

Coherent States for the Hydrogen Atom*

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Abstract

We obtained the coherent states for the hydrogen atom by transforming the problem onto the four oscillators in the parametric time at the classical level and quantizing these oscillators. We showed that for the coherent states the mean values of the physical position of the electron satisfy the Keplerian ellipsis and the dispersions of them oscillate in the parametric time.

1. Introduction

In 1926 Schrödinger constructed the coherent states for the harmonic oscillator [1]. These states satisfy the following properties:

They are the eigenstates of the lowering operator of the harmonic oscillator and the evolution of the eigenvalues are the same with the evolution of the classical dynamical variables.

They are the minimum uncertainties states without any dispersion during the evolution of the system in time.

Schrödinger also addressed the problem of the construction of the coherent states for the hydrogen atom.

There are two group of attempts to solve this problem. In the first group the authors tried to express the coherent states for the hydrogen atom as the superpositions of the stationary eigenfunctions of it. In this approach they discussed the evolution of the system in the physical time [2].

In the second group first Nieto and Simmons developed a general method for the constructions of the coherent states for different potentials [3]. Later Bhaumik et al.

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discussed the construction of the coherent states for hydrogen atom [4]. In this paper they transformed the time independent three dimensional hydrogen atom system onto the time independent four oscillator system by using the Kustaanheimo-Stiefel transformation [5-6] and constructed the coherent states by using the $SO(4)$ symmetry of the system. Before Duru and Kleinert also used the same transformation for the path integral quantization of the hydrogen atom and they pointed out that the four oscillator system evolve in a new parametric time instead of the physical time [7]. In 1988 Gerry discussed the same problem by considering evolution of the system in the parametric time [8]. Recently Toyoda and Wakayama also discussed the same problem by considering the $SU(2) \times SU(2)$ symmetry of the four oscillators [9].

Since the hydrogen atom has three degrees of freedom and the four oscillators system have the four degrees of freedom the authors of the references 4,8,9 eliminated the extra degree of the freedom by taking the conjugate momentum of this degree of freedom as zero. As a coincidence this condition gives the right energy spectra for the hydrogen atom, but it does not give the right wave functions.

In this work we discussed the solution this long standing problem by transforming the classical Kepler problem of to the four oscillators. Since the holomorphic coordinates are the classical analogue of the rising and lowering operators of the harmonic oscillators, we express the classical dynamics in terms of the holomorphic coordinates and quantize the system. Here we quantize the system by using the Schrödinger quantization and derive the coherent state wave functions in terms of the four oscillator states and the hydrogen wave functions in parabolic coordinates. We also evaluate the expectation values and the dispersions of the physical position of the particle [10].

2. Classical Coulomb Problem

Lagrangian of the electron in the Coulomb potential is given in the Cartan form as

$$L(\vec{x}, \vec{p}; t) = \vec{p} \cdot \frac{d\vec{x}}{dt} - \frac{1}{2m} \vec{p}^2 + \frac{e^2}{(|\vec{x}|)} \quad (1)$$

We add the free particle Lagrangian for a new degree of the freedom and this does not change the dynamics of the electron. Then the Lagrangian become

$$L(\vec{x}, x_4, \vec{p}, p_4; t) = \vec{p} \cdot \frac{d\vec{x}}{dt} + p_4 \cdot \frac{dx_4}{dt} - \frac{1}{2m} (p^2 + p_4^2) + \frac{e^2}{(|\vec{x}|)} \quad (2)$$

We define four vectors x_A and p_A such that

$$\begin{aligned} x_A &= (\vec{x}, x_4) \\ p_A &= (\vec{p}, p_4) \end{aligned} \quad (3)$$

The trajectories are parametrized in terms of the time t . We can parametrize the dynamics of the electron in a new time parameter s . Then the time t is also function of s . The new Lagrangian is

$$\mathcal{L}(x_A, p_A, t, p_0; s) = p_A \cdot \frac{dx_A}{dt} - \left(\frac{p_A^2}{2m} + \frac{e^2}{(|\vec{x}|)} \right) f(s) - p_0 \left[\frac{dt}{ds} - f(s) \right] \quad (4)$$

