Quantum Runge-Lenz Vector and the Hydrogen Atom, the hidden SO(4) symmetry

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Let's consider the Hydrogen atom and its Hamiltonian

\[ H = \frac{\| \vec{p} \|^2}{2 m_e} - \frac{\kappa}{r}, \]

where \( \vec{p} \) is the electron momentum, \( m_e \) its mass, \( \kappa \) a real positive constant, and \( r \) the distance of the electron from the proton located at the origin. We assume that the proton's mass is infinite. Classically, from the potential \( -\frac{\kappa}{r} \), one can derive a central force \( \vec{F} = -\frac{\kappa \vec{r}}{r^2} \) that drives the electron's motion.

Introducing the angular momentum

\[ \vec{L} = r \times \vec{p}, \]

one can further define the Runge-Lenz vector \( \vec{Z} \):

\[ \vec{Z} = \frac{1}{m_e} \vec{L} \times \vec{p} + \kappa \frac{\vec{r}}{r}. \]

It is well known that \( \vec{Z} \) is a constant of the motion, i.e. \( \frac{d}{dt} \vec{Z}(t) = 0 \). Switching to Quantum Mechanics, this condition reads

\[ [H, \vec{Z}] = 0. \]

where, for hermiticity purpose, the expression of \( \vec{Z} \) must be symmetrized

\[ \vec{Z} = \frac{1}{2 m_e} (\vec{L} \times \vec{p} - \vec{p} \times \vec{L}) + \kappa \frac{\vec{r}}{r}. \]

**Problem:** departing from the basic commutation rules between position \( \vec{r} \), momentum \( \vec{p} \) and angular momentum \( \vec{L} \) in tensor notation, and the expression of the Hamiltonian \( H \), demonstrate the following commutation rules between the quantum Hamiltonian, angular momentum and Runge-Lenz vector \( \vec{Z} \)

\[ [H, L_n] = 0 \quad \text{and} \quad [H, Z_n] = 0, \]
\[
[L_m, Z_n]_\pm = i \hbar \epsilon_{m, n, o} Z_o,
\]
\[
[Z_m, Z_n]_\pm = -2 \frac{i \hbar}{m_e} H \epsilon_{m, n, o} L_o.
\]

**Remark:** Since \(H\) commutes with both \(\vec{L}\) and \(\vec{Z}\), defining
\[
M_n = \sqrt{-\frac{m_e}{2 H}} Z_n,
\]
the commutation rules demonstrated can be rewritten as
\[
[L_m, L_n]_\pm = i \hbar \epsilon_{m, n, o} L_o,
\]
\[
[L_m, M_n]_\pm = i \hbar \epsilon_{m, n, o} M_o,
\]
\[
[M_m, M_n]_\pm = i \hbar \epsilon_{m, n, o} L_o.
\]

This set constitutes the Lie algebra of the SO(4) group (closely related to a Poincaré group in special relativity).

\[\nabla\text{ I Commutation rules and useful identities}\]

\[\nabla\text{ Quantum commutation rules basics and the Hamiltonian of the hydrogen atom}\]

Set macros for \(M = m_e\)

\>
restart;

\>
with(Physics) : with(Library) :

\>
interface(imaginaryunit = i) :

\>
macro(M = m_e):

Set the context: Cartesian coordinates, 3D Euclidean space, lowercase letters representing tensor indices, use automatic simplification (automatically apply simplify/size on everything). Here

\[V = \frac{1}{r}\] will represent the potential of the central force.

\>
Setup(coordinates = cartesian, hermitianoperators = \{X\}, realobjects = \{\hbar, \kappa, m_e\},

\>
automaticsimplification = true, dimension = 3, metric = Euclidean, spacetimeindices

\>
= lowercaselatin, mathematicalnotation = true, quiet)

\[
\left[\text{automaticsimplification} = \text{true}, \text{coordinatesystems} = \{X\}, \text{dimension} = 3, \right.
\]

\>
\[
\text{hermitianoperators} = \{X\}, \text{mathematicalnotation} = \text{true}, \text{metric} = \{(1, 1) = 1, (2, 2)\}
\]
Setting quantum (Hermitian) operators and related commutators:

- \( Z \) is Hermitian, but we derive that property further below.
- The potential \( V(X) \) of the hydrogen atom is assumed to commute with position, not with momentum - the commutation rule with \( p \) is derived further ahead.
- The commutator rules for angular momentum are an easy problem, we take them as the departure point.
- The last two commutators involving \( G(X) \) are for the differential operators approach only, not really part of the problem.

\[
\text{Setup}\{\text{quantum operators} = \{Z\}, \text{hermitian operators} = \{V, G, H, L, X, p\}, \text{algebra rules} = \{\}
\]

\[
\begin{align*}
%\text{Commutator} & \{X[k], X[l]\} = 0, \\
%\text{Commutator} & \{p[k], p[l]\} = 0, \\
%\text{Commutator} & \{X[k], p[l]\} = i \cdot h \cdot g_{-}[k, l], \\
%\text{Commutator} & \{L[j], L[k]\} = i \cdot h \cdot \text{LeviCivita}[j, k, n] \cdot L[n], \\
%\text{Commutator} & \{p[j], L[k]\} = i \cdot h \cdot \text{LeviCivita}[j, k, n] \cdot p[n], \\
%\text{Commutator} & \{X[j], L[k]\} = i \cdot h \cdot \text{LeviCivita}[j, k, n] \cdot X[n], \\
%\text{Commutator} & \{X[k], V(X)\} = 0, \\
%\text{Commutator} & \{V(X), G(X)\} = 0, \\
%\text{Commutator} & \{X[k], G(X)\} = 0 \} \\
\end{align*}
\]

