

CHAPTER VI

CONCLUSION

6.1 Summary

In chapter I, we briefly reviewed the propagator and Feynman path integral. 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 can be expressed in the path integral form

$$K(\vec{x}'', \vec{x}', t'', t') = \lim_{N \rightarrow \infty} \left(\frac{2\pi i \hbar \epsilon}{m} \right)^{-3N/2} \iint \dots \int \exp \left\{ \frac{i}{\hbar} \sum_{j=1}^N \left[\frac{m(\vec{x}_j - \vec{x}_{j-1})^2}{2\epsilon} - \epsilon V(\vec{x}_j) \right] \right\} d^3x_1 d^3x_2 \dots d^3x_{N-1} \quad (6.1)$$

or in a less restrictive notation as

$$K(\vec{x}'', \vec{x}', t'', t') = \int_{\vec{x}'}^{\vec{x}''} e^{\frac{i}{\hbar} S[\vec{x}'', \vec{x}']} \mathcal{D} \vec{x}(t) \quad (6.2)$$

Then, some simple examples which can be evaluated exactly by path integral formula have been examined in one dimension, such as the free particle and the harmonic oscillator.

In chapter II, the Green's function of the hydrogen atom has been reviewed in two dimensions by means of both configuration space and phase space path integral formalism. The path integral form of the two dimensional hydrogen atom problem is non gaussian and can be reduced to a gaussian integral by using the two key steps,

i) the reparameterization of path by a new time ii) the transformation of coordinates from Cartesian to parabolic. After using these two key steps we obtain the integral representation of the Green's function

$$G(\vec{x}, \vec{x}'; E) = 2^{-2} \int_0^{\infty} e^{\frac{ie\phi}{\hbar}} \frac{M\omega}{2\pi i \hbar \sin(\omega\phi)} \exp\left\{ \frac{iM}{\hbar 2 \sin(\omega\phi)} [(\vec{u}^2 + \vec{u}'^2) \cos(\omega\phi) - 2\vec{u} \cdot \vec{u}'] \right\} d\phi \quad (6.3)$$

where $M = 4m$ and $\omega = \left(-\frac{E}{2m}\right)^{\frac{1}{2}}$

In chapter III, the three dimensional hydrogen atom problem has been reviewed. Again, similar to the case of two dimensions, the path integral must be transformed into a gaussian integral by using the two key steps, the rescaling of time and the transformation of coordinates. But the transformation of coordinates is different from that used in two dimensions. In this problem we used the four dimensional KS transformation which transformed the variables $x(x, y, z)$ in R^3 into the variables $\vec{u}(u^1, u^2, u^3, u^4)$ in R^4 . Then, the Coulomb path integral is reduced to the four dimensional harmonic oscillator path integral and we obtained the integral representation of the Green's function

$$G(\vec{x}, \vec{x}'; E) = 2^{-4} \int_0^{\infty} \int_{-\infty}^{\infty} e^{\frac{ie\phi/\hbar}{F(\phi)}} F^4(\phi) \exp\left\{ -\pi F^2(\phi) [(\vec{u}^2 + \vec{u}'^2) \cos(\omega\phi) - 2\vec{u} \cdot \vec{u}'] \right\} \frac{1}{T^*} d\xi_N d\phi \quad (6.4)$$

In chapter IV, we consider the energy spectrum of the hydrogen atom from the exact Green's function. For the two dimensional Green's function we simplify the ϕ -integration by

transforming the parabolic coordinates (u^1, u^2) into polar coordinates (r, ϕ) . After carrying out the ϕ -integration we obtained the Green's function in the form

$$G(r'', \phi'', r', \phi'; k) = \sum_{l=-\infty}^{\infty} e^{il(\phi''-\phi')} G_l(r'', r'; k) \quad (6.5)$$

where

$$G_l(r'', r'; k) = \frac{m}{2\pi i \hbar} \frac{i^{2l+1} \Gamma(p+l+1/2)}{\Gamma(2l+1)} M_{p,l}(2ikr') W_{-p,l}(2ikr'') \quad (6.6)$$

