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Review

On Invariant Vectors in the Presence of Electric and Magnetic Fields

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Abstract: In this non-exhaustive review, we discuss the importance of invariant vectors in atomic physics, such as the Laplace–Runge–Lenz vector, the Redmond vector in the presence of an electric field, the Landau–Avron–Sivardièrevector when the system is subject to a magnetic field, and the supergeneralized Runge–Lenz vector for the two-center problem. The application to the Stark and Zeeman effects are outlined. The existence of constants of motion in the charge-dyon system is also briefly mentioned.

Keywords: symmetry; invariant vectors; Hermann–Bernoulli–Laplace–Runge–Lenz vector; Redmond invariant; dynamical symmetry; supergeneralized Runge–Lenz vector; Kustaanheimo–Stiefel transformation; charge-dyon system; MIC–Kepler problem

1. Introduction

The subject of invariants in physics, even restricted to the narrower field of atomic physics, is far too broad for any complete survey. The aim of the present article was accordingly rather more limited: attempting to review a a selection of works, starting from the Kepler problem and then considering the cases of electric and magnetic fields.

The German mathematician Noether showed, in 1918, that any invariance in a continuous group of transformations, of spatio-temporal nature or not, with n parameters, implies the existence of n conservation laws [1,2]. As Curie's principle (the symmetries of the causes are to be found in the effects) and Wigner's theorem (specifying how physical symmetries such as rotations, translations, as well as charge, parity, and time-reversal symmetries manifest themselves on the Hilbert space of states), Noether's theorem allows one to exploit the knowledge of the continuous symmetries of a system. Noether showed that, conversely, a conservation law is never accidental, but derives from the existence of a continuous symmetry. It is worth mentioning that the importance of Noether's contribution to science was only recognized around 1960.

In the case of mechanics problems, "dynamical" invariants are revealed, which cannot be associated with any continuous space–time symmetry and are, therefore, linked to the particular analytical properties of the interactions responsible for the motion. The first example of dynamical symmetry was discovered in 1710 by Hermann, who demonstrated [3,4] with the help of Bernoulli [5] that the motion of a mass in a Keplerian potential is characterized by two invariants: the angular momentum, which determines the plane of motion, and a second vector—called today the Laplace–Runge–Lenz vector—which fixes the orientation of the major axis of the elliptical orbit in its plane and whose modulus is proportional to the eccentricity of the orbit. Laplace exploited the existence of this vector [6], which was rediscovered by Hamilton [7], described by Runge in a didactic work [8], and finally, used by Lenz [9] and Pauli [10] to find the quantum properties of the hydrogen atom [11], characterized by a specific degeneracy of the energy levels called Coulomb degeneracy. In 1873, Bertrand showed that the orbit of a particle placed in central potential does not close

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Citation: Pain, J.-C. On Invariant Vectors in the Presence of Electric and Magnetic Fields. *Atoms* **2023**, *11*, 105. https://doi.org/10.3390/atoms11070105

Academic Editor: Alexander V. Demura and James F. Babb

Received: 21 April 2023
Revised: 11 July 2023
Accepted: 18 July 2023
Published: 20 July 2023

on itself, except if the potential is Keplerian or harmonic [12]: in the first case, there is a unique privileged direction in the plane of the orbit, which is precisely that of the Laplace vector; in the second case, there are two privileged directions, which are perpendicular and constitute the proper directions of the invariant tensor. According to Noether's theorem, a dynamical symmetry is associated with the Laplace vector: it is that of the $SO(4)$ group (with six parameters) of rotations in four-dimensional space, obtained by Fock [13] and Bargmann [14]. The symmetry of the isotropic harmonic oscillator in three dimensions was discovered in 1940 by Jauch and Hill [15] and is that of the $SU(3)$ group (with eight parameters) of unitary matrices 3×3 of determinant + 1. More than twenty years later, Redmond found an invariant in the presence of an electric field [16]. It is worth mentioning that there was a more-general finding that the Kepler system and the tri-dimensional harmonic oscillator (*stricto sensu*, the proper terminology would be "parabolic oscillator", "harmonic" applying rather to oscillations, but since this expression is widespread in the literature, we kept it throughout the paper.) with specific rational frequency ratios (1, 2 and 1/2) have common symmetries (which possess the combined Kepler/harmonic oscillator system as well), which are recognized in various fields of physics. In this framework, Alhassid et al. studied the spectrum of hydrogen subject to a certain class of perturbations, including the van der Waals and the diamagnetic interactions, and found a universal adiabatic invariant for this class [17]. Blümel et al. studied chaos for laser-cooled ions in a Paul trap. They discovered that the two-, three-, and four-ion crystals are stable until the Mathieu instability is reached. The authors proposed a simple model of radiofrequency heating, as well as a classification of the ion dynamics into four regimes: the crystal, the quasi-periodic regime, the chaotic regime, and the Mathieu regime [18]. Simonović and Nazmitdinov showed that a magnetic field gives rise to dynamical symmetries of a three-dimensional axially symmetric two-electron quantum dot with a parabolic confinement. The authors pointed out that such symmetries manifest themselves as near-degeneracies in the quantum spectrum at particular values of the magnetic field [19].

There are two main versions of the so-called two-center problem. The first one is the motion of an electron in the field of two stationary Coulomb centers of charges Z and Z' separated by a distance R, which is one of the most-fundamental problems in quantum mechanics. The second one is the motion of a planet in the gravitational field of two stationary stars of generally different masses, which is one of the most-important problems in celestial mechanics. Kryukov and Oks [20,21] derived a supergeneralized Runge–Lenz vector whose projection on the internuclear or interstellar axis is conserved.

A dyon is a hypothetical particle with both electric and magnetic charges. When its electric charge is zero, the particle is usually referred to as a magnetic monopole. Many grand unified theories predict the existence of both magnetic monopoles and dyons. Dyons were first proposed as a phenomenological alternative to quarks [22]. Schwinger extended the Dirac quantization condition [23] to the dyon and predicted the existence of a particle with the properties of the J/ψ meson prior to its discovery in 1974. There is much interest in the problem of bound states of a fermion in the field of a fixed Dirac monopole.

In Section 2, we introduce the Runge–Lenz vector in classical mechanics and discuss the Bertrand theorem. In Section 3, in the framework of the $SO(4)$ rotation group, the quantum mechanical analog to the Lenz vector is obtained and applied to the determination of the energy levels of the hydrogen atom and their degeneracy. In Section 4, the analogy between the Kepler and harmonic potentials is discussed and the Laplace invariant tensor is introduced. The Redmond invariant in the presence of an electric field is introduced in Section 5, and the Kryukov–Oks supergeneralized Runge–Lenz vector for the two-center problem is presented in Section 6. The Landau–Avron–Sivardière approach of the case of a magnetic field is discussed in Section 7, as well as the treatment of the hydrogen atom in crossed electric and magnetic fields. Finally, the dyon–dyon system is briefly evoked in Section 8 in the framework of the McIntosh–Cisneros (MIC)–Kepler problem. The linear Stark effect in the MIC–Kepler problem describing the interaction of charged particles with Dirac's dyon is considered.

2. The Kepler Problem: The Runge–Lenz Vector and Bertrand's Theorem

Let us consider a mass m subject to the (attractive) Kepler potential of a mass M. The reduced mass being $\mu = mM/(m+M)$, the potential reads

$$U(r) = -\frac{\alpha}{r} = -G\frac{Mm}{r} = -G\frac{\mu(m+M)}{r} = -\kappa\frac{\mu}{r}. \tag{1}$$

with $\alpha = \kappa\mu > 0$ and G the Cavendish gravitational constant. One, thus, has $\kappa = G(m+M)$. The potential has spherical symmetry and is independent of time. Therefore, kinetic energy and angular momentum have no explicit time dependence. We also know that, whatever the initial conditions, the orbit is an ellipse for the bound states (negative energy), a parabola for the zero-energy states, and a hyperbola for the positive-energy states.

2.1. The Runge–Lenz, Eccentricity, and Hamilton Vectors

As mentioned in the Introduction, the so-called Runge–Lenz vector was discovered by Hermann, transmitted by Bernoulli, used intensively by Laplace, exhumed by Runge at the beginning of the 20th Century, and used by Lenz and Pauli in quantum mechanics in order to study the hydrogen atom. Although the vector should, therefore, be called the Hermann–Bernoulli–Laplace–Runge–Lenz vector [4,5,24], we will, in the following, for simplicity and because it is the most-common way it is referred to in the literature, retain the denomination "Runge–Lenz" vector. The Runge–Lenz vector reads [25,26]

$$\mathbf{A} = \mathbf{v} \wedge \mathbf{L} - \alpha\frac{\mathbf{r}}{r} = \mathbf{v} \wedge \mathbf{L} - \alpha\mathbf{u}_r, \tag{2}$$

where $\mathbf{v}$ is the velocity of our system (mass m), $\mathbf{L} = \mu\mathbf{r} \wedge \mathbf{v}$ the angular momentum, and $\mathbf{u}_r = \mathbf{r}/r$ the radial unit vector. Throughout the paper, the symbol $\wedge$ denotes the vector product (note that the "cross" symbol is often used to represent the vector product. Since we use the cross symbol as a usual product in some equations or for the direct product of Lie algebras, to avoid confusion, we will use the "wedge" symbol throughout the paper, which corresponds to the French convention. It was introduced by Italian mathematicians Burali-Forti and Marcolongo in 1908 [27]):

$$\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} \wedge \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = \begin{pmatrix} a_2b_3 - a_3b_2 \\ a_3b_1 - a_1b_3 \\ a_1b_2 - a_2b_1 \end{pmatrix}. \tag{3}$$

There are other invariant vectors that are related to the Runge–Lenz vector.