\[
\text{algebra rules} = \{( [V(X), G(X)]_\_ = 0, [L_j, L_k]_\_ = i \cdot h \cdot epsilon_{j, k, n} \cdot L_n, [p_j, L_k]_\_ = 0, \}
\]

\[
\begin{align*}
&= i \cdot h \cdot epsilon_{j, k, n} \cdot p_n, [p_k, p_l]_\_ = 0, [X_k, L_j]_\_ = i \cdot h \cdot epsilon_{j, k, n} \cdot X_n, [X_k, G(X)]_\_ = 0, [X_k, V(X)]_\_ = 0, [X_k, p_l]_\_ = i \cdot h \cdot g_{k, p} \cdot [X_k, X_l]_\_ = 0, \}
\end{align*}
\]

\[
\text{hermitian operators} = \{G, H, L, V, p, x, y, z\}, \text{quantum operators} = \{G, H, L, V, Z, p, x, y, z\} \\
\]

Define the tensors

\[
\text{Define}\{p[k] = \{p_x, p_y, p_z\}, L[k] = \{L_x, L_y, L_z\}, Z[k] = \{Z_x, Z_y, Z_z\}, \text{quiet}\}
\]

\[
\{g_{a' \cdot k'}, \sigma_{a' \cdot k'}, X_{a' \cdot k'}, Z_{a' \cdot k'}, \partial_{a' \cdot k'}, g_{a', b', k'}, p_{a', b', c}\} \\
\]

\[
\text{CompactDisplay}(V(X), G(X)) \]

\[
V(X) \text{ will now be displayed as } V \\
G(X) \text{ will now be displayed as } G
\]

The Hamiltonian for the hydrogen atom

\[
\text{H} = \left( \frac{p[l]^2}{2 \cdot M} \right) - \kappa \cdot V(X)
\]

\[
H = \frac{p[l]^2}{2 \cdot m_e} - \kappa \cdot V
\]
\[ \textbf{Identities (I): } \partial_n(V) = -V^3 X_n, \quad V^3 X^2_l = V \quad \text{and} \quad \Box(V) = 0 \]

For a more compact calculus, we use the dimensionless potential \( V(X) \)
\[ V(X) = \frac{1}{\sqrt{X_0^2}} \]
(6)

The gradient of \( V(X) \) is
\[ \partial_n(V) = -\frac{1}{3} X_n \]
\[ \left( \frac{X_0^2}{2} \right) \]
(7)

So that
\[ \text{subs(} (\text{rhs = lhs)} \left( (6)^3 \right), (7) \text{)} \]
\[ \partial_n(V) = -V^3 X_n \]
(8)

Equivalently, \( V(X) \) can be written
\[ V = \frac{1}{\left( x^2 + y^2 + z^2 \right)^{1/2}} \]
(9)

from which one can deduce \( V^3 X^2_l = V \), that will often be used afterwards
\[ (9)^3 \cdot (x^2 + y^2 + z^2) \]
\[ V^3 \left( x^2 + y^2 + z^2 \right) = \frac{1}{\left( x^2 + y^2 + z^2 \right)^{1/2}} \]
(10)

And finally \( \Box(V) = 0 \)
\[ \text{subs(} \left( (\text{rhs = lhs)} \left( (9) \right), \left( x^2 + y^2 + z^2 \right) = X[l]^2 \right), (10) \text{)} \]
\[ V^3 X^2_l = V \]
(11)

And finally \( \Box(V) = 0 \)
\[ \text{subs(} \left( (\text{rhs = lhs)} \left( (9) \right), \left( x^2 + y^2 + z^2 \right) = X[l]^2 \right), (10) \text{)} \]
\[ \Box(V) = 0 \]
(13)
Identities (II): the commutation rules between $\vec{L}$, $\vec{p}$ and the potential $V(X)$

One has

$$L[q] = \text{LeviCivita}[q, m, n] \cdot X[m] \cdot p[n]$$

$$L_q = \epsilon_{m, n, q} X_m p_n$$ (14)

$$\text{Commutator}((14), V(X))$$

$$[L_q, V]_\_ = \epsilon_{m, n, q} X_m [p_n, V]_\_$$ (15)

These two commutators cannot be computed until providing more information - we set the equations here for use further below with a test function $G(X)$

$$\text{Commutator} = \text{Commutator}(p[q], V(X))$$

$$[p_q, V]_\_ = [p_q, V]_\_$$ (16)

$$\text{Commutator} = \text{Commutator}(p[q], V(X)^3)$$

$$[p_q, V^3]_\_ = [p_q, V^3]_\_$$ (17)

Set now differentialoperators and some commutators with the arbitrary test function $G(X)$, to be used in the alternative demonstrations based on using differentialoperators and to derive the commutation rules between $L$, $p$ and $V(X)$

$$\text{Setup}(\text{differentialoperators} = \{ [p[k], [x, y, z]] \}$$

$$[\text{differentialoperators} = \{ [p_k, [X]] \}]$$ (18)

