

Review

Dynamical Symmetries of the H Atom, One of the Most Important Tools of Modern Physics: SO(4) to SO(4,2), Background, Theory, and Use in Calculating Radiative Shifts

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Abstract: Understanding the hydrogen atom has been at the heart of modern physics. Exploring the symmetry of the most fundamental two body system has led to advances in atomic physics, quantum mechanics, quantum electrodynamics, and elementary particle physics. In this pedagogic review, we present an integrated treatment of the symmetries of the Schrodinger hydrogen atom, including the classical atom, the SO(4) degeneracy group, the non-invariance group or spectrum generating group SO(4,1), and the expanded group SO(4,2). After giving a brief history of these discoveries, most of which took place from 1935–1975, we focus on the physics of the hydrogen atom, providing a background discussion of the symmetries, providing explicit expressions for all of the manifestly Hermitian generators in terms of position and momenta operators in a Cartesian space, explaining the action of the generators on the basis states, and giving a unified treatment of the bound and continuum states in terms of eigenfunctions that have the same quantum numbers as the ordinary bound states. We present some new results from SO(4,2) group theory that are useful in a practical application, the computation of the first order Lamb shift in the hydrogen atom. By using SO(4,2) methods, we are able to obtain a generating function for the radiative shift for all levels. Students, non-experts, and the new generation of scientists may find the clearer, integrated presentation of the symmetries of the hydrogen atom helpful and illuminating. Experts will find new perspectives, even some surprises.

Keywords: symmetry; hydrogen atom; group theory; SO(4); SO(4,2); dynamical symmetry; non-invariance group; spectrum generating algebra; Runge-Lenz; Lamb shift

1. Introduction

1.1. Objective of This Paper

This pedagogic review is focused on the symmetries of the Schrodinger nonrelativistic hydrogen atom exclusively to give it the attention that we believe it deserves. The fundamental results of the early work are known and do not need to be derived again. However, having this knowledge permits us to use the modern language of group theory to do a clearer, more focused presentation, and to use arguments from physics to develop the proper forms for the generators, rather than dealing with detailed, mathematical derivations to prove results we know are correct.

There are numerous articles about the symmetry of the Schrodinger hydrogen atom, particularly the SO(4) group of the degenerate energy eigenstates, including discussions from classical perspectives. The spectrum generating group SO(4,1) and the non-invariance group SO(4,2) have been discussed, but, in many fewer articles, often in appendices, with different bases for the representations. For example, numerous papers employ Schrodinger wave functions in parabolic coordinates, not

with the familiar nlm quantum numbers, often with the emphasis on the details of the mathematical structures, not the physics, and with the emphasis on the potential role of the symmetry in elementary particle physics. Generators may be expressed in complex and unfamiliar terms, for example, in terms of the raising and lowering operators for quantum numbers characteristic of parabolic coordinates. Other approaches involve regularizing Schrodinger's equation by, for example, multiplying by r . The approach results in generators that are not always Hermitian or manifestly Hermitian, and the need for nonstandard inner products. Indeed, most of the seminal articles do not have the words "hydrogen atom" in the title but are focused on the prize down the road, understanding what was called at the time "the elementary particle zoo".

Yet, these foundational articles and books taken together present the information we have about the symmetry of the H atom, of which experts in the field are aware. On the other hand, to the non-expert, the student, or a researcher new to the field, it does not appear that the relevant information is in a form that is conveniently accessible. Since the hydrogen atom is the most fundamental physical system with an interaction, whose exploration and understanding has led to much of the progress in atomic physics, quantum physics, and quantum electrodynamics, we believe that a comprehensive treatment is warranted and, since most of the relevant papers were published four decades ago, is timely. Many younger physicists may not be acquainted with these results.

Unlike in a number of the foundational papers, here the operators are all Hermitian, and given in terms of the canonical position and momentum variables in the simplest forms. The transformations they generate are clearly explained, and we provide brief explanations for the group theory used in the derivations.

In most papers, a separate treatment for bound and scattering states is needed. In contrast we are able to clarify and simplify the exposition since we use a set of basis states which are eigenfunctions of the inverse of the coupling constant [1], that include both the bound states and the scattering states in a uniform way, and that employ the usual Cartesian position and momenta, with the usual inner product, with the exact same quantum numbers nlm as the ordinary bound states; a separate treatment for bound and scattering states is not required. In addition, we have two equivalent varieties of this uniform basis, one that is more suitable for momentum space calculations and one more suitable for configuration space calculations. This advantage again allows us to simplify the exposition.

We focus on the utility of group theoretic methods using our representation and derive expressions for the unitary transformation of group elements and some new results that allow for us to readily compute the first order radiative shift (Lamb shift) of a spinless electron, which accounts for about 95% of the total shift. This approach allows for us to obtain a generating function for the shifts for all energy levels. For comparison, we derive an expression for the Bethe log.

In summary, we present a unified treatment of the symmetries of the Schrodinger hydrogen atom, from the classical atom to $SO(4,2)$ that focuses on the physics of the hydrogen atom, that gives explicit expressions for all the manifestly Hermitian generators in terms of position and momenta operators in a Cartesian space, that explains the action of the generators on the basis states, which evaluates the Casimir operators characterizing the group representations, and that gives a unified treatment of the bound and continuum states in terms of wave functions that have the same quantum numbers as the ordinary bound states. We give an example of the use of $SO(4,2)$ in a practical application, the computation of the first order radiative shift in the hydrogen atom.

Hopefully, students and non-experts and the new generation of scientists will find this review helpful and illuminating, perhaps motivating some to use these methods in various new contexts. Senior researchers will find new perspectives, even some surprises and encouragements.

1.2. Outline of This Paper

In the remainder of Section 1 we give a brief historical account of the role of symmetry in quantum mechanics and of the work done in order to explore the symmetries of the Schrodinger hydrogen atom.

In Section 2, we provide some general background observations regarding symmetry groups and non-invariance groups and discuss the degeneracy groups for the Schrodinger, Dirac, and Klein-Gordon equations. We also introduce the uncommon $(Z\alpha)^{-1}$ eigenstates that allow us to treat the bound and scattering states in a uniform way, using the usual quantum numbers. In Section 3, the classical equations of motion of the nonrelativistic hydrogen atom in configuration and momentum space are derived from symmetry considerations. The physical meaning of the symmetry transformations and the structure of the degeneracy group $SO(4)$ is discussed. In Section 4, we discuss the symmetries using the language of quantum mechanics. In order to display the symmetries in quantum mechanics in the most elegant and uniform way we use a basis of eigenstates of the inverse of the coupling constant $(Z\alpha)^{-1}$. In Section 5 we discuss these wave functions in momentum and configuration space, how they transform and their classical limit for Rydberg states.

