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H-atom Ladder Operator Revisited

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An error laden note (Am. J. Phys., 34, 984,(1966)) concerning the ladder operator solution to the hydrogen atom electronic energy levels is corrected.

I. INTRODUCTION

The matrix formulation of the quantum mechanical solution to the energy levels of the hydrogen atom was obtained first by Pauli [1, 2] and incorporated into the ladder operator solution [3]. Some of the precursor commutator relations were summarized in [4].

Since the original note [3] contains several errors, this expanded discussion of the ladder operator for hydrogenic systems in written in extraordinary detail, contrary to current standards of writing.

II. THE HAMILTONIAN

The Hamiltonian for the proton-electron system colloquially called the hydrogen atom, when enlarged to include arbitrary atomic number (Z) so that the nuclear charge is Ze, is:

$$-\frac{\hbar^2}{2\mu}p^2 - \frac{Ze^2}{r} \tag{1}$$

where μ is the reduced mass of the atom/ion. However, for the purposes of this note, we re-phrase it as:

$$-\frac{\hbar^2}{2\mu}\vec{p}\cdot\vec{p} - \frac{Ze^2}{r} \tag{2}$$

We write it this way because the problem is intrinsically 3-dimensional in nature. The isoelectronic sequence hydrogen to helium plus one, to lithium plus two, etc., is included as the atomic number (Z) increases from one to two, to three, etc..

III. THE ANGULAR MOMENTUM

The standard separation of variables attack for this problem leads to separating the radial part of the solution from the angular part. Often, the angular part has been previously studied, starting from the definition of the angular momentum:

$$L = \vec{r}\times\vec{p} \tag{3}$$

leading to

$$L^2|\ell, m_\ell >= \ell(\ell+1)\hbar^2|\ell, m_\ell > \tag{4}$$

coupled with

$$L_z|\ell, m_\ell >= m_\ell\hbar|\ell, m_\ell > \tag{5}$$

which helps in focusing on the radial part which yields the eigenenergies of the system,

$$E_n = -\frac{Z^2e^4\mu}{\hbar^2n^2} \tag{6}$$

IV. THE RUNGE-LENZ VECTOR

Pauli *loc cit* was the first to use the Runge-Lenz vector to solve the hydrogen atomic problem in the Heisenberg/Dirac language.

$$\vec{A} = \left(\frac{1}{Ze^2\mu}\right)\left\{\vec{L}\times\vec{p} - \boldsymbol{i}\hbar\vec{p}\right\} + \frac{r}{\vec{r}} \tag{7}$$

The justification for this particular form of the operator equivalent of the Runge-Lenz vector can be found in this contribution [5].

V. COMMUTATORS

The commutators needed to effectuate a solution are difficult to obtain, but they are summarized as we will see below. We recall the commutator of angular momentum components as summarized here:

$$L\times L = -\boldsymbol{i}\hbar L \tag{8}$$

The cross product notation in Equation (8) is more understandable when written out in some detail.

$$L\times L = \begin{pmatrix} \hat{i} & \hat{j} & \hat{k} \\ L_x & L_y & L_z \\ L_x & L_y & L_z \end{pmatrix} = -\boldsymbol{i}\hbar\begin{pmatrix} L_x \\ L_y \\ L_z \end{pmatrix} \tag{9}$$

So

$$L\times L = \begin{pmatrix} L_y\cdot L_z - L_z\cdot L_y \\ L_x\cdot L_z - L_z\cdot L_x \\ L_x\cdot L_y - L_y\cdot L_x \end{pmatrix} = -\boldsymbol{i}\hbar\begin{pmatrix} L_x \\ L_y \\ L_z \end{pmatrix} \tag{10}$$

This means that

$$[L_y, L_z] = -\boldsymbol{i}\hbar L_x \tag{11}$$

etc.