In celestial mechanics, the eccentricity vector of a Kepler orbit [28,29] is the dimensionless vector with the direction pointing from apoapsis to periapsis (respectively, farthest and nearest points in the orbit of a planetary body about its primary body to the center of force) and with a magnitude equal to the orbit's scalar eccentricity. For Kepler orbits, the eccentricity vector is a constant of motion. It is of great interest in the analysis of almost-circular orbits, as perturbing (non-Keplerian) forces on an actual orbit will cause the osculating eccentricity vector to change continuously as opposed to the eccentricity, and the argument of periapsis parameters for which eccentricity zero (circular orbit) corresponds to a singularity. The eccentricity vector is

$$\mathbf{e} = \frac{\mathbf{v} \wedge \mathbf{L}}{\alpha} - \frac{\mathbf{r}}{|\mathbf{r}|}, \tag{4}$$

which follows immediately from the vector identity:

$$\mathbf{v} \wedge (\mathbf{r} \wedge \mathbf{v}) = (\mathbf{v} \cdot \mathbf{v})\mathbf{r} - (\mathbf{r} \cdot \mathbf{v})\mathbf{v}. \tag{5}$$

One has

$$\mathbf{e} = \frac{\mathbf{A}}{\mu\kappa} = \frac{1}{\kappa}(\mathbf{p} \wedge \mathbf{L}) - \mathbf{u}_r, \tag{6}$$

with $\mathbf{p} = \mu\mathbf{v}$. The Runge–Lenz vector $\mathbf{A}$ is directed from the center of force towards the periapsis, making it easy to visualize (Lenz and Pauli called it the "Achsenvektor") [30]. However, its physical dimension (SI units kg m^3 s^{-2}) does not endow it with any familiar meaning; the alternative invariant $\mathbf{A}/m$ is hardly better. If $\mathbf{e}$ is used instead of $\mathbf{A}$ in the derivation of the orbit equation, a simple equation appears, with an immediate physical meaning. This is why it is often considered that $\mathbf{e}$ should be preferred over $\mathbf{A}$ for didactic applications. In the literature, the only "eccentricity-like" vector referred to seems to be the one defined by Hamilton, $\mathbf{L} \wedge \mathbf{A}/L^2$: it is co-linear to $\mathbf{e}$, but has the dimension of a velocity or of a momentum according to the alternative definition of [31]. It does not coincide with a particular value of v or μv and, thus, has no special significance. More importantly, while the equations of motion have been obtained with all vectors, each one has its own mathematical simplicity (complexity) and physical meaning. Finally, the eccentricity vector naturally arises in solving the dynamical equation at an elementary level, without resorting to the Lagrangian formalism or group theory. The eccentricity vector also only arises in the case of an inverse-square law of force.

The vector product of $\mathbf{L}$ and $\mathbf{A}$ is an invariant. It is, thus, possible to deduce the invariant Hamilton $\mathbf{S}$ vector:

$$\mathbf{S} = \frac{1}{L^2}\mathbf{L} \wedge \mathbf{A} = \mathbf{v} - \frac{\alpha}{L^2}\mathbf{L} \wedge \mathbf{u}_r. \tag{7}$$

The Laplace vector indicates the direction of the periapsis. In the same way, the Hamilton vector is parallel to the velocity of the system at the periapsis [32–35].

2.2. The Bertrand Theorem

The Bertrand theorem [24,36–46] states that the orbit is closed only if the potential is in $1/r$ or harmonic r^2. In the Keplerian case, there are two privileged directions: the one relating the attractive center to the periapsis of the orbit and the perpendicular direction. The two directions play different roles. This justifies the existence of the vector $\mathbf{A}$. As mentioned above, the vector $\mathbf{A}$ is parallel to the big axis of the ellipse and indicates the direction of the periapsis. In the case of a harmonic (r^2) potential, there are also two privileged directions. The Binet formulas are, with $u = 1/r$, as follows:

- First Binet formula:

$$v^2 = C^2\left[u^2 + \left(\frac{du}{d\theta}\right)^2\right], \tag{8}$$

- Second Binet formula:

$$a_r = -C^2u^2\left[u + \frac{d^2u}{d\theta^2}\right], \tag{9}$$

where a_r is the acceleration and C the areal constant (twice the areal velocity, Kepler's second law). Let us consider a force proportional to r^n [47,48]:

$$a_r = -\kappa r^n \tag{10}$$

and a small perturbation ϵ to the circular trajectory of radius r_0 (corresponding to $d^2u/d\theta^2 = 0$):

$$C^2/r_0 = \kappa r_0^{n+2}. \tag{11}$$

One has

$$\frac{1}{r} = \frac{1}{r_0}(1 + \epsilon), \tag{12}$$

where $\epsilon \ll 1$. Using the second Binet formula, one obtains

$$\frac{d^2\epsilon}{d\theta^2} = -(n+3)(\epsilon + \beta\epsilon^2 + \gamma\epsilon^3) \tag{13}$$

where we have set $2\beta = -(n+2)$ and $6\gamma = (n+2)(n+1)$. We have to solve an equation describing a non-linear oscillation of variable ϵ. For that purpose, we can resort to a perturbative expansion of the solution and evaluate the apsidal angle of the orbits in the neighborhood of the circular one. At first order of approximation, in the vicinity of the circular trajectory, one has

$$\frac{d^2\epsilon_1}{d\theta^2} = -(n+3)\epsilon_1 \tag{14}$$

and, thus,

$$\epsilon_1 = M\cos(p\theta), \tag{15}$$

with $p^2 = n+3$. At the next (second) order, we obtain

$$\frac{d^2\epsilon_2}{d\theta^2} = -(n+3)\left\{\epsilon_2 - \beta\frac{M^2}{2}[1+\cos(2p\theta)]\right\} \tag{16}$$

yielding

$$\epsilon_2 = M\cos(p\theta) + M^2(G + A\cos(2p\theta)), \tag{17}$$

with $G = (n+2)/4$ and $A = -(n+2)/12$. Finally, at the third order, we look for solutions of the type

$$\epsilon_3 = M\cos(q\theta) + M^2[G + A\cos(2p\theta)] + M^3 B\cos(3p\theta) \tag{18}$$

satisfying the equation if and only if (the quantities n and q used in this section must not be confused with the parabolic quantum numbers (see Appendix A), and integer p must not be confused with the modulus of momentum vector $\mathbf{p}$):

$$q^2 = (-n+3)\left[1 - \frac{M^2}{12}(n-1)(n+2)\right] \tag{19}$$

where we have set

$$G = (n+2)/4 \tag{20}$$

as well as

$$B = (n+2)(n+3)/96. \tag{21}$$

The solution at third order, around the circular trajectory, is of the form $\epsilon = M\cos(q\theta) + O(M^2)$, where

$$q = \sqrt{n+3}\left[1 - \frac{M^2}{24}(n+2)(n-1)\right] \tag{22}$$

and the apsidal angle, equal to π/q, cannot be commensurable with π $\forall M \ll 1$, except if $n = 1$ or $n = -2$. Therefore, the orbits of a point subject to a central force proportional to the inverse of the power n of the distance between the active center and the point are closed if and only if $n = 1$ or $n = -2$.

3. The Runge–Lenz Vector in Quantum Mechanics

3.1. Construction of the SO(4) Rotation Group Quantum Mechanical Analog to the Runge–Lenz Vector

The resemblance between the Kepler problem of planetary motion and the charged particle in the Coulombic potential motivated us to understand symmetries possessed by such systems. The Hamiltonian can be written formally as

$$H = \frac{\mathbf{p}^2}{2\mu} - \frac{\alpha}{r}, \tag{23}$$

where μ is the reduced mass $Mm/(M+m)$, $\alpha = GMm = G\mu(M+m) = \kappa\mu$ (for Newton potential, see above), and $\alpha = Ze^2$ (for the Coulomb potential with $4\pi\epsilon_0$ set to unity). With **r**, **p**, and **L** as already established quantum mechanical operators, the classical Lenz vector **A** can be translated directly into quantum mechanics (vector **M**). There is only a bit of subtlety involved in its construction. We must take care in defining the cross-product (see Equation (3). We notice that $\mathbf{p} \wedge \mathbf{L} \neq -\mathbf{L} \wedge \mathbf{p}$. The classical Runge–Lenz operator is not Hermitian. Following the derivation of [49], we redefine **M** as a symmetric average. The quantum mechanical operator **M**, the extension of the classical Runge–Lenz vector, is defined as follows

$$\mathbf{M} = \frac{1}{2\mu}(\mathbf{p} \wedge \mathbf{L} - \mathbf{L} \wedge \mathbf{p}) - \alpha \mathbf{u}_r. \tag{24}$$

As expected, this vector commutes with the Hamiltonian, $[\mathbf{M}, H] = 0$, and defines a conserved quantity in the quantum mechanical analog of the classical Kepler problem. We find that

$$\mathbf{L}.\mathbf{M} = \mathbf{M}.\mathbf{L} = 0, \tag{25}$$

and

$$\mathbf{M}^2 = \frac{2H}{\mu}(\mathbf{L}^2 + \hbar^2) + \alpha^2 = 0. \tag{26}$$

From here, we look to understand how this new commuting operator relates to the physical system and all the existing conserved quantities. We examine the system in light of well-established geometrical symmetries.