In Section 6, we discuss the noninvariance or spectrum generating group of the hydrogen atom $SO(4,1)$ and relate it to the conformal group in momentum space. In Section 7, the enlarged spectrum generating group $SO(4,2)$ is introduced, with a discussion of the physical meaning of the generators. All of the physical states together form a basis for a unitary irreducible representation of these noninvariance groups. We derive manifestly Hermitian expressions in terms of the momentum and position canonical variables for the generators of the group transformations and obtain the values possible for the Casimir operators. We discuss the important subgroups of $SO(4,2)$.

In Section 8, we use the group theory of $SO(4,2)$ to determine the radiative shifts in energy levels due to the interaction of a spinless electron with its own radiation field, or equivalently with the quantum vacuum. In the nonrelativistic or dipole approximation the level shift contains a matrix element of a rotation operator of an $O(1,2)$ subgroup of the group $SO(4,2)$. We can sum this over all states, obtaining the character of the representation, yielding a single integral that is a generating function for the radiative shift for any level in the nonrelativistic or dipole approximation. A brief conclusion follows.

1.3. Brief History of Symmetry in Quantum Mechanics and Its Role in Understanding the Schrodinger Hydrogen Atom

The hydrogen atom is the fundamental two-body system and perhaps the most important tool of atomic physics and the continual challenge is to continually improve our understanding of the hydrogen atom and to calculate its properties to the highest accuracy possible. The current QED theory is the most precise of any physical theory [2]:

The study of the hydrogen atom has been at the heart of the development of modern physics...theoretical calculations reach precision up to the 12th decimal place...high resolution laser spectroscopy experiments...reach to the 15th decimal place for the 1S–2S transition...The Rydberg constant is known to six parts in 10^{12} [2,3]. Today, the precision is so great that measurement of the energy levels in the H atom has been used to determine the radius of the proton.

Continual progress in understanding the properties of the hydrogen atom has been central to progress in quantum physics [4]. Understanding the atomic spectra of the hydrogen atom drove the discovery of quantum mechanics in the 1920's. The measurement of the Lamb shift in 1947 and its explanation by Bethe in terms of atom's interaction with the quantum vacuum fluctuations ushered in a revolution in quantum electrodynamics [5–7]. Exploring the symmetries of the hydrogen atom has been an essential part of this progress. Symmetry is a concept that has played a broader role in physics in general; for example, in understanding the dynamics of the planets, atomic, and molecular spectra, and the masses of elementary particles.

When applied to an isolated system, Newton's equations of motion imply the conservation of momentum, angular momentum and energy. But the significance of these conservation laws was not really understood until 1911 when Emily Nother established the connection between symmetry

and conservation laws [8]. Rotational invariance in a system results in the conservation of angular momentum; translational invariance in space results in conservation of momentum; and translational invariance in time results in the conservation of energy. We will discuss Noether's Theorem in more detail in Section 2.

Another critical ingredient of knowledge, on which Noether based her proof, was the idea of an infinitesimal transformation, such as a infinitesimal rotation generated by the angular momentum operators in quantum mechanics. These ideas of infinitesimal transformations originated with the Norwegian mathematician Sophus Lie who was studying differential equations in the latter half of the nineteenth century. He studied the collection of infinitesimal transformations that would leave a differential equation invariant [9]. In 1918, German physicist and mathematician Hermann Weyl, in his classic book with the translated title "The Theory of Groups and Quantum Mechanics", would refer to this collection of differential generators leaving an operator invariant as a linear algebra, ushering in a little of the terminology of modern group theory [10]. Still this was a very early stage in understanding the role of symmetry in the language of quantum theory. When he introduced the new idea of a commutator on page 264, he put the word "commutator" in quotes. In the preface Weyl made a prescient observation: "... the essence of the new Heisenberg-Schrodinger-Dirac quantum mechanics is to be found in the fact that there is associated with each physical system a set of quantities, constituting a non-commutative algebra in the technical mathematical sense, the elements of which are the physical quantities themselves".

A few years later Eugene Wigner published in German, "Group Theory and Its Application to the Quantum Mechanics of Atomic Spectra [11]". One might ask why was this classic not translated into English until 1959. In the preface to the English edition, Prof. Wigner recalled: "When the first edition was published in 1931, there was a great reluctance among physicists toward accepting group theoretical arguments and the group theoretical point of view. It pleases the author that this reluctance has virtually vanished..." It was the application of group theory in particle physics in the early sixties, such as SU(3) and chiral symmetry, which reinvigorated interest in Wigner's book and the field in general. In the 1940's, Wigner and Bargmann developed the representation theory of the Poincare group that later provided an infrastructure for the development of relativistic quantum mechanics [11,12].

The progress in understanding the symmetries of the hydrogen atom, in particular, has some parallels to the history of symmetry in general: there were some decades of interest but after the 1930's interest waned for about three decades in both fields, until stimulated by the work on symmetry in particle physics.

Probably, the first major advance in understanding the role of symmetry in the classical treatment of the Kepler problem after Newton's discovery of universal gravitation, elliptical orbits, and Kepler's Laws, was made two centuries ago by Laplace when he discovered the existence of three new constants of the motion in addition to the components of the angular momentum [13]. These additional conserved quantities are the components of a vector which determines the direction of the perihelion of the motion (point closest to the focus) and whose magnitude is the eccentricity of the orbit. The Laplace vector was later rediscovered by Jacobi and has since been rediscovered numerous times under different names. Today it is generally referred to as the Runge-Lenz vector. However, the significance of this conserved quantity was not well understood until the nineteen thirties.

In 1924, Pauli made the next major step forward in understanding the role of symmetry in the hydrogen atom [14]. He used the conserved Runge-Lenz vector \mathbf{A} and the conserved angular momentum vector \mathbf{L} to solve for the energy spectrum of the hydrogen atom by purely algebraic means, a beautiful result, yet he did not explicitly identify that \mathbf{L} and \mathbf{A} formed the symmetry group SO(4) corresponding to the degeneracy. At this time, the degree of degeneracy in the hydrogen energy levels was believed to be n^2 for a state with principal quantum number n , clearly greater than the degeneracy due to rotational symmetry which is $(2l + 1)$. The n^2 degeneracy arises from the possible values of the angular momentum $l = 0, 1, 2, \dots, n - 1$, and the $2l + 1$ values of the angular momentum along the

azimuthal axis $m = -l, -l + 1, \dots, 0, 1, 2, l + 1$. The additional degeneracy was referred to as “accidental degeneracy [15].”

