

Hydrogen atom as a four-dimensional oscillator

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A coordinate transformation which exhibits the rotational invariance of the hydrogen atom in four-dimensional Hilbert space is introduced. The coordinates are shown to be directly related to the spherical polar and parabolic coordinates in position space. With the use of the transformation, the Schrödinger equation for the hydrogen atom left-multiplied by $4r$ is transformed into one for a four-dimensional harmonic oscillator. Solutions are obtained and related to the hydrogenic wave functions. Group-theoretical implications of the transformation and its application to the hydrogen Stark problem are briefly discussed.

I. INTRODUCTION

The degeneracy of the bound states of the nonrelativistic hydrogen atom is known to be linked with its rotational invariance in four-dimensional Euclidean space. Fock demonstrated this in his landmark paper¹ by making a stereographic projection of the momentum space onto a four-dimensional unit sphere. The momentum-space wave functions are obtained from the solutions of the four-dimensional Laplace equation. In the three-dimensional space, the Schrödinger equation for the hydrogen atom is separable in spherical polar and parabolic coordinates. While its separability in the former is related to the spherical symmetry of the central Coulomb potential, its separability in the latter is attributed to the "hidden" symmetry which is responsible for the degeneracy peculiar to the potential. It should be noted that the Fock coordinates are not canonical. They are projective momentum coordinates and do not seem to be directly related to either the spherical polar or the parabolic coordinates in three-dimensional position space. We have found a new coordinate transformation which not only exhibits the four-dimensional rotational invariance of the hydrogenic system but also relates *directly* to the separable coordinates mentioned above. In Sec. II, after being introduced, the new four-dimensional coordinates are used to transform the Schrödinger equation for the hydrogen atom into one for a four-dimensional harmonic oscillator. In solving the equation, we not only recover the energy spectrum and the wave functions in spherical polar coordinates but also obtain the hydrogenic wave functions as a linear combination of the oscillator wave functions in terms of products of Hermite polynomials. In Sec. III, we discuss briefly its group-theoretical implications and its application to the Stark effect of the hydrogen atom.

II. THE HYDROGENIC OSCILLATOR AND ITS SOLUTIONS

The new coordinates we use are given by

$$\begin{aligned} y_1 &= s \cos\alpha \cos\beta, \\ y_2 &= s \cos\alpha \sin\beta, \\ y_3 &= s \sin\alpha \cos\gamma, \\ y_4 &= s \sin\alpha \sin\gamma. \end{aligned} \quad (1)$$

These coordinates provide a parametrization of the four-dimensional rotation group and correspond to plane rotations in perpendicular spaces.² The coordinates in Eq. (1) can be shown to satisfy the commutation relations $[y_i, p_j] = i\hbar\delta_{ij}$, where $p_j = -i\hbar\partial/\partial y_j$, $i, j = 1, 2, 3, 4$. To reduce these coordinates to the three-dimensional spherical polar coordinates r, θ, φ , we set³

$$s = r^{1/2}, \quad 2\alpha = \theta, \quad \beta \pm \gamma = \varphi. \quad (2)$$

From Eqs. (1) and (2), we can establish the following relationships among the various coordinates⁴:

$$\begin{aligned} r &= y_1^2 + y_2^2 + y_3^2 + y_4^2 = s^2, \\ x &= r \sin\theta \cos\varphi = 2(y_1 y_3 \pm y_2 y_4), \\ y &= r \sin\theta \sin\varphi = 2(y_2 y_3 \mp y_1 y_4), \\ z &= r \cos\theta = y_1^2 + y_2^2 - y_3^2 - y_4^2, \\ \xi &= r + z = 2(y_1^2 + y_2^2), \\ \eta &= r - z = 2(y_3^2 + y_4^2), \\ \varphi &= \arctan(y_2 y_3 \mp y_1 y_4)/(y_1 y_3 \pm y_2 y_4). \end{aligned} \quad (3)$$

The two signs in Eq. (3) correspond to the two phase relations in Eq. (2).

Multiplying the Schrödinger equation $(H-E)\Psi = 0$, where H is the hydrogenic Hamiltonian, by $4r$ from the left and utilizing the above coordinate transformation, we obtain the equation for a four-dimensional harmonic oscillator as follows:

$$[-\hbar^2/(2M)\nabla_4^2 - 4Es^2 - 4Ze^2]\Psi = 0. \quad (4)$$

The four-dimensional Laplacian is given by

$$\nabla_4^2 = \sum_{i=1}^4 \frac{\partial^2}{\partial y_i^2} \quad (5)$$

$$\nabla_4^2 = \frac{\partial^2}{\partial s^2} + \left(\frac{3}{s}\right) \frac{\partial}{\partial s} - 4\vec{K}^2. \quad (6)$$