From the poles of the gamma function, we get the energy levels of the hydrogen atom in two dimensions

$$E_n = \frac{-me^4}{2\hbar^2(n+1/2)^2} \quad (6.7)$$

where $n = 0, 1, 2, \dots$

For the three dimensional Green's function, we must perform two integrations; the first integration is to project the oscillator propagator obtained in the KS coordinates back into the three dimensional physical space by eliminating the auxiliary variable ξ , and the last step is the integration over ϕ to get the Green's function in the energy domain. To eliminate the auxiliary variable ξ we transformed the KS variables (u^1, u^2, u^3, u^4) into the four dimensional polar coordinates $(r, \theta, \phi, \alpha)$. After carrying out the ϕ -integration we get the Green's function in a closed form

$$G(\vec{x}'', \vec{x}', E) = \frac{im}{2\pi \hbar} \frac{\Gamma(p+1)}{|\vec{x}'' - \vec{x}'|} \det \begin{vmatrix} M_{-p,1/2}(-ika) & W_{-p,1/2}(-ikb) \\ M'_{-p,1/2}(-ika) & W'_{-p,1/2}(-ikb) \end{vmatrix} \quad (6.8)$$



where
$$p = -\frac{ime^2}{\hbar^2 k^2}$$

The discrete energy spectrum arises from the poles of the gamma function in (6.8), that is $p+1 = -n$, $n = 1, 2, 3, \dots$ results in

$$E_n = -\frac{me^4}{2\hbar^2 n^2} \quad (n = 1, 2, 3, \dots) \quad (6.9)$$

which equivalent to the Bohr's energy levels of the hydrogen atom in three dimensions.

In chapter V, we have considered the wave functions of the hydrogen atom in three dimensions and we have shown to derive the wave functions from the Coulomb Green's function. The residues of the Green's function which represent the wave functions $\psi_n(\vec{x}')\psi_n^*(\vec{x})$ can be found from the formula

$$\text{Res}G(\vec{x}'', \vec{x}'; E) = \lim_{E \rightarrow E_n} (E - E_n) G(\vec{x}'', \vec{x}'; E) \quad (6.10)$$

By using this formula, the ground state and the excited state wave functions of the hydrogen atom can be found,

$$\lim_{E \rightarrow E_1} (E - E_1) G(\vec{x}'', \vec{x}'; E) = i\hbar \psi_{100}(\vec{r}'') \psi_{100}^*(\vec{r}') \quad (6.11)$$

and

$$\begin{aligned} \lim_{E \rightarrow E_2} (E - E_2) G(\vec{x}'', \vec{x}'; E) = & i\hbar \left\{ \psi_{200}(\vec{r}'') \psi_{200}^*(\vec{r}') + \psi_{210}(\vec{r}'') \psi_{210}^*(\vec{r}') \right. \\ & \left. + \psi_{211}(\vec{r}'') \psi_{211}^*(\vec{r}') + \psi_{21-1}(\vec{r}'') \psi_{21-1}^*(\vec{r}') \right\} \quad (6.12) \end{aligned}$$

or in the general form

$$\lim_{E \rightarrow E_n} (E - E_n) G(\vec{x}''; \vec{x}'; E) = i\pi \sum_{l=0}^{n-1} \sum_{m=-l}^l \Psi_{nlm}(\vec{r}'') \Psi_{nlm}^*(\vec{r}') \quad (6.13)$$

where

$$\begin{aligned} \Psi_{nlm}(\vec{r}) &= \frac{1}{\sqrt{\pi n}} \left(\frac{me^2}{\hbar^2} \right)^{3/2} \sqrt{\frac{(2l+1)(l-|m|)!(n-l-1)!}{(l+|m|)!(n+l)!}} e^{im\phi} P_l^m(\cos\theta) \\ &\times \left(\frac{2me^2 r}{\hbar^2} \right)^l e^{-\frac{me^2 r}{\hbar^2}} L_{n-l-1}^{2l+1} \left(\frac{2me^2 r}{\hbar^2} \right) \end{aligned} \quad (6.14)$$