Six years after Pauli’s paper, Hulthen used the new Heisenberg matrix mechanics to simplify the derivation of the energy eigenvalues of Pauli by showing that the sum of the squares $\mathbf{L}^2 + \mathbf{A}^2$ could be used to express the Hamiltonian and so could be used to find the energy eigenvalues [16]. In a one sentence footnote in this three page paper, Hulthen gives probably the most important information in his paper: Prof. Otto Klein, who had collaborated for years with Sophus Lie, had noticed that the two conserved vectors formed the generators of the Lorentz group, which we can describe as rotations in four dimensions, the fourth dimension being time. This is the non-compact group $SO(3,1)$, the special orthogonal group in four dimension whose transformations leave the magnitude $g_{\mu\nu}z^\mu z^\nu = -t^2 + x^2 + y^2 + z^2$ unchanged [17]. Klein’s perceptive observation triggered the introduction of group theory to understanding the hydrogen atom.

About a decade later, in 1935, the Russian physicist Vladimir Fock published a major article in *Zeitschrift für Physik*, the journal in which all the key articles about the hydrogen atom cited were published [18]. He transformed Schrodinger’s equation for a given energy eigenvalue from configuration space to momentum space, and did a stereographic projection onto a unit sphere, and showed that the bound state momentum space wave functions were spherical harmonics in four dimensions. He stated that this showed that rotations in four dimensions corresponded to the symmetry of the degenerate bound state energy levels in momentum space, realizing the group $SO(4)$, the group of special orthogonal transformations which leaves the norm of a four-vector $U_0^2 + U_1^2 + U_2^2 + U_3^2$ constant. By counting the number of four-dimensional spherical harmonics Y_{nlm} in momentum space ($m = -l, -l + 1, \dots, 0, 1, \dots, l$, where the angular momentum l can equal $l = n - 1, n - 2, \dots, 0$), he determined that the degree of degeneracy for the energy level characterized by the principal quantum number n was n^2 . It is interesting that Fock did not cite the work by Pauli, implying the four dimensional rotational symmetry in configuration space. Fock also presented some ideas about using this symmetry in calculating form factors for atoms.

A year later, the German-American mathematician and physicist Valentine Bargmann showed that for bound states ($E < 0$) Pauli’s conserved operators, the angular momentum \mathbf{L} and the Runge–Lenz vector \mathbf{A} , obeyed the commutation rules of the $SO(4)$ [12]. His use of commutators was so early in the field of quantum mechanics, that Bargmann explained the square bracket notation he used for a commutator in a footnote [19]. He gave differential expression for the operators, adapting the approach of Lie generators in the calculation of the commutators. He linked solutions to Schrodinger’s equation in parabolic coordinates to the existence of the conserved Runge–Lenz vector and was thereby able to establish the relationship of Fock’s results to the algebraic representation of $SO(4)$ for bound states implied by Fock and Pauli [12]. He also pointed out that the scattering states ($E > 0$) could provide a representation of the group $SO(3,1)$. In a note at the end of the paper, Bargmann, who was at the University in Zurich, thanked Pauli for pointing out the paper of Hulthen and the observation by Klein that the Lie algebra of \mathbf{L} and \mathbf{A} was the same as the infinitesimal Lorentz group, which is how he referred to a Lie algebra. Bargmann’s work was a milestone demonstrating the relationship of symmetry to conserved quantities and it clearly showed that to fully understand a physical system one needed to go beyond the usual ideas of geometrical symmetry. This work was the birth, in 1936, without much fanfare, of the idea of dynamical symmetry.

Little attention was paid to these developments until the 1960’s, when interest arose primarily because of the applications of group theory in particle physics, particularly modeling the mass spectra of hadrons. Particle physicists were faced with the challenge of achieving a quantitative description of hadron properties, particularly the mass spectra and form factors, in terms of quark models. Since little was known about quark dynamics they turned to group-theoretical arguments, exploring groups like $SU(3)$, chiral $U(3) \times U(3)$, $U(6) \times U(6)$, etc. The success of the eight-fold way of $SU(3)$ (special unitary group in three dimensions) of American physicist Murray Gell-Mann in 1962 brought attention to the

use of symmetry considerations and group theory as tools for exploring systems in which one was unsure of the exact dynamics [20].

In 1964, three decades after Fock's work, American physicist Julian Schwinger published a paper using $SO(4)$ symmetry to construct a Green function for the Coulomb potential, which he noted was based on a class he taught at Harvard in 1949 [21]. The publication was a response to the then current emphasis on group theory and symmetry, which led to, as Israeli physicist Yuval Ne'eman described it, "'the great-leap-forward' in particle physics during the years 1961–1966 [22]". Some of the principal researchers leading this effort were Ne'eman [23], Gell-Mann [20,24,25], Israeli physicist Y. Dothan [26], Japanese physicist Yochiri Nambu [27], and English-American Freeman Dyson [28]. Advantage was taken of the mathematical infrastructures of group theory developed years earlier [10–12,29,30].

Interest was particularly strong in systems with wave equations with an infinite number of components, which characterize non-compact groups. In about 1965, this interest in particle physics gave birth to the identification of $SO(4,1)$ and $SO(4,2)$ as Spectrum Generating Algebras that might serve as models for hadronic masses. The hydrogen atom was seen as a model to explore the infinite dimensional representations of non-compact groups. The first mention of $SO(4,1)$ was by Barut, Budini, and Fronsdal [31], where the H atom was presented as an illustration of a system characterized by non-compact representation, and so comprising an infinite number of states. The first mention of a six dimensional symmetry, referred to as the "non-compact group $O(6)$ ", appears to be by the Russian physicists I. Malin and V. Man'ko of the Moscow Physico-technical Institute [32]. In a careful three page paper, they showed that all of the bound states of the H atom energy spectrum in Fock coordinates provided a representation of this group, and they calculated the Casimir operators for their symmetric tensor representation in parabolic coordinates.

Very shortly thereafter, Turkish-American theoretical physicist Asim Barut and his student at University of Colorado, German theoretical physicist Hagen Kleinert, showed that including the dipole operator er as a generator led to the expansion of $SO(4,1)$ to $SO(4,2)$, and that all the bound states of the H atom formed a representation of $SO(4,2)$ [33]. This allowed them to calculate dipole transition matrix elements algebraically. They give a position representation of the generators based on the use of parabolic coordinates. The generators of the transformations are given in terms of the raising and lowering operators for the quantum numbers for solutions to the H atom in parabolic coordinates. The dilation operator is used to go from one $SO(4)$ subspace with one energy to a $SO(4)$ subspace with different energy and it has a rather complicated form. They also used $SO(4,2)$ symmetry to compute form factors [34].

