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AN ALTERNATIVE ALGEBRAIC METHOD FOR SOLVING THE RADIAL EQUATION FOR THE HIDROGEN ATOM

G.A.Estévez*[a], W.Solano-Torres[b] and
Peilian Lee, Z. Jiang, Y. Tao[c],
(a) Physics Department
University of Central Florida
Orlando, FL 32816 - 0993
(b) Departamento de Física
Universidad Nacional de Colombia
Santafé de Bogotá D.C., Colombia
A.A. No. 14490
(c) Basic Science Department
Anshan Institute of Iron and Steel Technology
Anshan, Liaoning
People´s Republic of China

ABSTRACT

A pair of ladder operators are introduced and use for solving the radial equation for the hydrogen atom. The energy eigenvalues as well explicit analytic expressions for the eigenfunctions of this particular Kepler problem are obtained after some algebraic manipulation of the operators.

1. INTRODUCTION

Algebraic techniques for solving quantum mechanics problems have been known for a long time[1-3] and are now standard texbook fare[3-6]. The importance of the operator algebra is often illustrated in the literature and textbooks on quantum mechanics by treating the cases of the linear simple harmonic oscillator and angular momentum problems[3-10]. Another example of an exactly solvable exercise in quantum mechanics is the eigenvalue problem corresponding to the radial equation for the Coulomb potential. Its solution employing ladder operators has received some attention[11-16]. The reported work on this problem concentrates mainly on the energy eigenvalue computation; even though formal solutions of the

* Permanent Addres : Department of Mathematics and Physical Sciences, Inter American University, Call Box 5100-41, San Germán, PR 00683, Puerto Rico, USA.

eigenfunctions are found in the literature[11,14-16], their identification with the eigensolutions expressed in terms of Laguerre polynomials is not usually explicitly shown. The purpose of this article is to employ Schrödinger's method of factorization[17-18] to develop an alternate pair of ladder operators which are particularly useful for computing the explicit form of the eigenfunctions of the hydrogen atom. The layout of this paper is as follows. In Section II the ladder operators for the radial differential equation corresponding to the hydrogen atom are introduced. The formal properties of these operators are also examined in thes section. Section III is devoted to the calculation of the eigenvalues and the explicit form of the eigenfunctions, and finally in Section IV some concluding remarks are made.

2. LADDER OPERATORS FOR THE RADIAL WAVE EQUATION

The radial differential equation for the nonrelativistic hydrogen atom is[4]

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) R + \frac{2\mu}{\hbar^2}\left[\frac{e^2}{r} - \frac{l(l+1)\hbar^2}{2\mu r^2}\right] R = -\frac{2\mu E}{\hbar^2} R \qquad (1)$$

where the symbols have their usual meaning; in particular l designates the orbital angular momentum quantum number and μ denotes the reduced mass of the electron-proton system.

In atomic units, where μ =1, e =1, and $\hbar$ =1, Eq.(1) becomes

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \frac{2}{r} - \frac{l(l+1)}{r^2}\right) R = WR \qquad (2)$$

with $W = -2E>0$. Because of the accidental degeneracy peculiar to the Coulomb potential there are different radial functions for distinct values of l corresponding to the same energy W. Denoting by R_{nl} the radial function coresponding to W_n and a given value of l, and defining the radial Hamiltonian operator $\hat{H}_l$ by the expression

$$\hat{H}_l = \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \frac{2}{r} - \frac{l(l+1)}{r^2} \qquad (3)$$

it is possible to recast the radial equation (2) in the compact form

$$\hat{H}_l R_{nl} = W_n R_{nl} \tag{4}$$

It is seen from this expression that W_n is an eigenvalue of $\hat{H}_l$. From the definition (3) it follows immediately that

$$\hat{H}_{l+1} = \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \frac{2}{r} - \frac{(l+1)(l+2)}{r^2} \tag{5}$$

Due to the symmetry property of the Coulomb potential the eigenvalue of $\hat{H}_l$ is simultaneously an eigenvalue of $\hat{H}_{l+1}$ but their eigenfunctions are different, thence

$$\hat{H}_{l+1} R_{n,l+1} = W_n R_{n,l+1} \tag{6}$$

We now introduce two operators $\hat{H}^+$ and $\hat{H}^-$ such that their product has the same eigenfunctions as $\hat{H}_l$. The eigenvalues H^+H^- of (or for that matter those of $\hat{H}^-\hat{H}^+$) may differ from the eigenvalues of $\hat{H}_l$. We write

$$\hat{H}^-_{l+1}\hat{H}^+_l = \hat{H}_l + C(l) \tag{7}$$

where C(l) is a scalar.