6.2 Discussion and Conclusion

As seen in chapter III, after using the two key steps of Duru and Kleinert, the path integral for the hydrogen atom problem can be performed exactly. The double integral representation of the Green's function can be written as

$$G(\vec{x}'', \vec{x}'; E) = 2^{-4} \iiint e^{ie^2 \sigma / \hbar} F^4(\sigma) \exp \left\{ -\pi F^2(\sigma) \left[(\vec{u}''^2 + \vec{u}'^2) \cos(\omega\sigma) - 2\vec{u}'' \cdot \vec{u}' \right] \right\} \frac{d\xi_N}{r'} d\sigma \quad (6.15)$$

Following Ho and Inomata's procedure, they transformed the four dimensional Cartesian variables (u^1, u^2, u^3, u^4) into the four dimensional polar variables $(r, \theta, \phi, \alpha)$ and they reduced (6.15) into the form

$$G(\vec{x}'', \vec{x}'; E) = \frac{\pi}{4} \int \exp \left\{ \frac{ie^2 \sigma}{\hbar} \right\} F^4(\sigma) \exp \left\{ -\pi F^2(\sigma) V \cos(\omega\sigma) \right\} I_0(\pi F^2(\sigma) u) d\sigma \quad (6.16)$$

where $V = r' + r''$ and $u = 2(r'r'')^{\frac{1}{2}} \cos \frac{\gamma}{2}$. In this thesis we follow Ho and Inomata's work until we arrive at Eq.(6.16).

In deed they still continued their work for completing the σ -integration. By transforming the modified Bessel function I_0 into the spherical Bessel function J_0 and then using the relation,

$$\sum_{l=0}^{\infty} (2l+1) J_{2l+1}(z) P_l(\cos \gamma) = z J_0(z \cos \frac{\gamma}{2}), \quad (6.17)$$

they could perform the σ -integration exactly and the result is (5)

$$G(\vec{x}'', \vec{x}'; E) = \sum_{l=0}^{\infty} G_l(r'', r'; E) P_l(\cos \gamma) \quad (6.18)$$

$$\text{where } G_l(r'', r'; E) = \Gamma(P+l+1) [8\pi \hbar r' r'' (2l+1)!]^{-1} M_{P, l+\frac{1}{2}}(2ikr') W_{-P, l+\frac{1}{2}}(\Gamma 2ikr'') \quad (6.19)$$

From the gamma function $\Gamma(P+l+1)$, they have shown that the energy spectrum of the hydrogen atom arises from the poles of gamma function, that is, $P+l+1 = -n$, results in

$$E_n = -\frac{me^4}{2\hbar^2 n^2} \quad (6.20)$$

But they did not show how to find the eigen functions from the exact Green's function in Eq. (6.18).

Following Duru and Kleinert's procedure, after using the transformation of variables from (u_1, u_2, u_3, u_4) to $(r, \theta, \varphi, \alpha)$, they also obtained the Green's function with the same result as that obtained by Ho and Inomata. However, they made the further transformation, by setting $\sigma = -i\tilde{\sigma}$ and substituting $\rho = \exp\left\{-\frac{2\omega\tilde{\sigma}}{\hbar}\right\}$. As a result, they obtained the final expression of the Green's function (8)

$$G(\vec{x}'', \vec{x}'; E) = -\frac{im}{\pi} P_0 \int_0^1 d\rho \frac{\rho^{-\nu}}{(1-\rho)^2} I_0\left(\frac{2P_0\sqrt{2\rho u}}{1-\rho}\right) e^{-P_0\frac{(1+\rho)V}{1-\rho}} \quad (6.21)$$

where $P_0 = \left(\frac{-2mE}{\hbar}\right)^{\frac{1}{2}}$ and $\nu = e^2/2\omega$. We see that from this integral representation of Green's function, it gives no information about the energy spectrum and eigen function of the hydrogen atom.

