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On the Schrödinger radial ladder operator

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Abstract. Using the radial ladder operators A_l^+ and A_l^- defined in solving the hydrogen atom radial equation with the factorisation method, we develop a new device by which the calculations on the average value of r^ν, the inner product of the radial wavefunctions and the matrix element of r are simplified and by which some new recurrence relations are derived.

1. Introduction

The factorisation method to solve the Schrödinger equation was proposed and discussed in the 1940s and 1950s. For a comprehensive review see [1] and references therein. It is an elegant and powerful device by which eigenvalues and eigenfunctions for some physically important solvable potentials can be obtained straightforwardly. Owing to the development of supersymmetry quantum mechanics (SSQM), this method has attracted fresh interest in recent years. Based on Witten's model [2] of SSQM, many papers explored various aspects [3] stemming from the factorisation which are very significant to quantum mechanics.

However, if we examine carefully the works published to date on the factorisation method, it can be found that some simple and useful consequences have not received sufficient attention. One of them is the application of the Schrödinger radial ladder operators.

It is well known that the angular momentum ladder operator and the creation and annihilation operators of the one-dimensional harmonic oscillator are very important to quantum mechanics. All these operators are the results of factorisation. We find that the Schrödinger radial ladder operators can be applied in order to greatly simplify practical quantum mechanics calculations. In this paper, we intend to adopt the familiar hydrogen atom to illustrate the point.

The paper is organised as follows. Section 2 presents the standard factorisation solving method of the hydrogen atom and gives the definition of the radial ladder operators. Section 3 discusses the calculation of the average value of the power of r. Section 4 investigates the inner product and orthogonality of the radial wavefunctions. Section 5 derives the recurrence relations for matrix elements of r. Section 6 summarises the conclusions of the present work.

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2. Solving the hydrogen atom radial equation by the factorisation method

We denote the reduced radial wavefunction of the hydrogen atom with a well defined value l of the angular momentum by $U_l(r)$, which satisfies a reduced radial Schrödinger equation

$$H_l U_l(r) \equiv \left(-\frac{d^2}{dr^2} - \frac{2}{r} + \frac{l(l+1)}{r^2} \right) U_l(r) = \varepsilon_l U_l(r) \tag{2.1}$$

and the boundary and normalising conditions

$$U_l(0) = U_l(\infty) = 0 \tag{2.2}$$

$$\int_0^\infty dr\, U_l^2(r) = 1 \tag{2.3}$$

where we adopt the atomic unit of length.

If we define two operators, according to the standard factorisation method [4], by

$$A_l^\pm \equiv \pm \frac{d}{dr} + \frac{l+1}{r} - \frac{1}{l+1} \tag{2.4}$$

which are adjoint to each other in the reduced radial wavefunctions space, then a little algebra shows that

$$\begin{aligned} H_l^+ &\equiv A_l^+ A_l^- = H_l + 1/(l+1)^2 \\ H_l^- &\equiv A_l^- A_l^+ = H_{l+1} + 1/(l+1)^2. \end{aligned} \tag{2.5}$$

$H_l^\pm$ are two Hermitian positive semidefinite operators. From (2.4) and (2.5) and considering the 'degeneracy theorem' of SSQM, we can immediately derive the following relationship between the eigenvalues and eigenfunctions of the two partner Hamiltonians $H_l^\pm$.

(i) The equation

$$A_l^- U_l^{(0)}(r) = 0 \tag{2.6}$$

has a normalisable solution which satisfies (2.2) and is the lowest eigenstate of H_l^+, corresponding to the eigenvalue zero, i.e.

$$H_l^+ U_l^{(0)}(r) = \varepsilon_l^{(+)(0)} U_l^{(0)}(r) \tag{2.7}$$

and

$$\varepsilon_l^{(+)(0)} = 0. \tag{2.8}$$

(ii) Apart from the lowest eigenstate of H_l^+, the partner Hamiltonians H_l^+ and H_l^- have identical bound state spectra, i.e. their eigenvalues satisfy

$$\varepsilon_l^{(-)(k)} = \varepsilon_l^{(+)(k+1)} \qquad k = 0, 1, 2, \ldots \tag{2.9}$$

where k is the number of the energy level above $\varepsilon_l^{(0)}$.