Lagrangians (4), (2) and have the same set of equations. We choose $f(s)$ as

$$\frac{dt}{ds} = f(s) = |\vec{x}| \quad (5)$$

Then \mathcal{L} becomes

$$\mathcal{L}(x_A, p_A, t, p_0; s) = p_A \cdot \frac{dx_A}{dt} - p_0 \frac{dt}{ds} - \left(\frac{|\vec{x}| p_A^2}{2m} + e^2 - p_0 |\vec{x}| \right) \quad (6)$$

Equation (6) is the Lagrangian of the electron in a 4 + 1 dimensional curved space under the potential $[-(p_0 |\vec{x}|) + e^2]$. This system is mapped onto the four harmonic oscillators under the Kustaanheimo-Stiefel transformation:

$$\begin{pmatrix} dx_1 + idx_2 \\ dx_3 + idx_4 \end{pmatrix} = 2(-2mp_0)^{-1/2} \begin{pmatrix} d\xi_A^* \xi_B + \xi_A^* d\xi_B \\ d\xi_A^* \xi_A - \xi_B^* d\xi_B \end{pmatrix} \quad (7)$$

The momenta are transformed as

$$\begin{pmatrix} p_{x_1} - ip_{x_2} \\ p_{x_3} - ip_{x_4} \end{pmatrix} = \frac{(-2mp_0)^{+1/2}}{|\xi_A|^2 + |\xi_B|^2} \begin{pmatrix} \xi_A p_{\xi_B} + \xi_B^* p_{\xi_A^*} \\ -\xi_B p_{\xi_B} + \xi_A^* p_{\xi_B^*} \end{pmatrix} \quad (8)$$

We define the complex spinors ξ and ξ^\dagger as

$$\begin{aligned} \xi &= \begin{pmatrix} \xi_A \\ \xi_B \end{pmatrix} \\ \xi^\dagger &= (\xi_A^*, \xi_B^*) \end{aligned} \quad (9)$$

Then the Lagrangian becomes

$$\mathcal{L} = p_\xi \frac{d\xi}{ds} + p_\xi \frac{d\xi^\dagger}{ds} + (-p_0) \frac{dt}{ds} - H \quad (10)$$

Where the Hamiltonian H is

$$H = \frac{(-2mp_0)^{1/2}}{2m} (p_\xi p_{\xi^\dagger} + \xi^\dagger \xi) - e^2 \quad (11)$$

H is the Hamiltonian of the four harmonic oscillators with the frequency $\omega = (-p_0/2m)^{1/2}$. We define the classical analogue of the rising and lowering operators of the harmonic oscillators. These are the holomorphic coordinates a and a^\dagger :

$$a = \frac{1}{\sqrt{2}} \begin{pmatrix} \xi_A^* + ip_{\xi_A} \\ \xi_A + ip_{\xi_A^*} \\ \xi_B^* + ip_{\xi_B} \\ \xi_B + ip_{\xi_B^*} \end{pmatrix}$$

$$a^\dagger = \frac{1}{\sqrt{2}} \left(\xi_A - ip_{\xi_A^*}, \xi_A^* - ip_{\xi_A}, \xi_B - ip_{\xi_B}, \xi_B^* - ip_{\xi_B^*} \right) \quad (12)$$

a and a^\dagger have four components. Then the Lagrangian is

$$\mathcal{L} = \frac{1}{2} \left(\frac{da^\dagger}{ds} a - a^\dagger \frac{da}{ds} \right) + (-p_o) \frac{dt}{ds} - (\omega a^\dagger a - e^2) \quad (13)$$

