# Computer Algebra in Physics: The hidden SO(4) symmetry of the hydrogen atom

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**Abstract**

Pauli first noticed the hidden SO(4) symmetry for the hydrogen atom in the early stages of quantum mechanics [1]. Starting from that symmetry, one can recover the spectrum of a spinless hydrogen atom and the degeneracy of its states without explicitly solving Schrödinger's equation [2], [3]. In this paper, we derive that SO(4) symmetry and spectrum using a computer algebra system (CAS). While this problem is well known [4], [5], its solution involves several steps of manipulating expressions with tensorial quantum operators, including simplifying them by taking into account a combination of commutator rules and Einstein's sum rule for repeated indices. Therefore, it is an excellent model to test the current status of CAS concerning this kind of quantum-and-tensor-algebra computations and to showcase the CAS technique. Generally speaking, when capable, CAS can significantly help with manipulations that, like non-commutative tensor calculus subject to algebra rules, are tedious, time-consuming and error-prone. The presentation also shows two alternative patterns of computer algebra steps that can be used for systematically tackling more complicated symbolic problems of this kind.

*Keywords:* Quantum mechanics; tensor calculus; commutator;

**PROGRAM SUMMARY/NEW VERSION PROGRAM SUMMARY**
*Program Title:* Maple specific worksheet
*CPC Library link to program files:* (to be added by Technical Editor)
*Developer's repository link:* To be provided later
*Code Ocean capsule:* (to be added by Technical Editor)
*Licensing provisions:* GPLv3
*Programming language:* Maple (Maplesoft)
*Supplementary material:* None
*Nature of problem(approx. 50-250 words):* See introduction and conclusions.
*Solution method(approx. 50-250 words):* See introduction and conclusions.
*Additional comments including restrictions and unusual features (approx. 50-250 words):* This article mirrors a Maple worksheet. As such, it is not an usual code intended to make a computation for a given set of parameters. It is rather a general template or guideline, useful to extend the present problem with new computations or, more generally, widely open to tackle new quantum mechanics problem involving tensor and commutator heavy calculus.

## 1. Introduction

In this work we derive, step-by-step, the SO(4) symmetry of the hydrogen atom and its spectrum using a computer algebra system (CAS). To the best of our knowledge, such a derivation using symbolic computation has not been shown before. The goal was to see whether this computation can be performed entering only the main definition formulas, followed by only simplification commands, and without using previous knowledge of the result. The presentation that follows showcases that approach, illustrating different techniques. The intricacy of this problem is in the symbolic manipulation and simplification of expressions involving noncommutative quantum tensor operators.

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The simplifications need to take into account commutator rules, symmetries under permutation of indices of tensorial subexpressions, and use Einstein's sum rule for repeated indices.

We performed the derivation using the Maple 2020 CAS with the Maplesoft Physics Updates v.913. Generally speaking, the default computational domains of CAS don't include tensors, noncommutative operators nor related simplifications. The exception is the Maple system, which is distributed with the Physics package, which extends that default domain to include those objects and related operations. Relevant for our purpose, Physics includes a Simplify command which takes into account custom algebra rules and the sum rule for repeated indices, and uses tensor-simplification algorithms [6] adapted to work on a noncommutative domain.

A few notes about notation: when working with a CAS, besides the expectation of achieving a correct result for a complicated symbolic calculation, readability is also an issue. It is desired that one be able to enter the definition formulas and computational steps to be performed (the *input*, shown in what follows preceded by a prompt >) in a way that resembles as closely as possible their paper and pencil representation, and that the results (the *output*, computed by the CAS) use easy-to-read, textbook mathematical-physics notation. The Maple Physics package implements such dedicated typesetting. In what follows, within text and in the *output*, noncommutative objects are displayed using a different color, e.g. $H$, vectors and tensor indices are displayed in the standard way, as in $\vec{L}$ and $L_q$, and commutators are displayed with a minus subscript, e.g. $[H, L_q]_-$. Although the Maple system optionally provides dedicated typesetting also for the *input*, we preferred to keep visible the Maple *input* syntax, allowing for comparison with paper and pencil notation and to transmit a more accurate picture of what it is like to work on a real problem using CAS. We collected the names of the handful of commands used together with a one line description for them in an Appendix at the end. Maple also implements the concept of *inert* representations of computations, which are activated only when desired. We use this feature in several places. Inert computations are entered by preceding the command with % and are displayed in grey. Finally, as is usual in CAS, every output has an equation label, which we use throughout the presentation to refer to previous intermediate results, both in text and in input lines.

In Sec.1, we present the standard formulation of the problem and the computational goal, which is the derivation of the formulas representing the SO(4) symmetry and related spectrum.

In Sec.2, we formulate the problem on a Maple worksheet by setting tensorial non-commutative operators representing position, linear and angular momentum, respectively $X_a$, $p_a$ and $L_a$, their commutation rules used as departure point, and the form of the quantum Hamiltonian $H$. That formulation is also used to derive a few related identities used in the sections that follow.

In Sec.3, we derive the conservation of both angular momentum and the Runge-Lenz quantum operator, respectively $[H, L_q]_-$ and $[H, Z_k]_-$. Taking advantage of the *differentialoperators* feature of the Physics package, we explore two equivalent approaches: first, using only a symbolic tensor representation $p_j$ of the momentum operator; second, using an explicit differential operator representation for it in configuration space, $p_j = -i\hbar\partial_j$. With the first approach, expressions are simplified only using the departing commutation rules and Einstein's sum rule for repeated indices. Using the second approach, $p_j$ represents an abstract non-commutative differentiation operator with respect to the coordinates which acts over expressions that involve a test function $G(X)$. In the end, $p_j$ is given an explicit form in coordinate representation the differentiation operations are performed and the test function $G(X)$is removed, yielding a result. Presenting both approaches is of interest as it offers two independent methods for performing the same computation, which is helpful to provide confidence in the results, a relevant issue when using computer algebra and in general.

In Sec.4, we derive $[L_m, Z_n]_- = i\hbar\epsilon_{mnu}Z_u$ and show that the classical relation between angular momentum and the Runge-Lenz vectors, $\vec{L} \,.\, \vec{Z} = 0$, due to the orbital momentum being perpendicular to the elliptic plane of motion in which the Runge-Lenz vector lies, still holds in quantum mechanics, where the components of these quantum vector operators do not commute.

In Sec.5, we derive $[Z_a, Z_b]_- = -\frac{2\mathrm{i}\hbar\epsilon_{abc}}{m_e} H L_c$ using the two alternative approaches described in Sec.3.

In Sec.6, we derive the well-known formula for the square of the Runge-Lenz vector, ${Z_k}^2 = \frac{2}{m_e} H(\hbar^2 + {L_a}^2) + \kappa^2$.

In Sec.7, we use the SO(4) algebra derived in the previous sections to obtain the spectrum of the hydrogen atom. Following the literature, this approach is limited to the bound states for which the energy is negative.

Some concluding remarks are presented at the end, and input syntax details are summarized in the Appendix. A Maple worksheet with the contents of this presentation, used to produce this article by exporting to LaTeX, can be downloaded from this Mapleprimes post: The-Hidden-SO4-Symmetry-Of-The-Hydrogen-Atom.

## 2. The hidden SO(4) symmetry of the hydrogen atom

Let's consider the hydrogen atom and its Hamiltonian

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

where $\vec{p}$ is the electron momentum, $m_e$ its mass, $\kappa$ a real positive constant, $r = \|\vec{r}\| \equiv \sqrt{{X_a}^2}$ the distance of the electron from the proton located at the origin, and $X_a$ is its tensorial representation with components $[x, y, z]$. We assume that the proton's mass is infinite. The electron and nucleus spin are not taken into account. Classically, from the potential $-\frac{\kappa}{r}$, one can derive a central force $\vec{F} = -\kappa\frac{\hat{r}}{r^2}$ that drives the electron's motion. Introducing the angular momentum

$$\vec{L} = \vec{r} \times \vec{p},$$

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

$$\vec{Z} = \frac{1}{m_e} \cdot (\vec{L} \times \vec{p}) + \kappa\frac{\vec{r}}{r}$$

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

$$[H, \vec{Z}]_- = 0$$

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

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

In what follows, departing from the Hamiltonian $H$, the basic commutation rules between position $\vec{r}$, momentum $\vec{p}$ and angular momentum $\vec{L}$ in tensor notation, we derive the following commutation rules between the quantum Hamiltonian, angular momentum and Runge-Lenz vector $\vec{Z}$

$$\begin{aligned}
[H, L_n]_- &= 0 \\
[H, Z_n]_- &= 0 \\
[L_m, Z_n]_- &= \mathrm{i}\hbar\epsilon_{mno} Z_o \\
[Z_m, Z_n]_- &= -2\frac{\mathrm{i}\hbar}{m_e} H \epsilon_{mno} L_o
\end{aligned}$$

Since $H$ commutes with both $\vec{L}$ and $\vec{Z}$, defining

$$M_n = \sqrt{-\frac{m_e}{2H}}\, Z_n,$$

these commutation rules can be rewritten as

$$\begin{array}{rcl} [L_m, L_n]_- & = & i\hbar\epsilon_{mno} L_o \\ [L_m, M_n]_- & = & i\hbar\epsilon_{mno} M_o \\ [M_m, M_n]_- & = & i\hbar\epsilon_{mno} L_o \end{array}$$

This set constitutes the Lie algebra of the SO(4) group.