(iii) The eigenfunctions of H_l^+ and H_l^- corresponding to the same eigenvalues are related by

$$\begin{aligned} A_l^- U_l^{(+)(k+1)}(r) &= (\varepsilon_l^{(-)(k)})^{1/2} U_l^{(-)(k)}(r) \\ A_l^+ U_l^{(-)(k)}(r) &= (\varepsilon_l^{(-)(k)})^{1/2} U_l^{(+)(k+1)}(r). \end{aligned} \tag{2.10}$$

Combining all these results with (2.5), we can straightforwardly write the solution of the hydrogen atom problem. Given l, the lowest energy of the hydrogen atom is evidently

$$\varepsilon_l^{(0)} = -1/(l+1)^2. \tag{2.11}$$

For different l, we can obtain the recurrence relation

$$\varepsilon_{l+1}^{(k)} = \varepsilon_l^{(k+1)}. \tag{2.12}$$

Using (2.12) k times altogether, we obtain

$$\varepsilon_l^{(k)} = \varepsilon_{l+1}^{(k-1)} = \ldots = \varepsilon_{l+k}^{(0)} = -1/(l+k+1)^2. \tag{2.13}$$

Hence, the familiar energy spectrum of the hydrogen atom is reproduced, i.e.

$$\varepsilon_{nl} \equiv \varepsilon_l^{(k)} = -1/n^2 \tag{2.14}$$

where

$$n = l+k+1 \qquad n = 1, 2, \ldots \tag{2.15}$$

is just the principal quantum number and k is the number of nodes of the radial wavefunction.

Equation (2.10) gives the recurrence relations

$$\begin{aligned} U_{n,l+1}^{(k-1)}(r) &= C_{nl}[A_l^- U_{n,l}^{(k)}(r)] \\ U_{n,l}^{(k)}(r) &= C_{nl}[A_l^+ U_{n,l+1}^{(k-1)}(r)] \end{aligned} \tag{2.16}$$

where

$$\begin{aligned} C_{nl} &= (\varepsilon_l^{(k)} - \varepsilon_l^{(0)})^{-1/2} \\ &= [1/(l+1)^2 - 1/n^2]^{-1/2}. \end{aligned} \tag{2.17}$$

It follows from (2.16) that the operator A_l^-, acting upon $U_{n,l}^{(k)}(r)$, decreases the number of the nodes by one and simultaneously increases the angular quantum number by one, while the operator A_l^+, acting upon $U_{n,l+1}^{(k-1)}(r)$, increases the number of the nodes by one and decreases the angular quantum number l by one. Therefore, we call them the Schrödinger radial ladder operators.

Given n, with $l = n-1$, the reduced wavefunction $U_{n,n-1}(r)$ (i.e. $U_l^{(0)}(r)$ in (2.6)) has no node and is called the key function, and satisfies

$$A_{n-1}^- U_{n,n-1}(r) = 0 \tag{2.18}$$

or explicitly

$$\left(-\frac{\mathrm{d}}{\mathrm{d}r} + \frac{n}{r} - \frac{1}{n}\right) U_{n,n-1}(r) = 0. \tag{2.19}$$

Solving the first-order differential equation, we can obtain a normalised key function

$$U_{n,n-1}(r) = (2/n)^{n+1/2}[(2n)!]^{-1/2} r^n \exp(-r/n). \tag{2.20}$$

Starting from the key function and using the recurrence relation (2.16), we can easily obtain all the reduced radial wavefunctions of the hydrogen atom bound states.

By comparison with the well known creation and annihilation operators, a^+ and a, of the one-dimensional oscillator, the radial ladder operators have some different properties, one of which is that their commutation relations are not constant. For instance,

$$[A_l^-, A_{l'}^+] = \frac{l'+l+2}{r^2} \tag{2.21}$$

$$[A_l^+, A_{l'}^+] = \frac{l-l'}{r^2} \tag{2.22}$$

$$[A_l^-, A_{l'}^-] = \frac{l'-l}{r^2}. \tag{2.23}$$

However, we find that the radial ladder operators are very useful in practical calculations on the hydrogen atom, as shown in the following sections.

3. The average value of the power of r

For convenience, in the following discussion we denote $U_{nl}(r)$ by $|nl\rangle$, the matrix elements of r^s by $\langle n'l'|r^s|nl\rangle$ and the average value of r^s simply by $\langle r^s\rangle_l$. With these notations, (2.16) and (2.18) can be written in the form

$$|n, l+1\rangle = C_{nl}A_l^-|n, l\rangle \tag{3.1}$$

$$|n, l\rangle = C_{nl}A_l^+|n, l+1\rangle \tag{3.2}$$

and

$$A_{n-1}^-|n, n-1\rangle = 0. \tag{3.3}$$

Note that $|nl\rangle$ satisfies the normalising condition, i.e.

$$\langle nl|nl\rangle = 1 \tag{3.4}$$

and the orthogonality is also satisfied, i.e.

$$\langle n'l'|nl\rangle = 0 \tag{3.5}$$

but only when $l = l'$ and $n \neq n'$.