The difference of the Lagrangians(10) and (13) is only a total derivative. Here $(\omega a^\dagger a - e^2)$ is the energy functional or the Hamiltonian of the four oscillators in the proper time parameter s . It is a constant and the value of it is zero. Then

$$p_o = -\frac{2me^2}{(a^\dagger a)^2} \quad (14)$$

3. Quantization of the Classical System

The Hamiltonian of the four oscillators system is

$$H = \omega (\hat{a}^\dagger \hat{a} + 2) \quad (15)$$

where \hat{a}^\dagger and \hat{a} are the canonical conjugate variables and they satisfy the commutation relations

$$[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij} \quad (16)$$

Then the eigenstates of \hat{a} are

$$|\alpha\rangle = e^{a^\dagger \alpha} |0\rangle \quad (17)$$

where α is the complex eigenvalue. The evolution of this state is given by

$$|\alpha(s)\rangle = e^{-iHs + \hat{a}^\dagger \alpha} |0\rangle \quad (18)$$

or

$$|\alpha(s)\rangle = e^{-i\omega(\hat{a}^\dagger a + 2)s + \hat{a}^\dagger \alpha} |0\rangle \quad (19)$$

The eigenstate $|\alpha\rangle$ can be expanded in terms of the oscillator states $|n\rangle$ as

$$|\alpha\rangle = \sum_{n_1, n_2, n_3, n_4} \frac{\alpha_+^{n_1} \alpha_-^{n_2} \beta_+^{n_3} \beta_-^{n_4}}{\sqrt{n_1! n_2! n_3! n_4!}} |n_1 n_2 n_3 n_4\rangle \quad (20)$$

Where the state $|n_1 n_2 n_3 n_4\rangle$ is defined as

$$|n_1 n_2 n_3 n_4\rangle = \frac{(a_+^\dagger)^{n_1} (a_-^\dagger)^{n_2} (b_+^\dagger)^{n_3} (b_-^\dagger)^{n_4}}{\sqrt{n_1! n_2! n_3! n_4!}} |0\rangle \quad (21)$$

Then $\alpha(s)$ becomes

$$\alpha(s) = e^{-i\omega s} \alpha \quad (22)$$

This is the same with the evolution of $a(s)$ in the classical dynamics of the system. Then $|\alpha(s)\rangle$ is

$$|\alpha(s)\rangle = \sum_{n_1, n_2, n_3, n_4} \frac{[\alpha_+(s)]^{n_1} [\alpha_-(s)]^{n_2} [\beta_+(s)]^{n_3} [\beta_-(s)]^{n_4}}{\sqrt{n_1! n_2! n_3! n_4!}} \times e^{-2i\omega s} |n_1 n_2 n_3 n_4\rangle \quad (23)$$

We express $|\alpha\rangle$ in terms of $|\xi, \xi^*\rangle$. First we express $|n_1 n_2 n_3 n_4\rangle$ in terms of the $|\xi, \xi^*\rangle$. The ground state $|0\rangle$ is the eigenstate of \hat{a} :

$$\hat{a} |0\rangle = 0 \quad (24)$$

or

$$\frac{1}{\sqrt{2}} \left(\xi^*/\sqrt{2} + \frac{\partial}{\partial \xi/\sqrt{2}} \right) \langle \xi, \xi^* | 0 \rangle = 0 \quad (25)$$

and

$$\frac{1}{\sqrt{2}} \left(\xi/\sqrt{2} + \frac{\partial}{\partial \xi^*/\sqrt{2}} \right) \langle \xi, \xi^* | 0 \rangle = 0 \quad (26)$$

The solution of these spinor equations is

$$\langle \xi, \xi^* | 0 \rangle = e^{-(\xi_A^* \xi_A + \xi_B^* \xi_B)/2} \quad (27)$$

Then $\langle \xi, \xi^* | n_1 n_2 n_3 n_4 \rangle$ is

$$\begin{aligned} \langle \xi, \xi^* | n_1 n_2 n_3 n_4 \rangle = & \left[\frac{1}{\sqrt{2}} \left(\xi_A/\sqrt{2} - \frac{\partial}{\partial \xi_A^*/\sqrt{2}} \right) \right]^{n_1} \times \left[\frac{1}{\sqrt{2}} \left(\xi_A^\dagger/\sqrt{2} - \frac{\partial}{\partial \xi_A/\sqrt{2}} \right) \right]^{n_2} \times \\ & \left[\frac{1}{\sqrt{2}} \left(\xi_B^*/\sqrt{2} - \frac{\partial}{\partial \xi_B^*/\sqrt{2}} \right) \right]^{n_3} \left[\frac{1}{\sqrt{2}} \left(\xi_B^*/\sqrt{2} - \frac{\partial}{\partial \xi_B^*/\sqrt{2}} \right) \right]^{n_4} \times \\ & e^{-(\xi_A^* \xi_A + \xi_B^* \xi_B)/2} \end{aligned} \quad (28)$$