Now, apply the differential operators found in the commutators above to $G(X)$

$$\text{lhs = ApplyProductsOfDifferentialOperators} @ \text{rhs} ((15) \cdot G(X))$$

$$[L_q, V]_\_ G = \epsilon_{m, n, q} X_m (p_n (V G) - V p_n (G))$$ (19)

$$\text{lhs = ApplyProductsOfDifferentialOperators} @ \text{rhs} ((16) \cdot G(X))$$

$$[p_q, V]_\_ G = p_q (V G) - V p_q (G)$$ (20)

$$\text{lhs = ApplyProductsOfDifferentialOperators} @ \text{rhs} ((17) \cdot G(X))$$

$$[p_q, V^3]_\_ G = p_q (V^3 G) - V^3 p_q (G)$$ (21)

The result of $p_l(G(X))$ is not known to the system at this point, we set equation to be used further below

$$p_l(G)$$ (22)

$$\text{ApplyProductsOfDifferentialOperators} (p[l] \cdot G(X)) = p[l] \cdot G(X)$$

$$p_l(G) = p_l G$$ (23)

Define now the momentum operator as an indexed procedure

$$p := \text{proc}(\ )$$

$$\text{local Ind := op(procname);}$$
\[
\text{return } \frac{h}{i} \cdot \text{Physics:} \cdot d \_ \text{Ind} \_ \text{args} ;
\]

end:

With this definition, we have

\[
> (19) \quad \left[ L_q, V \right]_- G = -i \epsilon_{m,n,q} \ h X_m \ \partial_n (V) \ G
\]

So that

\[
> \text{SubstituteTensor((8), (24))} \cdot \text{Inverse}(G(X))
\]

\[
\left[ L_q, V \right]_- = i \epsilon_{m,n,q} \ h X_m V^3 X_n
\]

Finally we get the first commutation rule:

\[
> \text{Simplify((25))}
\]

\[
\left[ L_q, V \right]_- = 0
\]

Likewise, from (20) we get the second commutation rule:

\[
> (20) \cdot \text{Inverse}(G(X))
\]

\[
\left[ p_q, V \right]_- = -i \ h \ \partial_q (V)
\]

\[
> \text{SubstituteTensor((8), (27))}
\]

\[
\left[ p_q, V \right]_- = i \ h V^3 X_q
\]

From (21) we get the third commutation rule we were looking for:

\[
> (21) \cdot \text{Inverse}(G(X))
\]

\[
\left[ p_q, V^3 \right]_- = -i \ h \ ( \partial_q (V) V^2 + V \partial_q (V) + V^2 \partial_q (V) )
\]

\[
> \text{lhs ((29))} = \text{Simplify(\text{SubstituteTensor((8), rhs ((29)))))}
\]

\[
\left[ p_q, V^3 \right]_- = 3 i \ h V^5 X_q
\]

In addition, we rewrite (23) as an identity to be used further below to remove \( \partial_j (G(X)) \). Equation (23), after defining \( p \) as a procedure in (24), becomes

\[
> (23) \quad -i \ h \ \partial_j (G) = p_j G
\]

\[
> \text{isolate ((23), } \partial_j (G(X)) \text{ )}
\]

\[
\partial_j (G) = \frac{i p_j G}{h}
\]

Add now these new commutation rules to the setup of the problem so that they are taken into account when using Simplify

\[
> (26), (28), (30)
\]

\[
\left[ L_q, V \right]_- = 0, \left[ p_q, V \right]_- = i \ h V^3 X_q, \left[ p_q, V^3 \right]_- = 3 i \ h V^5 X_q
\]

\[
> \text{Setup((33));}
\]
\[
\begin{align*}
\text{algebrarules} = \left\{ \begin{array}{c}
\left[ L_j, L_k \right]_\pm = i \hbar \epsilon_{j,k,n} L_n, \\
\left[ L_q, V \right]_\pm = 0, \\
\left[ X_j, L_k \right]_\pm = i \hbar \epsilon_{j,k,n} X_n, \\
\end{array} \right\}, \\
X_l = 0, \\
\left[ X_k, p_l \right]_\pm = i \hbar g_{k,l}, \\
\left[ X_k, G \right]_\pm = 0, \\
\left[ X_k, V \right]_\pm = 0, \\
\left[ p_j, L_k \right]_\pm = i \hbar \epsilon_{j,k,n} p_n, \\
\left[ p_j, p_l \right]_\pm = 0, \\
\left[ p_q, V^3 \right]_\pm = 3 i \hbar V^3 X_q, \\
\left[ p_q, V \right]_\pm = i \hbar V^3 X_q, \\
\left[ V, G \right]_\pm = 0
\end{align*}
\]

Undo differential operators to work using two different approaches, with and without differential operators

\[\text{Setup(differentialoperators = none)}\]

\[\text{[differentialoperators = none]}\] (35)

\[\nabla \text{II } \left[ H, L \right] = 0\]

Departing from the Hamiltonian of the hydrogen atom (5) and the definition of angular momentum (14)

\[\text{\textgreater{} (5); (14);}\]

\[H = \frac{p^2}{2 m_e} - \kappa V\]

\[L_q = \epsilon_{m,n,q} X_m p_n\] (36)

by taking their commutator we get

\[\text{\textgreater{} Commutator((5), (14))}\]

\[\left[ H, L_q \right] = \frac{-i \epsilon_{m,n,q} \hbar \left( -X_m V^3 X_n \kappa m_e + p_q p_n g_{l,m} \right)}{m_e}\] (37)

\[\text{\textgreater{} Simplify(37)}\]

\[\left[ H, L_q \right] = 0\] (38)

\[\nabla \text{III } \left[ H, Z \right] = 0\]