The papers of the Polish-American physicist Myron Bander and French physicist Claude Itzakson published in 1966, when both were working at SLAC (Stanford Linear Accelerator in California) provide the first mathematically rigorous and "succinct" review of the $O(4)$ symmetry of the H atom and provide an introduction to $SO(4,1)$ [35,36], which is referred to as a spectrum generating algebra SGA, meaning that it includes generators that take the basis states from one energy level to another. They use two approaches in their mathematical analysis, the first is referred to as "the infinitesimal method," based on the two symmetry operators, L and A and the $O(4)$ group they form, and the other, referred to as the "global method", first done by Fock, converts the Schrodinger equation to an integral equation with a manifest four dimensional symmetry in momentum space. They establish the equivalence of the two approaches by appealing to the solutions of the H atom in parabolic coordinates, and demonstrate that the symmetry operators in the momentum space correspond to the symmetry operators in the configuration space. As they note, the stereographic projection depends on the energy, so the statements for a $SO(4)$ subgroup are valid only in a subspace of constant energy. They then explore the expansion of the $SO(4)$ group to include scale changes so the energy can be changed, transforming between states of different principal quantum number, which correspond to different subspaces of $SO(4)$. To insure that this expansion results in a group, they include other transformations, which results in the the generators forming the conformal group $O(4,1)$. Their mathematical analysis introducing $SO(4,1)$ is based on the projection of a p dimensional space (4 in the case of interest) on a

paraboloid in $p + 1$ dimensions (5 dimensions). In their derivation they treat bound states in their first paper [35] and scattering states in the second paper [36].

As we have indicated the interest in the $SO(4,2)$ symmetry of the Schrodinger equation was driven by a program focused on developing equations for composite systems that had infinite multiplets of energy solutions and ultimately could lead to equations that could be used to predict masses of elementary particles, perhaps using other than four dimensions [27,35–40]. In 1969 Jordan and Pratt showed that one could add spin to the generators A and L , and still form a $SO(4)$ degeneracy group. By defining $J = \frac{1}{2}(L + A) + S$, they showed one could obtain a representation of $O(4,1)$ for any spin s [41].

In their review of the symmetry properties of the hydrogen atom, Bander and Itzakson emphasize this purpose for exploring the group theory of the hydrogen atom [35]:

The construction of unitary representations of non-compact groups that have the property that the irreducible representations of their maximal subgroup appear at most with multiplicity one is of certain interest for physical applications. The method of construction used here in the Coulomb potential case can be extended to various other cases. The geometrical emphasis may help to visualize things and provide a global form of the transformations.

Special attention was also given to solutions for the hydrogen atom from the two body Bethe-Salpeter equation for a proton and electron interacting by a Coulomb potential, since the symmetry was that of a relativistic non-compact group [27,40,42,43].

Finally in 1969, five years after it was published, Schwinger's form of the Coulomb Green's function based on the $SO(4)$ symmetry was used to calculate the Lamb shift by Michael Lieber, one of Schwinger's students at Harvard [21,44]. A year later, Robert Huff, a student of Christian Fronsdal at UCLA, focused on the use of the results from $SO(4,2)$ group theory to compute the Lamb shift [45]. He converted the conventional expression for the Lamb shift into a matrix element containing generators of $SO(4,2)$, and was able to perform rotations and scale changes to simplify and evaluate the matrix elements. After clever mathematical manipulation, he obtained an expression for the Bethe log in terms of a rapidly terminating series for the level shifts. He provided an appendix with a brief discussion of the fundamental of $SO(4,2)$ representations for the H atom, showing the expressions for the three generators needed to express the Schrodinger equation.

In the next few years, the researchers published a few mathematically oriented papers [41,46–50], a short book [51] dealing with the symmetries of the Coulomb problem, and a paper by Barut presenting a $SO(4,2)$ formulation of symmetry breaking in relativistic Kepler problems, with a 1 page summary of the application of $SO(4,2)$ for the non-relativistic hydrogen atom [34,52]. Bednar published a paper applying group theory to a variety of modified Coulomb potentials, which included some matrix elements of $SO(4,2)$ using hydrogen atom basis states with quantum numbers nlm [53]. There also was interest in application of the symmetry methods and dynamical groups in molecular chemistry [54] and atomic spectroscopy [55].

In the 1970's, researchers focused on developing methods of group theory and on understanding dynamical symmetries in diverse systems [56–58]. A book on group theory and its applications appeared in 1971 [59]. Barut and his collaborators published a series of papers dealing with the hydrogen atom as a relativistic elementary particle, leading to an infinite component wave equation and mass formula [60–63].

Papers on the classical Kepler problem, the Runge–Lenz vector, and $SO(4)$ for the hydrogen atom have continued to appear over the years, from 1959 to today. Many were published in the 1970's [64–70] and some since 1980, including [71–75]. Papers dealing with $SO(4,2)$ are much less frequent. In 1986 Barut, A. Bohm, and Ne'eman published a book on dynamical symmetries that included some material on the hydrogen atom [76]. In 1986, Greiner and Muller published the second edition of Quantum Mechanics Symmetries, which had six pages on the Hydrogen atom, covering only the $SO(4)$ symmetry [77]. The 2005 book by Gilmore on Lie algebras has 4 pages of homework problems

on the H atom to duplicate results in early papers [78]. The last papers I am aware of that used SO(4,2) were applications in molecular physics [79,80] and more general in scope [81]. Carl Wulfman published a book on dynamical symmetries in 2011, which provides a helpful discussion of dynamical symmetries for the hydrogen atom [82]. He regularizes the Schrodinger equation, essentially multiplying by r , obtaining Sturmian wave functions in parabolic coordinates. This approach allows for him to treat bound and scattering states for SO(4,2) at one time, but requires redefining the inner product, and leads to a non-Hermitian position operator.

1.4. The Dirac Hydrogen Atom

We have focused our discussion on the symmetries of the non-relativistic hydrogen atom described by the Schrodinger equation. Quantum mechanics also describes the hydrogen atom in terms of the relativistic Dirac equation, which we will only discuss briefly in this paper.

The gradual understanding of the dynamical symmetry of the Dirac atom parallels that of the Schrodinger atom, but it has received much less attention, probably because the system has less relevance for particle physics and for other applications. It was known that the rotational symmetry was present and that the equation predicted that the energy depended on the principal quantum number and the quantum number for the total angular momentum j , but not the spin s or orbital angular momentum l separately. This remarkable fact meant that, in some sense, angular momentum contributed the same to the total energy no matter whether it was intrinsic or orbital in origin. This degeneracy is lifted if we include the radiative interactions which leads to the Lamb shift.

In order to understand the symmetry group for the Dirac equation consider that for a given total angular momentum quantum number $J > 0$ there are two degenerate levels for each energy level of the Dirac hydrogen atom: one level has $l = J + 1/2$ and the other has $l = J - 1/2$. Since the l values differ by unity, the two levels have opposite parity. Dirac described a generalized parity operator K , which was conserved. For an operator Λ to transform one degenerate state into the other, it follows that the operator has to commute with J and have parity -1 . This means it has to anticommute with K , and so it is a conserved pseudoscalar operator.