The operator $4\vec{K}^2$ is the Casimir operator of the group $SO(4)$ and is given by⁵

$$4\vec{K}^2 = -\frac{\partial^2}{\partial \alpha^2} - (\tan \alpha - \cot \alpha) \frac{\partial}{\partial \alpha} \\ - \sec^2 \alpha \frac{\partial^2}{\partial \beta^2} - \cos^2 \alpha \frac{\partial^2}{\partial \gamma^2}.$$

Using the relations among the angular variables given in Eq. (2), we find $4\vec{K}^2 = 4\vec{L}^2$ where \vec{L} is the angular-momentum operator. By equating $-4E$ to $\frac{1}{2}M\omega^2$ and $4Ze$ to $N\hbar\omega$, where $N = n_1 + n_2 + n_3 + n_4 + 2$, and identifying the ground state $n = 1$ of the hydrogen atom as the zero-point oscillation $N = 2$ for the oscillator, we set $N = 2n$ and recover the energy spectrum $E = -p_c^2/(2Mn^2\hbar^2)$, where $p = Ze^2M$. It also follows that the frequency of the oscillator is given by $\omega_n = 2p_c/(Mn\hbar)$.⁶ It can easily be shown that the solution of Eq. (4) with the Laplacian given by Eq. (6) are the hydrogenic wave functions $\Psi_{nlm}(\vec{r})$. The solutions of Eq. (4) with the Laplacian given by Eq. (5) take the form

$$\Psi_{n_1 n_2 n_3 n_4} = C \exp(-p_c s^2/n\hbar^2) \Phi_{n_1 n_2 n_3 n_4}, \quad (7)$$

where C is a normalization constant and

$$\Phi_{n_1 n_2 n_3 n_4} = H_{n_1}(z_1)H_{n_2}(z_2)H_{n_3}(z_3)H_{n_4}(z_4). \quad (8)$$

The functions $H_n(z_i)$ are the Hermite polynomials in which we have set the argument $z_i = (2p_c/n\hbar)^{1/2}y_i$. In applications such as the treatment of the Stark effect, it is significant to note that the hydrogenic wave functions Ψ_{nlm} can be expressed as various combinations of the functions $\Phi_{n_1 n_2 n_3 n_4}$ given in Eq. (8). We have worked out the first few cases and they are given below: ($a = \hbar^2/p_c$)

$$\Psi_{100} = \frac{1}{\sqrt{\pi}a^{3/2}} \exp\left(-\frac{p_c s^2}{\hbar^2}\right) \Phi_{10000},$$

$$\Psi_{210} = \frac{1}{16\sqrt{2\pi}a^{3/2}} \exp\left(-\frac{p_c s^2}{2\hbar^2}\right) \\ \times (\Phi_{22000} + \Phi_{20200} - \Phi_{20020} - \Phi_{20002}),$$

$$\Psi_{21\pm 1} = \frac{1}{16\sqrt{\pi}a^{3/2}} \exp\left(-\frac{p_c s^2}{2\hbar^2}\right) \\ \times (\Phi_{21010} - \Phi_{20101} \pm i\Phi_{20110} \pm i\Phi_{21001}), \quad (9)$$

$$\Psi_{300} = \frac{1}{388\sqrt{3\pi}a^{3/2}} \exp\left(-\frac{p_c s^2}{3\hbar^2}\right) \\ \times (\Phi_{34000} + \Phi_{30400} + \Phi_{30040} + \Phi_{30004}),$$

$$\Psi_{310} = \frac{4\sqrt{2}}{729\sqrt{\pi}a^{3/2}} \exp\left(-\frac{p_c s^2}{3\hbar^2}\right) \\ \times [-\Phi_{34000} - \Phi_{30400} \\ + \Phi_{30040} - \Phi_{30004} \\ - 2(\Phi_{32200} - \Phi_{30022})].$$

III. SIGNIFICANCE OF THE TRANSFORMATION

Recently, there is a renewed interest in the Stark effect of the hydrogen atom.⁷⁻⁹ Our result will infuse further theoretical development of the problem in two respects. In the first place, as a result of the left-multiplying by $4r$, the Stark potential eFz becomes $4reFz$ in Eq. (4) and takes the form

$$H' = 4eF[(y_1^2 + y_2^2)^2 - (y_3^2 + y_4^2)^2]. \quad (10)$$

It is separable in the two pairs of coordinates y_1, y_2 and y_3, y_4 . By setting $\mu^2 = y_1^2 + y_2^2$ and $\nu^2 = y_3^2 + y_4^2$, it can easily be shown that the hydrogen Stark Hamiltonian takes the form of a pair of anharmonic oscillators in perpendicular spaces. The anharmonic oscillator has been investigated by Bender and Wu¹⁰ and its application to Stark effect has been discussed by Benassi *et al.*⁷ in terms of the squared parabolic coordinate defined in Ref. 3.