## 3. Setting the problem, commutation rules and useful identities

Formulating the problem requires loading the *Physics* package and its *Library* and *Vectors* subpackages, that contain additional manipulation commands; we set the imaginary unit to be represented by a lowercase Latin i letter instead of the default uppercase I.

> $with(Physics) : with(Library) : with(Vectors) : interface(imaginaryunit = i) :$

The context for this problem is Cartesian coordinates and a 3D Euclidean space where all of $\{\hbar, \kappa, m_e\}$ are real objects. We chose lowercase letters to represent tensor indices, the use of automatic simplification (i.e., *automatically simplify the size* of everything being displayed)

> $Setup(coordinates = cartesian, realobjects = \{\hbar, \kappa, m_e\}, automaticsimplification = true, dimension = 3, metric = Euclidean, spacetimeindices = lowercaselatin, quiet)$

$$[automaticsimplification = true, coordinatesystems = \{X\}, dimension = 3, metric = \{(1, 1) = 1, (2, 2) = 1, (3, 3) = 1\}, realobjects = \{\hbar, \kappa, m_e, \phi, r, \rho, \theta, x, y, z\}, spacetimeindices = lowercaselatin] \quad (1)$$

Next, we set the quantum Hermitian operators (not $Z$, we derive that property for it further below) and related commutators:

- the dimensionless potential $V = \frac{1}{r}$ is assumed to commute with position, not with momentum - the commutation rule with $p_k$ is derived in Sec.3.2;
- the commutator rules between position $X_n$ on the one hand, and linear $p_k$ and angular momentum $L_k$ on the other hand, are the departure point, entered using the inert form of the *Commutator* command. Tensors are indexed using the standard Maple notation for indexation, [].

> $Setup(quantumoperators = \{Z\}, hermitianoperators = \{V, H, L, X, p\}, algebrarules = \{\%Commutator(p[k], p[l]) = 0, \%Commutator(X[k], p[l]) = i\,\hbar\, g\_[k, l], \%Commutator(L[j], L[k]) = i\,\hbar\, LeviCivita[j, k, n]\, L[n], \%Commutator(p[j], L[k]) = i\,\hbar\, LeviCivita[j, k, n]\, p[n], \%Commutator(X[j], L[k]) = i\,\hbar\, LeviCivita[j, k, n]\, X[n], \%Commutator(X[k], V(X)) = 0\})$

$$\left[algebrarules = \left\{\left[L_j, L_k\right]_- = i\hbar\epsilon_{jkn}L_n, \left[p_j, L_k\right]_- = i\hbar\epsilon_{jkn}p_n, [p_k, p_l]_- = 0, \left[X_j, L_k\right]_- = i\hbar\epsilon_{jkn}X_n, [X_k, p_l]_- = i\hbar g_{kl}, [X_k, V(X)]_- = 0\right\}, hermitianoperators = \{H, L, V, p, x, y, z\}, quantumoperators = \{H, L, V, Z, p, x, y, z\}\right] \quad (2)$$

Define the *tensor* quantum operators representing the linear momentum, angular momentum and the Runge-Lenz vectors

> $Define(p[k], L[k], Z[k], quiet)$

$$\{\gamma_a, L_k, \sigma_a, Z_k, \partial_a, g_{ab}, p_k, \epsilon_{abc}, X_a\} \quad (3)$$

For readability, avoid redundant display of functionality

> $CompactDisplay((V, G)(X))$

$$V(X) \mathit{will\ now\ be\ displayed\ as}\ V$$

$$G(X)\ \mathit{will\ now\ be\ displayed\ as}\ G \tag{4}$$

The Hamiltonian for the hydrogen atom is entered as

> $H = \frac{p[l]^2}{2 \cdot m_e} - \kappa \cdot V(X)$

$$H = \frac{{p_l}^2}{2m_e} - \kappa V \tag{5}$$

### 3.1. *Definition of V(X) and related identities*

We use the dimensionless potential $V(X)$

> $V(X) = \frac{1}{(X[l]^2)^{\frac{1}{2}}}$

$$V = ({X_l}^2)^{-\frac{1}{2}} \tag{6}$$

The gradient of $V(X)$ is

> $d\_[n]((\mathbf{6}))$

$$\partial_n(V) = -({X_l}^2)^{-\frac{3}{2}}\, X_n \tag{7}$$

where we note that all these commands (including product and power), *distribute over equations*. So that

> $subs((rhs = lhs)((\mathbf{6})^3), (\mathbf{7}))$

$$\partial_n(V) = -V^3 X_n \tag{8}$$

Equivalently, from **(6)** one can deduce that will often be used afterwards

> $(rhs = lhs)(\frac{V(X)^3}{(\mathbf{6})^2})$

$$V^3 {X_l}^2 = V \tag{9}$$

### 3.2. *The commutation rules between linear and angular momentum and of the potential V(X)*

By definition

> $L[q] = LeviCivita[q, m, n] \cdot X[m] \cdot p[n]$

$$L_q = \epsilon_{mnq} X_m p_n \tag{10}$$

so

> $Commutator((\mathbf{10}), V(X))$

$$\left[L_q, V\right]_- = \epsilon_{mnq} X_m \left[p_n, V\right]_- \tag{11}$$

The commutator on the right-hand side cannot be computed by the CAS until providing more information. To derive the value of $[p_n, V]_-$we set $p_n$ as a *differentialoperator* and introduce an arbitrary test function $G(X)$

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

$$[differentialoperators = \{[p_k, [X]]\}] \tag{12}$$

Apply now to $G(X)$ the differential operator $p_n$ found in the commutator of the right-hand side of **(11)**

> $(lhs = ApplyProductsOfDifferentialOperators@rhs)((\mathbf{11}) \cdot G(X))$

$$\left[L_q, V\right]_- G = \epsilon_{mnq} X_m \left(p_n(VG) - V p_n(G)\right) \tag{13}$$

The result of $p_l(G(X))$ is not known to the system at this point. Define then an explicit representation for $p_n$ as the differential operator in configuration space $p_n = -i\hbar\partial_n$

> $p := u \to -i\,\hbar \cdot d\_[op(procname)](u)$

$$p := u \mapsto -\mathrm{i}\hbar\partial_{op(procname)}(u) \tag{14}$$

where in the above $op(procname)$ represents the indices with which the differential operator $p_n$ is called.With this definition, the right-hand side of **(13)** automatically evaluates to

> **(13)**

$$\left[L_q, V\right]_- G = -\mathrm{i}\epsilon_{mnq}\hbar X_m \partial_n(V)\, G \tag{15}$$

So that using **(8)** $\equiv \partial_n(V) = -V^3 X_n$ and multiplying by $G(X)^{-1}$,

> $SubstituteTensor(\mathbf{(8)}, \mathbf{(15)}) \cdot G(X)^{-1}$

$$\left[L_q, V\right]_- = \mathrm{i}\epsilon_{mnq}\hbar X_m V^3 X_n \tag{16}$$

from where we get the first commutation rule:

> $Simplify(\mathbf{(16)})$

$$\left[L_q, V\right]_- = 0 \tag{17}$$

Likewise, from the *inert* = *active* form of $[p_q, V(X)]_-$

> $(\%Commutator = Commutator)(p[q], V(X))$

$$\left[p_q, V\right]_- = \left[p_q, V\right]_- \tag{18}$$

by applying this equation to the test function $G(X)$ we get

> $(lhs = ApplyProductsOfDifferentialOperators@rhs)(\mathbf{(18)} \cdot G(X))$

$$\left[p_q, V\right]_- G = -\mathrm{i}\hbar\partial_q(V)\, G \tag{19}$$

> $SubstituteTensor(\mathbf{(8)}, \mathbf{(19)}) \cdot G(X)^{-1}$

$$\left[p_q, V\right]_- = \mathrm{i}\hbar V^3 X_q \tag{20}$$

In the same way, for $[p_q, V^3]_-$ we get

> $(\%Commutator = Commutator)(p[q], V(X)^3)$

$$\left[p_q, V^3\right]_- = \left[p_q, V^3\right]_- \tag{21}$$

> $(lhs = ApplyProductsOfDifferentialOperators@rhs)(\mathbf{(21)} \cdot G(X))$

$$\left[p_q, V^3\right]_- G = -\mathrm{i}\hbar\left(\partial_q(V)\, V^2 + V\partial_q(V)\, V + V^2\partial_q(V)\right) G \tag{22}$$

> $SubstituteTensor(\mathbf{(8)}, \mathbf{(22)}) \cdot G(X)^{-1}$

$$\left[p_q, V^3\right]_- = \mathrm{i}\hbar\left(V^3 X_q V^2 + V^4 X_q V + V^5 X_q\right) \tag{23}$$

> $(lhs = Simplify@rhs)(\mathbf{(23)})$

$$\left[p_q, V^3\right]_- = 3\mathrm{i}\hbar V^5 X_q \tag{24}$$

Adding now these new commutation rules to the setup of the problem, they will be taken into account in subsequent uses of *Simplify*

> **(17)**, **(20)**, **(24)**

$$\left[L_q, V\right]_- = 0, \left[p_q, V\right]_- = \mathrm{i}\hbar V^3 X_q, \left[p_q, V^3\right]_- = 3\mathrm{i}\hbar V^5 X_q \tag{25}$$

> *Setup*(**(25)**)

$$\Big[algebrarules = \Big\{\left[L_j, L_k\right]_- = \mathrm{i}\hbar\epsilon_{jkn}L_n, \left[L_q, V\right]_- = 0, \left[p_j, L_k\right]_- = \mathrm{i}\hbar\epsilon_{jkn}p_n, [p_k, p_l]_- = 0, \left[p_q, V\right]_- = \mathrm{i}\hbar V^3 X_q, \left[p_q, V^3\right]_- = 3\mathrm{i}\hbar V^5 X_q, \left[X_j, L_k\right]_- = \mathrm{i}\hbar\epsilon_{jkn}X_n, [X_k, p_l]_- = \mathrm{i}\hbar g_{kl}, [X_k, V]_- = 0\Big\}\Big] \tag{26}$$

Undo *differentialoperators* to work using two different approaches, with and without them.