The parity $(-1)^{l+J-1/2}$ is conserved in time, so the states are parity eigenstates. Using the two symmetry operators Λ and K , one can build a SU(2) algebra. If we include the O(3) symmetry due to the conservation of angular momentum, we obtain the full symmetry group $SU(2) \times O(3)$ which is isomorphic to SO(4) for the degeneracy of the Dirac hydrogen atom.

In 1950, M. Johnson and B. Lippman discovered the operator Λ [83]. Further work was done on understanding Λ by Biedenharn [84]. The Johnson–Lippman operator has been rediscovered and reviewed several times over the decades [85–87]. It has been interpreted in the non-relativistic limit as the projection of the Runge–Lenz vector onto the spin angular momentum [87–89]. The SO(4) group can be expanded to include all states, and then the spectrum generating group is SO(4,1) or SO(4,2) depending on the assumptions regarding relativistic properties and the charges present [33,38]. We will not discuss the symmetries of the Dirac H atom further.

2. Background

2.1. The Relationship between Symmetry and Conserved Quantities

The nature of the relationship between symmetry, degeneracy, and conserved operators is implicit in the equation

$$[H, S] = 0 \quad (1)$$

where H is the Hamiltonian of our system, S is a Hermitian operator, and the brackets signify a commutator if we are discussing a quantum mechanical system, or i times a Poisson bracket if we are discussing a classical system. If S is viewed as the generator of a transformation on H , then Equation (1) says the transformation leaves H unchanged. Therefore, we say S is a symmetry operator of H and

leaves the energy invariant. The fact that a non-trivial S exists means that there is a degeneracy. To show this, consider the action of the commutator on an energy eigenstate $|E\rangle$:

$$[H, S]|E\rangle = 0 \quad (2)$$

or

$$H(S|E\rangle) = E(S|E\rangle). \quad (3)$$

If S is nontrivial then $S|E\rangle$ is a different state from $|E\rangle$ but has the same energy eigenvalue. If we label all such degenerate states by

$$|E, m\rangle, m = 1, \dots, N \quad (4)$$

then clearly $S|E, m\rangle$ is a linear combination of degenerate states:

$$S|E, m\rangle = S_{ms}|E, s\rangle. \quad (5)$$

S_{ms} is a matrix representation of S in the subspace of degenerate states. In a classical Kepler system S generates an orbit deformation that leaves H invariant. The existence of a nontrivial S therefore implies degeneracy, in which multiple states have the same energy eigenvalue. We can show that the complete set of symmetry operators for H forms a Lie algebra by applying Jacobi's identity to our set of Hermitian operators S_i :

$$[H, S_i] = 0, \quad i = 1, \dots, L. \quad (6)$$

$$[S_j, [H, S_i]] + [S_i, [S_j, H]] + [H, [S_i, S_j]] = 0 \quad (7)$$

so

$$[H, [S_i, S_j]] = 0. \quad (8)$$

Therefore, the commutator of S_i and S_j is a symmetry operator of H . Either the commutator is a linear combination of all the symmetry operators $S_i, i = 1, \dots, L$:

$$[S_i, S_j] = C_{ij}^k S_k \quad (9)$$

or the commutator defines a new symmetry operator which we label S_{L+1} . We repeat this procedure until the Lie algebra closes as in Equation (9).

By exponentiation, we assume that we can locally associate a group of unitary transformations

$$e^{iS_i a^i} \quad (10)$$

for real a^i with our Lie algebra and so conclude that a group of transformations exists under which the Hamiltonian is invariant [90]. We call this the symmetry or degeneracy group of H . Our energy eigenstates states form a realization of this group.

It is possible to form scalar operators, called Casimir operators, from the generators of the group that commute with all the generators of the group, and, therefore, have numerical values. The values of the Casimir operators characterize the particular representation of the group. For example, for the rotation group in three dimensions, the generators are $L = (L_1, L_2, L_3)$ and the quantity $L^2 = L(L + 1)$ commutes with all of the generators. L can have any positive integer value for a particular representation. The Casimir operator for $O(3)$ is L^2 . The number of Casimir operators that characterize a group is called the rank of the group. $O(3)$ is rank 1 and $SO(4,2)$ is rank 3.

Now let us consider Equation (1) in a different way. If we view H as the generator of translations in time, then we recall that the total time derivative of an operator S_i is

$$\frac{dS_i}{dt} = \frac{i}{\hbar} [H, S_i] + \frac{\partial S_i}{\partial t} \quad (11)$$

where the commutator and the partial derivative give the implicit and explicit time dependence respectively. Provided that the symmetry operators have no explicit time dependence ($\frac{\partial S_i}{\partial t} = 0$), then Equation (11) implies that Equation (1) means that the symmetry operators S are conserved in time and $\frac{dS_i}{dt} = 0$. Conversely, we can say that conserved Hermitian operators with no explicit time dependence are symmetry operators of H . This very important relationship between conserved Hermitian operators and symmetry was first discovered by German mathematician Emmy Nother in 1917, and is called Nother's Theorem [8,91–95].

2.2. Non-Invariance Groups and Spectrum Generating Group

As we have discussed, the symmetry algebra contains conserved generators S_i that transform one energy eigenstate into a linear combination of eigenstates all with the same energy. In order to illustrate with hydrogen atom eigenstates:

$$S_i |nlm\rangle = \sum_{l',m'} S_{nlm}^{n'l'm'} |n'l'm'\rangle \quad (12)$$

where $|nlm\rangle$ refers to a state with energy E_n , angular momentum $l(l+1)$ and $l_z = m$.

A non-invariance algebra contains generators D_i that can be used to transform one energy eigenstate $|nlm\rangle$ into a linear combination of other eigenstates, with the same or a different energy, different angular momentum l , and different azimuthal angular momentum m :

$$D |nlm\rangle = \sum_{n',l',m'} D_{nlm}^{n'l'm'} |n'l'm'\rangle. \quad (13)$$

Because the set of energy eigenstates is complete, the action of the most general operator would be identical to that shown to Equation (13). Therefore this requirement alone is not sufficient to select the generators needed.

The goal is to expand the degeneracy group with its generators S_i into a larger group, so that some or all of the eigenstates form a representation of the larger group with the degeneracy group as a subgroup. Thus, we need to add generators G_i , such that the combined set of generators

$$\{S_i, G_j; \text{ for all } i, j\} \equiv \{D_k; \text{ for all } k\}$$

forms an algebra that closes

$$[D_i, D_j] = i\epsilon_{ijk} D_k. \quad (14)$$

This is the Lie algebra for the expanded group. To illustrate with a specific example, consider the $O(4)$ degeneracy group with six generators [96]. One can expand the group to $O(5)$ or $O(4,1)$ which has ten generators by adding a four-vector of generators. One component might be a scalar and the other three a three-vector. The question then is can some or all of the energy eigenstates provide a representation of $O(5)$? If so, then this would be considered a non-invariance group. The group might be expanded further in order to obtain generators of a certain type or to include all states in the representation. For the H atom the generators D_i can transform between different energy eigenvalues meaning between eigenfunctions with different principal quantum numbers.