3.2. The Algebra of the **M**, **L** *Generators*

The three components of **M**, like the three components of **L**, can be treated as generators of some infinitesimal transformations. With the goal of exploring the algebraic structure of these new generators, we work out their commutation relations (there are thirty-six in all). Some are known; indeed, $[L_i, L_j]$ are given by

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k \tag{27}$$

for $i, j, k = 1, 2, 3$, where ϵ_{ijk} is the Levi-Civita symbol:

$$\epsilon_{ijk} = \begin{vmatrix} \delta_{i1} & \delta_{i2} & \delta_{i3} \\ \delta_{j1} & \delta_{j2} & \delta_{j3} \\ \delta_{k1} & \delta_{k2} & \delta_{k3} \end{vmatrix} \tag{28}$$

and δ_{ij} the Kronecker symbol. The others are

$$\begin{aligned} [M_i, L_i] &= 0 \\ [M_i, L_j] &= i\hbar\epsilon_{ijk}M_k, \end{aligned} \tag{29}$$

and

$$[M_i, M_j] = -\frac{2i\hbar}{\mu}\epsilon_{ijk}HL_k. \tag{30}$$

The first set of these commutators (29) shows that **M** is a vector. M_i commutes with L_i since L_i generates rotation about the i axis, which has no effect on a vector pointed along that axis. On the other hand, if j is perpendicular to i, L_j induces a change in the direction of M_i. This is characterized by the second commutation relation in Equation (29), which implies that the direction of this change in M_j should be orthogonal to both M_j and L_i, in this case, along $-M_k$. The relation in Equation (30) breaks the closed algebra of the L and M operators together, since H is involved. We now make a useful substitution. Considering a degenerate subspace (manifold) of H with energy eigenvalue E (i.e., corresponding to a given value of n, due to the accidental degeneracy of level energies with respect to the

orbital quantum number ℓ), we can replace the Hamiltonian with the resulting energy eigenvalue and define $\mathbf{M}'$ such that

$$\mathbf{M}' = \left(-\frac{\mu}{2E}\right)^{1/2}\mathbf{M}. \tag{31}$$

The commutation relations remain unchanged with M replaced everywhere by M', with the exception of Equation (30), which now becomes

$$\left[M'_i, M'_j\right] = i\epsilon_{ijk}L_k, \tag{32}$$

the signature of a closed algebraic system.

3.3. Identifying the Closed Algebra of $\mathbf{L}$ and $\mathbf{M}'$ with the $SO(4)$ Group

We can relabel L_x, L_y, and L_z into L_1, L_2, and L_3. Substituting 1, 2, and 3 for x, y, and z allows for a natural extension beyond three dimensions. It is clear from Relations (31) and (32) that the $\mathbf{M}'$ matrices are merely generalized angular momentum operators in the fourth dimension. In four dimensions, we have $\binom{4}{2} = 6$ orthogonal angular momentum generators, where $\binom{n}{p} = n!/p(n-p)!$ is the usual binomial coefficient. Let us make the following associations:

$$\begin{array}{rcl} M'_x & = & L_{14}, \quad M'_y = L_{24}, \quad M'_z = L_{34}, \\ L_x & = & L_{23}, \quad L_y = L_{31}, \quad L_z = L_{12}, \end{array} \tag{33}$$

which can be summarized as

$$M'_i = L_{i4}, \ \ and \ \ L_i = \epsilon_{ijk}L_{jk} \tag{34}$$

We add a fictitious coordinate ω, so that the rotation in four-dimensional space is given by

$$\begin{pmatrix} x' \\ y' \\ z' \\ \omega' \end{pmatrix} = \exp\left[\sum_{i<j}\theta_{ij}L_{ij}\right]\begin{pmatrix} x \\ y \\ z \\ \omega \end{pmatrix}.$$

In order to obtain the energy, we can exploit the $SO(4)$ symmetry. It is easy to verify that the commutation relations in Section 4.3 still hold. In four dimensions, a degree of decoupling emerges: the maximal commuting set of operators includes two angular momentum operators at the same time: L_{12} with L_{34}, etc. Such a decoupling stems from the property that the two operators generate rotations in orthogonal, non-intersecting planes, defined by completely disjoint sets of vectors. This fact alludes to the structure of the group generated by the operators: the rotational group in four dimensions, $SO(4)$, of rank 2, which contains, as a subgroup, the rank 1 $SO(3)$ rotational group. We, therefore, generalized the closed algebra of $\mathbf{L}$ and $\mathbf{M}$ operators. The remarkable insight here is that a dynamical symmetry (as physically evidenced by eccentricities in closed orbits) is a mere artifact of rotational symmetry in a higher dimension.

3.4. Energy Levels of Hydrogen Atom

The partial decoupling of angular momentum operators in four dimensions hints at a decomposition of the $SO(4)$ group generated by the operators L and M [50,51]. Rank 2 $SO(4)$ groups by rule can be broken down into two completely decoupled rank 1 $SU(2)$ groups:

$$SO(4) \rightarrow SU(2) \times SU(2), \tag{35}$$

with three non-commuting generators each, yielding $3+3=6$ generators. We made then the following choice of basis:

$$\mathbf{I} = \frac{1}{2}(\mathbf{L} + \mathbf{M}') \tag{36}$$

and

$$\mathbf{K} = \frac{1}{2}(\mathbf{L} - \mathbf{M}') \tag{37}$$

with

$$\begin{aligned} \left[I_i, I_j\right] &= i\hbar\epsilon_{ijk} I_k, \\ \left[K_i, K_j\right] &= i\hbar\epsilon_{ijk} K_k, \\ [\mathbf{I}, \mathbf{K}] &= 0, \end{aligned} \tag{38}$$

$$[\mathbf{I}, H] = [\mathbf{K}, H] = 0. \tag{39}$$

Since both $\mathbf{I}$ and $\mathbf{K}$ constitute an $SU(2)$ known algebra, it is isomorphic to the group generated by angular momentum in three dimensions. We used our findings in Section 4.2 to obtain their possible eigenvalues. We can write states that are simultaneous eigenstates of H, I_z, and K_z:

$$|E; i, i_z, k, k_z\rangle. \tag{40}$$

and one has

$$I_z|E; i, i_z, k, k_z\rangle = i_z\hbar|E; i, i_z, k, k_z\rangle \tag{41}$$

for $i, k = 0, 1/2, 1, \cdots$. The corresponding Casimir operators, $\mathbf{I}^2$ and $\mathbf{K}^2$, are, respectively,

$$\mathbf{I}^2 = \frac{1}{4}(\mathbf{L} + \mathbf{M}')^2 \tag{42}$$

and

$$\mathbf{K}^2 = \frac{1}{4}(\mathbf{L} - \mathbf{M}')^2. \tag{43}$$

It is important to remember that Casimir operators are distinct from generators. They are actually functions of generators and, although they commute with all the generators of a group, are not considered to be in the set of commuting generators itself. A linear combination of these operators is diagonal in the basis of their common eigenvectors. The Casimir operators $\mathbf{I}^2$ and $\mathbf{K}^2$ commute with all the generators $(I_x, I_y, I_z, H, K_x, K_y, K_z)$. One has

$$\mathbf{I}^2|E; i, i_z, k, k_z\rangle = i(i+1)\hbar^2|E; i, i_z, k, k_z\rangle \tag{44}$$

and

$$\mathbf{K}^2|E; i, i_z, k, k_z\rangle = k(k+1)\hbar^2|E; i, i_z, k, k_z\rangle. \tag{45}$$

From $\mathbf{I}$ and $\mathbf{K}$, we can construct operators

$$C_1 = \mathbf{I}^2 - \mathbf{K}^2 \tag{46}$$

and

$$C_2 = \mathbf{I}^2 + \mathbf{K}^2, \tag{47}$$

which commute with all $so(4)$ generators and H. C_1 yields a constraint on the eigenvalues through

$$\begin{aligned} C_1 &= \mathbf{I}^2 - \mathbf{K}^2 \\ &= \frac{1}{4}(\mathbf{L}^2 + \mathbf{M}'^2 + \mathbf{L}.\mathbf{M}' + \mathbf{M}'.\mathbf{L}) \\ &= \mathbf{L}.\mathbf{M}' = 0. \end{aligned} \tag{48}$$

