CHAPTER II

THE HYDROGEN ATOM IN TWO DIMENSIONS

In this chapter we will examine the Green's function of the two dimensional hydrogen atom by means of path integration. The two dimensional hydrogen atom is a system in which an electron moves about a nucleus in a plane under the influence of an attractive Coulomb potential. It is a simple model that can be solved exactly by path integration. First, we study the Lagrangian path integral for the two dimensional hydrogen atom which has been solved by Inomata (7). The Hamiltonian path integral which has been solved by Duru and Klienert (8) will be discussed later.
The procedure consists of two steps; the rescaling of time parameter and the change of variables from Cartesian coordinates to parabolic coordinates.

2.1 Green's Function and Time Reparameterization.

Instead of considering the propagator $K(\vec{x}'', \vec{x}'; t'', t')$, we will determine its Fourier transform, the energy dependent Green's function

$$G(\vec{x}'', \vec{x}'; E) = \int_0^\infty K(\vec{x}'', \vec{x}'; \tau)\, e^{\frac{iE\tau}{\hbar}}\, d\tau \qquad (2.1)$$

which still contains all necessary information of a quantized system. For the two dimensional hydrogen atom problem, the propagator is given in the form,

$$K(\vec{x}'', \vec{x}' ; \tau) = \int_{x'}^{x''} \exp\left\{ \frac{i}{\hbar} \int_{0}^{\tau} L(\vec{x}, \dot{\vec{x}}) \, dt \right\} \mathcal{D} \vec{x}(t) \qquad (2.2)$$

with the Lagrangian

$$L(\vec{x}, \dot{\vec{x}}) = \frac{1}{2} m\dot{\vec{x}}^2 + \frac{e^2}{r} , \qquad (2.3)$$

$$\text{where} \qquad r = (x^2 + y^2)^{\frac{1}{2}} , \qquad (2.4)$$

or in the Hamiltonian path integral form (9)

$$K(\vec{x}'',\vec{x}' ; \tau) = \iint \exp\left\{ \frac{i}{\hbar} \int_{0}^{\tau} [\vec{p} \cdot \dot{\vec{x}} - H(\vec{p}, \vec{x})] dt \right\} \frac{1}{(2 \pi\hbar)^2} \mathcal{D}\vec{x}(t) \mathcal{D}\vec{p}(t)$$

$$(2.5)$$

with the Hamiltonian

$$H(\vec{p}, \vec{x}) = \frac{\vec{p}^{\,2}}{2m} - \frac{e^2}{r} \qquad (2.6)$$

On the polygonal basis, the Coulomb propagator (2.2) can be written as

$$K(\vec{x}'',\vec{x}' ; \tau) = \lim_{N \to \infty} \iint \cdots \int \exp \frac{i}{\hbar}\left\{ \sum_{j=1}^{N} \left[\frac{m(\Delta\vec{x}_j)^2}{2\tau_j} + \frac{e^2\tau_j}{\bar{r}_j} \right] \right\}$$

$$\times \prod_{j=1}^{N} \left(\frac{m}{2\pi i\hbar\tau_j}\right) \prod_{j=1}^{N-1} d^2x_j \qquad (2.7)$$

where $\tau_j = t_j - t_{j-1} = \varepsilon$ and $\bar{r}_j$ being the mid-point value of $\bar{r}_j$ to be specified later. Substituting (2.7) into (2.1) we obtain

$$G(\vec{x}'', \vec{x}'; E) = \lim_{N\to\infty} \int\int \ldots \int \exp\left\{ \frac{i}{\hbar} \sum_{j=1} \left[\frac{m(\Delta\vec{x}_j)^2}{2\tau_j} + \frac{e^2\tau_j}{\bar{r}_j} + E\tau_j \right] \right\}$$

$$\times \prod_{j=1}^{N} \left(\frac{m}{2\pi i\hbar\tau_j}\right) \prod_{j=1}^{N-1} d^2x_j \, d\tau \qquad (2.8)$$