Another way to view the expansion of the Lie algebra of the symmetry group is to consider additional generators D_i that are constants in time [97] but do not commute with the Hamiltonian so

$$\frac{dD_i}{dt} = 0 = \frac{i}{\hbar} [H, D_i] + \frac{\partial D_i}{\partial t}.$$

If we make the additional assumption that the time dependence of the generators is harmonic

$$\frac{\partial^2 D_i(t)}{\partial t^2} = \omega_{in} D_n(t).$$

then generators D_i , and the first and second partial derivatives with respect to time could close under commutation, forming an algebra. This approach does not tell us what generators to add, but, as we demonstrate in Section 7.5, it does reflect the behavior of the generators that have been added to form the spectrum generating group in the case of the hydrogen atom.

We may look for the largest set of generators D_i , which can transform the set of solutions into itself in an irreducible fashion (meaning no more generators than necessary). These generators form the Lie algebra for the non-invariance or spectrum generating algebra [32,98]. If the generators for the spectrum generating algebra can be exponentiated, then we have a group of transformations for the spectrum generating group. The corresponding wave functions form the basis for a single irreducible representation of this group. This group generates transformations among all the solutions for all energy eigenvalues and it is called the Spectrum Generating Group [99]. For the H atom, SO(4,1) is a spectrum generating group or non-invariance group, which can be reduced to contain one separate SO(4) subgroup for each value of n .

To get a representation of SO(4,1), we need an infinite number of states, which we have for the H atom. This group has been expanded by adding a five vector to form SO(4,2) because the additional generators can be used to express the Hamiltonian and the dipole transition operator. The group SO(p,q) is the group of orthogonal transformations that preserve the quantity $X = x_1^2 + x_2^2 + \dots + x_p^2 - \dots - x_{p+q}^2$, which may be viewed as the norm or a p+q-dimensional vector in a space that has a metric with p plus signs and q minus signs. The letters SO stand for special orthogonal, meaning the orthogonal transformations have determinant equal to +1.

In terms of group theory, there is a significant difference between a group like SO(4) and SO(4,1). SO(4) and SO(3) are both compact groups, while SO(4,1) and SO(4,2) are non-compact groups. A continuous group G is compact if each function $f(g)$, continuous for all elements g of the group G, is bounded. The rotation group in three dimensions O(3), which conserves the quantity $r^2 = x_1^2 + x_2^2 + x_3^2$, is an example of a compact group.

For a non-compact group, consider the Lorentz group O(3,1) of transformations to a coordinate system moving with a velocity v . The transformations preserve the quantity $r^2 - c^2t^2$. The matrix elements of the Lorentz transformations are proportional to $1/\sqrt{1-\beta^2}$, where $\beta = v/c$, and are not bounded as $\beta \rightarrow 1$. Therefore, r and ct may increase without bound, while the difference of the squares remains constant. Unitary representations of non-compact groups are infinite dimensional, for example, the representation of the non-invariance group SO(4,1) has an infinite number of states. Unitary representations of compact groups can be finite dimensional, for example, our representation of SO(4) for an energy level E_n has dimension n^2 .

In the nineteen sixties and later, the spectrum generating group was of special interest in particle physics, because it was believed it could provide guidance where the precise particle dynamics were not known. The hydrogen atom provided a physical system as a model. Because the application was in particle physics, there was less interest in exploring representations in terms of the dynamical variables for position and momentum.

The expansion of the group from SO(4,1) to SO(4,2) was motivated by the fact that the additional generators could be used to write Schrodinger's equation entirely in terms of the generators, and to express the dipole transition operator. This allowed for algebraic techniques and group theoretical methods to be used to obtain solutions, calculate matrix elements, and other quantities [33,38].

2.3. Basic Idea of Eigenstates of $(Z\alpha)^{-1}$

We briefly introduce the idea behind these states, since they are unfamiliar [1]. The full derivation is given in Section 4. Schrodinger's equation in momentum space for bound states can be written as

$$\left[p^2 + a^2 - \frac{2mZ\alpha}{r} \right] |a\rangle = 0.$$

where $a^2 = -2mE > 0$ and $Z\alpha$ is the coupling constant, which we will now view as a parameter. This equation has well behaved solutions for certain discrete eigenvalues of the energy or a^2 , namely

$$a_n^2 = -2mE_n$$

where $E_n = -\frac{1}{2} \frac{m(Z\alpha)^2}{n^2}$. We can write the eigenvalue condition equivalently as

$$\left(\frac{a_n}{mZ\alpha}\right) = \frac{1}{n}.$$

This last equation shows that solutions exist for certain values a_n of the RMS momentum a . To introduce eigenstates of $(Z\alpha)^{-1}$ we simply take a different view of this last equation and say that instead of quantizing a and obtaining a_n , we imagine that we quantize $(Z\alpha)^{-1}$, let a remain unchanged, obtaining

$$\frac{a}{m(Z\alpha)_n} = \frac{1}{n}.$$

Accordingly, now we can interpret Schrodinger's equation as an eigenvalue equation that has solutions for certain values of $(Z\alpha)^{-1}$ namely

$$(Z\alpha)_n^{-1} = \frac{m}{an}.$$

We have the same equation but can view the eigenvalues differently but equivalently. Instead of quantizing a we quantize $(Z\alpha)^{-1}$.

This roughly conveys the basic idea of eigenstates of the inverse of $(Z\alpha)$, but this simplified version does at all reveal the advantages of our reformulation because we have left the Hamiltonian unchanged. In Section 4, we transform Schrodinger's equation to an eigenvalue equation in a , so that the kernel is bounded, which means that there are no states with $E > 0$, no scattering states, and all states have the usual quantum numbers. Other important advantages to this approach will also be discussed.

2.4. Degeneracy Groups for Schrodinger, Dirac and Klein-Gordon Equations

The degeneracy groups for the bound states described by the different equations of the hydrogen atom are summarized in Table 1. The degeneracy (column 2) is due to the presence of conserved operators which are also symmetry operators (column 3), forming a degeneracy symmetry group (column 4). For example, The symmetry operators for the degeneracy group in the Schrodinger hydrogen atom are the angular momentum \mathbf{L} and the Runge-Lenz vector \mathbf{A} . In Section 3, it will be shown that together these are the generators for the direct product $SO(3) \times SO(3)$ which is isomorphic to $SO(4)$. Column 5 gives the particular representations present. These numbers are the allowed values of the Casimir operators for the group and they determine the degree of degeneracy (last column) and the corresponding allowed values of the quantum numbers for the degenerate states.