The combined operator $\hat{H}^-_{l+1}\hat{H}^+_l$ thus has a distinct eigenvalue for each different value of l, i.e., it is non-degenerate with respect to l; this is the main difference between $\hat{H}_l$ and the combined operator defined by Eq.(7). The reason different subscripts are employed for $\hat{H}^-$ and $\hat{H}^+$ will be apparent at the end of this section. The two first-order differential operators are defined as follows:

$$\hat{H}^-_{l+1} = \frac{d}{dr} + \frac{C_1(l)}{r} + C_2(l) \tag{8}$$

$$\hat{H}^+_l = \frac{d}{dr} + \frac{C_3(l)}{r} + C_4(l) \tag{9}$$

Substituting the last two expressions above into Eq.(7) and equating coefficients gives relationships from which the desired operators can be obtained. Different analytic forms of C(l) will give rise to distinct ladder operators. For instance, the choices $C(l) = -1/l^2$, and $C(l) = -1/(l+1)^2$ lead, respectively, to the sets of references 11 and 13. Now it can be shown that choosing $C(l)=-1/(l+1)^2$, the ladder operators generated agree with those of Ref.13, namely:

$$\hat{H}^-_{l+1} = \frac{d}{dr} + \frac{l+2}{r} - \frac{1}{l+1} \tag{10a}$$

$$\hat{H}^+_{l} = \frac{d}{dr} - \frac{l}{r} + \frac{1}{l+1} \tag{10b}$$

These two operators can be readily computed from Eqs.(8) and (9) in conjunction with Eq.(7).

Substitution of Eqs.(8) and (9) into Eq.(7) and equating coefficients on both sides of the resulting equation yield:

$$C_2 C_4 = -\frac{1}{(l+1)^2}, \qquad C_2 + C_4 = 0$$

$$C_1 + C_3 = 2, \qquad (C_1 - 1)\, C_3 = -l(l+1) \tag{11}$$

$$C_2 C_3 + C_1 C_4 = 2$$

To keep the notation uncluttered the argument l has been omitted on all the C's. The solution of the system of equations given by (11) is

$$C_1 = l+2, \qquad C_2 = -\frac{1}{l+1}, \qquad C_3 = -l, \qquad C_4 = \frac{1}{l+1} \tag{12}$$

Substitution of these results into Eqs.(8) and (9) yields Eqs.(10).

A useful additional relationship is

$$\hat{H}^+_l \hat{H}^-_{l+1} = \hat{H}_{l+1} + C(l) \tag{13}$$

It will be shown next that apart from proportionality constants

$$\hat{H}^+_l R_{nl}(r) \sim R_{n,l+1}(r) \tag{14}$$

$$\hat{H}^-_{l+1} R_{n,l+1}(r) \sim R_{n,l}(r) \tag{15}$$

Multiplying both sides of Eq.(7) from the left with $\hat{H}_l^+$ and acting with the resulting operator on the radial wavefunction R_{nl} renders the expresion

$$\hat{H}_l^+\hat{H}_{l+1}^-\hat{H}_l^+R_{nl} = \hat{H}_l^+[\hat{H}_l+C(l)]R_{nl} \qquad (16)$$

Employing the relationship (13) in conjunction wiht Eq.(4), Eq.(16) develops into

$$[\hat{H}_{l+1}+C(l)](\hat{H}_l^+R_{nl}) = [W+C(l)](\hat{H}_l^+R_{nl})$$

therefore

$$\hat{H}_{l+1}(\hat{H}_l^+R_{nl}) = W(\hat{H}_l^+R_{nl}) \qquad (17)$$

It is important to note that this is in the form of the eigenvalue equation (6). Equation (17) thus shows that $\hat{H}_l^+ R_{nl}$ is an eigenfunction of $\hat{H}_{l+1}$, thus proving Eq. (14). Equation (15) may be proved in a similar manner.

The mathematical entities $\hat{H}_l^+$ and $\hat{H}_{l+1}^-$ are thus the raising and lowering operators of the hydrogen-atom radial wavefunctions R_{nl} and $R_{n,l+1}$, respectively.