The last line used the relation from Equations (25) and (26). Actually, $C_1 = 0$ means that i and k are the same. This brings additional information (not given by $SU(2)$). We find the eigenvalues for operator C_2 with ease using Equations (44) and (45), yielding

$$C_2 = 2\mathbf{K}^2 \tag{49}$$

and

$$C_2|E; i, i_z, k, k_z\rangle = 2k(k+1)\hbar^2|E; i, i_z, k, k_z\rangle. \tag{50}$$

Combining Equations (25), (26), (31), (42), and (43), we derive a constant expression for C_2:

$$\begin{aligned} C_2 &= \mathbf{I}^2 + \mathbf{K}^2 = \frac{1}{2}\left(\mathbf{L}^2 + \mathbf{M}'^2\right) = \frac{1}{2}\left(\mathbf{L}^2 - \frac{\mu}{2E}\mathbf{M}'^2\right) \\ &= \frac{1}{2}\left[\mathbf{L}^2 - \frac{\mu}{2E}\left(\frac{2E}{\mu}(\mathbf{L}^2 + \hbar^2) + \alpha^2\right)\right] \\ &= -\frac{\hbar^2}{2} - \frac{\mu\alpha^2}{4E}. \end{aligned} \tag{51}$$

Equating Equations (49) and (50), we obtain our permissible energy levels for a hydrogenic atom:

$$E_k = -\mu\frac{\alpha^2}{2\hbar^2(2k+1)^2} \tag{52}$$

for $k = 0, 1/2, 1, \cdots$. Recalling that $\alpha = Ze^2$ and setting $2k + 1 = n$, for $n = 1, 2, 3, \cdots$, we recover the well-known expression:

$$E_n = -\mu\frac{\alpha^2}{2\hbar^2 n^2} \tag{53}$$

for $n = 1, 2, 3, \cdots$. The elegance of this method stems from the fact that, in addition to the hydrogen energy spectrum, the relevant constraints on various quantum numbers have emerged naturally as well. For instance, consider $\mathbf{L} = \mathbf{I} + \mathbf{K}$ from the initial definition of $\mathbf{I}$ and $\mathbf{K}$. Since $\mathbf{I} = \mathbf{K}$, we see that, by the triangular rule of vector addition, L can be at most $k + k = n - 1$, and its values extend to $|k - k| = 0$ in integer steps, as expected. In addition, following the algebra of $SU(2)$ groups, I_z and K_z, analogous to L_z, would each have $2k + 1 = n$ independent eigenvalues and eigenstates. The total degeneracy of an energy level, $n \times n = n^2$, is, therefore, also recovered [52].

4. Analogy with the Harmonic Potential: Invariant Tensor

Let us summarize the analogies between the Kepler and the harmonic oscillator problems [53]:

- The orbit is closed (Bertrand's theorem).
- The motion is periodic (degeneracy).
- There is a Laplace invariant.
- The motion has a dynamical symmetry higher than the rotation geometrical symmetry.
- For each value of the energy, one can find an infinity of classical orbits of different shapes.
- The separation of variables applies to several systems of coordinates.
- The quantum states are degenerate.

4.1. The Laplace Tensor

We have seen that the Runge–Lenz vector is an invariant of the Kepler motion. According to the reciprocal of the Noether theorem [1], a continuous symmetry can be associated with it. Such a symmetry was discovered by Fock and Bargmann in 1935: the Coulomb potential has an internal symmetry (or dynamical symmetry), isomorphic (for the bound states) to the one of the continuous group $SO(5)$ of the rotations in the four-dimensional

space. Such a group has six parameters, and there are indeed six constants of motion: the three components of the angular momentum and the three components of the Runge–Lenz vector. Actually, only five of these constants are independent, since the vectors **L** and **A** are orthogonal. The energy is not a constant of motion independent of the previous ones, since it can be calculated as a function of the invariants of A^2 and L^2, which are Casimir invariants of the $SO(4)$ group.

The harmonic potential also has a dynamical symmetry, isomorphic to the one of the continuous group $SU(3)$ of 3×3 matrices with determinant equal to one. This group has eight parameters. The eight corresponding constants of motion are the three components of the angular momentum and the five components of the symmetric Laplace tensor. Five of them are independent since **L** is an eigenvector of the Laplace tensor. Let us consider a mass μ in an isotropic harmonic potential:

$$\mathcal{U}(r) = \frac{1}{2}kr^2. \tag{54}$$

The equation of motion is

$$\mu \frac{d\mathbf{v}}{dt} = -k\mathbf{r}. \tag{55}$$

It is possible to define an invariant of the motion [54] as

$$\overline{\overline{\mathrm{A}}} = \frac{k}{2}\mathbf{r}^{\dagger}.\mathbf{r} + \frac{\mu}{2}\mathbf{v}^{\dagger}.\mathbf{v}, \tag{56}$$

$\mathbf{r}^{\dagger}$ and $\mathbf{r}$ being, respectively, the line and column representations of the vector. Let us set $\omega^2 = k/\mu$. The Laplace tensor reads [55–57]:

$$\overline{\overline{\mathrm{A}}} = \begin{pmatrix} \omega^2 x^2 + v_x^2 & \omega^2 xy + v_x v_y \\ \omega^2 xy + v_x v_y & \omega^2 y^2 + v_y^2 \end{pmatrix}, \tag{57}$$

where x and y are the coordinates of position operator $\mathbf{r}$ and v_x and v_y the coordinates of velocity $\mathbf{v}$. One has

$$\mathrm{Tr}\left(\overline{\overline{\mathrm{A}}}\right) = \lambda_1 + \lambda_2 = E \tag{58}$$

as well as

$$\mathrm{Det}\left(\overline{\overline{\mathrm{A}}}\right) = \lambda_1 \lambda_2 = \frac{1}{4}\omega^2 L^2 \tag{59}$$

yielding

$$\lambda_1 = \frac{1}{2}\left(E + \sqrt{E^2 - \omega^2 L^2}\right) \tag{60}$$

and

$$\lambda_2 = \frac{1}{2}\left(E - \sqrt{E^2 - \omega^2 L^2}\right) \tag{61}$$

and, finally,

$$E^2 = |\overline{\overline{\mathrm{A}}}|^2 + \frac{k}{2m}L^2. \tag{62}$$

We have

$$\begin{aligned} \mathbf{r}\overline{\overline{\mathrm{A}}}\mathbf{r} &= \begin{pmatrix} r\cos\theta & r\sin\theta \end{pmatrix} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \begin{pmatrix} r\cos\theta \\ r\sin\theta \end{pmatrix} \\ &= \lambda_1 r^2 \cos^2\theta + \lambda_2 r^2 \sin^2\theta \end{aligned} \tag{63}$$

and

$$\begin{aligned} \mathbf{r}\overline{\overline{\mathbf{A}}}\mathbf{r} &= \frac{k}{2}r^4 + \frac{\mu}{2}(\mathbf{r}.\mathbf{v})^2 \\ &= \frac{k}{2}r^4 + \frac{\mu}{2}\left(r^2v^2 - C^2\right). \end{aligned} \tag{64}$$

Eliminating v using the energy conservation gives

$$\frac{1}{r^2} = \frac{2\lambda_2}{\mu C^2}\cos^2\theta + \frac{2\lambda_1}{\mu C^2}\sin^2\theta. \tag{65}$$

If both eigenvalues are positive, the orbit is an ellipse with the semi-minor and semi-major axis given by

$$a^2 = \frac{\mu C^2}{2\lambda_2}, \quad b^2 = \frac{\mu C^2}{2\lambda_1}. \tag{66}$$

It is worth mentioning that the transformations of the group $SO(4)$ or $SU(3)$ enable one to change from an orbit of energy E to degenerated orbits of the same energy [58,59].

Analogies between the Kepler and harmonic motions were already known by Newton [60]. A mathematical transform from the one to the other was introduced in 1965 by Kustaanheimo and Stiefel [61].

4.2. The Kustaanheimo–Stiefel Transformation

The Kustaanheimo–Stiefel transformation is a particular case of the surjective application:

$$\mathbb{R}^4 \to \mathbb{R}^3 : (u_0, u_1, u_2, u_3) \longmapsto (x_0, x_2, x_3), \tag{67}$$

defined by

$$\begin{aligned} x_0 &= u_0^2 - pu_1^2 + tu_2^2 - ptu_3^2, \\ x_2 &= 2(u_0u_2 + pu_1u_3), \\ x_3 &= 2(u_0u_3 + u_1u_2), \end{aligned} \tag{68}$$

subject to the constraint $\omega = 0$ with

$$\omega = 2(u_1du_0 - u_0du_1 + tu_3du_2 - tu_2du_3), \tag{69}$$

where the parameters p and t can take the values ± 1. The transformation introduced by Kustaanheimo and Stiefel [62] corresponds to $p = t = -1$, while the cases $p = -t = -1$ and $p = -t = 1$ (or $p = t = 1$) correspond to two other (inequivalent) transformations.