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VI. COMMUTATORS INVOLVING ANGULAR MOMENTUM AND THE RUNGE-LENS VECTOR

Pauli lists the following commutators and relations in his paper:

$$[Pauli\ II] A_i L_i = L_i A_i \tag{12}$$

$$\begin{aligned}[Pauli\ I] A_x L_y - L_y A_x &= \boldsymbol{i}\hbar A_z \\ A_y L_z - L_z A_y &= \boldsymbol{i}\hbar A_x \\ A_z L_x - L_x A_z &= \boldsymbol{i}\hbar A_y\end{aligned} \tag{13}$$

$$[Pauli\ IV] 1 - A\cdot A = -\left(\frac{2E}{\mu Z^2 e^4}\right)(L^2 + \hbar^2) \tag{14}$$

$$[Pauli\ III]\,(A\times A)_j = -\left(\frac{2\boldsymbol{i}\hbar E}{\mu Z^2 e^4}\right) L_j \tag{15}$$

We define the up and down ladder operators following the angular momentum ladder operator example as

$$A_\pm = A_x \pm \boldsymbol{i} A_y \tag{16}$$

$$[A_\pm, L_z] = \mp \boldsymbol{i}\hbar A_\mp \tag{17}$$

$$[A_\pm, L^2] = \mp 2\hbar^2 A_\pm \mp 2\hbar A_\pm L_z \pm 2\hbar A_z L_\pm \tag{18}$$

or

$$[A_\pm, L^2] = \pm 2\hbar L_\pm A_z \mp 2\hbar A_\pm L_z \tag{19}$$

where $L_\pm = L_x \pm \boldsymbol{i} L_y$ are the up and down ladder operators for the angular momentum.

We know that

$$L^2|\ell, m_\ell >= \ell(\ell+1)\hbar^2|\ell, m_\ell > \tag{20}$$

and

$$L_z|\ell, m_\ell >= m_\ell\hbar|\ell, m_\ell > \tag{21}$$

Next, we note that

$$A_z L_z|\ell, m_\ell >= A_z m_\ell \hbar|\ell, m_\ell > \tag{22}$$

which says that $A_z|\ell, m_\ell >$ remains an eigenfunction of L_z

The question then becomes, what are the effects of $A_\pm$ on L_z and L^2? Equation 17 tells us

$$A_+ L_z - L_z A_+ = \boldsymbol{i}\hbar A_+ \tag{23}$$

so

$$A_+ L_z|\ell, m_\ell >= \boldsymbol{i}\hbar A_+|\ell, m_\ell > + L_z A_+ m_\ell \hbar|\ell, m_\ell >= (m_\ell + 1)\hbar A_+|\ell, m_\ell > \tag{24}$$

Therefore,

$$A_+|\ell, m_\ell > \to |\ell, m_\ell + 1 >$$

Equation 18 shows that

$$\begin{aligned}A_\pm L^2 - L^2 A_\pm &= \mp 2\hbar^2 A_\pm \mp 2\hbar A_\pm L_z \pm 2\hbar A_z L_\pm \\ -L^2 A_+|\ell,\ell > &= -A_+ L^2|\ell,\ell > -2\hbar^2 A_+|\ell,\ell > -2\hbar A_+ L_z|\ell,\ell > +2\hbar A_z L_+|\ell,\ell > \\ &= -A_+ L^2|\ell,\ell > -2\hbar^2 A_+|\ell,\ell > -2\hbar^2 \ell A_+|\ell,\ell > +2\hbar A_z \cancel{L_+|\ell,\ell >} \to 0 \\ &= -\ell(\ell+1)\hbar^2 A_+|\ell,\ell > -2\hbar^2 A_+|\ell,\ell > -2\hbar^2 \ell A_+|\ell,\ell > \\ &= \left\{-\ell(\ell+1)\hbar^2 - 2\hbar^2 - 2\hbar^2\ell\right\} A_+|\ell,\ell > \\ &= -\hbar^2\left\{\ell^2 + 3\ell + 2\right\} A_+|\ell,\ell >= -\hbar^2(\ell+1)((\ell+1)+1)A_+|\ell,\ell >\end{aligned} \tag{25}$$

which shows that $A_+|\ell, ? >$ is an eigenfunction of L^2 also, but laddered up once. Remember that $|\ell,\ell >$ has no higher L_z value, i.e. $|\ell, \ell+1>$ doesn't exist.