The Casimir operators, which are made from generators of the group, have to commute with all of the members of the group, and the only way this can happen is if they are actually constants for the representation. The generators are formed from the dynamical variables of the H atom, so the Casimir operators are invariants under the group composed of the generators, and their allowed numerical values reflect the underlying physics of the system and determine the appropriate representations of the group [9,82,100]. For example, L^2 is the Casimir operator for the group $O(3)$ and can have the values $l(l+1)$. The relationship between Casimir operators and group representations is true for all irreducible group representations, including the $SO(4)$ degeneracy group, as well as the spectrum generating group $SO(4,2)$ [43,53].

For the Schrodinger equation, there are n^2 states $|nlm\rangle$ that form a representation of the degeneracy group $SO(4)$ formed by \mathbf{L} and \mathbf{A} . These states correspond to the principal quantum number n , the n

different values of the angular momentum quantum number l , and $2l + 1$ different values of the z component of the angular momentum $l_z = m$.

For the Dirac equation, the $2(2J + 1)$ dimensional degeneracy group for bound states is realized by the total angular momentum operator \mathbf{J} , the generalized parity operator K , and the Johnson–Lippman operator Λ , which together form the Lie algebra for $SO(4)$.

For the fully relativistic Klein–Gordon equation, only the symmetry from rotational symmetry survives, leading to the degeneracy group $O(3)$. If the V^2 term, the four-potential term squared is dropped in a semi-relativistic approximation as we describe in Section 4.3, then the equation can be rewritten in the same form as the non-relativistic Schrodinger equation, so a Runge–Lenz vector can be defined and the degeneracy group is again $SO(4)$.

Table 1. In the table $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ is the orbital angular momentum; \mathbf{A} is the Runge–Lenz vector; $\mathbf{J} = \mathbf{L} + \sigma/2$ is the total angular momentum; K is the generalized parity operator; Λ is the conserved pseudoscalar operator.

Degeneracy Groups for Bound States in a Coulomb Potential					
Equation	Degeneracy	Conserved Quantities	Degeneracy Group	Representation	Dimension
Schrodinger	E indep. of l, l_z	\mathbf{A}, \mathbf{L}	$SO(4)$	$(\frac{n-1}{2}, \frac{n-1}{2})$	n^2
Klein-Gordon	E indep. of l_z	\mathbf{L}	$O(3)$	Casimir op. is $l(l+1)$	$2l+1$
Klein-Gordon without V^2 term	E indep. of l, l_z	\mathbf{A}, \mathbf{L}	$SO(4)$	$(\frac{n-1}{2}, \frac{n-1}{2})$	n^2
Dirac	E depends on J, n only	Λ, K, \mathbf{J}	$SO(4)$	$(1/2, J)$	$2(2J+1)$

3. Classical Theory of the H Atom

In order to discuss orbital motion and the continuous deformation of orbits we give this discussion in terms of classical mechanics, but much of it is valid in terms of the Heisenberg representation of quantum mechanics if the Poisson brackets are converted to commutators, as will be discussed in Section 4.

For a charged particle in a Coulomb potential, there are two classical conserved vectors: the angular momentum \mathbf{L} , which is perpendicular to the plane of the orbit, and the Runge–Lenz vector \mathbf{A} , which goes from the focus corresponding to the center of mass and force along the semi-major axis to the perihelion (closest point) of the elliptical orbit. The conservation of \mathbf{A} is related to the fact that non-relativistically the orbits do not precess. The Hamiltonian of our bound state classical system with an energy $E < 0$ is [17]

$$H = \frac{p^2}{2m} - \frac{Z\alpha}{r} = E \quad (15)$$

where m = mass of the electron, r is the location of the electron, p is its momentum, α is the fine structure constant, and E is the total non-relativistic energy.

The Runge–Lenz vector is

$$\mathbf{A} = \frac{1}{\sqrt{-2mH}} (\mathbf{p} \times \mathbf{L} - mZ\alpha \frac{\mathbf{r}}{r}) \quad (16)$$

where \mathbf{L} is the angular momentum. From Hamilton's equation, $H = E$, so

$$\mathbf{A} = \frac{\mathbf{p} \times \mathbf{L}}{a} - \frac{mZ\alpha}{a} \frac{\mathbf{r}}{r} \quad (17)$$

where a is defined by

$$a = \sqrt{-2mE}. \quad (18)$$

From the virial theorem, the average momentum $\langle p^2 \rangle = -2mE$ so a is the root mean square momentum. We are discussing bound states so $E < 0$. It is straightforward to verify that \mathbf{A} is conserved in time:

$$[\mathbf{A}, H] = \frac{d\mathbf{A}}{dt} = 0. \quad (19)$$

From the definition of \mathbf{A} and the definition of angular momentum

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \quad (20)$$

it follows that \mathbf{A} is orthogonal to the angular momentum vector

$$\mathbf{A} \cdot \mathbf{L} = 0. \quad (21)$$

Using the fact that \mathbf{A} and \mathbf{L} are conserved, we can easily obtain equations for the orbits in configuration and momentum space and the eccentricity, and other quantities, all usually derived by directly solving the equations of motion.

We will show that A and L are the generators of the group $O(4)$. If we introduce the linear combinations $N = \frac{1}{2}(L + A)$ and $M = \frac{1}{2}(L - A)$, we find that N and M commute reducing the nonsimple group $O(4)$ to $SU(2) \times SU(2)$, which we will discuss in Section 4.2 in the language of quantum mechanics.

3.1. Orbit in Configuration Space

In order to obtain the equation of the orbit one computes

$$\mathbf{r} \cdot \mathbf{A} = rA \cos\phi_r = -r \frac{mZ\alpha}{a} + \mathbf{r} \cdot \mathbf{p} \times \mathbf{L}. \quad (22)$$

Noting that $\mathbf{r} \cdot \mathbf{p} \times \mathbf{L} = L^2$, we can solve for r

$$r = \frac{L^2/mZ\alpha}{(a/mZ\alpha)A \cos\phi_r + 1}. \quad (23)$$

This is the equation of an ellipse with eccentricity $e = (a/mZ\alpha)A$ and a focus at the origin (Figure 1). To find e we calculate $\mathbf{A} \cdot \mathbf{A}$ using the identity $\mathbf{p} \times \mathbf{L} \cdot \mathbf{p} \times \mathbf{L} = p^2 L^2$ and obtain

$$A^2 = \frac{p^2 L^2}{a^2} - \frac{2mZ\alpha}{a^2} \frac{L^2}{r} + \left(\frac{mZ\alpha}{a}\right)^2. \quad (24)$$