The applications of the transformations (68) and (69) range from number theory to physics (classical and quantum mechanics, gauge theories, etc.). The Hurwitz matrix corresponding to (68) and (69) is connected to the problem of factoring the sum of four squared numbers. In classical mechanics, the Kustaanheimo–Stiefel transformation is used for the regularization of the Kepler problem [62]. In quantum mechanics, the latter transformation enables one to transform the Schrödinger equation for the three-dimensional hydrogen atom (in an electromagnetic field) into a Schrödinger equation for a four-dimensional isotropic harmonic oscillator (with quartic and sextic anharmonic terms) subject to a constraint [63–67]. Conversely, the mappings (68) and (69) may be used in some dimensional-reduction process for converting a dynamical system in $\mathbb{R}^4$ or $\mathbb{R}^2 \times \mathbb{R}^2$ into a dynamical system in $\mathbb{R}^3$.

When the Kustaanheimo–Stiefel transform is applied to the hydrogen atom in three dimensions, the constraint (69) manifests as a restriction on the oscillator quantum numbers in four dimensions. The usual procedure for determining this restriction is to compare the expressions for the energy eigenvalues for the oscillator and for the hydrogen atom and by demanding the consistency of the two [68], but Cahill demonstrated that it can be obtain in a direct and natural manner. His idea is not to treat the constraint as an operator

identity, but instead, to interpret it as a restriction on allowed energy states, acceptable wavefunctions being in the kernel of a specific operator [69].

In addition to the mathematical–physics interest, the transform has proven very useful in N-body simulations, where it helps to handle close encounters. At first sight, the formalism may seem rather cumbersome, with the role of the extra dimension being especially mysterious, but Saha showed how the Kustaanheimo–Stiefel transform can be interpreted as a rotation in three dimensions. For example, rotating a telescope from zenith to a chosen star in one rotation, the rotation axis and angle can be viewed as the Kustaanheimo–Stiefel transform of the star, and the non-uniqueness of the rotation axis encodes the extra dimension. This geometrical interpretation becomes obvious while writing the transform in quaternion form, which also enables one to derive concise expressions for regularized equations of motion [70].

It is worth mentioning that Yoshida proposed a derivation of the Kustaanheimo–Stiefel in parabolic coordinates (Appendix A). Through the latter derivation, it becomes clearer where and how the additional dimension is introduced and what the bilinear relation means [71].

4.3. Integrability and Similarity

A system with N degrees of freedom has at maximum $2N-1$ independent constants of motion. If there are N constants, the system is integrable. If there are $N+n$ ones, it is superintegrable and n-times degenerated. If $n = N-1$, the system is totally degenerated; this is the case of the Keplerian and harmonic motions [72].

Prince and Eliezer showed that the Laplace invariants are linked to the fact that the Kepler and harmonic motions are invariant by similarity, which explains, respectively, the third Kepler law and the isochronism of harmonic oscillations [73].

5. Invariant in the Presence of an Electric Field: The Redmond Invariant

Let us introduce, in the presence of an electric field $\mathbf{F} = F\mathbf{u}_z$, the so-called Redmond vector [16]:

$$\mathscr{R} = \mathbf{A} + \frac{1}{2}(\mathbf{r} \wedge \mathbf{F}) \wedge \mathbf{r} \tag{70}$$

and its projection on the z axis:

$$\mathscr{R}_z = A_z - \frac{1}{2}\left(x^2 + y^2\right)F. \tag{71}$$

The Redmond vector is not an invariant [74]. However, the quantity:

$$\mathscr{R}.\mathbf{F} = \mathbf{A}.\mathbf{F} + \frac{1}{2}[(\mathbf{r} \wedge \mathbf{F}) \wedge \mathbf{r}].\mathbf{F} \tag{72}$$

which, using the relation:

$$\mathbf{a} \cdot (\mathbf{b} \wedge \mathbf{c}) = \mathbf{b} \cdot (\mathbf{c} \wedge \mathbf{a}) - \mathbf{c} \cdot (\mathbf{a} \wedge \mathbf{b}) \tag{73}$$

is equal to

$$\mathscr{R}.\mathbf{F} = \mathbf{A}.\mathbf{F} - \frac{1}{2}(\mathbf{r} \wedge \mathbf{F})^2, \tag{74}$$

is an invariant. Indeed, for an electron, we have (since, in atomic units, the force $\mathbf{f}$ is related to the field $\mathbf{F}$ by $\mathbf{f} = -\mathbf{F}$):

$$\frac{d\mathbf{L}}{dt} = \mathbf{r} \wedge \mathbf{f} = -\mathbf{r} \wedge \mathbf{F} \tag{75}$$

and, thus,

$$\frac{d\mathbf{A}}{dt} = -[\mathbf{F} \wedge (\mathbf{r} \wedge \mathbf{v}) + \mathbf{v} \wedge (\mathbf{r} \wedge \mathbf{F})], \tag{76}$$

i.e.,

$$\frac{d\mathbf{A}}{dt}.\mathbf{F} = -\Big[(\mathbf{F}.\mathbf{r})(\mathbf{F}.\mathbf{v}) - \mathbf{r}.\mathbf{v}\,F^2\Big]. \tag{77}$$

We have also

$$\frac{1}{2}\frac{d}{dt}(\mathbf{r}\wedge\mathbf{F})^2 = (\mathbf{r}\wedge\mathbf{F}).(\mathbf{v}\wedge\mathbf{F}) \tag{78}$$

and using the formula (Binet–Cauchy identity):

$$(\mathbf{a}\wedge\mathbf{b}).(\mathbf{c}\wedge\mathbf{d}) = (\mathbf{a}.\mathbf{c}).(\mathbf{b}.\mathbf{d}) - (\mathbf{a}.\mathbf{d}).(\mathbf{b}\mathbf{c}), \tag{79}$$

we obtain zero [16]. The surface of the orbit precesses around the direction of the field, and its angle with the field oscillates around a given average value.

This invariant is interesting or the study of the classical Stark effect, i.e., the motion of an electron in an electric field [75].

6. Oks' Supergeneralized Runge–Lenz Vector for the Two-Center Problem

Let us consider the problem of two Coulomb centers of charges Z and Z' separated by a distance R. This is an example of the so-called "two-center problem". In the limit of large R, the problem of two Coulomb centers reduces to the problem of a hydrogenic ion in the nuclear charge Z in the uniform electric field $F = Z'/R^2$, which is another fundamental problem of quantum mechanics (its analog in celestial physics is the one-center Kepler problem in a uniform gravitational field).

This simpler problem has also a dynamical symmetry (which is linked to the fact that this problem allows the separation of variables in the parabolic coordinates). The corresponding integral of the motion in that case is the projection of a generalized Runge–Lenz vector on the internuclear axis. This generalized Runge–Lenz vector is the Redmond vector [16] (see Equation (70). After Redmond introduced it for this asymptotic case of the two-center problem, the challenge was to find a supergeneralization of the Runge–Lenz vector in the general (i.e., not necessarily asymptotic) case.

Throughout this section, we use atomic units $m = \hbar = e = 1$ to conform with the convention of the authors. Gurarie, assuming a charge Z_1 at $z = a$ and a charge Z_2 at $z = -a$ [76], considered the following Hamiltonian:

$$H = \frac{p^2}{2} - \frac{Z_1}{r_1} - \frac{Z_2}{r_2}, \tag{80}$$

r_1 and r_2 being the distances from each nucleus, and found the invariant vector:

$$\mathbf{A}^{(G)} = \mathbf{p}\wedge\mathbf{L} - Z_1\frac{\mathbf{r}-a\mathbf{u}_\alpha}{|\mathbf{r}-a\mathbf{u}_\alpha|} - Z_2\frac{\mathbf{r}+a\mathbf{u}_\alpha}{|\mathbf{r}+a\mathbf{u}_\alpha|}, \tag{81}$$

where $\mathbf{u}_\alpha$ is the unit vector from Z_1 to Z_2. It can be checked that, at large R, the Redmond vector is recovered.

Krivchenko and Liberman considered the Hamiltonian [77]:

$$H = \frac{p^2}{2} - \frac{Z_1}{r_1} - \frac{Z_2}{r_2} + \frac{Z_2}{R} \tag{82}$$

with Z_1 at the origin and Z_2 at $z = R$. They obtained (using parabolic coordinates) the following vector:

$$\mathbf{A}^{(KL)} = \mathbf{p}\wedge\mathbf{L} - Z_1\frac{\mathbf{r}_1}{|\mathbf{r}_1|} + Z_2\frac{\mathbf{r}_2}{|\mathbf{r}_2|} + Z_2\mathbf{u}_\alpha \tag{83}$$

but its projection on the axis is not preserved. This led Kryukov and Oks to introduce the supergeneralized Runge–Lenz vector for the two-center Coulomb problem [20]:

$$\mathbf{A}^{(KO)} = \mathbf{p} \wedge \mathbf{L} - \frac{L^2}{R}\mathbf{u}_\alpha - Z\frac{\mathbf{r}}{|\mathbf{r}|} - Z'\frac{\mathbf{R}-\mathbf{r}}{|\mathbf{R}-\mathbf{r}|} + Z'\mathbf{u}_\alpha, \tag{84}$$

the z axis going from Z to Z'.

