Feynman's theory has been powerless in solving the hydrogen atom problem, whose solution once symbolized the success of quantum mechanics has been left unsolved for some thirty years.

Historically, many physicists attempted to treat the hydrogen atom problem within the framework of Feynman approach. Gutzwiller(2) performed the path integration in phase space by using the semiclassical approximation. The Green's function evaluated approximately were found to give rise exactly to Bohr's formula for the bound state energy. The resdue values of approximate Green's function were shown to yield all the exact wave functions of the bound states, but this is the semi-classical not the analytical calculation of the Coulomb path integral.

A direct and analytical solution for the hydrogen atom problem via path integral then treated by Goovaerts and Devreese (3). They evaluated an integral transform of the propagator by means of the exact summation of a modified parturbation expansion to obtain the exact energy spectrum and to show a possible way of finding the wave functions, but the calculations are too complicated to be informative and the result is not given in a closed form. In 1979 Duru and Kleinert(4) proposed an important procedure for solving the hydrogen atom problem. The procedure consists of the following two key steps i) the reparameterization of paths in terms of a new time ii) the change of variables by the Kustaanheimo-Stiefel transformation. The transformation converts the phase space path integral of the three dimensional Coulomb problem into a four dimensional harmonic oscillator which is exactly solvable. According to Duru and Kleinert's ideas, Ho and Inomata (5) used these two key steps and performed the configuration space path integration. They obtained the Green's function of the hydrogen atom exactly with the same result as that of Duru and Kleinert. From this Green's function we can examine the energy spectrum of the hydrogen atom which is equivalent to Bohr's formula for the energy level of the hydrogen atom.

In the next section we will review the propagator and Feynman's path integral. Some sovable solutions which can be performed by path integral such as the free particle and the harmonic oscillator problems will be presented. In chapter II we will study the two dimensional hydrogen atom by means of both Lagrangian and Hamiltonian path integrations, and in chapter III the three dimensional hydrogen atom problem were treated. Then, in chapter IV and V, we show how to examine the energy spectrum and the wave functions of the hydrogen atom from the Green's function. The condusion will be contained in chapter VI.

1.2 The Propagator and Feynman's Path Integral

In quantum mechanics, the dynamical information of a quantum mechanical system is contained in the wave function. It is a function sometimes called probability amplitude that determined the waves associated with a particle. In practice, we can obtain this wave function by solving the Schroedinger's equation.

In Schroedinger's picture (6), there exists the state vector $|\psi(t)>$ evolves as

$$|\psi(t)> \quad = \quad U(t, t') \; |\psi(t')> \qquad (1.1)$$

where $U(t, t')$ is the time evolution operator satisfying the following properties,

i) $i\hbar \dfrac{\partial U(t,t')}{\partial t} = HU(t, t')$

ii) $U(t', t') = 1$

iii) $U(t'', t)U(t, t') = U(t'', t')$

iv) $U^{+}(t'', t') = U^{-1}(t'', t') = U(t', t'')$

and H is the Hamiltonian. If the Hamiltonian is not an explicit function of time then the evolution operator is of the form

$$U(t'', t') = \exp\left\{ -\frac{i}{\hbar}(t'', t')H \right\} \qquad (1.2)$$

In configuration representation (1.1) becomes

$$\langle \vec{x}'' | \psi(t'') \rangle = \int_{-\infty}^{\infty} \langle \vec{x}'' | U(t'', t') | \vec{x}' \rangle \langle \vec{x}' | \psi(t') \rangle \, d^3x' \qquad (1.3)$$

where the complete set

$$\int_{-\infty}^{\infty} | \vec{x}' \rangle \langle \vec{x}' | \, d^3 x' = 1 \qquad (1.4)$$

We can rewrite equation (1.3) as

$$\psi(\vec{x}'', t'') = \int_{-\infty}^{\infty} K(\vec{x}'', \vec{x}'; t'', t') \, \psi(\vec{x}', t') d^3x' \qquad (1.5)$$

where $k(\vec{x}'', \vec{x}' ; t'', t') = \langle \vec{x}'' | U(t'', t') | \vec{x}' \rangle$ (1.6)

$K(\vec{x}'', \vec{x}'; t'', t')$ is called the propagator or the probability amplitude of a particle to go from $\vec{x}'$ at time t' to $\vec{x}''$ at time t''.