3. COMPUTATION OF THE ENERGY LEVELS AND EIGENFUNCTIONS

The problem under consideration is that of finding the possible eigenvalues of Eq. (2) and the corresponding eigenfunctions. Employing the hypervirial theorem[19,20] it can be shown that for a given value W, the quantity l is bounded from above. Designating the maximum allowed value of l by l^*, the adder operator $\hat{H}_l^+$ when applied to the corresponding eigenfunction must give zero:

$$\hat{H}_{l^*}^+R_{n,l^*}=0 \qquad (18)$$

If $R_{n,l}$ is operated on by the combined operator of Eq. (7) with $l=l^*$, then

$$\hat{H}_{l^*+1}^-(\hat{H}_{l^*}^+R_{n,l^*}) = [\hat{H}_{l^*}+C(l^*)]R_{n,l^*} = [W+C(l^*)]R_{n,l^*} \qquad (19)$$

The quantity within parentheses on the left side of this equation vanishes due to condition (18). Since in this work $C(l^*) = -1/(l^*+1)^2$ it follows from Eq. (19) that

$$W = \frac{1}{(l^*+1)^2} \tag{20}$$

Let $n = l^* + 1$; since $E = -W/2$, we deduce from Eq. (20) that

$$E = -\frac{1}{2n^2} \tag{21}$$

This is the well-known expression for the possible bound-state energies of the hydrogen atom, expressed in atomic units; the quantity n is the principal quantum number. From the definition of $\hat{H}_l$ it is known that the minimum value that l can take on is zero. Thus for a given value of n, l encompasses the range from 0 to $l^* = n - 1$.

The radial function $R_{nl}(r)$ can now be computed. Consider first $R_{n,n-1}(r)$. Eq. (18) with $l^* = n - 1$ reads:

$$\hat{H}^+_{n-1} R_{n,n-1}(r) = 0 \tag{22}$$

If this expression is written out explicitly, one obtains

$$\left(\frac{d}{dr} - \frac{n-1}{r} + \frac{1}{n}\right) R_{n,n-1} = 0 \tag{23}$$

This is a first-order differential equation having the solution

$$R_{n,n-1}(r) = C e^{-r/n} r^{n-1} \tag{24}$$

C being a normalizing factor.
For every $l < l^*$, R_{nl} can be formally obtained by applying iteratively the operator $\hat{H}^-$ on $R_{n,n-1}$; thus

$$R_{nl}(r) = \left(\prod_{i=l+1}^{n-1} \hat{H}^-_l\right) R_{n,n-1} = \hat{H}^-_{l+1}\, \hat{H}^-_{l+2} \cdots \hat{H}^-_{n-2}\, \hat{H}^-_{n-1}\, R_{n,n-1} \tag{25}$$

The radial function $R_{nl}(r)$ should be expressed in terms of polynomials. First it will be shown that $R_{nl}(r)$ may be written as follows:

$$R_{nl}(r) = C(n,l)\, e^{-r/n}\, r^l \left(\sum_{k=0}^{n-l-1} A_k r^k\right) \tag{26}$$

where C(n,l) is chosen so as to normalize the radial function $R_{nl}(r)$. Equation (26) may be proved employing the method of induction, beginning by calculating $R_{n,n-2}$. Except for a proportionality constant the following can be written from (15)

$$R_{n,n-2} \sim \hat{H}^{-}_{n-2+1} R_{n,n-2+1} = \hat{H}^{-}_{n-1} R_{n,n-1} \tag{27}$$

Employing Eq. (10a.) with l = n - 2 in this expression yields (C=constant)

$$R_{n,n-2} = C'\left(\frac{d}{dr} + \frac{n}{r} - \frac{1}{n-1}\right) R_{n,n-1}$$

$$= C(n,n-2)\, e^{-r/n} r^{n-2} (2n-1) \left[1 - \frac{r}{n(n-1)}\right] \tag{28}$$

In similar fashion, if C" designates a new constant, then

$$R_{n,n-3} = C''\left(\frac{d}{dr} + \frac{n-1}{r} - \frac{1}{n-2}\right) R_{n,n-2} \tag{29}$$

$$= C(n,n-3)\, e^{-r/n} r^{n-3} (2n-3) \left[1 - \frac{2r}{n(n-2)} + \frac{2r^2}{n^2(n-2)(2n-3)}\right]$$

Assuming that the eigensolution R_{nl} may be written in the form given by Eq. (26), we propose to show that $R_{n,l-1}$ may be expressed as

$$R_{n,l-1}(r) = C(n,l-1)\, e^{-r/n} r^{l-1} \left(\sum_{k=0}^{n-l} B_k\, r^k\right) \tag{30}$$