> *Setup*(*differentialoperators* = *none*)

$$[differentialoperators = none] \tag{27}$$

## 4. Commutation rules between the Hamiltonian and each of the angular momentum and Runge-Lenz tensors

Departing from the Hamiltonian **(5)** $\equiv H = \frac{p_l^2}{2m_e} - \kappa V$ and the definition of angular momentum **(10)** $\equiv L_q = \epsilon_{mnq}X_m p_n$, by taking their commutator we get

> *Commutator*(**(5)**, **(10)**)

$$\left[H, L_q\right]_- = \frac{-\mathrm{i}\epsilon_{mnq}\hbar\left(-X_m V^3 X_n \kappa m_e + p_l p_n g_{lm}\right)}{m_e} \tag{28}$$

> *Simplify*(**(28)**)

$$\left[H, L_q\right]_- = 0 \tag{29}$$

### *4.1. The commutator between the Hamiltonian and Runge-Lenz tensor: algebraic approach*

Start from the definition of the quantum Runge-Lenz tensor

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

$$Z_k = \frac{\epsilon_{abk}\left(L_a p_b - p_a L_b\right)}{2m_e} + \kappa V X_k \tag{30}$$

This tensor is Hermitian

> **(30)** − *Dagger*(**(30)**)

$$Z_k - Z_k^{\dagger} = \frac{2\kappa V X_k m_e - 2\kappa X_k V m_e + \epsilon_{abk}\left(L_a p_b + L_b p_a - p_a L_b - p_b L_a\right)}{2m_e} \tag{31}$$

> *Simplify*(**(31)**)

$$Z_k - Z_k^{\dagger} = 0 \tag{32}$$

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

> (*%Commutator* = *Commutator*)(*L*[*a*], *p*[*b*])

$$[L_a, p_b]_- = \mathrm{i}\hbar\epsilon_{abn}p_n \tag{33}$$

the expression **(30)** for $Z_k$ can be simplified

> *Simplify*(**(30)**)

$$Z_k = \frac{i\hbar p_k}{m_e} + \kappa V X_k - \frac{\epsilon_{abk} p_a L_b}{m_e} \tag{34}$$

and the angular momentum removed from the the right-hand side using **(10)** $\equiv L_q = \epsilon_{mnq} X_m p_n$, so that $Z_k$ gets expressed entirely in terms of $p_k$, $X$ and $V$

> *Simplify*(*SubstituteTensor*(**(10)**, **(34)**))

$$Z_k = \frac{-i\hbar p_k + \kappa V X_k m_e - X_k {p_m}^2 + X_m p_k p_m}{m_e} \tag{35}$$

Taking the commutator between **(5)** $\equiv H = \frac{{p_l}^2}{2m_e} - \kappa V$, and this expression for $Z_k$ we have the starting point towards showing that $[H, Z_k]_- = 0$

> $\frac{2\,m_e}{\kappa\hbar}$ *Simplify*(*Commutator*(**(5)**, **(35)**))

$$\frac{2m_e\,[H, Z_k]_-}{\kappa\hbar} = \hbar V^3 X_k + \hbar V^5 {X_a}^2 X_k + 2i {X_a}^2 p_k V^3 + 2i V X_a X_k p_a V^2 - 2i X_a X_k p_a V^3 - 2i p_k V \tag{36}$$

In order to use the identities

> **(9)**, $V(X)^2 \cdot$ **(9)**

$$V^3 X_l^2 = V,\; V^5 X_l^2 = V^3 \tag{37}$$

we sort the products using the ordering shown in the left-hand sides

> *SortProducts*(**(36)**, $[V(X)^5, V(X)^3, X[a]^2]$)

$$\frac{2m_e\,[H, Z_k]_-}{\kappa\hbar} = \hbar V^3 X_k - 5\hbar V^5 {X_a}^2 X_k + 2i V^3 {X_a}^2 p_k + 2i V X_a X_k p_a V^2 - 2i X_a X_k p_a V^3 - 2i p_k V \tag{38}$$

> *SubstituteTensor*(**(37)**, **(38)**)

$$\frac{2m_e\,[H, Z_k]_-}{\kappa\hbar} = -4\hbar V^3 X_k + 2i V p_k + 2i V X_a X_k p_a V^2 - 2i X_a X_k p_a V^3 - 2i p_k V \tag{39}$$

> *Simplify*(**(39)**)

$$\frac{2m_e\,[H, Z_k]_-}{\kappa\hbar} = -2\hbar\left(V^3 X_k - V^5 {X_a}^2 X_k\right) \tag{40}$$

> $\frac{\kappa\hbar}{2m_e}$ *SubstituteTensor*(**(37)**, **(40)**)

$$[H, Z_k]_- = 0 \tag{41}$$

And this is the result we wanted to prove.

### 4.2. *The commutator between the Hamiltonian and Runge-Lenz tensor: alternative derivation using differential operators*

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

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

$$[differentialoperators = \{[p_k, [X]]\}] \tag{42}$$

So take the starting point **(36)**

> **(36)**

$$\frac{2m_e\,[H, Z_k]_-}{\kappa\hbar} = \hbar V^3 X_k + \hbar V^5 X_a{}^2 X_k + 2\mathrm{i} X_a{}^2 p_k V^3 + 2\mathrm{i} V X_a X_k p_a V^2 - 2\mathrm{i} X_a X_k p_a V^3 - 2\mathrm{i} p_k V \tag{43}$$

and to show that the right-hand side is equal to 0, multiply by a generic function $G(X)$ followed by transforming the products involving $p_n$ into the application of this differential operator $p_n = -i\hbar\partial_n$

> **(36)** $\cdot\, G(X)$

$$\frac{2m_e\,[H, Z_k]_-\,G}{\kappa\hbar} = \left(\hbar V^3 X_k + \hbar V^5 X_a{}^2 X_k + 2\mathrm{i} X_a{}^2 p_k V^3 + 2\mathrm{i} V X_a X_k p_a V^2 - 2\mathrm{i} X_a X_k p_a V^3 - 2\mathrm{i} p_k V\right) G \tag{44}$$

> *ApplyProductsOfDifferentialOperators*(**(44)**)

$$\begin{aligned}\frac{2m_e\,[H, Z_k]_-\,G}{\kappa\hbar} = {} & -2\hbar X_a X_k \left(\left(\partial_a(V)\, V^2 + V\partial_a(V)\, V + V^2\partial_a(V)\right) G + V^3\partial_a(G)\right) - 2\hbar V\partial_k(G) \\ & - 2\hbar\partial_k(V)\, G + 2\hbar X_a{}^2 \left(\left(\partial_k(V)\, V^2 + V\partial_k(V)\, V + V^2\partial_k(V)\right) G + V^3\partial_k(G)\right) \\ & + 2\hbar V X_a X_k \left((\partial_a(V)\, V + V\partial_a(V))\, G + V^2\partial_a(G)\right) + \hbar V^3 X_k G + \hbar V^5 X_a{}^2 X_k G\end{aligned} \tag{45}$$

> $\frac{1}{\hbar}$ *Simplify*(**(45)**)

$$\begin{aligned}\frac{2m_e\,[H, Z_k]_-\,G}{\hbar^2\kappa} = {} & 2 V X_a{}^2 \partial_k(V)\, G V + 2 V^2 X_a{}^2 \partial_k(V)\, G + G V^5 X_a{}^2 X_k + 2 V^3 X_a{}^2 \partial_k(G) \\ & - 2 V\partial_k(G) - 2\partial_k(V)\, G + G V^3 X_k + 2 X_a{}^2 \partial_k(V)\, G V^2 - 2 X_a X_k \partial_a(V)\, G V^2\end{aligned} \tag{46}$$

In addition, consider the application of $p_l$ to the test function $G(X)$

> $p[l]\, G(X)$

$$p_l G \tag{47}$$

> **(47)** = *ApplyProductsOfDifferentialOperators*(**(47)**)

$$p_l G = -\mathrm{i}\hbar\partial_l(G) \tag{48}$$

> *isolate*(**(48)**, $\partial_l(G(X))$)

$$\partial_l(G) = \frac{\mathrm{i} p_l G}{\hbar} \tag{49}$$

Using this identity **(49)** together with the derived identity **(8)**, followed by multiplying by $G(X)^{-1}$ to remove the test function from the equation, we get

> *Simplify*(*SubstituteTensor*(**(8)**, **(49)**, **(46)**) $\cdot\, G(X)^{-1}$)

$$\frac{2m_e\,[H, Z_k]_-}{\hbar^2\kappa} = -3 V^5 X_a{}^2 X_k + \frac{2\mathrm{i} V^3 X_a{}^2 p_k}{\hbar} - \frac{2\mathrm{i} V p_k}{\hbar} + 3 V^3 X_k \tag{50}$$

