The hydrogen atom in $\alpha$-dimensional space

Hua Li$^{1*}$, Hui Sun$^2$

$^1$ Department of Fundamental Courses, Academy of Armored Forces, Beijing, China
$^2$ Department of Physics, Beijing Normal University, Beijing, China

*Corresponding author e-mail: lihua9872@126.com

Abstract. The hydrogen atom system can be solved strictly by the eigenvalue equation and get analytical solutions, which is uncommon as a quantum mechanics system. In this study, we obtained wave functions and bound state energies of the hydrogen atom by the Schrödinger equation of the hydrogen atom in the noninteger-dimensional space. And we discussed dimensional behavior in binding energy, angular momentum, and radial density. The dimension $\alpha$ is given by the degree of anisotropy of the actual physical system. The excitons in solids are similar to the hydrogen atoms, except that the mass of their center positive charge is different, so the results obtained in this study were also applicable to excitons in anisotropic solids and hydrogenic impurities, which have application value.

1. Introduction

In the history of quantum mechanics, one of the most prominent achievements is explaining the chemical properties and periodicity of the hydrogen atoms’ spectra. Hydrogen atoms’ energy eigenvalue equation can be strictly solved with analytical solutions[1]. The hydrogen atom theory is the basis for complex atoms and molecular structures. In all kinds of quantum mechanics textbooks, researchers deduced the exact analytical solutions of hydrogen atoms in three-dimensional Euclidean space. By using fractal-dimensional space model, we solved the Schrödinger equations of the hydrogen atom in the fractional-dimensional space, and obtained the function of wave functions and bound state energies of the hydrogen atom about the dimensionality. Binding energy, angular momentum, and radial density were also discussed.

Quantum structures have quantum confinement effects on electrons. Quantum structures can be classified by dimensions: one-dimensional limited quasi-two-dimensional structure, commonly known as the quantum well; two-dimensional constrained quasi-one-dimensional structure, commonly known as quantum wire; three-dimensional restricted quasi-zero-dimensional structure, commonly known as a quantum dot[2]. These low-dimensional structures, such as quantum wells, quantum wires, superlattices, and quantum dots are anisotropic systems[3]. The effective masses of excitons in different lattice directions vary because they are anisotropic. Thus, it is very difficult to calculate in three-dimensional space. The traditional method of calculation is to use a variational approach or perturbation methods, and for convenience, usually, only one or several physical phenomena are considered. These calculations are tedious, and its accuracy depends on the properties of the wave function, and need to have numerical calculations to get the final result. In fractional space, however, the anisotropic interaction in 3-dimensional space are treated as isotropic in an effective fractional-dimensional system, and its dimension, $\alpha$, is given by the degree of anisotropy[3]. The excitons in the solid are similar to the hydrogen atoms unless the mass of the positive charge center is different[4-8].
Thus the results obtained in this paper are also applicable to exciton and hydrogen-like impurities in anisotropic solids. Using fractal spatial models to study hydrogen atoms can simplify the problem and guarantee the high accuracy, with a wide range of application value.

2. Fractional dimensional space model

As early as 1977, Frank H. Stillinger proposed the concept of fractional dimensional space, where the variations of physical quantities were discussed [9], and Laplace operator and angular momentum operator in a dimension space are given by

$$\nabla^2 = \frac{1}{r^{\alpha-1}} \frac{\partial}{\partial r} \left( \frac{1}{r^{\alpha-1}} \frac{\partial}{\partial r} \right) - \frac{l^2}{\hbar^2 r^2}$$  

(1)

where the angular momentum operator is characterized by

$$l^2 = -\frac{\hbar^2}{\sin^{\alpha-2} \theta} \frac{\partial}{\partial \theta} \left( \sin^{\alpha-2} \theta \frac{\partial}{\partial \theta} \right)$$  

(2)

Here, $\alpha$ is the Hausdorff dimension in fractional dimensional space. The position vector $\mathbf{r}$ in space is expressed by coordinates $r$ and $\theta$. $r$ is the radial distance, where $0 \leq r \leq \infty$, and $\theta$ is the deviation of the position vector $\mathbf{r}$ from the origin point in $\mathbf{a}$ space.

The integral formula in $\mathbf{a}$ space of fractional dimension is

$$\int_0^\infty \int \int_0^{2\pi} \int_0^{\pi} \sin^{\alpha-2} \theta \, d\theta$$  

(3)

The stationary Schrodinger equation of the electron under the Coulomb potential of the nucleus in the hydrogen atom can be expressed as:

$$\left( -\frac{\hbar^2}{2m_e} \nabla^2 - \frac{e^2}{r} \right) \psi = E \psi$$  

(4)

$$e_s = e(4\pi \varepsilon \varepsilon_0)^{-\frac{1}{2}} \text{ (SI)}$$  

(5a)

$$e_s = e \text{ (CGS)}$$  

(5b)

Using the Laplace Operator in the noninteger dimensional space, the stationary Schrodinger equation of the hydrogen atom is

$$\left[ -\frac{\hbar^2}{2\mu r^{\alpha-1}} \frac{\partial}{\partial r} \left( r^{\alpha-1} \frac{\partial}{\partial r} \right) + \frac{l^2}{2\mu r^2} - \frac{e^2}{4\pi \varepsilon \varepsilon_0 r} \right] \psi(r, \theta) = E \psi(r, \theta)$$  

(6)

The bound state energy and wave function of the hydrogen atom in the fraction dimensional model can be solved by the preceding equations.