According to Feynman's ideas, there are infinitely many paths of a particle to go from the initial point to the final point under restrictive conditions that $\vec{x}(t') = \vec{x}'$, $\vec{x}(t'') = \vec{x}''$. Each trajectory contributes to the total amplitude to go from $\vec{x}'$ to $\vec{x}''$. They contribute equal amounts to the total amplitude, but contribute at different phases. The phase of the contribution from a given path is the action S for that path in units of the quantum of action $\hbar$. That is, to summarise, the probability $P(\vec{x}'', \vec{x}')$ to go from a point $\vec{x}'$ at t' to the point $\vec{x}''$ at t'' is the absolute square $P(\vec{x}'', \vec{x}') = |K(\vec{x}'', \vec{x}' ; t'', t')|^2$ of an amplitude $K(\vec{x}'', \vec{x}'; t'', t')$ to go from $\vec{x}'$ to $\vec{x}''$. This amplitude is the sum of contribution $\varphi[\vec{x}(t)]$ from each path

$$K(\vec{x}'', \vec{x}', t'', t') = \sum_{\substack{\text{over all paths} \\ \text{from } \vec{x}' \text{ to } \vec{x}''}} \varphi[\vec{x}(t)] \qquad (1.7)$$

The contribution of a path has a phase propartional to the action S

$$\varphi[\vec{x}(t)] = \text{const } e^{\frac{1}{\hbar} S[\vec{x}(t)]} \qquad (1.8)$$

and

$$S = \int_{t'}^{t''} L(\vec{x}, \dot{\vec{x}})\, dt \qquad (1.9)$$

with the Lagrangian

$$L(\vec{x}, \dot{\vec{x}}) = \frac{1}{2} m\dot{\vec{x}}^2 - V(\vec{x}) \qquad (1.10)$$

Actually, we can not evaluate $K(\vec{x}'', \vec{x}' ; t'', t')$ from (1.7) directly because of their infinitely many paths contribution. Feynman (1) proposed another way to perform a new formalism of $K(\vec{x}'', \vec{x}' ; t'', t')$. By dividing the time variable into step of width $\varepsilon \to o$, this give us a set of value t_i spaced a distance ε apart between the values t' and t''. At each time t_i we select some special $\vec{x}_i$ and construct a path by connecting all points. It is possible to define a sum over all paths in this manner by taking a multiple integrals over all values of $\vec{x}_i$ for i between 1 and N-1, where

$$N\varepsilon = t'' - t'$$

$$\varepsilon = t_i - t_{i-1}$$

$$t_o = t'$$

$$t_N = t''$$

$$\vec{x}_o = \vec{x}' \quad ; \quad \vec{x}_N = \vec{x}''$$

The resulting equation is

$$K(\vec{x}'', \vec{x}' ; t'', t') = \lim_{N\to\infty} \iint\cdots\int \frac{e^{\frac{i}{\hbar} S[\vec{x}(t)]}}{A} \frac{d^3x_1}{A} \frac{d^3x_2}{A} \cdots \frac{d^3x_{N-1}}{A} \qquad (1.11)$$

where $S[\vec{x}(t)] = \int_{t'}^{t''} L(\vec{x}, \dot{\vec{x}})\, dt$ and the normalizing factor $A = \left(\frac{2\pi i\hbar\varepsilon}{m}\right)^{3/2}$.