As an application, Sanders and Oks used the robust perturbation theory [21,78] for calculating quadrupole corrections to the wave functions. This is important for the Stark effect and the asymmetry of hydrogenic spectral lines in plasmas. If, for the perturbed quantum system, there is an operator $\mathbf{A}$ that commutes with the Hamiltonian H and the parts of these operators $\mathbf{A_0}$ and H_0, characterizing the unperturbed quantum system, also commute, then the perturbation theory can be constructed in terms of the perturbation $(\mathbf{A} - \mathbf{A_0})$ to the operator $\mathbf{A_0}$, rather than in terms of the perturbation $(H - H_0)$ to the operator H_0. For calculating corrections to the wave functions (which are common for both $\mathbf{A_0}$ and H_0), the advantage is that the eigenvalues of the operator $\mathbf{A_0}$ are typically non-degenerate (which is not the case for the eigenvalues of the operator H_0). Therefore, for calculating the first-order corrections to the wave functions, it is sufficient to use the first order of the non-degenerate perturbation theory with respect to the perturbation $(\mathbf{A} - \mathbf{A_0})$, and it would not involve infinite summations. In distinction, for calculating the same corrections in terms of the perturbation $(H - H_0)$, one would have to proceed to the second order of the degenerate perturbation theory, involving infinite summations. Sanders and Oks chose the projection A_z of the super-generalized Runge–Lenz vector, derived by Kryukov and Oks [20], on the axis connecting the nucleus of the hydrogenic atom/ion with the perturbing ion. The operator of the unperturbed projection $A_z^{(0)}$ has the well-known eigenvalues q/n. According to Equation (12) from [21], the first non-vanishing term of the expansion of the operator $(A_z - A_z^{(0)})$ in terms of the small parameter n^2/R (here and below, we use atomic units) is $-L^2/R$. Then, the corrections to the wave functions are given by

$$-\frac{1}{R}\frac{(L^2)^{nq'_pm}_{nq_pm}}{A^{(0)}_{z,\alpha} - A^{(0)}_{z,\alpha'}} = -\frac{n}{R}\frac{(L^2)^{nq'_pm}_{nq_pm}}{(q_p - q'_p)} \tag{85}$$

where $q_p - q'_p = \pm 2$ with $q_p = n_1 - n_2$ and $q'_p = n'_1 - n'_2$ (not to be confused with the charge in Section 7.1). Sholin et al. showed that [79]:

$$\langle n_1 + 1, n_2 - 1, m|L^2|n_1 n_2 m\rangle = -\hbar[n_2(n - n_2)(n_1 + 1)(n - n_1 - 1)]^{1/2} \tag{86}$$

and

$$\langle n_1 - 1, n_2 + 1, m|L^2|n_1 n_2 m\rangle = -\hbar[n_1(n - n_1)(n_2 + 1)(n - n_2 - 1)]^{1/2}. \tag{87}$$

The state $|n_1 n_2 m\rangle$ can be expressed in terms of the normalized $O(4)$ state $|j_1 j_2 m_1 m_2\rangle$ (both representations are spherical wave functions in four dimensions) through the following relation (the parabolic quantum numbers are defined in Appendix A) [75]:

$$|n_1 n_2 m\rangle = (-1)^{\frac{2n_2+|m|-m}{2}}|j_1 j_2 m_1 m_2\rangle, \tag{88}$$

where j_1 and j_2 are the angular momenta associated with the operators:

$$\mathbf{J_1} = \frac{1}{2}(\mathbf{L} + \mathbf{M}) \tag{89}$$

and

$$\mathbf{J_2} = \frac{1}{2}(\mathbf{L} - \mathbf{M}) \tag{90}$$

and one has

$$j_1 = j_2 = j = \frac{n-1}{2}, \quad m_1 = \frac{m+n_2-n_1}{2} \quad and \quad m_2 = \frac{m+n_1-n_2}{2}. \tag{91}$$

One defines then

$$J_{1\pm} = J_{1x} \pm iJ_{1y}, \quad and, \quad J_{2\pm} = J_{2x} \pm iJ_{2y}, \tag{92}$$

as well as

$$M_+ = 2J_{1+} - L_+ = L_+ - 2J_{2+} \tag{93}$$

with $L_\pm = L_x \pm iL_y$ and

$$M_- = 2J_{1-} - L_- = L_- - 2J_{2-}, \tag{94}$$

yielding

$$\mathbf{M}.\mathbf{M} = \frac{1}{2}\left(M^+M^- + M^-M^+\right) + M_zM_z. \tag{95}$$

Sholin et al. obtained

$$\langle n_1 - 1, n_2, m+1|M_+|n_1n_2m\rangle = \hbar\sqrt{n_1(n-n_1)}, \tag{96}$$

$$\langle n_1, n_2 - 1, m+1|M_+|n_1n_2m\rangle = \hbar\sqrt{n_2(n-n_2)}, \tag{97}$$

$$\langle n_1 + 1, n_2, m-1|M_-|n_1n_2m\rangle = \hbar\sqrt{(n_1+1)(n-n_1-1)}, \tag{98}$$

and

$$\langle n_1, n_2 + 1, m-1|M_-|n_1n_2m\rangle = \hbar\sqrt{(n_2+1)(n-n_2-1)}. \tag{99}$$

We have also

$$\langle n_1 - 1, n_2, m+1|L_+|n_1n_2m\rangle = \hbar\sqrt{n_1(n-n_1)}, \tag{100}$$

$$\langle n_1, n_2 - 1, m+1|L_+|n_1n_2m\rangle = -\hbar\sqrt{n_2(n-n_2)}, \tag{101}$$

$$\langle n_1 + 1, n_2, m-1|L_-|n_1n_2m\rangle = \hbar\sqrt{(n_1+1)(n-n_1-1)}, \tag{102}$$

$$\langle n_1, n_2 + 1, m-1|L_-|n_1n_2m\rangle = -\hbar\sqrt{(n_2+1)(n-n_2-1)}, \tag{103}$$

$$\langle n_1, n_2, m|\mathbf{L}.\mathbf{L}|n_1n_2m\rangle = \frac{\hbar^2}{2}\left[n^2 - (n_1-n_2)^2 + |m|^2 - 1\right], \tag{104}$$

$$\langle n_1 + 1, n_2 - 1, m|\mathbf{L}.\mathbf{L}|n_1n_2m\rangle = -\hbar^2\sqrt{n_2(n-n_2)(n_1+1)(n-n_1-1)}, \tag{105}$$

$$\langle n_1 - 1, n_2 + 1, m|\mathbf{L}.\mathbf{L}|n_1n_2m\rangle = -\hbar^2\sqrt{n_1(n-n_1)(n_2+1)(n-n_2-1)}, \tag{106}$$

and

$$\langle n_1, n_2, m|\mathbf{L}.\mathbf{L} + \mathbf{M}.\mathbf{M}|n_1n_2m\rangle = \hbar^2\left(n^2-1\right). \tag{107}$$

As mentioned by Sanders and Oks, the non-diagonal matrix elements of the operator L_x in parabolic coordinates were reproduced in Gavrilenko's article [80]. In addition, the non-diagonal matrix elements of the operators $L_\pm$ can also be deduced from their proportionality (with the n-manifold) to the non-diagonal matrix elements of the operators $(x+iy)$. As a consequence, the non-diagonal matrix elements of the operator L^2 in parabolic coordinates can be obtained using their similar proportionality to the non-diagonal matrix

elements of the operator $(x^2 + y^2)$. The latter matrix elements were calculated, for instance, by Clark [81]. It is important to mention that Sanders and Oks [78] provided corrections to the Sholin tables from [82], which were used by many authors to calculate the asymmetry of hydrogenic spectral lines in plasmas.

7. Invariants in the Presence of a Magnetic Field

7.1. The Landau–Avron–Sivardière Approach

In the case of an external magnetic field, much less is known. Liberman did not provide any invariant in that case, but obtained series expansions, revealing some underlying symmetry [83]. The equation of motion of a charge q in the uniform field $\mathbf{B}$ is

$$\mu \frac{d\mathbf{v}}{dt} = q\mathbf{v} \wedge \mathbf{B}. \tag{108}$$

Integrating with respect to time, we obtain

$$\mu\mathbf{v} = q\mathbf{r} \wedge \mathbf{B} + \mathbf{k}, \tag{109}$$

where $\mathbf{k} = \mu\mathbf{v}_0 - \mathbf{B} \wedge \mathbf{r}_0$ is the time-invariant Landau vector ($\mathbf{r}_0 = \mathbf{r}(t = 0)$ and $\mathbf{v}_0 = \mathbf{v}(t = 0)$). Combining Equations (108) and (109), one obtains

$$\frac{d^2\mathbf{r}}{dt^2} + \frac{q^2B^2}{\mu^2}\mathbf{r} = \frac{q}{\mu^2}\mathbf{k} \wedge \mathbf{B}, \tag{110}$$

which means that the motion of q is harmonic: the center C of the elliptic orbit is given by $\mathbf{OC} = (\mathbf{k} \wedge \mathbf{B})/(qB^2)$, and the orbit is in fact a circle, since, according to Equation (108), the tangential acceleration is zero and the normal acceleration is constant. However [84], it is not necessary to know how to solve Equation (110). Multiplying Equation (109) by $\mathbf{B}$,