Because of the nongaussian type of the integral, we can not carry out this path integral directly. Therefore we must reduce it into a gaussian form. The first step of the reduction procedure is to apply the time rescaling, for each short time interval,

$$\tau_j \to \sigma_j = \frac{\tau_j}{\bar{r}_j} \qquad (2.9)$$

In the limit $N \to \infty$ the local scaling relation

$$dt \to ds = \frac{dt}{r(t)} \qquad (2.10)$$

and notice that

$$\tau = \sum_{j=1}^{N} \tau_j \qquad (2.11)$$

The small change in τ may be described by

$$\Delta\tau = \sum_{j=1}^{N} \tau_j - \sum_{j=1}^{N-1} \tau_j = \tau_N \qquad (2.12)$$

from (2.9) we get

$$\Delta\tau = \bar{r}_N\sigma_N \qquad (2.13)$$

Again, in the limit $N \to \infty$, there follows

$$d\tau = r'' d\sigma \tag{2.14}$$

where $d\sigma$ is the limiting value of σ_N , that is, the value of ds at r".

With the newly scaled time variable, the Green's function (2.8) can be expressed as

$$G(\vec{x}'', \vec{x}';E) = \lim_{N\to\infty} \iiint\cdots\int \exp\left\{ \frac{i}{\hbar} \sum_{j=1}^{N} \left[\frac{m(\Delta\vec{x}_j)^2}{2\bar{r}_j\sigma_j} + e^2\sigma_j + E\bar{r}_j\sigma_j \right] \right\}$$

$$\times \prod_{j=1}^{N} \left(\frac{m}{2\pi i\hbar\sigma_j\bar{r}_j} \right) \prod_{j=1}^{N-1} d^2x_j r'' d\sigma \tag{2.15}$$

We see that the appearance of the radial variable in the denominator of the kinetic energy term still keeps the path integral in (2.15) nongaussian type. The next step of the reduction procedure is to eleminate a residual effect from the kinetic term by transforming the integration variables from Cartesian coordinates to parabolic coordinates.

2.2 The Levi-Civitá Transformation and the Coulomb Green's Function from the Lagrangian Path Integral.

The Green's function (2.15) expressed in terms of the new time parameter, may be put into the form

$$G(\vec{x}'',\vec{x}',E) = \int_0^\infty \exp\left\{ \frac{ie^2\sigma}{\hbar} \right\} Q(\vec{x}'', \vec{x}'; \sigma)\, d\sigma \tag{2.16}$$

where

$$Q(\vec{x}'', \vec{x}';\sigma) = \lim_{N\to\infty} \int\int \cdots \int \exp\left\{ \frac{i}{\hbar} \sum_{j=1}^{N} S(\sigma_j) \right\}$$

$$\times \prod_{j=}^{N} \left(\frac{m}{2\pi i \hbar \tau_j}\right) \prod_{j=1}^{N-1} (\bar{r}_j)^{-1} \, d^2 x_j \tag{2.17}$$

and

$$S(\sigma_j) = \frac{m(\Delta\vec{x}_j)^2}{2\bar{r}_j \sigma_j} + E\,\bar{r}_j \sigma_j \tag{2.18}$$

Thus the problem is reduced to evaluate the path integral $Q(\vec{x}'',\vec{x}',\sigma)$ with the short time action (2.18).

To convert the non gaussian path integral (2.17) into a gaussian form, the Levi-Civita transformation (10) is used for mapping from Cartesian coordinates $\vec{x}(x, y)$ to parabolic coordinates $\vec{u}(\xi, \eta)$ in two dimensions,

$$\begin{aligned} x &= \xi^2 - \eta^2, \\ y &= 2\xi\eta . \end{aligned} \tag{2.19}$$

In the matrix representation,

$$x = A(u) \cdot \vec{u} \tag{2.20}$$

or

$$x^a = \sum_{b=1}^{2} A^{ab}(u) u^b \tag{2.21}$$

where $x^1 = x$, $x^2 = y$, $u^1 = \xi$, $u^2 = \eta$ and

$$A(u) = \begin{bmatrix} u^1 & -u^2 \\ u^2 & u^1 \end{bmatrix} \qquad (2.22)$$

The transformation matrix (2.22) is orthogonal in the sense that

$$\tilde{A}(u) \;.\; A(u) = rI \qquad (2.23)$$

where $r = \vec{u}^2 = \xi^2 + \eta^2$ (2.24)