Using Equation 24, we have

$$\begin{aligned}
A_-L^2 - L^2A_- &= +2\hbar^2 A_- + 2\hbar A_-L_z - 2\hbar A_z L_- \\
-L^2A_-|\ell,-\ell> &= -A_-L^2|\ell,-\ell> +2\hbar^2 A_-|\ell,-\ell> +2\hbar A_-L_z|\ell,-\ell> -2\hbar A_zL_-|\ell,-\ell> \\
-L^2A_-|\ell,-\ell> &= -A_-L^2|\ell,\ell> +2\hbar^2 A_-|\ell,-\ell> -2\hbar^2\ell A_-|\ell,-\ell> -2\hbar A_z\cancelto{0}{L_-|\ell,-\ell>} \\
-L^2A_-|\ell,-\ell> &= -\ell(\ell+1)\hbar^2 A_-|\ell,-\ell> +2\hbar^2 A_-|\ell,-\ell> -2\hbar^2\ell A_-|\ell,-\ell> \\
&= -\left\{\ell(\ell+1)\hbar^2 - 2\hbar^2 + 2\hbar^2\ell\right\} A_-|\ell,-\ell> \\
&= -\hbar^2\left\{\ell^2+3\ell-2\right\} A_-|\ell,-\ell> = -\hbar^2\left\{(??????)\right\} A_-|\ell,-\ell>
\end{aligned} \tag{26}$$

Clearly, something is wrong here! According to Burkhardt and Leventhal, the up ladder operator is (supressing $\hbar^2$)

$$L^2A_+|\ell,\ell> = (A_+L^2 - 2A_zL_+ + 2A_+ + 2A_+L_z|\ell,\ell>$$

while the second (down)ladder operator should be

$$L^2A_-|\ell,-\ell> = (A_-L^2 + 2A_zL_- + 2A_- - 2A_-L_z)|\ell,-\ell> \tag{27}$$

Then, using their formulation, we have

$$L^2A_-|\ell,-\ell> = (A_-\ell(\ell+1) + \cancelto{0}{2A_zL_-} + 2A_- + 2\ell A_-)|\ell,-\ell>$$

so far

$$L^2A_-|\ell,-\ell> = (\ell(\ell+1) + 2 + 2\ell)A_-|\ell,-\ell>$$

$$L^2A_-|\ell,-\ell> = (\ell^2 + 3\ell + 2)A_-|\ell,-\ell>$$

$$L^2A_-|\ell,-\ell> = (\ell+1)(\ell+2)A_-|\ell,-\ell>$$

Returning to Equation 26 and changing one sign as shown, we have

$$\begin{aligned}
A_-L^2 - L^2A_- &= +2\hbar^2 A_- \overset{+}{\cancel{-}}2\hbar A_-L_z - 2\hbar A_z L_- \\
-L^2A_-|\ell,-\ell> &= -A_-L^2|\ell,-\ell> +2\hbar^2 A_-|\ell,-\ell> +2\hbar A_-L_z|\ell,-\ell> -2\hbar A_zL_-|\ell,-\ell> \\
-L^2A_-|\ell,-\ell> &= -A_-L^2|\ell,\ell> +2\hbar^2 A_-|\ell,-\ell> -2\hbar^2\ell A_-|\ell,-\ell> -2\hbar A_z\cancelto{0}{L_-|\ell,-\ell>} \\
-L^2A_-|\ell,-\ell> &= -\ell(\ell+1)\hbar^2 A_-|\ell,-\ell> +2\hbar^2 A_-|\ell,-\ell> -2\hbar^2\ell A_-|\ell,-\ell> \\
&= -\left\{\ell(\ell+1)\hbar^2 + 2\hbar^2 + 2\hbar^2\ell\right\} A_-|\ell,-\ell> \\
&= -\hbar^2\left\{\ell^2+3\ell+2\right\} A_-|\ell,-\ell> = -\hbar^2(\ell+1)(\ell+2)A_-|\ell,-\ell>
\end{aligned} \tag{28}$$

This means that their sign was right and mine was wrong!