First, we calculate the average values of r^s in the key function $|n, n-1\rangle$, which are simple and useful to illustrate the technique.

Step (i). From the definition of the radial ladder operators, we have

$$\tfrac{1}{2}(A_{n-1}^+ + A_{n-1}^-) = \frac{n}{r} - \frac{1}{n} \tag{3.6}$$

and hence

$$\left\langle \frac{1}{r} \right\rangle_{n-1} = \frac{1}{2n}\langle A_{n-1}^+ + A_{n-1}^-\rangle_{n-1} + \frac{1}{n^2}. \tag{3.7}$$

However, from (3.3) we know that

$$\langle A_{n-1}^-\rangle_{n-1} = 0 \tag{3.8}$$

and

$$\langle A_{n-1}^{+}\rangle_{n-1}=0. \tag{3.9}$$

Thus

$$\left\langle\frac{1}{r}\right\rangle_{n-1}=\frac{1}{n^2}. \tag{3.10}$$

Step (ii). Multiplying both sides of (3.6) by r, we obtain

$$\tfrac{1}{2}r(A_{n-1}^{+}+A_{n-1}^{-})=n-r/n \tag{3.11}$$

and hence

$$\langle r\rangle_{n-1}=n^2-\tfrac{1}{2}n\langle r(A_{n-1}^{+}+A_{n-1}^{-})\rangle_{n-1}. \tag{3.12}$$

By means of (3.3) and considering

$$[r, A_{n-1}^{+}]=-1 \tag{3.13}$$

we have

$$\langle r\rangle_{n-1}=n(n+\tfrac{1}{2}). \tag{3.14}$$

Step (iii). In general, multiplying both sides of (3.6) by r^s with any s and using a similar method as above, we immediately obtain a recurrence relation

$$\langle r^s\rangle_{n-1}=n(n+\tfrac{1}{2}s)\langle r^{s-1}\rangle_{n-1}. \tag{3.15}$$

If $s>0$, using (3.15) s times altogether, we arrive at the final result. However, if $s<0$, it has to be used in the reverse order, i.e.

$$\langle r^s\rangle_{n-1}=\frac{1}{n[n+\frac{1}{2}(s+1)]}\langle r^{s+1}\rangle_{n-1} \qquad \text{for } s<0. \tag{3.16}$$

Since it is necessary that the average value of r^s is positive, the restriction must be imposed on s that

$$s>-2n-1. \tag{3.17}$$

For an arbitrary $|nl\rangle$ we have

$$\tfrac{1}{2}\langle r^s(A_l^{+}+A_l^{-})\rangle_l=(l+1)\langle r^{s-1}\rangle_l-(l+1)^{-1}\langle r^s\rangle_l. \tag{3.18}$$

Since $A_l^{-}|nl\rangle\neq 0$ if $l\neq n-1$, the previous method is not available. However, when $l+1<n-1$, we have

$$\begin{aligned}\tfrac{1}{2}\langle r^s(A_l^{+}+A_l^{-})\rangle_l&=\tfrac{1}{2}C_{nl}^{2}(\langle A_l^{-}r^sA_l^{+}A_l^{+}\rangle_{l+1}+\langle A_l^{-}r^sA_l^{-}A_l^{+}\rangle_{l+1})\\&=\tfrac{1}{2}C_{nl}^{2}(\langle A_l^{-}A_l^{+}r^sA_l^{+}\rangle_{l+1}+\langle A_l^{-}r^s(A_l^{-}A_l^{+})\rangle_{l+1}+\langle A_l^{-}[r^s, A_l^{+}]A_l^{+}\rangle_{l+1}).\end{aligned} \tag{3.19}$$

Substituting (2.5) into (3.19) and considering (2.17), we get

$$\tfrac{1}{2}\langle r^s(A_l^{+}+A_l^{-})\rangle_l=\tfrac{1}{2}(\langle r^sA_l^{+}+A_l^{-}r^s\rangle_{l+1}-s\langle r^{s-1}\rangle_l). \tag{3.20}$$

Since

$$r^sA_l^{-}+A_l^{-}r^s=(-s+2l+2)r^{s-1}-2(l+1)^{-1}r^s \tag{3.21}$$

we finally obtain a recurrence relation for the average value

$$(l+1)^{-1}\langle r^s\rangle-(l+1+\tfrac{1}{2}s)\langle r^{s-1}\rangle_l=(l+1)^{-1}\langle r^s\rangle_{l+1}-(l+1-\tfrac{1}{2}s)\langle r^{s-1}\rangle_{l+1}. \tag{3.22}$$

Taking $s=0$, from (3.22) we can immediately obtain

$$\langle r^{-1}\rangle_l = \langle r^{-1}\rangle_{l+1} = \ldots = \langle r^{-1}\rangle_{n-1} = 1/n^2 \tag{3.23}$$

which are just the results given by the virial theorem.