Applying **(37)** $\equiv V^3 X_l{}^2 = V,\ V^5 X_l{}^2 = V^3$

> $\frac{\hbar^2\kappa}{2m_e}$ *SubstituteTensor*(**(37)**, **(50)**)

$$[H, Z_k]_- = 0 \tag{51}$$

Add to the setup these derived commutation rules between the Hamiltonian, angular momentum and Runge-Lenz tensors

> **(29)**, **(51)**

$$\left[H, L_q\right]_- = 0,\ [H, Z_k]_- = 0 \tag{52}$$

> $Setup((\mathbf{52}))$

$$\left[algebrarules = \left\{\left[H, L_q\right]_- = 0, [H, Z_k]_- = 0, \left[L_j, L_k\right]_- = \mathrm{i}\hbar\epsilon_{jkn}L_n, \left[L_q, V\right]_- = 0, \left[p_j, L_k\right]_- = \mathrm{i}\hbar\epsilon_{jkn}p_n, [p_k, p_l]_- = 0, \left[p_q, V\right]_- = \mathrm{i}\hbar V^3 X_q, \left[p_q, V^3\right]_- = 3\mathrm{i}\hbar V^5 X_q, \left[X_j, L_k\right]_- = \mathrm{i}\hbar\epsilon_{jkn}X_n, [X_k, p_l]_- = \mathrm{i}\hbar g_{kl}, [X_k, V]_- = 0\right\}\right] \tag{53}$$

Reset *differentialoperators* in order to proceed to the next section working without them

> $Setup(differentialoperators = none)$

$$[differentialoperators = none] \tag{54}$$

## 5. Commutation rules between the angular momentum and the Runge-Lenz tensors

Departing from the definition of these tensors, introduced in the previous sections

> $(\mathbf{10})$; $(\mathbf{35})$

$$L_q = \epsilon_{mnq}X_m p_n$$

$$Z_k = \frac{-\mathrm{i}\hbar p_k + \kappa V X_k m_e - X_k {p_m}^2 + X_m p_k p_m}{m_e} \tag{55}$$

the left-hand side of the identity to be proved is the left-hand side of the commutator of these two equations

> $m_e\, Commutator((\mathbf{10}), (\mathbf{35}))$

$$m_e \left[L_q, Z_k\right]_- = \epsilon_{mnq}\hbar\Big(\mathrm{i}X_m\left(-g_{kn}V + V^3 X_n X_k\right)\kappa m_e + \hbar g_{km}p_n - 2\mathrm{i}X_k p_a p_n g_{am} - \mathrm{i}X_m p_k p_a g_{an} + \mathrm{i}X_m {p_a}^2 g_{kn} + \mathrm{i}X_a\left(g_{am}p_k + g_{km}p_a\right)p_n\Big) \tag{56}$$

> $Simplify((\mathbf{56}))$

$$m_e\left[L_q, Z_k\right]_- = -\hbar\left(\mathrm{i}VX_a\kappa m_e + \hbar p_a - \mathrm{i}X_a {p_m}^2 + \mathrm{i}X_m p_a p_m\right)\epsilon_{akq} \tag{57}$$

By eye, the right-hand side of **(57)** is similar to the right-hand side of the definition of $Z_k$ in **(55)**, so introduce this definition directly into the right-hand side of **(57)**. For that purpose, isolate $X_k {p_m}^2$

> $isolate((\mathbf{55}), X[k]\cdot p[m]^2)$

$$X_k {p_m}^2 = -Z_k m_e - \mathrm{i}\hbar p_k + \kappa V X_k m_e + X_m p_k p_m \tag{58}$$

> $SubstituteTensor((\mathbf{58}), (\mathbf{57}))$

$$m_e\left[L_q, Z_k\right]_- = \mathrm{i}\hbar\left(-Z_a m_e + X_b p_a p_b - X_m p_a p_m\right)\epsilon_{akq} \tag{59}$$

Simplifying, we get the desired result, and we substitute the *active* by the *inert* form of *Commutator* for posterior use of this formula without having the *Commutator* automatically executed.

> $Simplify((\mathbf{59}))$

$$m_e\left[L_q, Z_k\right]_- = -\mathrm{i}\hbar Z_a m_e \epsilon_{akq} \tag{60}$$

> $\dfrac{1}{m_e}\, subs(Commutator = \%Commutator, (\mathbf{60}))$

$$\left[L_q, Z_k\right]_- = -\mathrm{i}\hbar\epsilon_{akq}Z_a \tag{61}$$

Set now this algebra rule to be available to the system when convenient

> $Setup((\mathbf{61}))$

$$\left[algebrarules = \left\{\left[H, L_q\right]_- = 0, [H, Z_k]_- = 0, \left[L_j, L_k\right]_- = \mathrm{i}\hbar\epsilon_{jkn}L_n, \left[L_q, Z_k\right]_- = -\mathrm{i}\hbar\epsilon_{akq}Z_a, \left[L_q, V\right]_- = 0, \left[p_j, L_k\right]_- = \mathrm{i}\hbar\epsilon_{jkn}p_n, [p_k, p_l]_- = 0, \left[p_q, V\right]_- = \mathrm{i}\hbar V^3 X_q, \left[p_q, V^3\right]_- = 3\mathrm{i}\hbar V^5 X_q, \left[X_j, L_k\right]_- = \mathrm{i}\hbar\epsilon_{jkn}X_n, [X_k, p_l]_- = \mathrm{i}\hbar g_{kl}, [X_k, V]_- = 0\right\}\right] \tag{62}$$

### *5.1. The scalar product between the quantized angular momentum and the Runge-Lenz tensors*

Classically, the orbital momentum is perpendicular to the elliptic plane of motion, while the Runge-Lenz vector lies in that plane, so that $\vec{L}_{Classical} \cdot \vec{Z}_{Classical} = 0$. In quantum mechanics, from **(61)** $\equiv [L_q, Z_k]_- \neq 0$ but $\vec{L} \cdot \vec{Z} = \vec{Z} \cdot \vec{L} = 0$ still holds. To verify that, take the definition **(30)** of the quantum Runge-Lenz vector and multiply it by $L_k$

> **(30)** . $L[k]$

$$L_k Z_k = \frac{\epsilon_{abk} (L_a p_b L_k - p_a L_b L_k)}{2 m_e} + \kappa V X_k L_k \tag{63}$$

> *Simplify*(**(63)**)

$$L_k Z_k = \kappa L_a V X_a \tag{64}$$

Using **(10)** $\equiv L_q = \epsilon_{mnq} X_m p_n$,

> *lhs*(**(64)**) = *SubstituteTensor*(**(10)**, *rhs*(**(64)**))

$$L_k Z_k = \kappa \epsilon_{amn} X_m p_n V X_a \tag{65}$$

> *Simplify*(**(65)**)

$$L_k Z_k = 0 \tag{66}$$

and due to **(61)** $\equiv [L_q, Z_k]_- = -\hbar \mathrm{i} Z_a \epsilon_{akq}$, reversing the order in the product,

> *SortProducts*(**(66)**, $[Z[k], L[k]]$)

$$Z_k L_k = 0 \tag{67}$$

## 6. Commutation rules between the components of the Runge-Lenz tensor

Here again the starting point is **(35)**, the definition of the quantum Runge-Lenz tensor

> *SubstituteTensorIndices*($k = q$, **(35)**)

$$Z_q = \frac{-\mathrm{i}\hbar p_q + \kappa V X_q m_e + X_m p_q p_m - X_q {p_m}^2}{m_e} \tag{68}$$

The commutator $[Z_k, Z_q]_-$is computed via

> $m_e^2$ (*lhs* = *Expand*@*rhs*)(*Commutator*(**(35)**, **(68)**))

$$\begin{aligned} m_e^2 \left[Z_k, Z_q\right]_- = \hbar \Big( & -\left(g_{ak} p_a p_q - g_{mq} p_k p_m - g_{kq} ({p_a}^2 - {p_m}^2)\right) \hbar + \mathrm{i} g_{mq} X_m {p_a}^2 p_k + \mathrm{i} g_{am} X_a p_k p_m p_q + \mathrm{i} g_{kq} X_m {p_a}^2 p_m + \mathrm{i} g_{mq} X_a p_a p_k p_m \\ & - \mathrm{i} g_{ak} X_m p_a p_m p_q - \mathrm{i} g_{am} X_m p_a p_k p_q - 2\mathrm{i} g_{am} X_q p_a p_k p_m - 2\mathrm{i} g_{mq} X_k {p_a}^2 p_m + 2\mathrm{i} g_{ak} X_q {p_m}^2 p_a - \mathrm{i} g_{ak} X_a {p_m}^2 p_q \\ & - \mathrm{i} g_{kq} X_a {p_m}^2 p_a + 2\mathrm{i} g_{am} X_k p_a p_m p_q + \mathrm{i} V^3 X_k X_m X_q p_m \kappa m_e + 3\hbar V^5 {X_a}^2 X_k X_q \kappa m_e - 3\hbar V^5 {X_m}^2 X_k X_q \kappa m_e \\ & - 2\mathrm{i} X_k p_m V^3 X_m X_q \kappa m_e - \mathrm{i} X_a p_q V^3 X_a X_k \kappa m_e - \mathrm{i} V^3 X_a X_q p_a X_k \kappa m_e + 2\mathrm{i} X_q p_a V^3 X_a X_k \kappa m_e + \mathrm{i} X_m p_k V^3 X_m X_q \kappa m_e \\ & + 2\mathrm{i} V X_k p_m \kappa m_e g_{mq} - \mathrm{i} X_m p_k V \kappa m_e g_{mq} - \mathrm{i} V X_m p_m \kappa m_e g_{kq} - 2\mathrm{i} V X_q p_a \kappa m_e g_{ak} + \mathrm{i} V X_a p_q \kappa m_e g_{ak} + \mathrm{i} V X_a p_a \kappa m_e g_{kq} \Big) \end{aligned} \tag{69}$$