As noted in the introduction, the original note had several errors in it, and this is the most important error. The down ladder operator in the note is wrong. For that reason, we here re-derive the commutator of the down ladder operator with the L^2.

VII. THE COMMUTATOR OF A_- AND L^2, RE-DERIVED

We re-compute a commutator,

$$A_-L^2 - L^2A_- = A_-(L_x^2 + L_y^2 + L_z^2) - (L_x^2 + L_y^2 + L_z^2)A_- \tag{29}$$

$$A_-L^2 - L^2A_- = (A_x - iA_y)(L_x^2 + L_y^2 + L_z^2) - (L_x^2 + L_y^2 + L_z^2)(A_x - iA_y) \tag{30}$$

$$\begin{aligned} A_-L^2 - L^2A_- &= \\ A_x(\cancel{L_x^2} + L_y^2 + L_z^2) &- iA_y(L_x^2 + \cancel{L_y^2} + L_z^2) \\ -(\cancel{L_x^2} + L_y^2 + L_z^2)A_x &- (L_x^2 + \cancel{L_y^2} + L_z^2)(-iA_y) \end{aligned} \tag{31}$$

Remember the commutators

$$A_kL_j - L_jA_k = i\hbar\epsilon_{k,j,l}A_l \tag{32}$$

where $\epsilon_{j,k,l}$ is the Levi-Civita epsilon.

$$\begin{aligned} A_xL_y - L_yA_x &= \boldsymbol{i}\hbar A_z \\ A_yL_z - L_zA_y &= \boldsymbol{i}\hbar A_x \\ A_zL_x - L_xA_z &= \boldsymbol{i}\hbar A_y \\ A_yL_x - L_xA_y &= -\boldsymbol{i}\hbar A_z \\ A_zL_y - L_yA_z &= -\boldsymbol{i}\hbar A_x \\ A_xL_z - L_zA_x &= -\boldsymbol{i}\hbar A_y \end{aligned} \tag{33}$$

$$\begin{aligned} A_-L^2 - L^2A_- &= \\ A_xL_y^2 + A_xL_z^2 &- iA_yL_x^2 - iA_yL_z^2 \\ -(L_y^2A_x + L_z^2A_x) &- (L_x^2(-iA_y) + L_z^2(-iA_y)) \end{aligned} \tag{34}$$

$$\begin{aligned} &A_-L^2 - L^2A_- = \\ &\cancel{A_xL_y}L_y \to \underbrace{A_xL_y} - L_yA_x = \boldsymbol{i}\hbar A_z \\ &+\cancel{A_xL_z}L_z \to \underbrace{A_xL_z} - L_zA_x = -\boldsymbol{i}\hbar A_y \\ &-i\cancel{A_yL_x}L_x \to \underbrace{A_yL_x} - L_xA_y = -\boldsymbol{i}\hbar A_z \\ &-i\cancel{A_yL_z}L_z \to \underbrace{A_yL_z} - L_zA_y = \boldsymbol{i}\hbar A_x \\ &-L_y\cancel{L_yA_x} \to A_xL_y - \underbrace{L_yA_x} = \boldsymbol{i}\hbar A_z \\ &-L_z\cancel{L_zA_x} \to A_xL_z - \underbrace{L_zA_x} = -\boldsymbol{i}\hbar A_y \\ &+iL_x\cancel{L_xA_y} \to A_yL_x - \underbrace{L_xA_y} = -\boldsymbol{i}\hbar A_z \\ &+iL_z\cancel{L_zA_y} \to A_yL_z - \underbrace{L_zA_y} = \boldsymbol{i}\hbar A_x \end{aligned} \tag{35}$$