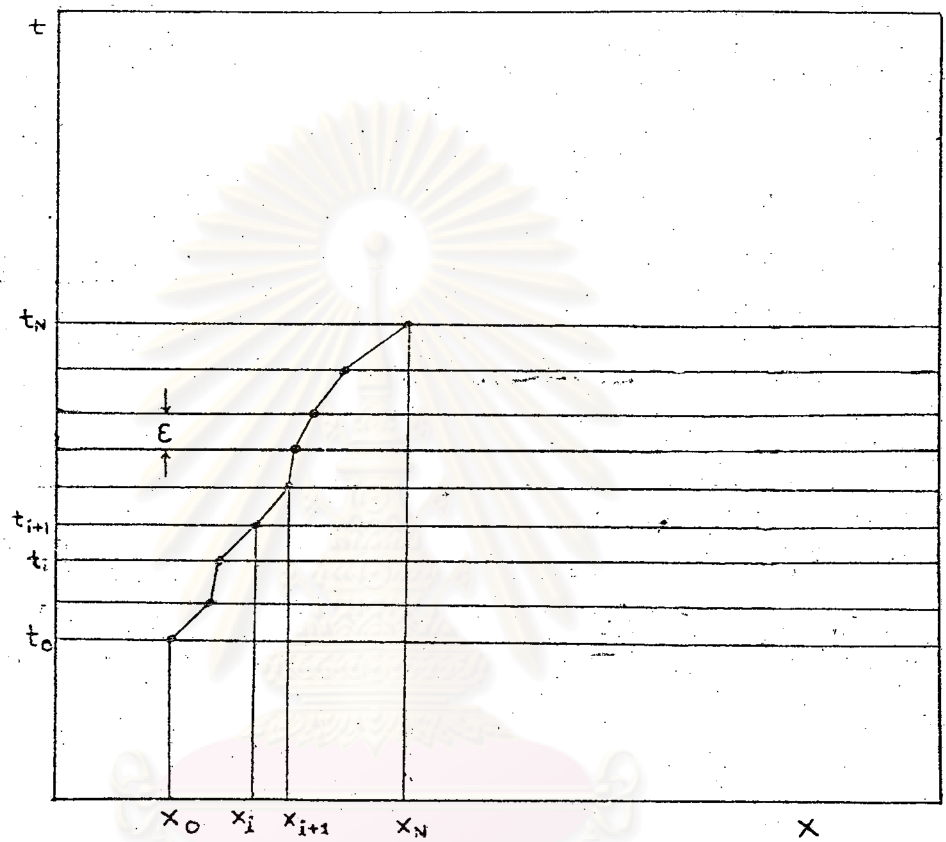

Fig. 1 The sum over paths is defined as a limit, in which at first the path is specified by giving only its coordinate x at a large number of specified times separated by very small intervals ε . The path sum is then an integral over all these specific coordinates. Then to achieve the correct measure, the limit is taken as ε approaches 0.

For the small time slices

$$S(t_j\,,\,t_{j-1}) \;=\; \int_{t_{j-1}}^{t_j} L(\vec{x},\dot{\vec{x}})\,dt$$

$$\sim \frac{m}{2\varepsilon}(\vec{x}_j-\vec{x}_{j-1})^2 - \varepsilon V(\vec{x}_j) \qquad (1.12)$$

so that (1.11) can be written as

$$K(\vec{x}'',\vec{x}';t'',t') = \lim_{N\to\infty}\left(\frac{m}{2i\pi\hbar\varepsilon}\right)^{(3/2)N}\iint\cdots\int \exp\frac{i}{\hbar}\left\{\sum_{j=1}^{N}\left(\frac{m}{2\varepsilon}(\vec{x}_j-\vec{x}_{j-1})^2 - \varepsilon V(\vec{x}_j)\right)\right\} \times d^3x_1\,d^3x_2\ldots d^3x_{N-1} \qquad (1.13)$$

Feynman wrote this sum over all paths in a less restrictive notation as

$$K(\vec{x}'',\vec{x}';t'',t') = \int_{\vec{x}'}^{\vec{x}''} e^{\frac{i}{\hbar}S[\vec{x}'',\vec{x}']}\,\mathcal{D}\vec{x}(t) \qquad (1.14)$$

which he called a path integral. Next sections we consider the path integral of the free particle and the harmonic oscillator in one dimension.