3. Organization of the Text

The bound state energy and wave function of hydrogen atom in fractional dimensional space

Using the separation variable method, we can denote the wave function as $\psi(r, \theta) = R(r)\Theta(\theta)$. Substituting the equation for Eq.6, we have

$$R''(r) + \frac{\alpha-1}{r} R'(r) + \left[ \frac{2\mu}{\hbar^2} \left( E + \frac{e^2}{4\pi \varepsilon \varepsilon_0 r} \right) - \frac{l(l+\alpha-2)}{r^2} \right] R(r) = 0$$  

(7)

$$\Theta''(\theta) + (\alpha - 2) \cot \theta \Theta'(\theta) + l(l + \alpha + 2) \Theta(\theta) = 0$$  

(8)

While we denote $R(r) = r^l e^{-kr} u(r)$ and $x = 2kr$, the radial Eq.7 can be transformed into the confluent hypergeometric equation:

$$x u''(x) + (b - x) u'(x) - au(x) = 0$$  

(9)
where $b = 2l + \alpha - 1$, $\alpha = l + \frac{\alpha - 1}{2} - \frac{B}{k^2}$, and $\alpha = 2\mu E/\hbar^2 B = \frac{\mu e^2}{4\pi\varepsilon_0\hbar^2}$ and $0 \leq r \leq \infty$. The solution of the equation can be expressed as a confluent hypergeometric function $M(\alpha, b, x)$. When $\alpha$ is non-negative integer or $\alpha = n + l + 1$ ($n = 1, 2, 3, ..., l = 0, 1, 2, ..., n - 1$), the wave function satisfies bound state condition (i.e. quadratic integrality), thus the confluent hypergeometric function $M(\alpha, b, x)$ can transform into a polynomial $M(-n + l + 1, 2l + \alpha - 1, 2k_n r)$, where $k_n = 1/[n + (\alpha - 3)/2]a_e$, which determines the value of the quantum number $(n, l)$, the bound state energy level, and orbit radius:

$$E_n = -\frac{E_e}{(n + \frac{\alpha - 3}{2})^2}$$

$$a_n = \left(n + \frac{\alpha - 3}{2}\right)^2 a_e$$

where $a_e$ is the effective Bohr radius, $E_e = -\frac{\mu e^2}{2\hbar^2}$. The confluent hypergeometric function $M(\alpha, b, x)$ and generalized Laguerre polynomials can be used to calculate the radial distribution function $R_{nl}$:

$$M(-m, y + 1, x) = \left[m\frac{\Gamma(y + 1)}{\Gamma(y + m + 1)}\right] L_n^m(x)$$

where $m$ is a positive integer and $y$ is a parameter. The radial distribution function $R_{nl}$ can thus be expressed as:

$$R_{nl} = M_{nl}(\alpha)r^l e^{-\kappa r} L_{n-l-1}^{2l+\alpha-2}(2k_n r)$$

where normalization factor can be expressed as:

$$M_{nl}(\alpha) = \left(\frac{4}{a_e}\right)^{l+\frac{\alpha}{2}} \times \left(\frac{(n-l-1)!}{(2n+\alpha-3)^{2l+\alpha-2}\Gamma(n+l+\alpha-2)}\right)^{1/2}$$

In which $n, l$ are the main quantum number and the angular momentum quantum number respectively, and $R_{nl}$ satisfies the normalization condition $\int_{0}^{\infty} r^{n-l-1} |R_{nl}|^2 dr = 1$. The radial density can be obtained by the integrated equation.

Denote $x = \cos \theta$ ($-1 \leq x \leq 1$) and $\lambda = \frac{\alpha}{2} - 1$, Eq.8 can be transformed into the Gegenbauer equation

$$(1 - x^2)\theta''(x) - (2\lambda + 1)x\theta'(x) + l(l+2\lambda)\theta(x) = 0$$

The solution can be transformed into Gegenbauer polynomials $\theta_l(\theta) = H(\alpha)C^{\alpha/2-1}_l(\cos \theta)$, where the normalizion factor is

$$H(\alpha) = \left\{\begin{array}{ll}
\frac{\Gamma(\alpha/2 - 1)}{l^{(1/2)}(l \neq 0)} & \text{or} \frac{l^{(1/2)}(l = 0)}{\Gamma(2\alpha/2)^{1/2}}
\end{array}\right.$$