Secondly, instead of the parabolic coordinates which have been considered to be convenient for perturbative calculations, our result provides an alternative way for such calculations. In terms of the coordinates given in Eq. (1), the evaluation of the matrix element $\langle n'l'm' | H' | nlm \rangle$ can be reduced to the evaluation of matrix elements of y_i^k , $k = 2$ or 4 involving the oscillator wave functions of the same frequency $\omega = 2p_c/M\hbar$. In order

to see this, we define

$$\begin{aligned} |nmi\rangle &= \Phi_n \left(\left(\frac{2p_c}{n\hbar^2} \right)^{1/2} y_i \right) \\ &= \exp \left(-\frac{p_c y_i^2}{n\hbar^2} \right) H_n \left(\left(\frac{2p_c}{n\hbar^2} \right)^{1/2} y_i \right), \end{aligned} \quad (11)$$

$$\begin{aligned} |n1i\rangle &= \Phi_n \left(\left(\frac{2p_c}{\hbar^2} \right)^{1/2} y_i \right) \\ &= \exp \left(-\frac{p_c y_i^2}{\hbar^2} \right) H_n \left(\left(\frac{2p_c}{\hbar^2} \right)^{1/2} y_i \right). \end{aligned} \quad (12)$$

Introducing the scaling operator $S_i(1/n^{1/2})$, we have

$$S_i(1/n^{1/2}) \Phi_n \left(\left(\frac{2p_c}{\hbar^2} \right)^{1/2} y_i \right) = n^{1/4} \Phi_n \left(\left(\frac{2p_c}{n\hbar^2} \right)^{1/2} y_i \right). \quad (13)$$

From Eqs. (9) through (13), we then have

$$\begin{aligned} \langle n'n'i | y_i^k | nmi \rangle &= (nn')^{-1/4} \langle n'1i | S_i^* (1/n'^{1/2}) y_i^k S_i(1/n^{1/2}) | n1i \rangle \\ &= (nn')^{-1/4} \langle n'1i | S_i(n'^{1/2}/n^{1/2}) y_i^k | n1i \rangle \\ &= (nn')^{-1/4} \sum_{n''} \langle n'1i | S_i(n'^{1/2}/n^{1/2}) | n''1i \rangle \\ &\quad \times \langle n''1i | y_i^k | n1i \rangle. \end{aligned} \quad (14)$$

The matrix element of the form $\langle n'1i | S_i(n'^{1/2}/n^{1/2}) | n''1i \rangle$ has been evaluated by Englefield.¹¹ Further investigation and evaluation of Eq. (14) in connection with the hydrogenic Stark effect will be the subject of a future publication. However, it can immediately be seen on the basis of the form of H' given in Eq. (10) that all matrix elements between wave functions symmetric in the two pairs of variables y_1, y_2 and y_3, y_4 vanish.

As a concluding remark, it should be pointed out that the solutions $\Psi_{n_1 n_2 n_3 n_4}$ in Eq. (7) are the basic functions in a four-dimensional Hilbert space for realizing the ladder representations of the Lie algebra $L(2, 2)$ of the group $U(2, 2)$ in terms of the variables given in Eq. (1).¹² Its unimodular subgroup $SU(2, 2)$ is the universal covering group of $SO(4, 2)$, the dynamical group of the nonrelativistic hydrogen atom.¹³ For a fixed pair of numbers $N_1 = n_1 + n_2 + 1$ and $N_2 = n_3 + n_4 + 1$, these solutions form an orthonormal set.

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We believe our transformation provides a new way of geometrizing the Coulomb field.

³F. Ravndal and T. Toyoda, Nucl. Phys. B **3**, 312 (1967). These authors pointed out that the two choices of phase relations $\varphi = \beta \pm \gamma$ are associated with the dynamical algebra of the chiral group $SU(2) \times SU(2)$.

⁴In terms of our transformation, the coordinates in Ref. 3 should read $x_1 = 2\mu\nu \cos\varphi$, $x_2 = 2\mu\nu \sin\varphi$, and $x_3 = \mu^2 - \nu^2$.

⁵M. J. Englefield, *Group Theory and the Coulomb Problem* (Wiley-Interscience, New York, 1972). Appendix C gives the expression for the Casimir operator $4\vec{K}^2$.

⁶By making a termwise comparison between the Schrödinger equations for the two-dimensional harmonic oscillator and the hydrogen atom, one obtains the frequency $\omega_n = p_c/Mn\hbar$. See p. 76 of Ref. 5.

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¹¹See Ref. 5, Eq. (6.16) on p. 93, or Eq. (6.20) on p. 95.

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¹³Note added in proof. It has been brought to our attention after the submission of this paper that A. O. Barut, C. K. E. Schneider, and R. Wilson, J. Math. Phys. **20**, 2244 (1979) related the Kepler motion and the oscillatory motion by the Kustaanheimo-Steifel transformation.