which becomes

$$\begin{aligned} &A_-L^2 - L^2A_- = \\ &(\cancel{A_xL_y}L_y \to (L_yA_x + \boldsymbol{i}\hbar A_z)L_y \\ &+\cancel{A_xL_z}L_z \to (L_zA_x - \boldsymbol{i}\hbar A_y)L_z \\ &-i\cancel{A_yL_x}L_x \to (L_xA_y - \boldsymbol{i}\hbar A_z)L_x \\ &-i\cancel{A_yL_z}L_z \to (L_zA_y + \boldsymbol{i}\hbar A_x)L_z \\ &-L_y\cancel{L_yA_x} \to L_y(A_xL_y - \boldsymbol{i}\hbar A_z) \\ &-L_z\cancel{L_zA_x} \to L_z(A_xL_z + \boldsymbol{i}\hbar A_y) \\ &+iL_x\cancel{L_xA_y} \to L_x(A_yL_x + \boldsymbol{i}\hbar A_z) \\ &+iL_z\cancel{L_zA_y} \to L_z(A_yL_z - \boldsymbol{i}\hbar A_x) \end{aligned} \tag{36}$$

so

$$\begin{aligned} A_-L^2 - L^2A_- = &(\cancel{L_yA_x} + \boldsymbol{i}\hbar A_z)L_y + (\cancel{L_zA_x} - \boldsymbol{i}\hbar A_y)L_z - i(\xcancel{L_xA_y} - \boldsymbol{i}\hbar A_z)L_x - i(L_zA_y + \boldsymbol{i}\hbar A_x)L_z \\ &-L_y(\cancel{A_xL_y} - \boldsymbol{i}\hbar A_z) - L_z(\cancel{A_xL_z} + \boldsymbol{i}\hbar A_y) + iL_x(\xcancel{A_yL_x} + \boldsymbol{i}\hbar A_z) + iL_z(A_yL_z - \boldsymbol{i}\hbar A_x) \end{aligned}$$

and

$$\frac{A_-L^2 - L^2A_-}{\hbar} = \boldsymbol{i}\overline{\underline{A_zL_y}} - \boldsymbol{i}\,\overline{\underbrace{A_yL_z}} - \overline{A_zL_x} + \underline{A_xL_z} + \overbrace{\underline{L_y\boldsymbol{i}A_z}} - \boldsymbol{i}\underbrace{L_zA_y} - L_xA_z - i^2\overbrace{L_zA_x} \tag{37}$$

The output from Maxima (after dividing by $\hbar$)is:

$$-i\underbrace{L_z\cdot A_y} + \overbrace{L_z\cdot A_x} + i\overbrace{\underline{L_y\cdot A_z}} - L_x\cdot A_z + i\,\overline{\underline{A_z\cdot L_y}} - \overline{A_z\cdot L_x} - i\,\overline{\underbrace{A_y\cdot L_z}} + \underline{A_x\cdot L_z} \tag{38}$$

(where we highlight terms to show sign equivalence).

Therefore, we have, to get to our goal $(A_zL_- + A_- - A_-L_z)$, to choose judiciously how we gather and invert terms. To do this, we reorder the terms to show how they suggest approaching our target:

$$\begin{aligned}\frac{A_-L^2 - L^2A_-}{\hbar} &= iA_zL_y - A_zL_x \to A_z(iL_y - L_x) \to -A_zL_- \\ &\quad +A_x - iA_yL_z \to (A_x - iA_y)L_z \to A_-L_z \\ &\quad +iL_yA_z - iL_zA_y - L_xA_z + L_zA_x\end{aligned} \tag{39}$$