The angular distribution function satisfies the normalization condition:

$$\int_{0}^{\pi} \theta_l(\theta) \times \sin^{\alpha - 2} \theta d\theta = \delta_{ll'}$$

where $l, l' = 0, 1, 2, 3, ..., n - 1$. As $\theta(\theta)$ is symmetric: $\theta(-x) = (-1)^l \theta_l(x)$, the wave function parity $P_{nl}(r, \theta) = R_{nl}(r)\theta_l(\theta)$ depends on the angular momentum quantum number $l$. When $\alpha = 3$, $\theta_l(x)$ turns into the Legendre polynomials $\theta_l(\theta) = (l + 1/2)^{1/2}P_l(\cos \theta)$; when $\alpha = 2$, $\theta_l(\theta)$ turns into the Chebyshev polynomials of the first kind: $\theta_l(\theta) = (2/\pi)^{1/2}T_l(\cos \theta)$ for
\( l \neq 0 \), and \( \Theta_l(\theta) = (1/\pi)^{1/2}T_l(\cos \theta) \) for \( l = 0 \); in the one-dimensional case, the form of the Coulomb potential is more complex, which can be expressed by \( \delta \) potential.

4. Dimensional behavior

4.1. Bound state energies

In the case of integer dimension, the results obtained by the Eq. 10 were \( E_n = -\frac{\mu e_s^2}{2\hbar^2 e_s^2 n^2} \) for \( \alpha = 3 \), and \( E_n = -\frac{\mu e_s^4}{2\hbar^2 e_s^2 n^2(n-1/2)^2} \) for \( \alpha = 2 \). Especially for the ground state \( (n = 1) \), it can be seen from the following Fig. 1, \( E_n^{(\alpha=2)} = 4E_{n}^{(\alpha=3)} \), which is a well-known result in quantum mechanics. when \( \alpha = 1 \), the binding energy goes to infinity, \( E_n^{(1D)} = \infty \).

![Figure 1. Hydrogen atom bound-state energies as a functions of dimension \( \alpha \).](image)

4.2. Radial density

The analytical formulas of the wave function have been given in the third part. The distribution of radial density on interval \( r \sim r + dr \) is determined by the radial distribution function, which is defined as \( \mathbf{P}_{nl}(r) = r^{\alpha-1}[R_{nl}(r)]^2 \) in \( \alpha \) dimensional space. When the derivative of radial density, \( \frac{dP_{10}(r)}{dr} = 0 \), equals to zero, the exciton radius \( r_e \) can be obtained. The exciton radius can also be obtained according to the Eq. 11 when \( n = 1 \):

\[
r_e = \left(\frac{\alpha-1}{2}\right) a_e \tag{18}
\]

The exciton radius is \( r_e(3D) = a_e \) for \( \alpha = 3 \), \( r_e(2D) = a_e/4 \) for \( \alpha = 2 \), and \( r_e(1D) = 0 \) for \( \alpha = 1 \), which is caused by the essence of Coulomb action.

4.3. Angular momentum

According to the angular momentum operator of the Eq.6 and the wave function, the eigenvalue equation of the angular momentum operator can be obtained:

\[
\hat{l}^2\psi_{nl}(r, \theta) = l(l + \alpha - 2)\hbar^2\psi_{nl}(r, \theta) \tag{19}
\]

The eigenvalues of angular momentum are related to the dimension \( \alpha \):
\[ |l| = \sqrt{l(l + \alpha - 2)\hbar} \]  \tag{20}

Angular momentum quantum number range is \( l = 0, 1, 2, 3 \ldots, n - 1 \). Especially, when \( \alpha = 3 \), \( |l| = \sqrt{l(l + 1)\hbar} \).

5. Discussion

In the preceding paragraphs, a hydrogen atom in fractional dimension is solved in detail. The excitons in the solid are similar to the hydrogen atoms unless the mass of the positive charge center is different. Low-dimensional structures are anisotropic systems. The effective masses of excitons in different lattice directions vary because they are anisotropic. Thus, it is very difficult to calculate in three-dimensional space. However, the anisotropy in three-dimensional system can be regarded as isotropic in the fractal dimension. Therefore, using the fractal dimensional model method to deal with excitons, and some low-dimensional structures in anisotropic solids can simplify the problem with high accuracy.

Thus, the results obtained in this study can extend to further studies on anisotropic solid excitons, hydrogen-like impurities and some low-dimensional quantum structure.

6. Conclusion

By using the fractal dimensional space model, and solving the Schrödinger equation of hydrogen atoms in the fractal space, we obtained the analytic solution of the bound state energy and the wave function of the hydrogen atom concerning the dimensional variables and discussed the variation. Bound state energy varies concerning the main quantum number and the dimension, and the wave function, the dimension and its parity depends on the angular momentum quantum number \( l \).

Meanwhile, due to the advantages of the fractal dimensional method in anisotropy systems, the results we obtained can be generalized to the exciton and hydrogen-like impurities in anisotropic solids and some low-dimensional quantum structures.

Acknowledgments

We are thankful to the National Natural Science Foundation of China (Grant No. 10574011 and 10974017) for providing financial assistance during the process of this work.

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