1.3 The Path integral of a Free Particle

From (1.13) we can use it to compute the propagator of a free particle. The Lagrangian for a free particle is

$$L(\vec{x}\,,\dot{\vec{x}}) = \frac{1}{2}m\dot{\vec{x}}^2 \qquad (1.15)$$

Thus with the helps of (1.13) the propagator for a free particle in one dimension is

$$K(\vec{x}'', \vec{x}' \; ; \; t'', t') = \lim_{N\to\infty} \int\int \ldots \int \exp\left\{ \frac{im}{2\hbar\varepsilon} \sum_{j=1}^{N} (x_j - x_{j-1})^2 \right\}$$

$$\left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{N/2} dx_1 dx_2 \ldots dx_{N-1} \qquad (1.16)$$

It is the integral of the form $\int_{-\infty}^{\infty} \exp(-ax^2 + bx)dx$ which called a gaussian integral. Since the integral of a gaussian is again gaussian, we may carry out the integrations on one variable after the other and with the helps of the formula

$$\int_{-\infty}^{\infty} \left(\frac{2\pi i\hbar\varepsilon}{m}\right)^{-\frac{1}{2}} \exp\left\{ \frac{im}{2\hbar\varepsilon} \left((x_2 - x_1)^2 + (x - x_o)^2 \right) \right\} dx_1$$

$$= \left(\frac{2\pi i\hbar 2\varepsilon}{m}\right)^{-\frac{1}{2}} \exp\left\{ \frac{m(x_2 - x_o)^2}{2i\hbar(2\varepsilon)} \right\} \qquad (1.17)$$

After the integrations are completed, the limit may be taken. The result is

$$K(\vec{x}'', \vec{x}' \; ; \; t'', t') = \left[\frac{2\pi i\hbar(t''-t')}{m}\right]^{\frac{1}{2}} \exp\left\{ \frac{im}{2\hbar} \frac{(x''-x')^2}{(t''-t')} \right\} (1.18)$$

1.4 The Harmonic Oscillator

In principle, if the path integral still be a gaussian form, it is possible to carry out the integral over all paths in a way which described in the previous section. But in real practice, it is too complicated to perform, for example, the harmonic oscillator problem. We will present an alternative calculation of the propagator of the harmonic oscillator in the following ways.

Let $\bar{x}(t)$ be the classical path between the end points. This is the path which is the extremum for the action S,

$$S_{cl}[x(t)] = S[\bar{x}(t)] \tag{1.19}$$

We can represent x in term of $\bar{x}$ and y

$$x = \bar{x} + y \tag{1.20}$$

Namely, instead of definding a point on the path by its distance x(t) from an arbitrary axis, we measure instead the deviation y(t) from the classical path as shown in Fig. 2

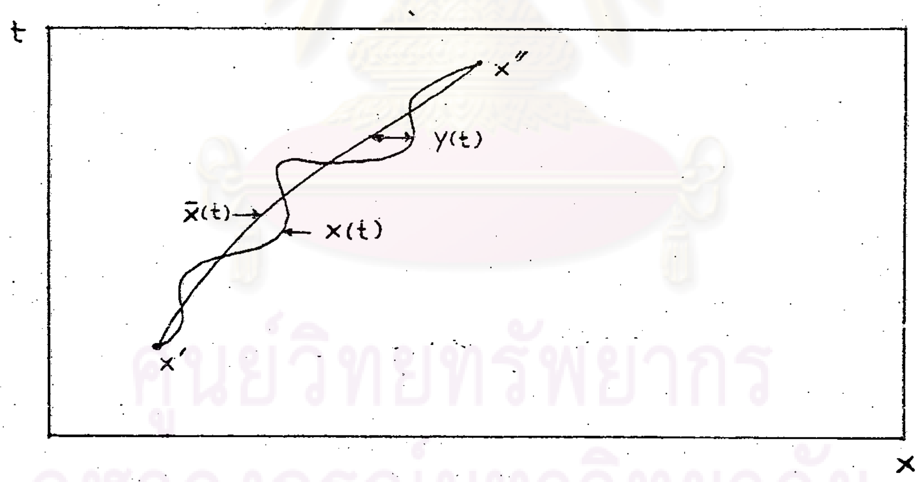

Fig. 2 The difference between the classical path $\bar{x}(t)$ and some possible alternative path y(t). The end point y(t") = y(t') = 0.