This one is less easy. Start from the definition of the quantum Runge-Lenz vector

\[Z[k] = \frac{1}{2 M} \cdot \text{LeviCivita}[a, b, k] \cdot (L[a] \cdot p[b] - p[a] \cdot L[b]) + \kappa \cdot V(X) \cdot X[k]\]

\[Z_k = \frac{\epsilon_{a,b,k} \left( L_a p_b - p_a L_b \right)}{2 m_e} + \kappa V X_k\] (39)

Since the system now knows about the commutation rule between linear and angular momentum,

\[\text{\textgreater{} (%Commutator = Commutator)(L[a], p[b])}\]

\[\left[ L_a, p_b \right] = i \hbar \epsilon_{a,b,n} p_n\] (40)

the expression (39) for
$Z_k$ can be simplified

> Simplify(39)

$$Z_k = \frac{i\hbar p_k}{m_e} + \kappa V X_k - \frac{\epsilon_{a, b, k} p_a L_b}{m_e}$$  \hspace{1cm} (41)$$

and the angular momentum removed from the the right-hand side so that $Z_k$ gets expressed entirely in terms of $p_k, X$ and $V$

> (14)

$$L_q = \epsilon_{m, n, q} X_m p_n$$  \hspace{1cm} (42)$$

> Simplify(SubstituteTensor((14), (41)))

$$Z_k = -i\hbar p_k + \kappa V X_k m_e + X_m p_k p_m - X_k p_n^2$$  \hspace{1cm} (43)$$

Taking the commutator between the Hamiltonian (5) and this expression for $Z_k$ we have the starting point towards showing that $[H, Z_k] = 0$

> Simplify(Commutator((5), (43)))

$$[H, Z_k] = \frac{1}{2m_e} \left( \kappa \hbar \left( \hbar V^2 X_k + \hbar V^5 X_a^2 X_k - 2i p_k V + 2i V X_a X_k p_a V^2 
+ 2i X_b^2 p_k V^3 - 2i X_a X_k p_a V^3 \right) \right)$$  \hspace{1cm} (44)$$

For the term with $V^5$ we use the derived identity (11)

> (11)

$$V^3 X_l^2 = V$$  \hspace{1cm} (45)$$

> $$(X)^2 \cdot (11) \cdot X[k]$$

$$V^5 X_l^2 X_k = V^3 X_k$$  \hspace{1cm} (46)$$

> SubstituteTensor((46), (44))

$$[H, Z_k] = \frac{\kappa \hbar \left( \hbar V^5 X_k - i p_k V + i X_b^2 p_k V^3 + i V X_a X_k p_a V^2 - i X_a X_k p_a V^3 \right)}{m_e}$$  \hspace{1cm} (47)$$

> Simplify((47))

$$[H, Z_k] = \frac{\kappa \hbar \left( 2 \hbar V^5 X_k - i p_k V + i X_b^2 p_k V^3 \right)}{m_e}$$  \hspace{1cm} (48)$$

Another term with $V^5$ appeared

> SubstituteTensor((46), (48))

$$[H, Z_k] = \frac{\kappa \hbar \left( 2 \hbar V^5 X_k - i p_k V + i X_b^2 p_k V^3 \right)}{m_e}$$  \hspace{1cm} (49)$$

Make $X_b$ and $V$ be contiguous to further apply (11)
\[ \begin{align*}
\text{SortProducts (49), } [p[k], X[b]] \\quad & \quad \left[ [H, Z_k] = \frac{\kappa \hbar \left( 2 \hbar V^3 X_k - i p_k V + i \left( p_k X_b^2 + 2 i \hbar g_{b,k} X_b \right) V \right)}{m_e} \right] (50) \\
\text{Simplify (50)} \quad & \quad \left[ [H, Z_k] = \frac{-i \hbar \kappa \left( p_k V - p_k V^3 X_b^2 \right)}{m_e} \right] (51) \\
p[k] \cdot (45) \quad & \quad p_k V^3 X_i^2 = p_k V (52) \\
\text{SubstituteTensor (52, 51)} \quad & \quad \left[ [H, Z_k] = 0 \right] (53)
\end{align*} \]

And this is the result we wanted to prove. In the next section there is an alternative derivation that could be seen as more abstract or more direct, depending on the point of view.

\begin{itemize}
\item \textbf{Alternative approach using differential operators}
\end{itemize}

As done in the previous section when deriving the commutators between linear and angular momentum, on the one hand, and the central potential \( V \) on the other hand, the idea here is again to use differential operators taking advantage of the ability to compute with them as operands of a product, that get applied only when it appears convenient for us.

\[ \begin{align*}
\text{Setup (differentialoperators } = \{ [p[k], [x, y, z]] \} \} \\
\left[ \text{differentialoperators } = \{ [[p_k, [X]]] \} \right] (54)
\end{align*} \]

So take the starting point (44)

\[ \begin{align*}
[H, Z_k] &= \frac{1}{2 m_e} \left( \kappa \hbar \left( \hbar V^3 X_k + \hbar V^5 X_a^2 X_k - 2 i p_k V + 2 i V X_a X_k p_a V^2 \right. \\
&\quad \left. + 2 i X_b^2 p_k V^3 - 2 i X_a X_k p_a V^3 \right) \right) \quad (55)
\end{align*} \]

and to show that the left-hand side is equal to 0, multiply by a generic function \( G(X) \) followed by transforming the products involving \( p_k \) by the application of this differential operator.