> $\frac{\mathrm{i}}{\hbar}$ *Simplify*(**(69)**)

$$\begin{aligned} \frac{\mathrm{i} m_e^2 \left[Z_k, Z_q\right]_-}{\hbar} = & -{X_a}^2 X_q p_k V^3 \kappa m_e + {X_a}^2 X_k p_q V^3 \kappa m_e - 3 X_k p_q V \kappa m_e + 3 X_q p_k V \kappa m_e \\ & - X_m {p_a}^2 p_m g_{kq} + X_a {p_m}^2 p_a g_{kq} + X_k {p_a}^2 p_q - X_q {p_a}^2 p_k \end{aligned} \tag{70}$$

In order to use **(9)** $\equiv V^3 {X_l}^2 = V$, sort the products in **(70)** using the ordering $V^3 {X_a}^2$

> *Normal*(*SortProducts*(**(70)**, $[V(X)^3, X[a]^2]$))

$$\frac{\mathrm{i}m_e^2\left[Z_k,Z_q\right]_-}{\hbar}=V^3X_a{}^2X_kp_q\kappa m_e-V^3X_a{}^2X_qp_k\kappa m_e-3X_kp_qV\kappa m_e+3X_qp_kV\kappa m_e-X_mp_a{}^2p_mg_{kq}+X_ap_m{}^2p_ag_{kq}+X_kp_a{}^2p_q-X_qp_a{}^2p_k \tag{71}$$

> *SubstituteTensor*((**9**), (**71**))

$$\frac{\mathrm{i}m_e^2\left[Z_k,Z_q\right]_-}{\hbar}=VX_kp_q\kappa m_e-\kappa m_eVX_qp_k-3X_kp_qV\kappa m_e+3X_qp_kV\kappa m_e-X_mp_a{}^2p_mg_{kq}+X_ap_m{}^2p_ag_{kq}+X_kp_a{}^2p_q-X_qp_a{}^2p_k \tag{72}$$

Regarding the term quadratic in the momentum, from the expression for the Hamiltonian (**5**) $\equiv H=\frac{p_l{}^2}{2m_e}-\kappa V$,
> *isolate*((**5**), $p[l]^2$)

$$p_l{}^2=2\left(\kappa V+H\right)m_e \tag{73}$$

In order to use this equation (**73**) to substitute $p_l{}^2$ into the expression (**72**) for $[Z_k,Z_q]_-$ and *not* receive noncommutative products with $H$ in between the position $X_k$ and momentum $p_q$operators (that would require further using, afterwards, of the commutator between $H$and $p_q$) , sort first the products in (**72**) positioning all square of momentums $p^2$ to the right of occurrences of $p$
> *SortProducts*((**72**), $[p[a],p[k],p[m],p[q],p[a]^2,p[m]^2]$)

$$\frac{\mathrm{i}m_e^2\left[Z_k,Z_q\right]_-}{\hbar}=VX_kp_q\kappa m_e-\kappa m_eVX_qp_k-3X_kp_qV\kappa m_e+3X_qp_kV\kappa m_e-X_mp_mp_a{}^2g_{kq}+X_ap_ap_m{}^2g_{kq}+X_kp_qp_a{}^2-X_qp_kp_a{}^2 \tag{74}$$

> *SubstituteTensor*((**73**), (**74**))

$$\frac{\mathrm{i}m_e^2\left[Z_k,Z_q\right]_-}{\hbar}=VX_kp_q\kappa m_e-\kappa m_eVX_qp_k-3X_kp_qV\kappa m_e+3X_qp_kV\kappa m_e-X_mp_m2\left(\kappa V+H\right)m_eg_{kq}+X_ap_a2\left(\kappa V+H\right)m_eg_{kq}+X_kp_q2\left(\kappa V+H\right)m_e-X_qp_k2\left(\kappa V+H\right)m_e \tag{75}$$

> $\frac{\hbar}{\mathrm{i}\,m_e^2}$ *Simplify*((**75**))

$$\left[Z_k,Z_q\right]_-=\frac{2\mathrm{i}\hbar\left(-X_kp_qH+X_qp_kH\right)}{m_e} \tag{76}$$

Finally, from the definition of the angular momentum (**10**) $\equiv L_q=\epsilon_{mnq}X_mp_n$, multiplying by $\epsilon_{abc}$ we can construct an expression for $X_ap_bH-X_bp_aH$ in terms of $L_q$
> *LeviCivita*$[a,b,q]\cdot$ (**10**)

$$\epsilon_{abq}L_q=\epsilon_{abq}\epsilon_{mnq}X_mp_n \tag{77}$$

> *Simplify*((*rhs* = *lhs*)((**77**)))

$$X_ap_b-X_bp_a=\epsilon_{abq}L_q \tag{78}$$

> *Expand*((**78**) $\cdot$ *H*)

$$X_ap_bH-X_bp_aH=\epsilon_{abq}HL_q \tag{79}$$

> *SubstituteTensor*((**79**), (**76**))

$$\left[Z_k,Z_q\right]_-=\frac{-2\mathrm{i}\hbar\epsilon_{ckq}HL_c}{m_e} \tag{80}$$

Which is the identity we wanted to prove.

### 6.1. *Alternative derivation using differential operators*

Set again the *differentialoperator* representation for the momentum operator $p_k$

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

$$[differentialoperators = \{[p_k, [X]]\}] \tag{81}$$

and apply the expression **(69)** for $[Z_k, Z_q]_-$to the test function $G(X)$

> $ApplyProductsOfDifferentialOperators(\mathbf{(69)} \cdot G(X))$

$$\begin{aligned} m_e^2 \left[Z_k, Z_q\right]_- G = \hbar \Big(&-\kappa m_e \hbar X_a \left(\left(\partial_q(V)\, V^2 + V \partial_q(V)\, V + V^2 \partial_q(V)\right) X_a X_k G + g_{aq} V^3 X_k G + g_{kq} V^3 X_a G + V^3 X_a X_k \partial_q(G)\right) \\ &- \kappa m_e \hbar V^3 X_a X_q \left(g_{ak} G + X_k \partial_a(G)\right) \\ &+ 2\kappa m_e \hbar X_q \left(\left(\partial_a(V)\, V^2 + V \partial_a(V)\, V + V^2 \partial_a(V)\right) X_a X_k G + 4 V^3 X_k G + V^3 X_a X_k \partial_a(G)\right) \\ &+ \kappa m_e \hbar X_m \left(\left(\partial_k(V)\, V^2 + V \partial_k(V)\, V + V^2 \partial_k(V)\right) X_m X_q G + g_{km} V^3 X_q G + g_{kq} V^3 X_m G + V^3 X_m X_q \partial_k(G)\right) \\ &+ \kappa m_e \hbar V^3 X_k X_m X_q \partial_m(G) \\ &- 2\kappa m_e \hbar X_k \left(\left(\partial_m(V)\, V^2 + V \partial_m(V)\, V + V^2 \partial_m(V)\right) X_m X_q G + 4 V^3 X_q G + V^3 X_m X_q \partial_m(G)\right) \\ &- g_{kq} \hbar^3 X_m \partial_m(\square(G)) - \hbar^3 g_{mq} X_a \partial_a(\partial_k(\partial_m(G))) + g_{kq} \hbar^3 X_a \partial_a(\square(G)) - 2\hbar^3 g_{am} X_k \partial_a\left(\partial_m\left(\partial_q(G)\right)\right) \\ &+ 2\hbar^3 g_{mq} X_k \partial_m(\square(G)) + \hbar^3 g_{ak} X_a \partial_q(\square(G)) + \hbar^3 g_{ak} X_m \partial_a\left(\partial_m\left(\partial_q(G)\right)\right) + \hbar^3 g_{am} X_m \partial_a\left(\partial_k\left(\partial_q(G)\right)\right) \\ &- 2\hbar^3 g_{ak} X_q \partial_a(\square(G)) - \hbar^3 g_{am} X_a \partial_k\left(\partial_m\left(\partial_q(G)\right)\right) - g_{mq} \hbar^3 \partial_k(\partial_m(G)) + g_{ak} \hbar^3 \partial_a\left(\partial_q(G)\right) \\ &- \hbar^3 g_{mq} X_m \partial_k(\square(G)) + 2\hbar^3 g_{am} X_q \partial_a(\partial_k(\partial_m(G))) + -3\hbar V^5 X_m{}^2 X_k X_q \kappa m_e G + 3\hbar V^5 X_a{}^2 X_k X_q \kappa m_e G \\ &+ \kappa m_e g_{ak} \hbar V X_a \partial_q(G) + \kappa m_e g_{kq} \hbar V X_a \partial_a(G) + 2\kappa m_e g_{mq} \hbar V X_k \partial_m(G) - 2\kappa m_e g_{ak} \hbar V X_q \partial_a(G) \\ &- \kappa m_e g_{mq} \hbar X_m \left(\partial_k(V)\, G + V \partial_k(G)\right) - \kappa m_e g_{kq} \hbar V X_m \partial_m(G)\Big) \end{aligned} \tag{82}$$