$\mathbf{v}$ is known from Equation (108). The nature of the motion is then found easily. Let us choose a new origin C with $\mathbf{OC} = \mathbf{a}$ such that the new Landau vector $\mathbf{K}$ is zero. We have, setting $\mathbf{r} = \mathbf{a} + \mathbf{R}$ and $\mathbf{v} = \mathbf{V} = d\mathbf{R}/dt$:

$$\mu\mathbf{V} = q\mathbf{R} \wedge \mathbf{V}. \tag{111}$$

and combining Equations (109) and (111):

$$\mathbf{a} = \frac{1}{qB^2}(\mathbf{k} \wedge \mathbf{B}) = \mathbf{r}_0 + \frac{\mu}{qB^2}\mathbf{v}_0 \wedge \mathbf{B} \tag{112}$$

and

$$\mathbf{a} \wedge \mathbf{k} = \frac{\mu v^2}{qB^2}\mathbf{B} + \mathbf{L}, \tag{113}$$

where $\mathbf{L} = \mu\mathbf{r} \wedge \mathbf{v} + qr^2\mathbf{B}/2$ is the angular momentum $\mathbf{r} \wedge \mathbf{p}$, $\mathbf{p} = \mu\mathbf{v} + \mathbf{A}$ and $\mathbf{A} = (\mathbf{B} \wedge \mathbf{r})/2$ is the vector potential in the symmetric gauge. The invariance of $\mathbf{L}$ is a consequence of the rotational symmetry around $\mathbf{B}$ [85,86], and it is easy to show that

$$L = \frac{qB}{2}(a^2 - R^2). \tag{114}$$

In the case of the motion of a charge in the field of a magnetic dipole, the motion may occur in the plane of symmetry of the dipole. If the motion is bound, the orbit fills a circular crown, the axis of which carries the dipole: no privileged direction exists in the plane, and no dynamical invariant can be found.

In the case of the motion of a charge in a magnetic monopole, there is a privileged direction in space different from the one of the cone axis: the direction of the periapsis. Such a direction is the one of a dynamical invariant, which could be determined by Kerner [87–89].

The corresponding dynamical symmetry is the one of the $SO(4,2)$ group of matrices acting in the four-dimensional space and conserving the pseudo-norm $x^2 + y^2 - z^2 - t^2$.

7.2. The Zeeman Effect

The symmetry of the quadratic Zeeman effect was investigated by different authors [81,90–92]. In [93], on the motion of a charge in a magnetic field, Sivardière considered the Zeeman effect for the harmonic oscillator and showed that the motion is epicyclic.

In a very interesting work, Yuzbashyan et al., motivated by the renewed interest in non-trivial degeneracies of a simple spin Hamiltonian, proposed a general approach to extract all non-trivial symmetries from the energy spectrum [94].

7.3. The Spectrum of the Hydrogen Atom in Electric and Magnetic Fields

The effect of a magnetic field on spectral line shapes, with or without an additional electric field, is an important topic of atomic physics (see, for example, the non-exhaustive list of references: [95–104]), for astrophysical or magnetic-fusion applications, both from the theoretical side and for the interpretation of Z-pinch experiments, for instance.

A consistent treatment of the splitting of the hydrogen atom in crossed weak electric and magnetic fields was given by Demkov et al. [105]. In that work, only the first-order perturbation theory was considered. The resulting formula for the energy corrections valid for arbitrary mutual orientation of the fields **F** and **B** was [106]:

$$E^{(1)} = n'e_1 + n''e_2, \tag{115}$$

where n' and n'' belong to the set $\{-j, -j+1, \cdots, j\}$, with $j = (n-1)/2$, and e_1 and e_2 are absolute values (in atomic units) of the operator:

$$\mathbf{e_1} = \frac{\mathbf{B}}{2c} - \frac{3}{2}n\mathbf{F} \tag{116}$$

where c is the speed of light in vacuum, and

$$\mathbf{e_2} = \frac{\mathbf{B}}{2c} + \frac{3}{2}n\mathbf{F}. \tag{117}$$

The zero-order wave functions are eigenvectors of $I_{1\alpha}$ and $I_{2\alpha}$:

$$I_{1\alpha}\psi_{nn'n''} = n'\psi_{nn'n''} \tag{118}$$

and

$$I_{2\alpha}\psi_{nn'n''} = n''\psi_{nn'n''} \tag{119}$$

where

$$I_{i\alpha} = \frac{\mathbf{I_i}.\mathbf{e_i}}{e_i}, \tag{120}$$

where the operators $\mathbf{I_1}, \mathbf{I_2}$ are connected to **L** and **M** via

$$\mathbf{I_1} = \frac{\mathbf{L} + \mathbf{M}}{2} \tag{121}$$

and

$$\mathbf{I_1} = \frac{\mathbf{L} - \mathbf{M}}{2}, \tag{122}$$

exactly as Equations (36) and (37). In general, first-order Formula (115) completely removes the degeneracy. Second-order corrections lead only to small energy shifts. The latter was calculated by Solov'ev [107] using the dynamical symmetry group $O(4,2)$ of atomic hydrogen. The problem becomes much more involved if the two fields are perpendicular ($\mathbf{F} \perp \mathbf{B}$, when $e_1 = e_2 = e$. The first-order correction $E^{(1)}$ depends then only on the set

of quantum numbers $n' + n = q$, implying a residual n-fold $(n - q)$ degeneracy. The second-order perturbation theory removes the degeneracy:

$$\begin{aligned} E &= -\frac{1}{2n^2} + E^{(1)} + \frac{F^2 n^4}{16}\left[3q^2 - 17n^2 - 19 - \frac{6}{1+\gamma^2}(n^2 - 3q^2 - 1)\right] \\ &\quad + \frac{H^2 n^2}{16c^2}(3n^2 + 1 - q^2 + \epsilon), \end{aligned} \tag{123}$$

where $\gamma = 3ncF/H$ and ϵ is the eigenvalue of the operator:

$$b(I_{1\alpha} - I_{2\alpha})^2 - 16 I_{1\beta} I_{2\beta}. \tag{124}$$

In the above formula, $I_{1\beta}$ is the projection of operator $\mathbf{I_i}$ on a direction belonging to the plane ($\mathbf{e}_1$, $\mathbf{e}_2$) and orthogonal to $\mathbf{e}_i$. The parameter b is given by the formula:

$$b = \gamma^2 - 1 - \frac{2}{1+\gamma^2}. \tag{125}$$

In fact, b grows monotonously when the ration F/H is increased. The extreme values $b = -3$ and $b = \infty$ correspond to purely magnetic and electric perturbations (quadratic Zeeman and Stark effects). In these limits, the quantum number q turns into the magnetic quantum number m (in the case where $F = 0$) or into $n_1 - n_2$, where n_1 and n_2 are parabolic quantum numbers (in the case where $H = 0$).

7.4. Magnetic Monopole

The existence of isolated magnetic monopoles was first suggested by Dirac in 1931 [23] and could explain the quantization of the charge. Since there is still no known experimental or observational evidence that magnetic monopoles exist, they remain an active field of research. The magnetic field of a particle of charge q in $\mathbf{r} = r\mathbf{u_r}$ is spherical and reads [89]

$$\mathbf{B} = g\frac{\mathbf{r}}{r^3} \tag{126}$$

and the equation of motion is

$$\mu\frac{d\mathbf{v}}{dt} = \delta\frac{\mathbf{L}}{\mu r^3}, \tag{127}$$

where $\delta = -qg$, $\mathbf{L} = \mu\mathbf{r} \wedge \mathbf{v}$ is not an invariant, but the Poincaré vector $\mathbf{J} = \mathbf{L} + \alpha\mathbf{u}_r$ is one [108].

8. The Charge-Dyon System

A dyon is a hypothetical particle in four-dimensional theories with both electric and magnetic charges. A dyon with a zero electric charge is usually referred to as a magnetic monopole. Many grand unified theories predict the existence of both magnetic monopoles and dyons. Dyons were introduced by Schwinger in 1969 as a phenomenological alternative to quarks [22]. He extended the Dirac quantization condition [23] to the dyon and used the model to predict the existence of a particle with the properties of the J/ψ meson prior to its discovery in 1974. There is much interest in the problem of bound states of a fermion in the field of a fixed Dirac monopole or in a 't Hooft–Polyakov monopole [109,110]. In theoretical physics, the 't Hooft–Polyakov monopole is a topological soliton, similar to the Dirac monopole, but without the Dirac string. The allowed charges of dyons are restricted by the Dirac quantization condition. This states, in particular, that their magnetic charge must be integral and that their electric charges must all be equal modulo one. It was shown that a constant homogeneous electric field completely removes the degeneracy of the energy levels on the orbital quantum number [111]. An important property is that the charge-dyon system possesses hidden symmetry, the corresponding group being $SO(4)$ for the discrete spectrum and $SO(3,1)$ for the continuous spectrum. It was shown that the

problem of the charge-dyon system due to hidden symmetry can be factorized not only in spherical, but also in parabolic coordinates [111].