Then $\langle \xi, \xi^\dagger | \alpha \rangle$ becomes

$$\langle \xi, \xi^\dagger | \alpha \rangle = e^{-(\xi_A^* \xi_A + \xi_B^* \xi_B)/2 + \xi_A(\alpha_1 - i\alpha_2) + \xi_A^*(\alpha_1 + i\alpha_2) + \xi_A(\beta_1 - i\beta_2) + \xi_A^*(\beta_1 + i\beta_2) - (\alpha_1^2 + \alpha_2^2 + \beta_1^2 + \beta_2^2)} \quad (29)$$

We expand $\langle \xi, \xi^\dagger | \alpha \rangle$ as

$$\begin{aligned} \langle \xi, \xi^\dagger | \alpha \rangle &= \sum_{n_{12}, m_{12}} \frac{(\alpha_+ \alpha_-)^{n_{12}} (\alpha_+ / \alpha_-)^{m_{12}}}{\sqrt{(n_{12} + m_{12})! (n_{12} - m_{12})!}} e^{2im_{12} \arg \xi_A} |\xi_A|^{2|m_{12}|} \\ &\times L_{n_{12} - |m_{12}|}^{2|m_{12}|} \left(|\xi_A|^2 \right) \sum_{n_{34}, m_{34}} \frac{(\beta_+ \beta_-)^{n_{34}} (\beta_+ / \beta_-)^{m_{34}}}{\sqrt{(n_{34} + m_{34})! (n_{34} - m_{34})!}} \\ &\times e^{2im_{34} \arg \xi_B} |\xi_B|^{2|m_{34}|} L_{n_{34} - |m_{34}|}^{2|m_{34}|} \left(|\xi_B|^2 \right) \end{aligned} \quad (30)$$

where the numbers n_{ij} and m_{ij} are defined as

$$\begin{aligned} n_{ij} &= (n_i + n_j)/2 \\ m_{ij} &= (n_i - n_j)/2 \end{aligned} \quad (31)$$

Since the Kustaanheimo-Stiefel transformation is double valued, the coherent states are symmetric under the transformation $\xi \rightarrow -\xi$ or $\alpha \rightarrow -\alpha$ and $\beta \rightarrow -\beta$. Then $\langle \xi, \xi^\dagger | \alpha \rangle$ becomes

$$\begin{aligned} \langle \xi, \xi^\dagger | \alpha \rangle^S &= \sum_{n_{12}, m_{12}} \frac{(\alpha_+ \alpha_-)^{n_{12}} (\alpha_+ / \alpha_-)^{m_{12}}}{\sqrt{(n_{12} + m_{12})! (n_{12} - m_{12})!}} e^{2im_{12} \arg \xi_A} |\xi_A|^{2|m_{12}|} \times \\ &L_{n_{12} - |m_{12}|}^{2|m_{12}|} \left(|\xi_A|^2 \right) \sum_{n_{34}, m_{34}} \left[\frac{1 + (-1)^{n_{12} + n_{34}}}{2} \right]^{1/2} \frac{(\beta_+ \beta_-)^{n_{34}} (\beta_+ / \beta_-)^{m_{34}}}{\sqrt{(n_{34} + m_{34})! (n_{34} - m_{34})!}} \times \\ &e^{2im_{34} \arg \xi_B} |\xi_B|^{2|m_{34}|} L_{n_{34} - |m_{34}|}^{2|m_{34}|} \left(|\xi_B|^2 \right) \end{aligned} \quad (32)$$