> $\dfrac{1}{3\,\hbar^2}\, Simplify(\mathbf{(82)})$

$$\begin{aligned} \frac{m_e^2 \left[Z_k, Z_q\right]_- G}{3\hbar^2} = &\frac{\kappa m_e V X_d \partial_k(V)\, G V X_q X_d}{3} - \frac{\kappa m_e V X_d \partial_q(V)\, G V X_k X_d}{3} - \frac{2\kappa m_e V X_k \partial_d(V)\, G V X_q X_d}{3} \\ &+ \frac{2\kappa m_e V X_q \partial_d(V)\, G V X_k X_d}{3} + \frac{\kappa m_e V^2 X_d \partial_k(V)\, G X_q X_d}{3} - \frac{\kappa m_e V^2 X_d \partial_q(V)\, G X_k X_d}{3} \\ &- \frac{2\kappa m_e V^2 X_k \partial_d(V)\, G X_q X_d}{3} + \frac{2\kappa m_e V^2 X_q \partial_d(V)\, G X_k X_d}{3} + \frac{\kappa m_e X_d \partial_k(V)\, G V^2 X_q X_d}{3} \\ &- \frac{\kappa m_e X_d \partial_q(V)\, G V^2 X_k X_d}{3} - \frac{2\kappa m_e X_k \partial_d(V)\, G V^2 X_q X_d}{3} + \frac{2\kappa m_e X_q \partial_d(V)\, G V^2 X_k X_d}{3} \\ &- \frac{\kappa m_e V^3 X_d{}^2 X_k \partial_q(G)}{3} + \frac{\kappa m_e V^3 X_d{}^2 X_q \partial_k(G)}{3} - \frac{\kappa m_e G V^3 X_k X_q}{3} + \frac{\hbar^2 X_k \partial_q(\square(G))}{3} \\ &- \frac{\hbar^2 X_q \partial_k(\square(G))}{3} + m_e \left(V X_k \partial_q(G) - V X_q \partial_k(G) - \frac{X_q \partial_k(V)\, G}{3}\right) \kappa \end{aligned} \tag{83}$$

Recalling **(8)** $\equiv \partial_n(V) = -V^3 X_n$ and **(49)** $\equiv \partial_l(G) = \frac{\mathrm{i}}{\hbar} p_l G$

> $3\,\hbar\, Simplify(SubstituteTensor(\mathbf{(8)}, \mathbf{(49)}, \mathbf{(83)}))$

$$\frac{m_e^2 \left[Z_k, Z_q\right]_- G}{\hbar} = -\mathrm{i}\kappa m_e V^3 X_d{}^2 X_k p_q G + \mathrm{i}\kappa m_e V^3 X_d{}^2 X_q p_k G + \hbar^3 X_k \partial_q(\square(G)) - \hbar^3 X_q \partial_k(\square(G)) + 3\mathrm{i} m_e \kappa \left(V X_k p_q G - V X_q p_k G\right) \tag{84}$$

Evaluating the term $\partial_q(\square(G(X)))$

> $p[a]\, p[l]^2 \cdot G(X)$

$$p_l{}^2 p_a G \tag{85}$$

> (85) = *ApplyProductsOfDifferentialOperators*((85))

$$p_l{}^2 p_a G = \mathrm{i}\hbar^3 \partial_a(\square(G)) \tag{86}$$

> *isolate*((86), $\partial_a(\square(G(X)))$)

$$\partial_a(\square(G)) = \frac{-\mathrm{i} p_l{}^2 p_a G}{\hbar^3} \tag{87}$$

Inserting this result into the expression **(84)** for $[Z_k, Z_q]_-$and removing the test function multiplying by $G(X)^{-1}$
> *Simplify*(*SubstituteTensor*((87), (84)) $\cdot\, G(X)^{-1}$)

$$\frac{m_e^2 \left[Z_k, Z_q\right]_-}{\hbar} = \mathrm{i}\kappa m_e V^3 X_d{}^2 X_q p_k + \mathrm{i}\left(3 V X_k p_q \kappa m_e - 3\kappa m_e V X_q p_k - \kappa m_e V^3 X_d{}^2 X_k p_q - X_k p_d{}^2 p_q + X_q p_d{}^2 p_k\right) \tag{88}$$

This expression can be factored
> *Factor*((88))

$$\frac{m_e^2 \left[Z_k, Z_q\right]_-}{\hbar} = -\mathrm{i}\left(-3 V \kappa m_e + p_d{}^2 + \kappa m_e V^3 X_d{}^2\right)\left(-X_q p_k + X_k p_q\right) \tag{89}$$

Using the identity **(9)** $\equiv V^3 X_l{}^2 = V$for the potential
> $\frac{\hbar}{m_e^2}$ *SubstituteTensor*((9), (89))

$$\left[Z_k, Z_q\right]_- = \frac{-\mathrm{i}\hbar\left(-2 V \kappa m_e + p_d{}^2\right)\left(-X_q p_k + X_k p_q\right)}{m_e^2} \tag{90}$$

Next using
> (73), (78)

$$p_l{}^2 = 2\left(\kappa V + H\right) m_e, X_a p_b - X_b p_a = \epsilon_{abq} L_q \tag{91}$$

> *SubstituteTensor*((91), (90))

$$\left[Z_k, Z_q\right]_- = \frac{-2\mathrm{i}\hbar \epsilon_{ckq} H L_c}{m_e} \tag{92}$$

> *evalb*((80) − (92))

$$true \tag{93}$$

Which is the expected result. Set now differential operators to *none*.
> *Setup*(*differentialoperators* = *none*)

$$[differentialoperators = none] \tag{94}$$

## 7. The square of the norm of the Runge-Lenz vector

Taking the square of the definition of $Z_k$ and simplifying

> $(\mathbf{30})^2$

$$Z_k^{\,2} = \left(\frac{\epsilon_{abk}\,(L_a p_b - p_a L_b)}{2 m_e} + \kappa V X_k\right)\left(\frac{\epsilon_{cdk}\,(L_c p_d - p_c L_d)}{2 m_e} + \kappa V X_k\right) \tag{95}$$

> $2 m_e^2\, Simplify((\mathbf{95}))$

$$2 m_e^2 Z_k^{\,2} = 2\kappa\hbar^2 V^3 X_a^{\,2} m_e - 6\kappa\hbar^2 V m_e + 2\kappa^2 V^2 X_a^{\,2} m_e^2 - 4\epsilon_{abc} X_a p_b L_c V \kappa m_e - p_a p_b L_b L_a + 2 p_a^{\,2} L_b^{\,2} - p_a L_b L_a p_b \tag{96}$$

Using the algebraic properties of the potential

> $(\mathbf{9}),\ V(X)^{-1}\cdot(\mathbf{9})$

$$V^3 X_l^{\,2} = V,\ V^2 X_l^{\,2} = 1 \tag{97}$$

the expression **(96)** for $Z_k^{\,2}$ becomes

> $SubstituteTensor((\mathbf{97}), (\mathbf{96}))$

$$2 m_e^2 Z_k^{\,2} = -4\kappa\hbar^2 V m_e + 2\kappa^2 m_e^2 - 4\epsilon_{abc} X_a p_b L_c V \kappa m_e - p_a p_b L_b L_a + 2 p_a^{\,2} L_b^{\,2} - p_a L_b L_a p_b \tag{98}$$

The term having $\epsilon_{abc}$ can be simplified using the expression of the momentum operator

> $(rhs = lhs)((\mathbf{10}))$

$$\epsilon_{mnq} X_m p_n = L_q \tag{99}$$

> $(\mathbf{99})\cdot L[q]\cdot V(X)$

$$\epsilon_{mnq} X_m p_n L_q V = L_q^{\,2} V \tag{100}$$

> $SubstituteTensor((\mathbf{100}), (\mathbf{98}))$

$$2 m_e^2 Z_k^{\,2} = -4\kappa\hbar^2 V m_e + 2\kappa^2 m_e^2 - 4 L_c^{\,2} V \kappa m_e - p_a p_b L_b L_a + 2 p_a^{\,2} L_b^{\,2} - p_a L_b L_a p_b \tag{101}$$

Reordering **(101)** to have the two terms with four operators sorted as $p_a p_b L_a L_b$

> $Simplify(SortProducts((\mathbf{101}), [p[a], p[b], L[a], L[b]]))$

$$2 m_e^2 Z_k^{\,2} = -4\kappa\hbar^2 V m_e + 2\kappa^2 m_e^2 - 4 L_a^{\,2} V \kappa m_e - 2 p_a p_b L_a L_b + 2 p_a^{\,2} L_b^{\,2} + 2\hbar^2 p_a^{\,2} \tag{102}$$

Considering now the resulting single term $p_a p_b L_a L_b$, it can be shown it is equal to zero using the definition **(10)** $\equiv L_q = \epsilon_{mnq} X_m p_n$

> $p[a]\, p[b]\, L[a]\, L[b]$

$$p_a p_b L_a L_b \tag{103}$$

> $(\mathbf{103}) = SubstituteTensor((\mathbf{10}), (\mathbf{103}))$

$$p_a p_b L_a L_b = \epsilon_{amn}\epsilon_{bef} p_a p_b X_m p_n X_e p_f \tag{104}$$

> $Simplify((\mathbf{104}))$

$$p_a p_b L_a L_b = 0 \tag{105}$$

Taking this result into account, we have, for $Z_k^{\,2}$

> $subs((\mathbf{105}), (\mathbf{102}))$

$$2 m_e^2 Z_k^{\,2} = -4\kappa\hbar^2 V m_e + 2\kappa^2 m_e^2 - 4 L_a^{\,2} V \kappa m_e + 2 p_a^{\,2} L_b^{\,2} + 2\hbar^2 p_a^{\,2} \tag{106}$$

Substituting now **(73)** $\equiv p_l{}^2 = 2(\kappa V + H)m_e$
> $\frac{1}{2\,m_e^2}$ *SubstituteTensor*(**(73)**, **(106)**)

$$Z_k{}^2 = \frac{2\hbar^2 H m_e + \kappa^2 m_e^2 - 2L_a{}^2 V \kappa m_e + 2\,(\kappa V + H)\,m_e L_b{}^2}{m_e^2} \tag{107}$$

Equalizing the repeated indices, the right-hand side can be factored
> $(lhs = Factor@rhs)(EqualizeRepeatedIndices(\mathbf{(107)}) - \kappa^2) + \kappa^2$

$$Z_k{}^2 = \frac{2H\left(\hbar^2 + L_a{}^2\right)}{m_e} + \kappa^2 \tag{108}$$

Which is the result we wanted to demonstrate.