In this research, we follow Ho and Inomata's procedure, but instead of using the transformation of (6.17) to perform the δ -integration, we use the relation

$$I_0(au) = \frac{\partial}{\partial u} (uI_1(au)) \quad (6.22)$$

for completing the σ -integration and we obtain the Green's function in a closed form

$$G(\vec{x}'', \vec{x}'; E) = \frac{mi}{2\pi\hbar} \frac{\Gamma(P+1)}{|\vec{x}'' - \vec{x}'|} \det \begin{vmatrix} M_{-P, \frac{1}{2}}(-ika) & W_{-P, \frac{1}{2}}(-ikb) \\ M'_{-P, \frac{1}{2}}(-ika) & W'_{-P, \frac{1}{2}}(-ikb) \end{vmatrix} \quad (6.23)$$

From this Green's function, the energy levels of the hydrogen atom can be found from the poles of gamma function $\Gamma(P+1)$ which corresponds to

$$E_n = -\frac{me^4}{2\hbar^2 n^2} \quad (6.24)$$

and we can verify that its residues

$$\text{Res } G(\vec{x}'', \vec{x}'; E) = \lim_{E \rightarrow E_n} (E - E_n) G(\vec{x}'', \vec{x}'; E) \quad (6.25)$$

represent the usual spherical wave function $\psi_{n\ell m}(\vec{r})$ of the hydrogen atom. This wave function can be easily derived from the Schroedinger's equation. Furthermore, the Green's function in Eq. (6.23) corresponds to the Green's function that obtained by Hostler without using path integral. By solving Schroedinger's equation, Hostler obtained the Green's function in the form (15)

$$G(\vec{x}'', \vec{x}'; E) = -\frac{\Gamma(P+1)}{4\pi |\vec{x}'' - \vec{x}'|} \det \begin{vmatrix} M_{-P, \frac{1}{2}}(-ika) & W_{-P, \frac{1}{2}}(-ikb) \\ M'_{-P, \frac{1}{2}}(-ika) & W'_{-P, \frac{1}{2}}(-ikb) \end{vmatrix} \quad (6.26)$$

which still contains all informations about the energy spectrum and the wave function of the hydrogen atom in three dimensions. Strictly speaking, however, all expressions of $G(\vec{x}'', \vec{x}'; E)$, Eq. (6.18), (6.21) and (6.23) are equivalent, but our expression (Eq. (6.23)) is more compacted and also equivalent to the Green's function that is obtained by Hostler without using path integral.

The solution of the hydrogen atom problem has already been well-known. The energy spectrum and the wave functions for the hydrogen atom can be obtained rather easily from the Schroedinger's wave equation. Therefore, the solution itself is not particularly important. The main problem is whether path integration can be carried out for the hydrogen atom. The only path integral known to be soluble is of the gaussian type. In order to succeed in the path integration, one has to succeed in reducing the path integral to a gaussian path integral. The path integral for the harmonic oscillator is the simplest that can be directly reduced to a gaussian path integral. The presence of the Coulomb potential in the integrand makes the path integral non-gaussian so that its direct path integration becomes hopeless. What is shown in this dissertation is a procedure which converts the Coulomb path integral into an oscillator path integral which is exactly path-integrable. The keys of the technical breakthrough for the hydrogen atom problem are the position-dependent time rescaling and the mapping of the three dimensional space on to a four dimensional space. Finding the exact path integration procedure does not remain to be a theorist's academic satisfaction. The success of the transformation procedure certainly encourages further studies of contact transformation in path integral.