The radial function $R_{n,l-1}$ is uniquely generated from R_{nl} employing the ladder operator $\hat{H}^{-}_{l}$. We write

$$R_{n,l-1}(r) = C^*\, \hat{H}^{-}_{l} R_{nl} = C^*\left(\frac{d}{dr} + \frac{l+1}{r} - \frac{1}{l}\right) R_{nl}$$

$$R_{n,l-1}(r) = C(n,l-1)\left(\frac{d}{dr} + \frac{l+1}{r} - \frac{1}{l}\right)\left\{e^{-r/n} r^{l} \left(\sum_{j=0}^{n-l-1} A_j\, r^j\right)\right\}$$

Performing the indicated operations in the last expression above yields

$$R_{n,l-1}(r) = C(n,l-1)\,e^{-r/n}r^{l-1}\left(\left[\sum_{j=0}^{n-l-1}(j+2l+1)A_j\,r^j\right]\right.$$

$$\left. - \left(\frac{1}{n}+\frac{1}{l}\right)\sum_{j=0}^{n-l-1}A_j r^{j+1}\right.$$

When this last equation is put in the form (30) the following relationships between the old and the new coefficients are achieved:

$$B_0 = (2l+1)\,A_0$$

$$B_k = (k+2l+1)\,A_k - \left(\frac{1}{n}+\frac{1}{l}\right)A_{k-1} \qquad (K=1,\ldots\ldots,n-l-1) \qquad (31)$$

$$B_{n-l} = -\left(\frac{1}{n}+\frac{1}{l}\right)A_{n-l-1}$$

The ansatz (26) has been thus justified. For completeness sake it is next shown that the radial function R_{nl} for the hydrogen atom obtained above agrees with the one deduced employing the usual power-series solution method. It suffices to show that the coefficients of the polynomial in (26) are related by the following recursion formula[21] valid for $K \leq n-l-1$

$$A_{k+1} = \left(\frac{2}{n}\right)\frac{k+1+l-n}{(k+1)(k+2l+2)}A_k \qquad (32)$$

Note that if instead of r a new measure of length ρ defined by (ao = Bohr radius)

$$\rho = \frac{r\sqrt{8\mu|E|}}{\hbar} = \frac{2r}{na_0} \qquad (33)$$

is employed, (in atomic units $\rho = 2r/n$), the recursion relation would be

$$A_{k+1} = \frac{k+1+l-n}{(k+1)(k+2l+2)}A_k \qquad (34)$$

The proof of Eq. (32) can also be performed employing the method of induction. When $l = n - 2$, the parameter K can take on only two values : 0 and 1. From the expression within

square brackets in Equation (28) it is seen that $A_0 = 1$, $A_1 = -1/[n(n-1)]$, thus

$$A_1 = -\frac{A_0}{n(n-1)} \tag{35}$$

which is just Eq. (32) with $l = n - 2$ and $k = 0$. Similarly when $l=n-3$, the three polynomial coefficients in the expression within square brackets in Eq. (29) also satisfy the recursion formula (32).

Assuming that all coefficients A_k in the expression for R_{nl} given by Eq.(26) satisfy (32), it is necessary to show that the coefficients B_k in $R_{n,l-1}$ satisfy (32) as well. The recursion formula for the coefficients B_k in the expression for $R_{n,l-1}$ reads:

$$B_{k+1} = \left(\frac{2}{n}\right)\frac{k+l-n}{(k+1)(k+2l)}B_k \tag{36}$$

From the middle expression of Eq. (31)

$$B_{k+1} = (k+2l+2)A_{k+1} - \left(\frac{1}{n}+\frac{1}{l}\right)A_k$$

The ratio of succeeding terms is thus

$$\frac{B_{k+1}}{B_k} = \frac{(k+2l+2)A_{k+1} - \left(\frac{1}{n}+\frac{1}{l}\right)A_k}{(k+2l+1)A_k - \left(\frac{1}{n}+\frac{1}{l}\right)A_{k-1}} \tag{37}$$

Substituting in this expression the relationships between the coefficients A_k given by Eq. (32), Eq. (36) is obtained. This concludes the proof.

4. CONCLUDING REMARKS

Employing the simple and elegant method of factorization two ladder operators were constructed and used for solving the radial equation corresponding to a hydrogen-atom system. The possible energy states of this system were determined employing an almost wholly algebraic procedure involving the use of the ladder operators. The operators introduced in this article can be safely applied to the case $l = 0$, in contradistinction to the ladder operators advocated in Ref.11. Further, their application to the computation of the explicit analytic form of the eigensolutions of the radial equation for the hydrogen atom appears to be more convenient. The insight

gained by the student may be helpful, at an advanced level, in the treatment of the creation and annihilation operators in quantum-field theory. The above features should render this article especially useful to undergraduate students of physics.

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