## 8. The atomic hydrogen spectrum

We now have all the algebra to reconstruct the hydrogen spectrum. Following the literature, this approach is limited to the bound states for which the energy is negative. Assuming an eigenstate of $H$ with negative eigenvalue $E$, we replace the Hamiltonian $H$ by $E$, and look for the possible values of $E$. Another way to state the same thing is that the analysis is restricted to the subspace of energy $E$. The operator $M_n = \sqrt{-\frac{m_e}{2E}}\,Z_n$, is introduced as mentioned in Sec.1. The operators $J$ and $K$, to be used soon after, are added to the formulation of the problem
> $Setup(hermitianoperators = \{M, J, K\})$

$$[hermitianoperators = \{H, J, K, L, M, V, p, x, y, z\}] \tag{109}$$

> $Define(M[n], J[n], K[n], quiet)$

$$\{\gamma_a, J_n, K_n, L_k, M_n, \sigma_a, Z_k, \partial_a, g_{ab}, p_k, \epsilon_{abc}, X_a\} \tag{110}$$

The domain for $m_e$ and $E$ is set via
> $Assume(m_e > 0, E < 0)$

$$\{E :: (-\infty, 0)\}, \{m_e :: (0, \infty)\} \tag{111}$$

from where
> $M[n] = \sqrt{-\frac{m_e}{2E}}Z[n]$

$$M_n = \frac{\sqrt{-\frac{2m_e}{E}}\,Z_n}{2} \tag{112}$$

> $simplify(isolate(\mathbf{(112)}, Z[n]))$

$$Z_n = \frac{M_n\sqrt{2}\,\sqrt{-E}}{\sqrt{m_e}} \tag{113}$$

Recalling the commutation rules **(92)** $\equiv [Z_k, Z_q]_- = -\frac{2i\hbar\epsilon_{akq}HL_a}{m_e}$ and **(113)** above with $E$ replacing $H$
> $SubstituteTensor(H = E, \mathbf{(113)}, \mathbf{(92)})$

$$\left[\frac{M_k\sqrt{2}\,\sqrt{-E}}{\sqrt{m_e}}, \frac{M_q\sqrt{2}\,\sqrt{-E}}{\sqrt{m_e}}\right]_- = \frac{-2i\hbar\epsilon_{ckq}EL_c}{m_e} \tag{114}$$

> *Simplify*((**114**))

$$-\frac{2E\left[M_k, M_q\right]_-}{m_e} = \frac{-2\mathrm{i}\hbar\epsilon_{ckq}EL_c}{m_e} \tag{115}$$

Isolating the commutator, the expression (**92**) for $[Z_k, Z_q]_-$appears rewritten in terms of the $M_k$ as
> *isolate*((**115**), *Commutator*($M[k]$, $M[q]$))

$$\left[M_k, M_q\right]_- = \mathrm{i}\hbar\epsilon_{ckq}L_c \tag{116}$$

Likewise, inserting (**113**) $\equiv Z_n = \frac{M_n\sqrt{2}\sqrt{-E}}{\sqrt{m_e}}$ into the expression (**61**) $\equiv [L_q, Z_k]_- = -\hbar\mathrm{i}\epsilon_{akq}Z_a$, we get it rewritten in terms of $L_q, M_k$
> *Simplify*(*SubstituteTensor*((**113**), (**61**)))

$$\frac{\sqrt{2}\sqrt{-E}\left[L_q, M_k\right]_-}{\sqrt{m_e}} = \frac{-\mathrm{i}\hbar\epsilon_{akq}M_a\sqrt{2}\sqrt{-E}}{\sqrt{m_e}} \tag{117}$$

> *isolate*((**117**), *Commutator*($L[q]$, $M[k]$))

$$\left[L_q, M_k\right]_- = -\mathrm{i}\hbar\epsilon_{akq}M_a \tag{118}$$

Add these two newly derived commutators to the setup
> *Setup*((**116**), (**118**))

$$\Big[algebrarules = \Big\{\left[H, L_q\right]_- = 0, [H, Z_k]_- = 0, \left[L_j, L_k\right]_- = \mathrm{i}\hbar\epsilon_{jkn}L_n, \left[L_q, M_k\right]_- = -\mathrm{i}\hbar\epsilon_{akq}M_a, \left[L_q, Z_k\right]_- = -\mathrm{i}\hbar\epsilon_{akq}Z_a,$$
$$\left[L_q, V\right]_- = 0, \left[M_k, M_q\right]_- = \mathrm{i}\hbar\epsilon_{ckq}L_c, \left[p_j, L_k\right]_- = \mathrm{i}\hbar\epsilon_{jkn}p_n, [p_k, p_l]_- = 0, \left[p_q, V\right]_- = \mathrm{i}\hbar V^3X_q, \left[p_q, V^3\right]_- = 3\mathrm{i}\hbar V^5X_q,$$
$$\left[X_j, L_k\right]_- = \mathrm{i}\hbar\epsilon_{jkn}X_n, [X_k, p_l]_- = \mathrm{i}\hbar g_{kl}, [X_k, V]_- = 0\Big\}\Big] \tag{119}$$

These commutators (**118**), (**116**), together with the departing commutator
> (*%Commutator* = *Commutator*)($L[m]$, $L[n]$)

$$[L_m, L_n]_- = \mathrm{i}\hbar\epsilon_{amn}L_a \tag{120}$$

constitute a closed form, the algebra of the SO(4) group, that is, the rotation group in dimension 4.

We now define the two operators $J$ and $K$ as follows
> $J[m] = \frac{1}{2}\cdot(L[m] + M[m])$

$$J_m = \frac{L_m}{2} + \frac{M_m}{2} \tag{121}$$

> $K[m] = \frac{1}{2}\cdot(L[m] - M[m])$

$$K_m = \frac{L_m}{2} - \frac{M_m}{2} \tag{122}$$

Because $M$ and $L$ both commute with $H$ (since $M$ is proportional to $Z$ up-to a commutative factor), it is straightforward to see that $J$ and $K$ also commute with $H$. They are therefore constants of the motion. Additionally, because at this point (see (**119**)) the system already knows about the commutators (**116**) $\equiv [M_k, M_q]_-$ and (**118**) $\equiv [L_q, M_k]_-$, the commutator between the components of $J_m$ results in
> *Commutator*((**121**), *SubstituteTensorIndices*($m = n$, (**121**)))

$$[J_m, J_n]_- = \frac{\mathrm{i}}{4}\left(\left(L_a + 2M_a\right)\epsilon_{amn} + \epsilon_{cmn}L_c\right)\hbar \tag{123}$$

> *Simplify*(**(123)**)

$$[J_m, J_n]_- = \frac{\mathrm{i}}{2}\epsilon_{amn}\hbar\left(L_a + M_a\right) \tag{124}$$

> *SubstituteTensor*((*rhs* = *lhs*)(**(121)**), **(124)**)

$$[J_m, J_n]_- = \mathrm{i}\epsilon_{amn}\hbar J_a \tag{125}$$

In a similar manner
> *Commutator*(**(122)**, *SubstituteTensorIndices*(*m* = *n*, **(122)**))

$$[K_m, K_n]_- = \frac{\mathrm{i}}{4}\left(\left(L_a - 2M_a\right)\epsilon_{amn} + \epsilon_{cmn}L_c\right)\hbar \tag{126}$$

> *Simplify*(**(126)**)

$$[K_m, K_n]_- = \frac{\mathrm{i}}{2}\epsilon_{amn}\hbar\left(L_a - M_a\right) \tag{127}$$

> *SubstituteTensor*((*rhs* = *lhs*)(**(122)**), **(127)**)

$$[K_m, K_n]_- = \mathrm{i}\epsilon_{amn}\hbar K_a \tag{128}$$

Also
> *Commutator*(**(121)**, *subs*(*m* = *n*, **(122)**))

$$[J_m, K_n]_- = \frac{\mathrm{i}}{4}\hbar\left(\epsilon_{amn}L_a - \epsilon_{cmn}L_c\right) \tag{129}$$