This gives the condition

$$n_{12} + n_{34} = 2n \quad (33)$$

We parametrize ξ_A and ξ_B in the spherical coordinates as

$$(\xi_A \xi_B) = \sqrt{r} (-2mp_0)^{1/2} \begin{pmatrix} \sin \theta/2 e^{i(\psi+\varphi)/2} \\ \cos \theta/2 e^{i(\psi-\varphi)/2} \end{pmatrix} \quad (34)$$

where ψ is the angle corresponds to x_4 and we sum over the values of all ψ . This is

$$\langle \xi, \xi^\dagger | \alpha \rangle_{\text{physical}}^S = \int_0^{2\pi} \frac{d\psi}{2\pi} \langle \xi, \xi^\dagger | \alpha \rangle^S \quad (35)$$

This gives

$$\begin{aligned} \langle \xi, \xi^\dagger | \alpha \rangle_{\text{physical}}^S = & \\ \sum_{n'_1, n'_2, m} & \frac{(\alpha_+ \alpha_- \beta_+ \beta_-)^{n'_1 + n'_2 + m} (\alpha_+ \alpha_- / \beta_+ \beta_-)^{n'_1 - n'_2} \left(\frac{\alpha_+ / \alpha_-}{\beta_+ / \beta_-} \right)^m}{\sqrt{n'_1! (n'_1 + |m|)! n'_2! (n'_2 + |m|)!}} e^{im\varphi} \left[\frac{(-2mp_0)^{1/2} r \sin \theta}{2} \right]^{|m|} \\ & L_{n'_1}^{|m|} \left[(-2mp_0)^{1/2} r \sin^2 \theta / 2 \right] L_{n'_2}^{|m|} \left[(-2mp_0)^{1/2} r \cos^2 \theta / 2 \right] \end{aligned} \quad (36)$$

where n'_1 , n'_2 and m are the quantum numbers in the parabolic coordinates and these are defined as

$$\begin{aligned} n'_1 &= n_{12} - |m_{12}| \\ n'_2 &= n_{34} - |m_{12}| \end{aligned} \quad (37)$$

$$m = 2 |m_{12}|$$

This is the expression of the coherent states in terms of the hydrogen wave functions in parabolic coordinates.

4. Kepler Orbits

To obtain the Kepler orbits for the hydrogen atom we evaluate the expectation values of \vec{r} and r . The expectation values of \vec{r} is expressed in terms of the α_+ , α_- , β_+ , β_- as

$$\begin{aligned} \langle \vec{r} \rangle &= (-2mp_0)^{-1/2} \times \\ & \{ (\alpha_+^* + \alpha_-) \left[(\beta_+ + \beta_-^*) (\hat{e}_1 - i\hat{e}_2) + (\alpha_+ + \alpha_-^*) \hat{e}_3 / 2 \right] + \\ & (\beta_+^* + \beta_-) \left[(\alpha_+ + \alpha_-^*) (\hat{e}_1 + i\hat{e}_2) + (\beta_+ + \beta_-^*) \hat{e}_3 / 2 \right] \} \end{aligned} \quad (38)$$

We parametrize α_\pm and β_\pm as

$$\begin{aligned} \alpha_\pm(s) &= |\alpha_\pm| e \\ \beta_\pm(s) &= |\beta_\pm| e^{i\omega s + i\Delta_\pm} \end{aligned} \quad (39)$$

Then $\langle \vec{r} \rangle$ becomes

$$\langle \vec{r} \rangle = \vec{a} \cos 2(\omega s - \Phi) + \vec{b} \sin 2(\omega s - \Phi) + \vec{c} \quad (40)$$

where \vec{a} , \vec{b} and \vec{c} are

$$\vec{a} = (-2mp_o)^{+1/2} [(|\alpha_+\beta_-| + |\alpha_-\beta_+|) \hat{e}'_1 + \cos \varphi (|\alpha_+\alpha_-| + |\beta_+\beta_-|) \hat{e}_3/2]$$

$$\vec{b} = (-2mp_o)^{+1/2} [(|\alpha_+\beta_-| - |\alpha_-\beta_+|) \hat{e}'_2 + \sin \varphi (|\alpha_+\alpha_-| + |\beta_+\beta_-|) \hat{e}_3/2]$$

$$\vec{c} = (-2mp_o)^{+1/2} [2(|\alpha_+\beta_+| + |\alpha_-\beta_-|) \cos \varphi \hat{e} + 2(|\alpha_+\beta_+| - |\alpha_-\beta_-|) + \sin \varphi \hat{e}'_2 + (|\alpha_+|^2 + |\alpha_-|^2 - |\beta_+|^2 - |\beta_-|^2) \hat{e}_3/2] \quad (41)$$