At each t the variables x and y differ by the constant $\bar{x}$. Therefore, clearly $dx_j = dy_j$ for each specific point t_j in the subdivision of time. In general we may say $\mathcal{D}x(t) = \mathcal{D}y(t)$. The integral for the action can be written as

$$S[x(t)] = \int_{t'}^{t''} [a(t)(\dot{\bar{x}}^2 + 2\dot{\bar{x}}\dot{y} + y^2) + \ldots] dt \qquad (1.21)$$

If all terms which do not involve y are collected the resulting integral is just $S[\bar{x}(t)] = S[_{C\ell} x(t)]$. Further more, all terms which contain y as a linear factor are collected, the resulting integral vanishes. The function $\bar{x}(t)$ is so chosen that satisfies the variational principle, the propagator $K(\vec{x}'', \vec{x}' ; t'', t')$ can be written as

$$K(\vec{x}'', \vec{x}'; t'', t') = e^{\frac{i}{\hbar} S_{C\ell}[\vec{x}(t)]} \int_{o}^{o} \exp\left\{ \frac{i}{\hbar} \int_{t'}^{t''} [a(t)\dot{y}^2 + b(t)\dot{y}y + c(t)y^2] dt \right\} \mathcal{D}y(t) \qquad (1.22)$$

where $$\int_{o}^{o} \mathcal{D}y(t) = \lim_{N\to\infty} \int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} dy_1 dy_2 \ldots dy_{N-1} (A)^{-N/2} \qquad (1.23)$$

For the harmonic oscillator, the Lagrangian as

$$L(\vec{x}, \dot{\vec{x}}) = \frac{m}{2}(\dot{\vec{x}}^2 - \omega^2\vec{x}^2) \qquad (1.24)$$

so that

$$K(x'', x' ; t'', t') = \int_{x'}^{x''} \exp\left\{ \frac{i}{\hbar} \int_{t}^{t''} dt \frac{m}{2}(\dot{x}^2 - \omega^2 x^2) \right\} \mathcal{D}x(t)$$

$$= e^{\frac{i}{\hbar} S_{C\ell}[x(t)]} \int_{0}^{0} \exp\left\{ \frac{i}{\hbar} \int_{0}^{\tau} \frac{m}{2}(\dot{y}^2 - \omega^2 y^2) dt \right\} \mathcal{D}y(t)$$

$$= e^{\frac{i}{\hbar} S_{C\ell}[x(t)]} F(\tau) \qquad (1.25)$$

where $\tau = t'' - t'$. The action $S_{C\ell}[x(t)]$ can be performed exactly, the result is

$$S_{C\ell}[x(t)] = \frac{im\omega}{2\hbar \sin(\omega\tau)} \left[(x''^2 + x'^2) \cos(\omega\tau) - 2x''x' \right] \qquad (1.26)$$

Since all paths $y(t)$ go from 0 at $t = t'$ to 0 at $t = t''$, such paths can be written as a Fourier Sine series with a foundamental period of τ

$$y(t) = \sum_{n} a_n \sin\left(\frac{n\pi t}{\tau}\right) \qquad (1.27)$$

The function $F(\tau)$ in equation (1.25) can be written as

$$F(\tau) = J \int\int \cdots \int \exp\left\{ \sum_{n=1}^{N} \frac{im}{2\hbar}\left[\left(\frac{n\pi}{\tau}\right)^2 - \omega^2\right] a_n^2 \right\} \frac{da_1}{A} \frac{da_2}{A} \cdots \frac{da_N}{A} \qquad (1.28)$$

where J is the Jacobian of transformation which is a constant . After integration and taking the limit $N \to \infty$ we find

$$F(\tau) = \left[\frac{m}{2\pi i\hbar \sin(\omega\tau)}\right]^{\frac{1}{2}} \qquad (1.29)$$

Finally , the harmonic oscillator's propagator can be performed exactly in the form :

$$K(x'', x'; t'', t') = \left[\frac{m\omega}{2\pi i\hbar \sin(\omega\tau)}\right]^{\frac{1}{2}} \exp\left\{\frac{im}{2\hbar \sin(\omega\tau)}\left[(x''^2 + x'^2)\cos(\omega\tau) - 2x'x''\right]\right\} \qquad (1.30)$$