Then the space interval obey the following transformation rule

$$\Delta\vec{x}_j = 2A(\bar{u}_j) \,.\, \Delta\vec{u}_j \qquad (2.25)$$

where $\bar{u}_j^a = \frac{1}{2}(u_j^a + u_{j-1}^a)$; $\Delta\vec{u}_j = \vec{u}_j - \vec{u}_{j-1}$

and $A(\bar{u}_j) = \begin{bmatrix} \bar{u}_j^1 & -\bar{u}_j^2 \\ \bar{u}_j^2 & \bar{u}_j^1 \end{bmatrix}$ (2.26)

The mid-point value $\bar{r}_j$ has been introduced earlier, and it is specified more explicitly by choosing

$$\bar{r}_j = \bar{u}_j^2 = (\bar{u}_j^1)^2 + (\bar{u}_j^2)^2 \qquad (2.27)$$

so that $\tilde{A}(\bar{u}_j) . A(\bar{u}_j) = \bar{r}_j I$ (2.28)

Then
$$\left.\begin{aligned} (\Delta\vec{x}_j)^2 &= 4\bar{r}_j\,(\Delta\vec{u}_j)^2 \\ \left.\frac{\partial(x,\,y)}{\partial(u^1,u^2)}\right|_j &= 4\bar{r}_j \end{aligned}\right\} \tag{2.29}$$

and from (2.29) we find that

$$d^2x_j = 4\bar{r}_j d^2u_j \tag{2.30}$$

Now performing the change of variables with the aid of (2.29) and (2.30) at each short time interval, we obtain the integral form

$$Q(\vec{u}'',\vec{u}';\sigma) = \lim_{N\to\infty} \frac{1}{2}\int\int\cdots\int \exp\left\{\frac{i}{\hbar}\sum_{j=1}^{N}\left[\frac{2m}{\sigma_j}(\Delta\vec{u}_j)^2 + E(\bar{u}_j)^2\sigma_j\right]\right\}$$

$$\times \prod_{j=1}^{N}\left(\frac{4m}{2\pi i\hbar\sigma_j}\right)\prod_{j=1}^{N-1} d^2u_j \tag{2.31}$$

This expression is obviously equivalent to the path integral for and isotropic oscillator of mass $M = 4m$ and frequency $\omega = (-E/2m)^{\frac{1}{2}}$ in two dimensions. This path integral can be evaluated in the usual fashion as shown in chapter I. The result is

$$Q(\vec{u}'',\vec{u}';\sigma) = \left(\frac{M\omega}{8\pi i\hbar}\right)\operatorname{cosec}(\omega\sigma)\exp\left\{\frac{iM\omega}{2\hbar}\left[(\vec{u}''^2+\vec{u}'^2)\cot(\omega\sigma) - 2\vec{u}'\cdot\vec{u}''\operatorname{cosec}(\omega\sigma)\right]\right\} \tag{2.32}$$

2.3 The Hamiltonian Path Integral

Consider the phase space path integral in two dimensions

$$K(\vec{x}'',\vec{x}';t'',t') = \iint \mathcal{D}\vec{x}(t)\mathcal{D}\vec{p}(t)\frac{1}{(2\pi\hbar)^2}\exp\left\{\frac{i}{\hbar}\int_{t'}^{t''}dt\left[\vec{p}\cdot\dot{\vec{x}} - \frac{\vec{p}^2}{2m} - V(\vec{x})\right]\right\} \tag{2.33}$$

if the integration over momentum variables were done, (2.33) may be reduced to

$$K(\vec{x}'',\vec{x}';t'',t') = \int \mathcal{D}\vec{x}(t)\exp\left\{\frac{i}{\hbar}\int_{t'}^{t''}dt\left(\frac{m\dot{\vec{x}}^2}{2} - V(\vec{x})\right)\right\} \tag{2.34}$$

which is the propagator in the Lagrangian path integral form. After reparameterization of the time variable