(we report the Maxima output here approximately following the printed equations, from the output of code shown in the Appendix)

$$-i\,Lz \cdot Ay + Lz \cdot Ax + i\,Ly \cdot Az - Lx \cdot Az - Az \cdot L\_minus + A\_minus \cdot Lz$$

and we notice that our target involves reading right to left (in operator order) L_i followed by A_i, meaning that the last four terms are in the wrong order. We employ the commutators to correct this ordering

$$\begin{aligned}\frac{A_-L^2 - L^2A_-}{\hbar} &= iA_zL_y - A_zL_x \to A_z(iL_y - L_x) \to -A_zL_- \\ &\quad +A_x - iA_yL_z \to (A_x - iA_y)L_z \to A_-L_z \\ &\quad +i\cancel{L_yA_z} \nearrow A_zL_y + iA_x \\ &\quad -i\cancel{L_zA_y} \nearrow A_yL_z - iA_x \\ &\quad -\cancel{L_xA_z} \nearrow A_zL_x - iA_y \\ &\quad +\cancel{L_zA_x} \nearrow A_xL_z + iA_y\end{aligned} \tag{40}$$

$$-i\,Lz \cdot Ay + Lz \cdot Ax - Lx \cdot Az + i\,Az \cdot Ly - Az \cdot L\_minus - \%hbar\,Ax + A\_minus \cdot Lz$$

$$Lz \cdot Ax - Lx \cdot Az + i\,Az \cdot Ly - Az \cdot L\_minus - i\,Ay \cdot Lz - 2\,\%hbar\,Ax + A\_minus \cdot Lz$$

$$Lz \cdot Ax + i\,Az \cdot Ly - Az \cdot Lx - Az \cdot L\_minus - i\,Ay \cdot Lz + i\,\%hbar\,Ay - 2\,\%hbar\,Ax + A\_minus \cdot Lz$$

$$i\,Az \cdot Ly - Az \cdot Lx - Az \cdot L\_minus - i\,Ay \cdot Lz + 2\,i\,\%hbar\,Ay + Ax \cdot Lz - 2\,\%hbar\,Ax + A\_minus \cdot Lz$$

which becomes

$$\begin{aligned}\frac{A_-L^2 - L^2A_-}{\hbar} &= iA_zL_y - A_zL_x \to A_z(iL_y - L_x) \to -A_zL_- \\ &\quad +A_x - iA_yL_z \to (A_x - iA_y)L_z \to A_-L_z \\ &\quad +i(A_zL_y + iA_x) \to i\,\underbrace{A_zL_y}\,-A_x \\ &\quad -i(A_yL_z - iA_x) \to -i\,\overbrace{A_yL_z}\,-A_x \\ &\quad -(A_zL_x - iA_y) \to -\underbrace{A_zL_x}\,+iA_y \\ &\quad +(A_xL_z + iA_y) \to \overbrace{A_xL_z}\,+iA_y\end{aligned} \tag{41}$$

and finally(?)

$$\begin{aligned}\frac{A_-L^2 - L^2A_-}{\hbar} &= iA_zL_y - A_zL_x \to A_z(iL_y - L_x) \to -A_zL_- \\ &\quad +A_x - iA_yL_z \to (A_x - iA_y)L_z \to A_-L_z \\ &\quad -A_zL_- + iA_y - A_x \\ &\quad +A_-L_z + iA_y - A_x\end{aligned} \tag{42}$$

$$-2\,Az \cdot L\_minus + 2\,i\,\%hbar\;Ay - 2\,\%hbar\;Ax + 2\,A\_minus \cdot Lz$$

$$-2\,Az \cdot L\_minus + 2\,A\_minus \cdot Lz - 2\,\%hbar\;A\_minus$$

$$\frac{A_-L^2 - L^2A_-}{\hbar} = -2A_zL_- + 2A_-L_z - 2(A_x - iA_y) \tag{43}$$

or

$$\frac{A_-L^2 - L^2A_-}{\hbar} = -2A_zL_- + 2A_-L_z - 2A_- \tag{44}$$

which is Equation 27.