\[ \begin{align*}
[H, Z_k] G &= \frac{1}{2 m_e} \left( \kappa \hbar \left( \hbar V^3 X_k + \hbar V^5 X_a^2 X_k - 2 i p_k V + 2 i V X_a X_k p_a V^2 \right. \\
&\quad \left. + 2 i X_b^2 p_k V^3 - 2 i X_a X_k p_a V^3 \right) \right) (56)
\end{align*} \]

\[ \begin{align*}
[H, Z_k] G &= -\frac{1}{m_e} \left( \kappa \hbar \left( \hbar V \partial_k(G) + \hbar \partial_k(V) \right) G - \hbar V X_a X_k \left( \partial_a(V) \right) V \right) \quad (57)
\end{align*} \]
+ \partial_a (V) G + V^2 \partial_a (G) \right) - \hbar X_b^2 \left( \left( \partial_k (V) V^2 + \partial_k (V) V + V^2 \partial_k (V) \right) G \\
+ V^3 \partial_k (G) \right) + \hbar X_a X_k \left( \left( \partial_a (V) V^2 + \partial_a (V) V + V^2 \partial_a (V) \right) G + V^3 \partial_a (G) \right) \\
- \left( \frac{\hbar V^3 X_k G}{2} - \frac{\hbar V^5 X_a^2 X_k G}{2} \right) \right) \\
> \text{Simplify(} (57) \text{)} \\
[H, Z_k]_\hbar G = - \frac{1}{m_e} \left( \hbar^2 \kappa \left( V \partial_k (G) + \partial_k (V) G - X_b^2 \partial_k (V) G V^2 - V X_b^2 \partial_k (V) G V \right) \\
- V^2 X_b^2 \partial_k (V) G - V^3 X_b^2 \partial_k (G) + X_a X_k \partial_a (V) G V^2 - \frac{G V^3 X_k}{2} \\
- \frac{G V^5 X_a^2 X_k}{2} \right) \right) \\

Use now the derived identities for the gradients of $V$ and $G$ and then remove the generic function $G$ from the equation by multiplying by the inverse of $G$ \\
> (8); (32); \\
\partial_n (V) = -V^3 X_n \\
\partial_l (G) = \frac{ip_l G}{\hbar} \\
> \text{Simplify(SubstituteTensor(} (8), (32), (58) \text{) \cdot Inverse(} G (X) \text{) )} \\
[H, Z_k]_\hbar = - \frac{\hbar \kappa \left( i V p_k - i V^3 X_a^2 p_k - \frac{3 \hbar V^2 X_k}{2} + \frac{3 \hbar V^5 X_a^2 p_k}{2} \right)}{m_e} \\

To show that the right-hand side is actually 0, recalling (11) \\
> (11) \\
V^3 X_l^2 = V \\
> (\text{rhs} = \text{lhs})((11) \cdot p[k]) \\
V p_k = V^3 X_l^2 p_k \\
> \text{Simplify(SubstituteTensor(} (62), (46) \text{), (60) \text{) )} \\
[H, Z_k]_\hbar = 0 \\

Reset differentialoperators in order to proceed to the next section working without differential operators \\
> Setup(differentialoperators = none) \\
[\text{differentialoperators = none}] 
>
\[ \begin{align*}
\mathbf{IV} \quad & [L_m, Z_n]_- = i \hbar \epsilon_{m, n, k} Z_k
\end{align*} \]

Strategy:

1. Express \( L_m \) and \( Z_k \) in terms of \( X_a \) and \( p_b \) from previous sections.
2. Construct the left-hand and right-hand sides of \( [L_q, Z_k]_- = -i \hbar \epsilon_{k, q, u} Z_u \), the formula we want to prove.
3. Simplify the result.

Step 1 got accomplished in the previous sections.

\[ L_q = \epsilon_{m, n, q} X_m p_n \]  \hspace{1cm} (65)

\[ Z_k = -i \hbar p_k + \kappa V X_k m_e + X_m p_k p_m - X_k p_n^2 \]  \hspace{1cm} (66)

Step 2.

The left-hand side of the identity to be proved is the left-hand side of their commutator.

\[ \text{Commutator}((14), (43)) \]

\[ [L_q, Z_k]_- = \frac{1}{m_e} \left( \epsilon_{m, n, q} \hbar \left( i X_m \left( -g_{k, n} V + V^3 X_n X_k \right) \kappa m_e + \hbar g_{k, m} p_n - i X_m p_k p_a g_{a, n} \right) + i X_m p_{b, k}^2 g_{k, n} - 2 i X_k p_{b, n} g_{b, m} + i X_a \left( g_{a, m} p_k + g_{k, m} p_a \right) p_n \right) \]  \hspace{1cm} (67)

The right-hand side of \([L_q, Z_k]_- = -i \hbar \epsilon_{k, q, u} Z_u\) to be proved is given by

\[ i \hbar \cdot \text{LeviCivita}[q, k, u] \cdot \text{SubstituteTensorIndices}(k = u, (43)) \]

\[ -i \hbar \epsilon_{k, q, u} Z_u = \frac{i \hbar \epsilon_{k, q, u} \left( i p_u - \kappa V X_u m_e + X_u p_n^2 - X_m p_u p_m \right)}{m_e} \]  \hspace{1cm} (68)

Step 3.