$$dt \rightarrow rds$$

$$S(t) = \int^{t}\frac{d\tau}{r(\tau)} \tag{2.35}$$

and using $V(x) = -\frac{e^2}{r}$ for the hydrogen atom problem , we obtain

$$K(\vec{x}'',\vec{x}';t'',t') = \iint \mathcal{D}\vec{x}(t)\mathcal{D}\vec{p}(t)\frac{1}{(2\pi\hbar)^2}$$

$$\exp\left\{\frac{i}{\hbar}\int_{S'}^{S''}ds\left[\vec{p}(S)\cdot\dot{\vec{x}}(S) - r(S)\frac{\vec{p}^2}{2m} + e^2\right]\right\} \tag{2.36}$$

where $S(t') = S'$; $S(t'') = S''$ and $\frac{dx(S)}{ds} = \dot{x}(S)$.

Notice that the initial and final times of the path t' and t'' are fixed. Therefore, the parameter S'' and S' are path dependence quantities. We can display explicitly this dependence by incorporating the constant

$$t'' - t' = \int_{S'}^{S''} r(S)ds \qquad (2.37)$$

into the integral as follows

$$K(\vec{x}'',\vec{x}';t'',t') = \int_{S'}^{\infty} r''ds''\delta\left(t''-t'-\int_{S'}^{S''} r(s)ds\right)\exp\left\{\frac{i}{\hbar}e^2(S''-S')\right\}$$

$$\times \int \mathcal{D}\vec{x}(t)\mathcal{D}\vec{p}(t)\frac{1}{(2\pi\hbar)^2}\exp\left\{\frac{i}{\hbar}\int_{S'}^{S''} ds\left(\vec{p}\cdot\dot{\vec{x}}-\frac{r\vec{p}^{\,2}}{2m}\right)\right\}$$

$$(2.38)$$

Upon using a Fourier representation of the δ-function, (2.38) becomes

$$K(\vec{x}'',\vec{x}';t'',t') = \int\frac{dE}{(2\pi\hbar)}\exp\left\{-\frac{iE}{\hbar}(t''-t')\right\} r''\iint\frac{1}{(2\pi\hbar)^2}\mathcal{D}\vec{p}(t)\mathcal{D}\vec{x}(t)$$

$$\int_{S'}^{\infty} dS''\, e^{\frac{i}{\hbar}e^2(S''-S')} \times \exp\left\{\frac{i}{\hbar}\int_{S'}^{S''} ds\left(\vec{p}\cdot\dot{\vec{x}}-\frac{r\vec{p}^{\,2}}{2m}+Er\right)\right\}$$

$$= \int\frac{dE}{(2\pi\hbar)}\exp\left\{-\frac{iE}{\hbar}(t''-t')\right\} G(\vec{x}'',\vec{x}';E) \qquad (2.39)$$

where

$$G(\vec{x}'',\vec{x}';E) = \frac{r''}{(2\pi\hbar)^2}\iint \mathcal{D}\vec{p}(t)\mathcal{D}\vec{x}(t)\int_{S'}^{\infty} dS''\, e^{\frac{i}{\hbar}e^2(S''-S')}$$

$$\exp\left\{\frac{i}{\hbar}\int_{S'}^{S''} dS\left(\vec{p}\cdot\dot{\vec{x}}-\frac{r\vec{p}^{\,2}}{2m} + Er\right)\right\} \qquad (2.40)$$

which can be written as

$$G(\vec{x}'', \vec{x}';E) = \int_{S'}^{\infty} dS''\, e^{\frac{i}{\hbar}e^2(S''-S')} Q(\vec{x}'';\vec{x}'; S'',S') \qquad (2.41)$$

where $$Q(\vec{x}'',\vec{x}';S'',S') = \frac{r''}{(2\pi\hbar)^2}\iint \mathcal{D}\vec{p}(t)\mathcal{D}\vec{x}(t)$$

$$\exp\left\{\frac{i}{\hbar}\int_{S'}^{S''} dS\left(\vec{p}\cdot\dot{\vec{x}}-\frac{\vec{p}^{\,2}r}{2m} + Er\right)\right\} \qquad (2.42)$$