VIII. THE BALMER FORMULA

Assume that there is a maximum value to ℓ which we denote as ℓ^*. Since

$$A_-A_+|\ell^*, \ell^* >= 0$$

since the A_+ operator would yield $|\ell^*+1, \ell^*+1>$ which contradicts that ℓ^* is a maximum value. we have

$$(A_x - iA_y)(A_x + iA_y)|\ell^*, \ell^* >= 0 \tag{45}$$

$$\left(A_xA_x + A_yA_y + A_zA_z + i(A_xA_y - A_yA_x) - A_zA_z\right)|\ell^*, \ell^* >= 0 \tag{46}$$

$$\left(\vec{A}\cdot\vec{A} + i[A_x, A_y] - A_z^2\right)|\ell^*, \ell^* >= 0 \tag{47}$$

But as shown in Appendix II,

$$A_x \cdot A_y - A_y \cdot A_x = -\left(\frac{2\boldsymbol{i}\hbar E}{\mu Z^2 e^4}\right)L_z \tag{48}$$

so, also employing Equation 14 we obtain

$$\left(1 + \frac{2E}{\mu Z^2 e^4}(L^2 + \hbar^2) - i\frac{2i\hbar E}{\mu Z^2 e^4}L_z\right)|\ell^*, \ell^* >= 0 \tag{49}$$

which leads to the infamous

$$E_n = -\frac{\mu Z^2 e^4}{2\hbar^2(\ell^* + 1)^2} \tag{50}$$

where $n = \ell^* + 1$.

IX. COMMENTARY

The fact that the original paper contained several errors is quit disturbing. Refereeing is supposed to reassure the reader that what s/he is reading has been vetted and is substantially correct. In this case, the conclusions were right, but the methodology failed. Clearly, the referee assumed that my commutator was correct.

X. REMARKS

The original paper which is the genesis of this posting, was published in *Am. J. Phys.*, volume 34, page 984, in 1966! It's mandatory brevity, I believe, is the reason that it is not being read [6] and incorporated into the standard 1st year quantum chemistry classes. Perhaps, an alternative view is that ladder operators are of limited interest to chemists. Since the paper has several errors [7], perhaps it's a blessing that it remains unread!

There is an extensive literature on this subject, based on differential equations [8], and other (more advanced) mathematical subjects too numerous to address here.

XI. APPENDIX 1

The following Maxima code is self explanatory. It pauses at the creating of the LaTeX input of the final commutator (Equation 38, *vide infra*). After that, the reorganization of the terms proceeds to its final conclusion. Other paths could be taken.

```
reset() + kill(all);

dotscrules:true$

Lxsq:Lx.Lx$
Lysq: Ly.Ly$
Lzsq: Lz.Lz$
Lsq: Lxsq+Lysq+Lzsq$

Aminus:(Ax-%i*Ay);
AminusLsq : Aminus.Lsq$
LsqAminus : Lsq.Aminus$
print ("expanded initial form")$
comm:(AminusLsq-LsqAminus),expand;
comm: substitute(Lx.Lx.Ax =Lx.Ax.Lx,comm)$
comm: substitute(Ly.Ly.Ay =Ly.Ay.Ly,comm)$
comm: substitute(Lz.Lz.Az =Lz.Az.Lz,comm)$
comm: substitute(Ax.Lx.Lx =Lx.Ax.Lx,comm)$
comm: substitute(Ay.Ly.Ly =Ly.Ay.Ly,comm)$
print ("expanded after i,i exchanged form")$
comm: substitute(Az.Lz.Lz =Lz.Az.Lz,comm);


comm: substitute(%i*Lz.(Lz.Ay) =%i*(Lz.(Ay.Lz)-%i*%hbar*Lz.Ax),comm),expand;
comm: substitute(%i*Ay.(Lz^^2) =%i*(Lz.(Ay.Lz)+%i*%hbar*Ax.Lz),comm),expand;

comm: substitute(Lx.Lx.Ay =(Lx.(Ay.Lx)+%i*%hbar*Lx.Az),comm),expand;
comm: substitute(%i*Ay.Lx^^2 =%i*(Lx.Ay.Lx-%i*%hbar*Az.Lx),comm),expand;

print ("3  x-y *Ly(Ly.Ax) ")$
comm:substitute(Ax.Ly^^2=Ly.Ax.Ly+%i*%hbar*Az.Ly,comm),expand;
comm:substitute((Ly^^2).Ax=Ly.Ax.Ly-%i*%hbar*Ly.Az,comm),expand;


comm: substitute(((Lz^^2).Ax) =Lz.(Ax.Lz)+%i*%hbar*Lz.Ay,comm),expand;
comm: substitute((Ax.Lz^^2) =Lz.Ax.Lz-%i*%hbar*Ay.Lz,comm),expand;


comm:comm/%hbar$
comm:expand(comm);
```

