

FURTHER STUDY ON THE SOLUTION OF SCHRÖDINGER EQUATION OF HYDROGEN-LIKE ATOM

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ABSTRACT

In this work the Schrödinger equation of the hydrogen-like atom is analytically solved. Three sets of analytical solution are obtained if the factor r^{-1} is not neglected. The first solution is the same as the traditional radial wave function; another one diverges; the last one is far different from the traditional solution. On the consideration of the finite size of the nucleus, the third wave function does not diverge while r approaches to zero. Its radial wave function has below characteristics: (1) the angular-momentum quantum number l must be greater than the principal quantum number n ; (2) l must not be 0 or 1; (3) the electron-cloud distribution differs from the traditional one; (4) the electron is closer to the nucleus by comparison with that in traditional results. On the other hand, the validity of solutions needs to be verified experimentally.

1. INTRODUCTION

In the traditional quantum mechanics, factor r^{-1} was always neglected in the solving the Schrödinger equation of the hydrogen-like atom because the wave function diverges while r approaches to zero. Based on the previous works^[1,2], the Schrödinger equation of the hydrogen-like atom is analytically solved further here.

2. MODEL AND RESULTS

For the simplest system of two bodies with a Coulomb interaction being similar to that of the hydrogen atom, the corresponding Schrödinger equation is:

$$\left(-\frac{\hbar^2}{8\pi^2\mu}\nabla^2 - \frac{Ze^2}{r}\right)\Psi(\theta, \phi, r) = E\Psi(\theta, \phi, r)$$

The wave function $\psi(r)$ is an eigen-solution of energy E and angular momentum (l, m) in the form of:

$$\Psi(\theta, \phi, r) = Y_{lm}(\theta, \phi)R_n(r)$$

Let $R_n(r) = R(r)/r$, the radial equation is:

$$R(r)'' + [\varepsilon + \varepsilon_0 r^{-1} - L(L+1)r^{-2}]R(r) = 0$$

with $\varepsilon = 8\pi^2\mu E/\hbar^2$ and $\varepsilon_0 = 8\pi^2\mu Ze^2/\hbar^2$.

If $E < 0$ for $r \rightarrow \infty$, the equation is reduced to:

$$R(r)'' - \beta^2 R(r) = 0$$

The corresponding solution is:

$$R(r) = C(r)\exp(\pm\beta r)$$

where

$$\beta = \sqrt{-\varepsilon} = \sqrt{-\frac{8\pi^2\mu E}{\hbar^2}}$$

If $R(r) = C(r)\exp(\beta r)$, it represents an unbound state. On the other hand, if $R(r) = C(r)\exp(-\beta r)$ and let

$$R(r) = r^n \exp(-\beta r)U(r)$$

It yields

$$\left[U'' + (2nr^{-1} - 2\beta)U' + (\varepsilon_0 - 2n\beta)r^{-1}U \right] + [n(n-1) - L(L+1)]r^{-2}U = 0$$

When $n(n-1) - L(L+1) = 0$, the above equation can be simplified to:

$$U'' + (2nr^{-1} - 2\beta)U' + (\varepsilon_0 - 2n\beta)r^{-1}U = 0$$

For $n(n-1) - L(L+1) = 0$, there are two situations:

(a) $n = L + 1$, there is:

$$rU'' + [2(L+1) - 2\beta r]U' + [\varepsilon_0 - 2(L+1)\beta]U = 0$$

The solution is exactly the same as the tradition solution obtained long time ago.

(b) $n = -L$, there is

$$rU'' - (2L + 2\beta r)U' + (2L\beta + \varepsilon_0)U = 0$$

The solution is:

$$R(r) = r^{-L} \exp(-\beta r)U(r)$$

Please do not worry that the $(1/r) \rightarrow \infty$ if $r \rightarrow 0$! Before r approaches zero, the interaction potential of two particles should be changed from Ze^2/r to another form in the nuclear type because a nucleus has a finite size.

Let above equation take a general form:

$$rU'' - (b + ar)U' + \left(\frac{ab}{2} + c\right)U = 0$$

Its solution is:

$$U = \sum_{m=0}^{\infty} \alpha_m r^m$$

The recursion relation is

$$(m+1)(b-m)\alpha_{m+1} = a[(b/2 + c/a) - m]\alpha_m$$

and the solution is as below:

$$\begin{aligned} U &= \alpha_0 + \frac{[b/2 + c/a]}{b} \alpha_0 ar + \frac{[b/2 + c/a][b/2 + c/a - 1]}{b(b-1)2!} \alpha_0 a^2 r^2 + \dots \\ &= \frac{\Gamma[b/2 + c/a]}{\Gamma[b]} \sum_{m=0}^{b-1} \frac{\Gamma[b-m]}{\Gamma[(b/2 + c/a) - m]m!} \alpha_0 a^m r^m \end{aligned}$$

From

$$\frac{b}{2} + \frac{c}{a} = l + \frac{\varepsilon_0}{2\beta}$$

there also has three situations as below.

(i) $b < b/2 + c/a$ (or $l < \varepsilon_0/2\beta$), $\alpha_m = 0$, $m = 0, 1, 2, \dots, 2l$. Let $m = 2l + 1 + k$, where $k = 0, 1, 2, \dots$,

The recursion relation is:

$$(k+1)(2l+2+k)\alpha_{k+2+2l} = 2\beta(k+1+l - \varepsilon_0/2\beta)\alpha_{k+1+2l}$$

Let $c/a = \varepsilon_0/2\beta = n$, we have:

$$(k+1)(2l+2+k)\alpha_{k+2+2l} = 2\beta(k+1+l-n)\alpha_{k+1+2l}$$

The solution is as below:

$$U(r) = r^{1+2l} \sum_{k=0}^{\infty} \chi_k r^k$$

with

$$\chi_k = \alpha_{k+1+2l} = \frac{\Gamma(2l+2)}{\Gamma(l+1-n)} \frac{\Gamma(k+1+l-n)}{\Gamma(2l+2+k)k!} (2\beta)^k \chi_0$$

This solution is exactly the same as the traditional radial wave function.