Setting $s=1$, we have

$$\begin{aligned}\langle r\rangle_l &= \sum_{k=l}^{n-2}(k+1) + \langle r\rangle_{n-1} \\ &= \tfrac{1}{2}[3n^2 - l(l+1)]\end{aligned} \tag{3.24}$$

which is a very useful result.

When $s<0$, (3.21) should be rewritten as

$$[(l+1)+\tfrac{1}{2}(s+1)]\langle r^s\rangle_l - (l+1)^{-1}\langle r^{s+1}\rangle_l = [(l+1)-\tfrac{1}{2}(s+1)]\langle r^s\rangle_{l+1} - (l+1)^{-1}\langle r^{s+1}\rangle_{l+1} \tag{3.25}$$

for which, considering the necessity of the positive average value, we can also obtain the restriction

$$s > -2l-3. \tag{3.26}$$

4. Orthogonality and inner product calculation

As pointed out in the previous section, the radial wavefunctions are orthogonal to one another if they have the same angular quantum number l, which can be proved as follows.

If $n>n'$ and $l=n'-1$, then by means of (3.2) and (3.3), we have

$$\langle n', n'-1|n, n'-1\rangle = C_{n,n'-1}\langle n', n'-1|A^+_{n'-1}|n, n'\rangle = 0. \tag{4.1}$$

If $n>n'$ and $l<n'-1$, then by successive applications of (3.2) and (3.3) we have

$$\begin{aligned}\langle n'l|nl\rangle &= C_{nl}\langle n', l|A^+_l|n, l+1\rangle = C_{nl}C^{-1}_{n'l}\langle n', l+1|n, l+1\rangle = \ldots \\ &= C_{nl}C_{n,l+1}\ldots C_{n,n'-2}C^{-1}_{n',n'-2}\ldots C^{-1}_{n'l}\langle n', n'-1|n, n'-1\rangle \\ &= 0\end{aligned} \tag{4.2}$$

where (4.1) is used in the last step. Although we consider $n>n'$ only, the proof is universal.

For any inner product $\langle n'l'|nl\rangle$, we can derive a recurrence relation. For definiteness we set $l<n-1$ and then have

$$\langle n'l'|nl\rangle = C_{nl}\langle n'l'|A^+_l|n, l+1\rangle. \tag{4.3}$$

Setting

$$A^+_l = b^{(+)}_l A^+_l + b^{(-)}_l A^-_{l-1} + b^{(0)}_l \tag{4.4}$$

from (2.4) it can be obtained that

$$b^{(+)}_l = (2l+3)/(l+l'+3) \tag{4.5}$$

$$b^{(-)}_l = (l-l')/(l+l'+3) \tag{4.6}$$

$$b^{(0)}_l = (2l+3)(l-l')/(l'+1)(l+1)(l+2). \tag{4.7}$$

Substituting (4.4) into (4.3), we obtain

$$\begin{aligned}\langle n'l'|nl\rangle = {} & b^{(+)}_l C_{nl}C^{-1}_{n'l}\langle n', l'+1|n, l+1\rangle + b^{(0)}_l C_{nl}\langle n'l'|n, l+1\rangle \\ & + b^{(-)}_l C_{nl}C^{-1}_{n,l+1}\langle n', l'|n, l+2\rangle.\end{aligned} \tag{4.8}$$

Equation (4.8) is just the required recurrence relation which seems to be quite complex. In fact, it enables us not only to simplify the calculation of the inner product, but also to derive the general formula in some cases. We illustrate the point with two examples.

(i) If $l' = n' - 1$ and $l = n - 2$, then since

$$\langle n', n'|n, n-1\rangle = 0 \tag{4.9}$$

and

$$\langle n', n'-1|n, n\rangle = 0 \tag{4.10}$$

we obtain

$$\langle n', n'-1|n, n-2\rangle = b^{(0)}_{n-1} C_{n,n-2}\langle n', n'-1|n, n-1\rangle. \tag{4.11}$$

Therefore we need only to calculate a simple integral of two key wavefunctions.