Take one minus the other one and the right-hand side must be equal to 0.

\[ \text{Simplify}((69)) \]

\[ [L_q, Z_k]_- + i \hbar \epsilon_{k, q, u} Z_u = 0 \]  \hspace{1cm} (70)
\[ \nabla V \left[ Z_m, Z_n \right] = -\frac{2i\hbar}{m_e} H \epsilon_{m, n, o} L_{o} \]

Here again the starting point is (43), the definition of the quantum Runge-Lenz vector.

> SubstituteTensorIndices \((k = q, (43))\)

\[ Z_q = \frac{-i\hbar p_q + \kappa V X_q m_e + X_m p_q p_m - X_q p_n^2}{m_e} \quad (71) \]

In this section the strategy is the same as in the previous section: construct the left-hand and right-hand sides of \[ Z_m, Z_n \] = \( -\frac{2i\hbar}{m_e} H \epsilon_{m, n, o} L_{o} \), then take one minus the other one, and show that the right-hand side is equal to 0.

Start with the left-hand side \[ Z_m, Z_n \]

> Commutator ((43), (71))

\[ \left[ Z_k, Z_q \right] = \frac{1}{m_e} \left( -2i\hbar g_{b, m} X_q p_b p_k p_m + \kappa m_e X_m (i\hbar p_k \left(-V m, q + V^3 X_m X_q\right) + i\hbar \right) \]

\[ -g_{k, q} V + V^3 X_q X_k p_m + 2i\hbar g_{b, k} X_q p_b p_n^2 - i\hbar X_m \left( g_{a, k} p_q p_a p_m \right) \]

\[ + g_{a, m} p_k p_q p_a + \hbar^2 V^3 X_k X_q \kappa m_e - \hbar^2 V^3 X_q X_k \kappa m_e + i\hbar X_k \left( g_{a, m} p_q \right) \]

\[ + g_{m, q} p_a \right) p_k p_m + 2i\hbar g_{a, n} X_k p_n p_q p_a - 2i\hbar g_{n, q} X_k p_n p_b^2 + i\hbar X_q \left( 2p_b V^3 X_b \right) \]

\[ + V^3 \left( 3i\hbar + 2p_b X_b \right) - \left( 3i\hbar V^5 X_b + 2 V^3 p_b \right) X_b \right) X_k \kappa m_e \]

\[- 2i\hbar V X_q p_b + m_e g_{b, k} - \hbar^2 p_n^2 g_{k, q} + \hbar^2 p_k p_m g_{m, q} - \hbar^2 p_q p_a g_{a, k} + \hbar^2 g_{k, q} \]

\[ + \left( 2i\hbar X_k \right) \left( V p_n g_{n, q} + g_{m, q} X_n \right) + \left( 2p_n^3 X_n + V^3 \left( 3i\hbar + 2p_n X_n \right) \right) X_q \]

\[ - iX_k \left( p_q V^3 X_q + V^3 X_q p_a \right) X_k + iV X_a \left( g_{a, k} p_q + g_{k, q} p_a \right) \kappa m_e - iX_a \left( g_{a, k} p_q \right) \]
Now the right-hand side, constructed from the definition of the angular momentum
\[ L_q = \epsilon_{m,n,q} X_m p_n \]  
\[ (73) \]
Multiply by \( \frac{-2i\hbar \epsilon_{k,q,u} H}{m_e} \)
\[ \frac{-2i\hbar \epsilon_{k,q,u} H L_u}{m_e} = \frac{-2i\hbar \epsilon_{k,q,u} \epsilon_{m,n,u} H X_m p_n}{m_e} \]  
\[ (74) \]
Replace the Hamiltonian \( H \) by its expression quadratic in the momentum
\[ H = \frac{p_l^2}{2m_e} - \kappa V \]  
\[ (75) \]
\[ \text{lhs } (74) = \text{SubstituteTensor } (5, \text{rhs } (74)) \]
\[ \frac{-2i\hbar \epsilon_{k,q,u} H L_u}{m_e} = \frac{-2i\hbar \epsilon_{k,q,u} \epsilon_{m,n,u} \left( \frac{p_l^2}{2m_e} - \kappa V \right) X_m p_n}{m_e} \]  
\[ (76) \]
Now set up the problem, taking \((72)\) minus \((76)\)
\[ Z_k Z_q \]  
\[ + \frac{2i\hbar \epsilon_{k,q,u} H L_u}{m_e} = \frac{1}{m_e^2} \left( \hbar \left( iX_m \left( g_{a,k} p_q p_a + g_{m,q} p_a \right) p_k p_m \right) + 2i \epsilon_{k,q,u} \epsilon_{m,n,u} \left( \frac{p_l^2}{2m_e} - \kappa V \right) X_m p_n m_e \right) - iX_m \left( g_{k,q} p_b^2 p_m + g_{b,q} p_b^2 \right) + 2i g_{a,n} X_k p_n p_q p_a \]
\[ + 2i \epsilon_{k,q,u} \epsilon_{m,n,u} \left( \frac{p_l^2}{2m_e} - \kappa V \right) X_m p_n m_e - 2i g_{n,q} X_k p_n p_b^2 - iX_m \left( g_{a,k} p_q \right) + g_{k,q} p_a^2 + iX_m \left( g_{k,q} p_b^2 p_m + g_{m,q} p_b^2 \right) + \hbar V^3 X_k X_q \kappa m_e \]
\[ - \hbar V^3 X_q X_k \kappa m_e - 2i g_{b,m} X_q p_b p_k p_m - 2i V X_q p_b \kappa m_e g_{b,k} - iX_m \left( p_q V^3 X_a \right) \]
\[ + V^3 X_q p_a \right) X_k \kappa m_e + 2i g_{b,k} X_q p_b p_n^2 + iV X_a \left( g_{a,k} p_q + g_{k,q} p_a \right) \kappa m_e \]
\[ + \hbar g_{m, q} p_k p_m - \hbar g_{a, k} p_q p_a + \hbar g_{k, q} p_b^2 - \hbar g_{k, q} p_n^2 + \left( i X_m p_k \left( -g_{m, q} V + V^3 X_m X_q \right) + \left( -g_{k, q} V + V^3 X_k X_q \right) p_m \right) + 2 i X_k \left( V p_n g_{n, q} - \frac{2 p_n V^3 X_n + V^3 \left( 3 i \hbar + 2 p_n X_n \right) - \left( 3 i \hbar V^5 X_n + 2 V^3 p_n \right) X_q \right) \right) \]