(ii) $b = b/2 + c/a$. The recursion relation is

$$(m+1)\alpha_{m+1} = 2\beta\alpha_m$$

The solution is as below:

$$U(r) = \alpha_0 \exp(2\beta r)$$

It diverges when r is enough large, we do not discuss it again.

(iii) $b > b/2 + c/a$ (or $l > \epsilon_0/2\beta$). Let $n = \epsilon_0/2\beta$ with $n = 1, 2, 3, \dots, l-1$. Because $l > n$, so that $l \neq 0, 1$

$$\begin{aligned} l=2, n=1 \\ l=3, n=1,2 \\ l=4, n=1,2,3, \\ \dots \end{aligned}$$

The solution is:

$$U(r) = \sum_{m=0}^{n+l} \alpha_m r^m$$

Where $\beta = 1/(nr_H)$, r_H is the Bohr radius and

$$\alpha_m = \frac{\Gamma(l+n)}{\Gamma(2l)} \frac{\Gamma(2l-m)}{\Gamma(l+n-m)m!} (2\beta)^m \alpha_0$$

$$R(r) = r^{-l} \exp(-\beta r) U(r)$$

This solution is quite different from the traditional solution. For example:

$$U(r) = \alpha_0 \left[1 + \frac{3}{2} \frac{r}{r_H} + \left(\frac{r}{r_H}\right)^2 + \frac{1}{3} \left(\frac{r}{r_H}\right)^3 \right] \text{ for } l=2, n=1$$

$$U(r) = \alpha_0 \left[1 + \frac{4}{3} \frac{r}{r_H} + \frac{4}{5} \left(\frac{r}{r_H}\right)^2 + \frac{4}{15} \left(\frac{r}{r_H}\right)^3 + \frac{2}{45} \left(\frac{r}{r_H}\right)^4 \right] \text{ for } l=3, n=1$$

$$U(r) = \alpha_0 \left[1 + \frac{5}{6} \frac{r}{r_H} + \frac{1}{3} \left(\frac{r}{r_H}\right)^2 + \frac{1}{12} \left(\frac{r}{r_H}\right)^3 + \frac{1}{72} \left(\frac{r}{r_H}\right)^4 + \frac{1}{720} \left(\frac{r}{r_H}\right)^5 \right] \text{ for } l=3, n=2$$

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In $r < r_0$ region, $R_n(r) = u(r)/r$. We have

$$u(r)'' + \left[\frac{8\pi^2 \mu}{h^2} (E + U(r)) - L(L+1)r^{-2} \right] u(r) = 0$$

where

$$U(r) = \begin{cases} -\frac{e^2}{r} & r > r_0 \\ U_0 & r < r_0 \end{cases}$$

Energy $E_n = -2\pi^2\mu Z^2 e^4/n^2 h^2$, where $n = m - l$, and $n = 1, 2, 3, \dots$, the wave function $u(r) = u_{nl}(r)$

$$u_{nl}(r) = \begin{cases} \sum \alpha_n r^m & r > r_0 \\ A_j_l(K_n r) & r < r_0 \end{cases}$$

with

$$K_n = \left[\frac{8\pi^2\mu(U_0 - |E_n|)}{h^2} \right]^{1/2}$$

where $j_l(K_n r)$ is spherical Bessel function

3. DISCUSSION

From the results obtained above, it is not necessary to abnegate the factor r^{-l} just in the traditional quantum mechanics to solve the Schrödinger equation of the hydrogen-like atom. Because there is not the problem about the wave function to be divergence while r approaches to zero. Based on the previous works ^[1,2], the Schrödinger equation of the hydrogen-like atom could be analytically solved further. When the finite size (existing a radius r_0) of a nucleus is considered the factor r^{-l} could not be necessary to neglect. If the wave function is even existed in the region of less than radius r_0 , the electron should be captured by the nucleus. In this case it seems that a nuclear process is generated and a dineutron could be confirmed on this work as the observation of beta-delayed two-neutron radioactivity in 1979 ^[3]. If not, the probability of electron in the close-by the radius r_0 of nucleus should be very large that a nuclear reaction could be generated very easily.

In this work three sets of analytical solution are obtained if the factor r^{-l} is not neglected. The first solution is the same as the traditional radial wave function; another one diverges; the last one is far different from the traditional solution. On the consideration of the finite size of the nuclear, the third wave function does not diverge while r approaches to zero. Its radial wave function has below characteristics: (1) the angular-momentum quantum number l must be greater than the principal quantum number n ; (2) l must not be 0 or 1; (3) the electron-cloud distribution differs from the traditional one; (4) the electron is closer to the nuclear by comparison with that in traditional results. On the other hand, the validity of solutions needs to be verified experimentally.

4. CONCLUSION

The radial wave function obtained by us in this work has below characteristics: (1) The angular-momentum quantum number l must be greater than the principal quantum number n ; (2) l must not be 0 or 1; (3) The electron-cloud distribution differs from the traditional one; (4) The electron is closer to the nuclear by comparison with that in traditional results. On the other hand, the validity of solutions needs to be verified experimentally.

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