> *Simplify*(**(129)**)

$$[J_m, K_n]_- = 0 \tag{130}$$

Both $J$ and $K$ have the symmetry of a rotation operator in two independent 3 dimension spaces. $H$ then has the symmetry of the group $\mathrm{SO}(3) \otimes \mathrm{SO}(3)$. Furthermore, one knows that the possible eigenvalues for the rotation operators $J$ and $K$ are $j(j+1)\hbar^2$ and $k(k+1)\hbar^2$, with $j, k \in \{0, \frac{1}{2}, 1, \frac{3}{2}, 2, ...\}$. Computing now $J^2$
> *Expand*(**(121)**$^2$)

$$J_m^{\ 2} = \frac{L_m^{\ 2}}{4} + \frac{L_m M_m}{2} + \frac{M_m^{\ 2}}{4} \tag{131}$$

Recalling **(66)** $\equiv L_k Z_k = 0$, and considering that $M$ is proportional to $Z$, we have that $L_m M_m = 0$
> *subs*($L[m]\,M[m] = 0$, **(131)**)

$$J_m^{\ 2} = \frac{L_m^{\ 2}}{4} + \frac{M_m^{\ 2}}{4} \tag{132}$$

Likewise, for $K^2$, from **(122)** $\equiv K_m = \frac{L_m}{2} - \frac{M_m}{2}$
> *Expand*(**(122)**$^2$)

$$K_m^{\ 2} = \frac{L_m^{\ 2}}{4} - \frac{L_m M_m}{2} + \frac{M_m^{\ 2}}{4} \tag{133}$$

> *subs*($L[m]\,M[m] = 0$, **(133)**)

$$K_m^{\ 2} = \frac{L_m^{\ 2}}{4} + \frac{M_m^{\ 2}}{4} \tag{134}$$

So that
> **(132)** − **(134)**

$$J_m^2 - K_m^2 = 0 \tag{135}$$

That is, $J_m^2 = K_m^2$, which means they share the same eigenvalues, say $j(j+1)\hbar^2$ for a given eigenstate of $H$ with the considered eigenvalue $E$. Next, inserting **(113)** $\equiv Z_n = \frac{M_n \sqrt{2}\sqrt{-E}}{\sqrt{m_e}}$ into **(108)** $\equiv Z_k^2 = \frac{2H(\hbar^2+L_a^2)}{m_e} + \kappa^2$ we get an expression for $M_k^2$
> *SubstituteTensor*($H = E$, **(113)**, **(108)**)

$$-\frac{2EM_k^2}{m_e} = \frac{2E\left(\hbar^2 + L_a^2\right)}{m_e} + \kappa^2 \tag{136}$$

> $-\frac{m_e}{2E}$ **(136)**

$$M_k^2 = -\frac{2\hbar^2 E + 2EL_a^2 + \kappa^2 m_e}{2E} \tag{137}$$

Substituting this result into **(132)** $\equiv J_m^2 = \frac{L_m^2}{4} + \frac{M_m^2}{4}$ and simplifying we get
> *Simplify*(*SubstituteTensor*(**(137)**, **(132)**))

$$J_m^2 = -\frac{\hbar^2}{4} - \frac{\kappa^2 m_e}{8E} \tag{138}$$

Taking the average value of $J_m^2$ over an eigenvector, $J_m^2$ can be replaced by its eigenvalue $j(j+1)\hbar^2$
> *subs*($J[m]^2 = j\,(j+1)\,\hbar^2$, **(138)**)

$$j\,(j+1)\,\hbar^2 = -\frac{\hbar^2}{4} - \frac{\kappa^2 m_e}{8E} \tag{139}$$

from where the possible values of the energy are
> *isolate*(**(139)**, $E$)

$$E = -\frac{\kappa^2 m_e}{2\hbar^2\,(2j+1)^2} \tag{140}$$

Assuming $n = 2j+1$, a positive integer and $j \in \{0, \frac{1}{2}, 1, \frac{3}{2}, 2, ...\}$,the spectrum for an hydrogen atom is thus
> *subs*($\{2\,j+1 = n, E = E(n)\}$, **(140)**)

$$E(n) = -\frac{\kappa^2 m_e}{2\hbar^2 n^2} \tag{141}$$

Which is the energy spectrum for a spinless hydrogenoid system.

### Conclusions

In this presentation, we derived, step-by-step, the SO(4) symmetry of the hydrogen atom and its spectrum using the computer algebra Maple system. The derivation was performed without departing from the results, entering only the main definition formulas in eqs. **(1)**, **(2)** and **(5)**, followed by using a few simplification commands - mainly *Simplify*, *SortProducts* and *SubstituteTensor* - and a handful of Maple basic commands, *subs*, *lhs*, *rhs* and *isolate*. The computational path that was used to get the results of sections 2 to 8 is not unique. Instead of searching for the shortest path, we prioritized clarity and illustration of the techniques that can be used to work on problems like this one.

This problem is mainly about simplifying expressions using two different techniques. First, expressions with noncommutative operands in products need reduction with respect to the commutator algebra rules that have been set. Second, products of tensorial operators require simplification using the sum rule for repeated indices and the symmetries of tensorial subexpressions. Those techniques, which are part of the Maple Physics simplifier, together with the *SortProducts* and *SubstituteTensor* commands for sorting the operands in products to apply tensorial identities, sufficed. The derivations were performed in a reasonably small number of steps.

Two different computational strategies - with and without differential operators - were used in sections 3 and 5, showing a way to verify results, a relevant issue in general when performing complicated algebraic manipulations. The Maple Physics' ability to handle differential operators as noncommutative operands in products (as frequently done in paper and pencil computations) facilitates readability and ease in entering the computations. The complexity of those operations is then handled by one *Physics:-Library* command, *ApplyProductsOfDifferentialOperators* (see eqs. **(45)** and **(82)**).

It is interesting to note: a) the ability of the system to factor expressions involving products of noncommutative operands (see eqs. **(89)** and **(108)**) and b) the adaptation of the algorithms for simplifying tensorial expressions [6] to the noncommutativity domain, used throughout this presentation.

Also worth mentioning, the use of equation labels can reduce the whole computation to entering the main definitions, followed by applying a few commands to equation labels. That approach helps to reduce the chance of typographical errors to a very strict minimum. Likewise, the fact that commands and equations distribute over each other allows cumbersome manipulations to be performed in simple ways, as done, for instance, in eqs. **(8)**, **(9)** and **(13)**. Additionally , it was helpful to have the display of each intermediate result automatically expressed using standard mathematical physics notation.

Finally, if this work focused on a well-known case, the employed tools can be used to tackle a wide range of hot topics research in the quantum mechanics field, and beyond. To give but a few examples, recently (work in progress - see related Mapleprimes post [7]), we reproduced the calculus performed in [8]. This paper evaluates the constraints of magnetostatic traps for neutral cold atoms and Bose Einstein condensates. Besides, the overall possibilities includes the general framework of periodically driven systems, notably requiring Taylor development to approximate commutators [9]. The calculus could be extended to Lie superalgebra in the field of Anderson localization for disordered media, see [10] and supplemental material. Note that the present calculus are performed using an Euclidean metric. This feature could however easily be extended to any arbitrary metric, openings-up a wide range of possibilities to what can now be done with a computer, replacing pencil and paper.

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## Appendix A. Appendix

In this presentation, the input lines are preceded by a prompt > and the commands used are of three kinds: some basic Maple manipulation commands, the main Physics package commands to set the context of a formulation and simplify expressions, and two commands of the *Physics:-Library* to perform specialized operations in expressions.

### The basic Maple commands used

- *interface* is used once at the beginning to set the letter used to represent the imaginary unit (default is I but we used i).

- *isolate* is used in several places to isolate a variable in an expression, for example isolating $x$ in $ax + b = 0$ results in $x = -\frac{b}{a}$
- *lhs* and *rhs* respectively get the left-hand side $A$and right-hand side $B$of an equation $A = B$
- *subs* substitutes the left-hand side of an equation by the right-hand side in a given target, for example $subs(A = B, A + C)$ results in $B + C$
- @ is used to compose commands. So $(A \circ B)(x)$ is the same as $A(B(x))$. This command is useful to express an abstract combo of manipulations, for example as in **(108)** $\equiv$ ($lhs = Factor \circ rhs$).

### The Physics commands used

- *Setup* is used to set algebra rules as well as the dimension of space, type of metric, and conventions as the kind of letter used to represent indices.
- *Commutator* computes the commutator between two objects using the algebra rules set using *Setup*. If no rules are known to the system, it outputs a representation for the commutator that the system understands.
- *CompactDisplay* is used to avoid redundant display of the functionality of a function.
- The input $d\_[n]$ represents the $\partial_n$ tensorial differential operator.
- *Define* is used to define tensors, with or without specifying its components.
- *Dagger* computes the Hermitian transpose of an expression.
- *Normal, Expand, Factor* respectively normalizes, expands and factorizes expressions that involve products of noncommutative operands.
- *Simplify* performs simplification of tensorial expressions involving products of noncommutative factors taking into account Einstein's sum rule for repeated indices, symmetries of the indices of tensorial subexpressions and custom commutator algebra rules.
- *SortProducts* uses the commutation rules set using *Setup* to sort the non-commutative operands of a product in an indicated ordering.

### The Physics:-Library commands used

- *Library:-ApplyProductsOfDifferentialOperators* applies the differential operators found in a product to the product operands that appear to its right. For example, applying this command to $pV(X)m_e$ results in $m_e \cdot p(V(X))$
- *Library:-EqualizeRepeatedIndices* equalizes the repeated indices in the terms of a sum, so for instance applying this command to ${L_a}^2 + {L_b}^2$ results in $2 \cdot {L_a}^2$

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