So the starting point to prove that \( Z_k, Z_q = 2 i \hbar \epsilon_{k, q, u} H L u \) is

\[
\frac{2 i \hbar \epsilon_{k, q, u} H L u}{m_e} + \left[ Z_k, Z_q \right] - \frac{1}{m_e} \left( \hbar \left( \hbar V^5 X_j^2 X_k X_q X_k m_e \right) - i \kappa X^2 X_k p_k V^3 m_e \right)
\]

\[
+ i \kappa X^2 X_k p_q V^3 m_e + i \kappa X^2 X_k p_k V^3 m_e - i \kappa X^2 X_k X_k X^2 p_j V^3 m_e
\]

\[
- i \kappa X X_k^2 X_q p_g V^3 m_e - i g_{k, q} X c p_c p_d + i g_{k, q} X h p_a p_b + 2 i X q p_d p_p
\]

\[
- 2 i X q p_a p_k \right) \right]
\]

were the proof is achieved showing that the right-hand side of this equation is indeed equal to 0.

Start checking the repeated indices, as we would do by hand

> Check((78), all)

The products in the given expression check ok.

The repeated indices per term are: \([\{\ldots, \{\ldots, \ldots\} \}, \{\ldots\}\), the free indices are: \(\{\ldots\}\)

\[
([\{u\}], \{k, q\}) = ([\{a, b, c, d, g, j\}], \{k, q\})
\]

Check in which terms - that involve \( V - \) are these repeated indices appearing

> for term in select(has, map (op, indets ((78), `+`)), V) do

term = Check(term, repeated, quiet)
od

\[
- i \kappa X_k p_q V m_e = [\emptyset]
\]

\[
- i \kappa X_b^2 X_q p_k V^3 m_e = [\{b\}]
\]

\[
- i \kappa V X g X k X_q p_g V^3 m_e = [\{g\}]
\]

\[
i \kappa X_q p_k V m_e = [\emptyset]
\]

\[
i \kappa X_b^2 X_k p_q V^3 m_e = [\{b\}]
\]

\[
i \kappa X_j X k X_q p_j V^3 m_e = [\{j\}]
\]

(80)
\[ \hbar V^5 X_j^2 X_k X_q \kappa m_e = [ \{ j \} ] \] (80)

We see that there are terms with \( X_j^2 \) and terms with \( X_b^2 \), so \( j = b \) results in a simplification

> SubstituteTensorIndices ([ \{ j \} ], (78))

\[
\frac{2i \hbar \epsilon_{k,q,u} H L_u + [Z_k Z_q]_m e}{m_e} = -\frac{1}{m_e} \left( \hbar V^5 X_b^2 X_k X_q \kappa m_e - i \kappa X_b^2 X_q p_k V^3 m_e \right)
\]

\[
+ i \kappa X_b^2 X_q p_k V^3 m_e + i \kappa X_q p_k V m_e - i \kappa X_b X_q X_p p_b V^3 m_e
\]

\[
- i \kappa V X_k X_q p_g V^2 m_e - ig_{k,q} X_c p_c p_d + ig_{k,q} X_b p_a V + 2i X_q p_d p_k
\]

\[
- 2 i X_q p_a^2 p_k \right)
\] (81)

> Simplify (81)

\[
\frac{2i \hbar \epsilon_{k,q,u} H L_u + [Z_k Z_q]_m e}{m_e}
\]

\[
= \frac{i \hbar \kappa \left( X_b^2 X_q p_k V^3 - X_b^2 X_k p_q V^3 - X_q p_k V + X_k p_q V \right)}{m_e}
\] (82)

There are two terms with \( V^3 \) that could be removed using

> (11)

\[
V^3 X_j^2 = V
\] (83)

but for that to be possible, in (82) we need to have \( V \) to the left of \( X_b^2 \). So sort the products indicating the desired ordering of operands, then simplify