Thus, the problem is reduced to evaluate the path integral (2.42) with the new time variable S. Now, using the canonical transformation as in section II

$$\left.\begin{aligned} x_1 &= u_1^2 - u_2^2\,, & P_1 &= \frac{1}{2u^2}(u_1P_{u1} + u_2P_{u2}) \\ x_2 &= 2u_1u_2\,, & P_2 &= \frac{1}{2u^2}(-u_2P_{u1} + u_1P_{u2}) \end{aligned}\right\} \qquad (2.43)$$

where $u^2 = u_1^2 + u_2^2 = r$ and consider the transformation of the path integral from $\vec{x}$, $\vec{p}$ to $\vec{u}$, $\vec{P}_u$ with

$$dx = 2\begin{pmatrix} u_1 & u_2 \\ -u_2 & u_1 \end{pmatrix} du \qquad (2.44)$$

$$dp = \frac{1}{2u^2}\begin{bmatrix} u_1 & u_2 \\ -u_2 & u_1 \end{bmatrix} dP_u \tag{2.44}$$

one has

$$d^2p = \frac{1}{4u^2}\, d^2Pu = \frac{1}{4r} d^2P_u$$

$$(2.45)$$

$$d^2x = 4u^2d^2u = 4rd^2x$$

$$\text{So that} \quad d^2xd^2p = d^2ud^2P_u \tag{2.46}$$

The functional measure $\mathcal{D}\vec{p}\mathcal{D}\vec{x}$, does not simply transform like (2.46) but its satisfies

$$\frac{\mathcal{D}\vec{p}\mathcal{D}\vec{x}}{(2\pi\hbar)^2} = \frac{1}{4r''}\,\frac{1}{(2\pi\hbar)^2}\,\mathcal{D}\vec{u}\mathcal{D}\vec{P}_u \tag{2.47}$$

because d^2P_N is not accompanied by d^2x_N which $\vec{x}_N = \vec{x}''$ is the fixed end points. After using the canonical change of variables from $(\vec{x}, \vec{p})$ to $(\vec{u}, \vec{P}_u)$ then the expression (2.42) becomes

$$Q(\vec{u}'',\vec{u}';s''s') = \frac{1}{4}\iint \frac{\mathcal{D}\vec{P}_u}{(2\pi\hbar)^2}\mathcal{D}\vec{u}\exp\left\{\frac{i}{\hbar}\int_{s'}^{s''} ds\left[\vec{P}_u\cdot\dot{\vec{u}} - \frac{\vec{P}_u^2}{8m} + E\vec{u}^2\right]\right\} \tag{2.48}$$

The path integral appears in (2.48) is obviously the propagator of the two dimensional harmonic oscillator in $\vec{u}(s)$ coordinates with mass $M = 4m$ and frequency $\omega = (-E/2m)^{\frac{1}{2}}$. This is the gaussian functional integral can be performed in the usual fashion, the result is

$$Q(\vec{u}'',\vec{u}',\sigma) = \frac{1}{4}\left[\frac{M\omega}{2\pi i\hbar \sin\omega\sigma}\right] \exp\left\{\frac{i}{\hbar}\frac{M\omega}{2\sin\omega\sigma}\left[(\vec{u}''^2+\vec{u}'^2)\cos\omega\sigma - 2\,\vec{u}'\cdot\vec{u}''\right]\right\} \qquad (2.49)$$

where $\sigma = S'' - S'$.

The Green's function (2.41), expressed in terms of the new time parameter can be put into the form

$$G(\vec{x}'',\vec{x}';E) = \int_0^\infty d\sigma\, e^{\frac{i}{\hbar}e^2\sigma}\left[\frac{M\omega}{8\pi i\hbar \sin\omega\sigma}\right] \exp\left\{\frac{i}{\hbar}\frac{M}{2\sin\omega\sigma}\left[(\vec{u}''^2+\vec{u}'^2)\cos\omega\sigma - 2\vec{u}'\cdot\vec{u}''\right]\right\} \qquad (2.50)$$

Eq. (2.50) is the integral representation of the Coulomb Green's function in parabolic coordinates. In order to get the information about the energy spectrum of the hydrogen atom from this Green's function, one must try to carry out the σ-integration which can be done by transforming the parabolic variables (u_1, u_2) into polar variables (r, φ). The detail of the procedure will be shown in chapter IV.