The unit vectors \hat{e}'_1 and \hat{e}'_2 are

$$\begin{aligned} \hat{e}'_1 &= \hat{e}_1 \cos(\Delta - \delta) + \hat{e}_2 \sin(\Delta - \delta) \\ \hat{e}'_2 &= -\hat{e}_1 \sin(\Delta - \delta) + \hat{e}_2 \cos(\Delta - \delta) \end{aligned} \quad (42)$$

The phase angles Φ , Δ , δ and φ are related to the δ_{\pm} and Δ_{\pm} by

$$\begin{aligned} 2\Phi &= (\Delta_+ + \Delta_- + \delta_+ + \delta_-)/2 \\ \varphi &= (\Delta_+ + \Delta_- - \delta_+ - \delta_-)/2 \\ \delta &= \delta_+ - \delta_- \\ \Delta &= \Delta_+ - \Delta_- \end{aligned} \quad (43)$$

For an elliptic orbit \vec{b} and \vec{c} must be perpendicular and parallel to \vec{a} respectively. For the satisfaction of the first condition $\vec{a} \perp \vec{b}$ we choose $\varphi = 0$. The condition $\vec{a} \parallel \vec{b}$ requires that

$$\alpha_+^2 + |\beta_+|^2 - |\alpha_-|^2 - |\beta_-|^2 = 0 \quad (44)$$

This condition is equivalent to $p_4 = 0$ or $p_\psi = 0$ and this is expressed in terms of the quantum numbers m_{12} and m_{34} as

$$m_{12} = -m_{34} \quad (45)$$

Then $\langle \vec{r} \rangle$ describes an ellipse. The major axis a and eccentricity ϵ is given by

$$|\vec{a}| = (-2mp_o)^{-1/2} \left[\left(|\alpha_+|^2 + |\alpha_-|^2 + |\beta_+|^2 + |\beta_-|^2 \right) / 2 \right]^2$$

$$\epsilon = 2 (|\alpha_+ \alpha_-| + |\beta_+ \beta_-|) / |\vec{a}| \quad (46)$$

The expectation value of r is

$$\langle r \rangle = \frac{1}{me^2} \left[\left(|\alpha_+|^2 + |\beta_+|^2 + |\alpha_-|^2 + |\beta_-|^2 + 2 \right) / 2 \right]^2 \times$$

$$[1 + \cos 2(\omega s - \Phi)] \quad (47)$$

This gives the value of the a as

$$a = \frac{1}{4me^2} \left(|\alpha_+|^2 + |\beta_+|^2 + |\alpha_-|^2 + |\beta_-|^2 + 2 \right)^2 \quad (48)$$

The difference between the $|\vec{a}|$ and a comes from the quantum corrections.

The dispersions of x_1, x_2, x_3 and r are evaluated in the same way. The results are

$$(\Delta x)_s^2 = (\Delta y)_s^2 = \frac{a^{3/2}}{\sqrt{me^2}} (1 + \epsilon \cos 2(\omega s - \Phi)) - \frac{a}{me^2}$$

$$(\Delta x_3)_s^2 = (\Delta r)_s^2 = \frac{a^{3/2}}{\sqrt{me^2}} (1 + \epsilon \cos 2(\omega s - \Phi)) - \frac{a}{2me^2} \quad (49)$$

5. Conclusion

In this study we derived the coherent states for the hydrogen atom by transforming the problem onto the four oscillators and quantizing this system. These states are parametrized by three complex eigenvalues and expressed as the superpositions of the hydrogen wave functions in elliptic coordinates.

We showed that the expectation values of the position operator and their dispersions oscillate with the same frequency and the center of the wave packet travel along the Keplerian ellipse.

The technique developed in here may be applied to the other potentials for which the quantum mechanical problem can be transformed to the oscillator.

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