The following code continues the computation, back substituting in the same order as shown above. Lots of print statements are included so that it is clear how we are copying the hand calculations.

```
print(" (Az.Lx=%i*(Az.Ly)+Az.Lminus; OK")$
comm:substitute(Az.Lx=%i*(Az.Ly)+Az.L_minus,comm),expand;
print("LaTeX:")$
tex(comm);
print (" ")$
```

```
print("1 ; Ax.Lz=%i*(Ay.Lz)+A_minus.Lz; OK")$
comm:substitute(Ax.Lz=%i*(Ay.Lz)+A_minus.Lz,comm),expand;
print("LaTeX:")$
tex(comm);
print (" ")$

print (" 2; %i*Ly.Az=%i*(Az.Ly+%i*%hbar*Ax)")$
comm:substitute(%i*Ly.Az=%i*(Az.Ly+%i*%hbar*Ax),comm),expand;
tex(comm)$
print (" ")$

print ("3; %i*Lz.Ay=%i*(Ay.Lz-%i*%hbar*Ax); OK")$
comm:substitute(%i*Lz.Ay=%i*(Ay.Lz-%i*%hbar*Ax),comm),expand;
print("LaTeX:")$
tex(comm);


print (" 4; Lx.Az= Az.Lx-%i*%hbar*Ay")$
comm:substitute(Lx.Az= Az.Lx-%i*%hbar*Ay,comm),expand;
print (" ")$
print("LaTeX:")$
tex(comm);
print (" ")$

print ("5; Lx.Az = Az.Lx + %i*%hbar*Ay")$
comm:substitute(Lz.Ax = Ax.Lz + %i*%hbar*Ay,comm),expand;
print (" ")$
print("LaTeX:")$
tex(comm);
print (" ")$

print (" 6; Az.Lx=Az.L_minus + %i*Az.Ly")$
comm:substitute(Az.Lx=Az.L_minus + %i*Az.Ly,comm),expand;
print (" ")$

print("7 ; Ax.Lz=%i*(Ay.Lz)+A_minus.Lz; OK")$
comm:substitute(Ax.Lz=%i*(Ay.Lz)+A_minus.Lz,comm),expand;
tex(comm);
print (" ")$

print("7a ; Ax=%i*Ay+A_minus; OK")$
comm:substitute(Ax=%i*Ay+A_minus,comm),expand;
tex(comm);
```

XII. APPENDIX 2

We expand Equation 15 as:

$$A \times A = \begin{pmatrix} A_y \cdot A_z - A_z \cdot A_y \\ A_x \cdot A_z - A_z \cdot A_x \\ A_x \cdot A_y - A_y \cdot A_x \end{pmatrix} = -\left(\frac{2i\hbar E}{\mu Z^2 e^4}\right)\begin{pmatrix} L_x \\ L_y \\ L_z \end{pmatrix} \tag{51}$$

The z-component of the cross product, $(A \times A)_z$, is the third, i.e., lowest one.

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