> SortProducts ((82), \( [p_k p_q, X_k, X_q, X_b] \))

\[
\frac{2i \hbar \epsilon_{k,q,u} H L_u + [Z_k Z_q]_m e}{m_e} = \frac{1}{m_e} \left( -i \hbar \kappa \left( -p_k X_b^2 + i \hbar g_{k,q} X_b^2 \right)
\]

\[
+ 2i \hbar g_{b,k} X_b \right) V^3 + \left( p_q X_k X_b^2 + i \hbar g_{k,q} X_b^2 + 2i \hbar g_{b,q} X_k X_b \right) V^3 + \left( p_q X_q \right)
\]

\[
+ i \hbar g_{q,k} \right) V - \left( p_q X_k + i \hbar g_{k,q} V \right) \right)
\] (84)

> Simplify (84)

\[
\frac{2i \hbar \epsilon_{k,q,u} H L_u + [Z_k Z_q]_m e}{m_e}
\]

\[
= \frac{-i \hbar \kappa \left( p_k V X_q - p_k V^3 X_b^2 X_q + p_q V^3 X_b^2 X_k - p_q V X_k \right)}{m_e}
\] (85)

> SubstituteTensor ((83), (85))

\[
\frac{2i \hbar \epsilon_{k,q,u} H L_u + [Z_k Z_q]_m e}{m_e} = \frac{-i \hbar \kappa \left( p_k V X_q - V p_k X_q + V p_q X_k - p_q V X_k \right)}{m_e}
\] (86)

> Simplify (86)
\[
\frac{2 \mathrm{i} \hbar \epsilon_{k, q, u} H L_u + [Z^k, Z^q]_{-} m_e}{m_e} = 0
\]

which is the identity we wanted to prove. In the next section the same result is obtained using differential operators.

\section*{Alternative approach using differential operators}

The main idea: make \( p_k \) be a differential operator, then make (78)

\[
\frac{2 \mathrm{i} \hbar \epsilon_{k, q, u} H L_u + [Z^k, Z^q]_{-} m_e}{m_e} = -\frac{1}{m_e^2} \left( \hbar \left( \hbar V^5 X^2_j X^k_q \kappa m_e \right. \right.

- i \kappa X^2_b X^q_p V^3 m_e + i \kappa X^2_b X^p_k p V^3 m_e + i \kappa X^p_k p V m_e - i \kappa X^p_k V m_e

\left. + i \kappa X_j^k X^q X^p_j p v^3 m_e - i \kappa X_j^k X^p_j p v^3 m_e \right)

\]

by a generic function \( G(X) \), apply the products of differential operators, then use the tensorial simplification equations

\[
\delta_n(V) = -V^3 X^n \\
\delta_l(G) = \frac{i p_l G}{\hbar} \\
V^3 X^2 = V
\]

The goal is again to show that the right-hand side of (78) is equal to 0, so set \( p_k \) to be a differential operator, multiply (78) by a generic function \( G(X) \) followed by applying \( p_k \) where it corresponds

\section*{Setup (differentialoperators = \( \{ [p[k], [x, y, z]] \} \))}

\[\text{differentialoperators} = \{ [p_k, [X]] \}\]

\section*{ApplyProductsOfDifferentialOperators ((91))}

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\[
\frac{(2i\hbar\epsilon_{k,q,u}H L_u + [Z_k Z_q] - m_e) G}{m_e} = \frac{1}{m_e^2} \left( \hbar \left( g_{k,q} \hbar^3 X_k \partial_b (\Box (G)) \right) \right.
\]

We want to show that the right-hand side is equal to 0; start simplifying with respect to algebra rules and using Einstein's sum rule for repeated indices

> **Simplify** ([92])

\[
\frac{(2i\hbar\epsilon_{k,q,u}H L_u + [Z_k Z_q] - m_e) G}{m_e} = \frac{1}{m_e^2} \left( \hbar^2 \kappa \left( -X_k X_l X_q \partial_l (V) G V^2 \right) \right.
\]

Next, using (8), the gradient of \( V \) can be removed

> **SubstituteTensor** ([94], [93])

\[
\frac{(2i\hbar\epsilon_{k,q,u}H L_u + [Z_k Z_q] - m_e) G}{m_e} = \frac{1}{m_e^2} \left( \hbar^2 \kappa \left( -X_k X_l X_q V^3 X_l G V^2 \right) \right.
\]

> **Simplify** ([95])

\[
\frac{(2i\hbar\epsilon_{k,q,u}H L_u + [Z_k Z_q] - m_e) G}{m_e} = \frac{1}{m_e^2} \left( \hbar^2 \kappa \left( -X_k X_l X_q V^3 X_l G V^2 \right) \right.
\]
\[ \frac{\hbar^2\kappa}{m_e} \left( -V^3 X_a^2 X_k \partial_q (G) + V^3 X_a^2 X_k \partial_k (G) + VX_k \partial_q (G) - VX_k \partial_k (G) \right) \]

From (32) the gradient of \( G \) can be removed

> (32)

\[ \frac{i p_l G}{\hbar} \]

(97)

> Simplify(SubstituteTensor((32), (96)))

\[ \frac{\left( 2i \hbar \epsilon_{k, q, u} H L_u + \left[ Z_k, Z_q \right]_{m_e} \right) G}{m_e} \]

(98)

And there are still two terms of the form \( X^2 V^3 \) that can be removed using (11)

> (11)

\[ V^3 X_l^2 = V \]

(99)

> SubstituteTensor((11), (98))

\[ \frac{\left( 2i \hbar \epsilon_{k, q, u} H L_u + \left[ Z_k, Z_q \right]_{m_e} \right) G}{m_e} = 0 \]

(100)

And since \( G \) is just an arbitrary test function, the above is already the result (87) we wanted to obtain.

>