(ii) If $l' = n' - 2$ and $l = n - 2$, we can obtain

$$\begin{aligned}\langle n', n'-2|n, n-2\rangle &= b^{(+)}_{n-2} C_{n,n-2} C^{-1}_{n',n'-2}\langle n', n'-1|n, n-1\rangle + b^{(0)}_{n-2} C_{n,n-2}\langle n', n'-2|n, n-1\rangle \\ &= [b^{(+)}_{n-2} C_{n,n-2} C^{-1}_{n',n'-2} + b^{(0)}_{n-2} b^{(0)}_{n'-1} C_{n,n-2} C_{n',n'-2}]\langle n', n'-1|n, n-1\rangle\end{aligned} \tag{4.12}$$

where (4.11) is used. In this case we also need only to calculate a simple integral of two key functions.

5. Matrix elements of r

In many practical calculations of quantum physics, the matrix elements of r are very important. By means of the ladder operators, we can derive some useful recurrence relations.

First, it is readily verified that

$$2lA^+_{l-1} = (2l+1)A^+_l + A^-_l - 2(2l+1)/r. \tag{5.1}$$

Multiplying (5.1) from the right by $|n'l\rangle$ and simultaneously from the left by $\langle n, l|r$, we have

$$2l\langle n, l|rA^+_{l-1}|n'l\rangle = (2l+1)\langle nl|rA^+_l|n'l\rangle + \langle nl|rA^-_l|n'l\rangle - l(2l+1)\langle nl|n'l\rangle. \tag{5.2}$$

Since

$$\langle nl|n'l\rangle = 0 \qquad n \neq n' \tag{5.3}$$

and

$$[r, A^+_l] = -1 \tag{5.4}$$

we obtain

$$2l\langle nl|rA^+_{l-1}|n'l\rangle = (2l+1)\langle nl|A^+_l r|n'l\rangle + \langle nl|rA^-_l|n'l\rangle. \tag{5.5}$$

Using (3.1) and (3.2), we finally obtain

$$C^{-1}_{n',l-1} 2l\langle nl|r|n', l-1\rangle = C^{-1}_{nl}(2l+1)\langle n, l+1|r|n'l\rangle + C^{-1}_{n'l}\langle nl|r|n', l+1\rangle. \tag{5.6}$$

Interchanging n and n', we obtain another relation

$$C^{-1}_{n,l-1} 2l\langle n', l|r|n, l-1\rangle = C^{-1}_{n'l}(2l+1)\langle n', l+1|r|nl\rangle + C^{-1}_{nl}\langle n'l|r|n, l+1\rangle. \tag{5.7}$$

Equations (5.6) and (5.7) are two recurrence relations which were given by Infeld and Hull [1]. If we can determine the matrix element corresponding to the highest angular quantum number l, then we can calculate all matrix elements of r by using these formulae successively. When $n > n'$, for example, to find such a starting point merely requires the calculation of $\langle n', n'-1|r|nn'\rangle$ which can also be obtained by means of ladder operators.

Since

$$r(A^+_{n'-1} + A^-_{n'}) = (2n'+1) - \frac{2n'+1}{n'(n'+1)} r \tag{5.8}$$

and

$$\begin{aligned}\langle n', n'-1|r(A^+_{n'-1} + A^-_{n'})|nn'\rangle &= \langle n', n'-1|[r, A^+_{n'-1}]|n, n'\rangle + C^{-1}_{nn'}\langle n', n'-1|r|n, n'+1\rangle \\ &= -\langle n', n'-1|n, n'\rangle + C^{-1}_{nn'}\langle n', n'-1|r|n, n'+1\rangle \end{aligned} \tag{5.9}$$

then, combining (5.8) and (5.9), we obtain

$$\begin{aligned}\langle n', n'-1|r|nn'\rangle &= \frac{2n'(n'+1)^2}{2n'+1}\langle n', n'-1|n, n'\rangle - \frac{n'(n'+1)}{2n'+1} C^{-1}_{nn'}\langle n', n'-1|r|n, n'+1\rangle. \end{aligned} \tag{5.10}$$

This is also a new recurrence relation. Applying (5.10) and (4.8) successively, the starting point can be found.

6. Conclusions

From the above discussions we can see that, although the radial ladder operators are more complex than the angular momentum ladder operators and the creation and annihilation operators of the one-dimensional harmonic oscillator, their application does simplify calculations of the average values and matrix elements. By using the device developed in this work, we can avoid lengthy integrals and do not require a detailed knowledge of complicated special functions.

Since there is a close connection between the ladder operators and the factorisation, the development of SSQM based on factorisations should stimulate more attention to the radial ladder operators.

In this paper, as an example, we have discussed only the hydrogen atom but we believe that these methods can be generalised to other solvable potentials. The results will be given elsewhere.

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