8.1. Classical Approach of the Charged Monopole Problem

In the case of the so-called "augmented charged monopole problem", the monopole creates the potential:

$$\frac{\delta^2}{2\mu r^2}. \tag{128}$$

Such an additive modification of the Coulomb potential by a repulsive inverse-square potential was introduced a long time ago [112,113] in order to enhance the dynamical symmetry. Thus, in addition to the Lorentz force, the monopole creates a central force $\mathbf{f}$ deriving from the potential $U(r)$, and the equation of motion reads

$$\mathbf{f} = \mu\frac{d\mathbf{v}}{dt} = \delta\frac{\mathbf{L}}{\mu r^3} - \frac{dU}{dr}\mathbf{u}_r. \tag{129}$$

Taking the vector product of the latter equation with $\mathbf{J} = \mathbf{L} + \delta\mathbf{u}_r$ and using

$$\frac{d\mathbf{u}_r}{dt} = \frac{1}{\mu r^2}\mathbf{L} \wedge \mathbf{u}_r, \tag{130}$$

we obtain

$$\frac{d\mathbf{v}}{dt} \wedge \mathbf{J} - \left(r^2\frac{dU}{dr} + \frac{\delta^2}{mr}\right)\frac{d\mathbf{u}_r}{dt} = \mathbf{0}. \tag{131}$$

If the coefficient of $d\mathbf{u}_r/dt$ is equal to a constant γ, that is, if

$$U(r) = -\frac{\gamma}{r} + \frac{\delta^2}{2\mu r^2}, \tag{132}$$

then a direct integration of Equation (131) provides the following invariant Laplace-like vector:

$$\mathbf{A} = \mathbf{v} \wedge \mathbf{J} - \gamma\mathbf{u}_r = \mathbf{v} \wedge \mathbf{L} - \delta\frac{\mathbf{L}}{\mu r} - \gamma\mathbf{u}_r. \tag{133}$$

8.2. Quantum Mechanical MIC–Kepler Problem

The integrable MIC–Kepler system was constructed by Zwanziger [112] and rediscovered by McIntosh and Cisneros [113]. This system is described by the Hamiltonian:

$$H_0 = \frac{\hbar^2}{2\mu}(i\nabla + s\mathbf{A})^2 + \frac{\hbar^2 s^2}{2\mu r^2} - \frac{\gamma}{r}, \tag{134}$$

where

$$\nabla \wedge \mathbf{A} = \frac{\mathbf{r}}{r^3}. \tag{135}$$

Its distinctive peculiarity is the hidden symmetry given by the following constants of motion:

$$I = \frac{\hbar}{2\mu}[(i\nabla + s\mathbf{A}) \wedge \mathbf{J} - \mathbf{J} \wedge (i\nabla + s\mathbf{A})] + \gamma\frac{\mathbf{r}}{r}, \tag{136}$$

with

$$\mathbf{J} = -\hbar(i\nabla + s\mathbf{A}) \wedge \mathbf{r} + \frac{\hbar s\mathbf{r}}{r}. \tag{137}$$

These constants of motion, together with the Hamiltonian, form the quadratic symmetry algebra of the Coulomb problem. The operator $\mathbf{J}$ defines the angular momentum of the system, while the operator $\mathbf{I}$ is the analog of the Runge–Lenz vector. For the negative values of energy, the constants of motion form the $so(4)$ algebra, whereas for positive values of energy, they build the $so(3,1)$ one. Due to the hidden symmetry, the MIC–Kepler

problem could be factorized in a few coordinate systems, e.g., in the spherical and parabolic ones. Hence, the MIC–Kepler system is a generalization of the Coulomb problem in the presence of a Dirac monopole. It can be considered as a one-parameter deformation family of the standard Kepler problem with the property that it retains its dynamical symmetries. Physically, the deformation parameter δ can be interpreted as the magnetic charge of the particle at rest and measures the pitch of the cone on which the trajectory lies. Actually, its genuine mathematical interpretation is as a cohomology class [114] of the symplectic structure [115]. The global symmetry group of the problem is either $SO(4)$, $E(3)$, or $SO(3,1)$, depending on whether the energy is negative, zero, or positive. The motion obeys the three Kepler laws. The monopole number s satisfies Dirac's charge quantization rule, $s = 0, \pm 1/2, \pm 1, \cdots$. The MIC–Kepler system could be constructed by the reduction of the four-dimensional isotropic oscillator by the use of the so-called Kustaanheimo–Stiefel transformation (see Section 4.2), both on classical and quantum mechanical levels [116–119]. In a similar way, reducing the two- and eight- dimensional isotropic oscillator, one can obtain the two- [120,121] and five-dimensional [122–124] analogs of the MIC–Kepler system. An infinitely thin solenoid providing the system the spin $1/2$ plays the role of the monopole in the two-dimensional case, whereas, in the five-dimensional case, this role is performed by the $SU(2)$ Yang monopole [125], endowing the system with the isospin. All the above-mentioned systems have Coulomb symmetries and can be solved in spherical and parabolic coordinates, both in the discrete and continuous parts of the energy spectra [126–128]. Finally, it is worth mentioning that there are generalizations of MIC–Kepler systems on a three-dimensional sphere [129].

9. Conclusions

In this review, we discussed the importance of invariant vectors in atomic physics, such as the Runge–Lenz vector, the Redmond vector in the presence of an electric field, and the Landau–Avron–Sivardière vector when the system is subject to a magnetic field. The supergeneralized vector for the two-center problem is probably the most-important recent result on the subject. The existence of constants of motion in the charge-dyon system was also briefly introduced. It is worth mentioning that Yoshida [130] discussed the main known ways of generalizing the Runge–Lenz vector [131,132]. De Castro Moreira generalized the Landau vector in some physical situations where it is possible to define a "potential" linear momentum [133]. From a more-general viewpoint, the author discussed the conditions for the introduction of the concept of a "generalized" linear (angular) momentum in analogy with the concept of mechanical energy. Oks reviewed classical studies of the oscillatory–precessional motion of an electron in the field of an electric dipole (the latter representing the polar molecule) with or without external magnetic or electric fields [134]. In future work, we plan to discuss the case of the anisotropic harmonic oscillator and, especially, its connections with the effect of an external electric field on the energy levels of a hydrogen atom [135,136].

Funding: This research received no external funding.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: The data presented in this study are available upon request from the corresponding author. The data are not publicly available due to privacy and ethical restrictions.

Acknowledgments: I am indebted to Pichai Ramedevi for her wonderful lectures on "Group theory methods in physics" at the Indian Institute of Technology in Bombay. I also would like to thank Alexander Demura for a careful reading of the manuscript and for very useful suggestions.

Conflicts of Interest: The author declares no conflict of interest.

Abbreviations

The following abbreviations are used in this manuscript:

MIC McIntosh and Cisneros

Appendix A. Parabolic Quantum Numbers

Here, the parabolic quantum numbers are defined [137]. The Schrödinger equation for the unperturbed one-electron system can also be separated into parabolic coordinates, a fact related to the accidental degeneracy of level energies with respect to the orbital quantum number ℓ (atomic units are used in the following equation):

$$H_0|nqm\rangle = -\frac{Z^2}{2n^2}|nqm\rangle, \tag{A1}$$

where n is the principal quantum number, m is the orbital magnetic quantum number ($-n+1 \leq m \leq n-1$), and $q = n_1 - n_2$ with $-n+1 \leq m \leq n-1$ is the parabolic (or electric) quantum number depending on two positive integers n_1 and n_2, which obey the equation $n = n_1 + n_2 + |m| + 1$. Each parabolic state $|nqm\rangle$ has a residual degeneracy of two due to the invariance of the Hamiltonian with respect to the sign of the orbital magnetic quantum number. A parabolic state can be represented equivalently as $|nn_1n_2m>$ or $|nqm>$, but the latter form presents the advantage of significantly simplifying the summation over the quantum numbers. Solving for n_1 and n_2, we obtain

$$2n_1 = n - 1 - |m| + q \geq 0 \quad \text{and} \quad 2n_2 = n - 1 - |m| - q \geq 0. \tag{A2}$$

For fixed quantum numbers n and m, the above relations imply that the allowed values of q vary linearly between $-n+1+|m|$ and $n-1-|m|$ with an incremental step of two. Alternatively, for fixed quantum numbers n and q, the allowed values of m vary between $-n+1+|q|$ and $n-1-|q|$ with a step of two. For instance, the total degeneracy of the shell n may be evaluated in parabolic coordinates using the sums:

$$2n^2 = 2\sum_{m=-n+1}^{n-1}\sum_{q=-n+1+|m|}^{n-1-|m|}\zeta(q,m) = 2\sum_{q=-n+1}^{n-1}\sum_{m=-n+1+|q|}^{n-1-|q|}\zeta(q,m) \tag{A3}$$

where the factor of two is due to the degeneracy with respect to the electron spin. The quantity $\zeta(q,m)$, defined as

$$\zeta(q,m) = \frac{1}{2}\left[1-(-1)^{q+m-n}\right] \tag{A4}$$

is used to account for the double-increment over q or m.

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