Substituting E for the Hamiltonian Equation (15) gives the usual result

$$\frac{a}{mZ\alpha} A = e = \sqrt{\frac{2EL^2}{m(Z\alpha)^2} + 1}. \quad (25)$$

The length r_c of the semi-major axis is the average of the radii at the turning points

$$r_c = \frac{r_1 + r_2}{2}. \quad (26)$$

Using the orbit equation we find

$$r_c = \frac{L^2}{mZ\alpha} \frac{1}{1 - e^2} \tag{27}$$

or

$$r_c = -\frac{Z\alpha}{2E} = \frac{mZ\alpha}{a^2}. \tag{28}$$

The energy depends only on the length of the semi-major axis r_c , not on the eccentricity. This important result is a consequence of the symmetry of the problem. It is convenient to parameterize the eccentricity in terms of the angle ν (see Figure 1) where

$$e = \sin \nu \tag{29}$$

From this definition and from Equations (25), (27), and (28) follow the useful results

$$L = r_c a \cos \nu, \quad A = r_c a \sin \nu \tag{30}$$

which immediately imply

$$L^2 + A^2 = (r_c a)^2 = \left(\frac{mZ\alpha}{a}\right)^2. \tag{31}$$

This equation is the classical analogue of an important quantum mechanical result first obtained by Pauli and Hulthen allowing us to determine the energy levels from symmetry properties alone [14,16]. From Figure 1, it is apparent that this equation is a statement of Pythagoras’s theorem for right triangles.

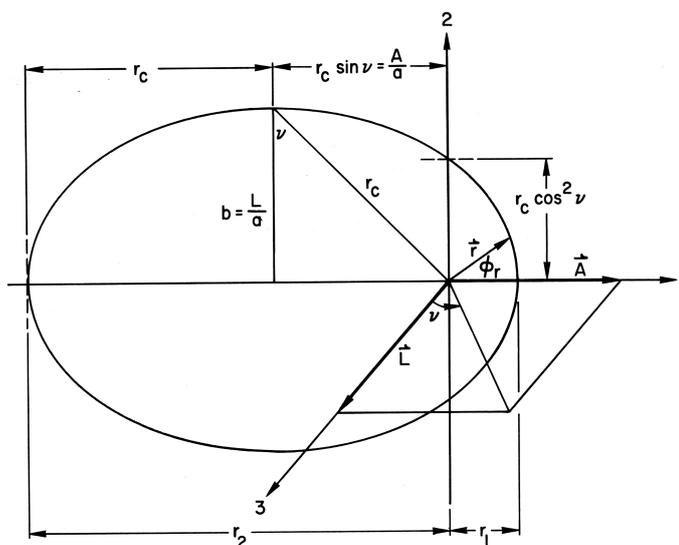


Figure 1. Classical Kepler orbit in configuration space. The orbit is in the 1–2 plane (plane of the paper). One focus, where the proton charge is located, is the origin. The semi-minor axis is $b = r_c \sin \nu$. The semi-major axis is r_c .

The energy equation (Equation (15)) and the orbit equation (Equation (23)) respectively may be rewritten in terms of a , r , and ν :

$$\frac{r_c}{r} = \frac{p^2 + a^2}{2a^2} \tag{32}$$

$$r = \frac{r_c \cos^2 \nu}{1 + \sin \nu \cos \phi_r}. \tag{33}$$

3.2. The Period

To obtain the period, we use the geometrical definition of the eccentricity

$$e = \sqrt{1 - (b/r_c)^2} \quad (34)$$

where b is the semi-minor axis. Using $e = \sin \nu$ we find

$$b = r_c \cos \nu \quad (35)$$

so from Equation (30), we obtain

$$L = ab. \quad (36)$$

From classical mechanics, we know the magnitude of the angular momentum is equal to twice the mass times the area swept out by the radius vector per unit time. The area of the ellipse is $\pi b r_c$. If the period of the classical motion is T , then $L = 2m\pi b r_c / T$. Therefore, the classical period is

$$T = 2\pi \frac{m r_c}{a} = 2\pi \sqrt{\frac{m(Z\alpha)^2}{-8E^3}}. \quad (37)$$

and the classical frequency $\omega_{cl} = 2\pi/T$ is

$$\omega_{cl} = \frac{a}{m r_c}. \quad (38)$$

3.3. Group Structure $SO(4)$

The generators of our symmetry operations form the closed Poisson bracket algebra of $O(4)$:

$$[L_i, L_j] = i\epsilon_{ijk} L_k, \quad [L_i, A_j] = i\epsilon_{ijk} A_k, \quad [A_i, A_j] = i\epsilon_{ijk} L_k. \quad (39)$$

The brackets mean i times the Poisson bracket, which is the classical limit of a commutator. The first bracket says that the angular momentum generates rotations and forms a closed Lie algebra corresponding to $O(3)$. The second bracket says that the Runge-Lenz vector transforms as a vector under rotations generated by the angular momentum. The last commutator says that the multiple transformations generated by the Runge-Lenz vector are equivalent to a rotation. Taken together the commutators form the Lie algebra of $O(4)$. The connected symmetry group for the classical bound state Kepler problem is obtained by exponentiating our algebra giving the symmetry group $SO(4)$. The scattering states with $E > 0$ form an infinite dimensional representation of the non-compact group $SO(3,1)$.

We now want to determine the nature of the transformations generated by A_i and L_i . Clearly, $L \cdot \delta\omega$ generates a rotation of the elliptical orbit about the axis $\delta\omega$ by an amount $\delta\omega$. To investigate the transformations generated by $A \cdot \delta\nu$ we assume a particular orientation of the orbit, namely that it is in the 1–2 (or x-y) plane and that A is along the 1-axis (see Figure 1). The more general problem is obtained by a rotation generated by L_i . For an example, we choose a transformation with $\delta\nu$ pointing along the 2-axis, so that $A \cdot \delta\nu = A_2 \delta\nu$. The change in A is defined by δA , where

$$\delta A = i[A \cdot \delta\nu, A]. \quad (40)$$

From the Poisson bracket relations, we find for this particular case:

$$\delta A_1 = L_3 \delta\nu, \quad \delta A_2 = 0, \quad \delta A_3 = -L_1 \delta\nu \quad (41)$$

For our orbit, $L_1 = 0$ so $\delta A_3 = 0$. We perform a similar computation to find δL . We find we can characterize the transformation by

$$\begin{aligned} \delta A_1 &= L_3 \delta v & \text{or} & & \delta A &= L \delta v \\ \delta L_3 &= -A_1 \delta v & \text{or} & & \delta L &= -A \delta v \\ \delta e &= \sqrt{1 - e^2} \delta v & \text{or} & & \delta(\sin \nu) &= \cos \nu \delta v \end{aligned} \quad (42)$$

Recalling $e = \sin \nu$ and Equation (30), we see that these transformations are equivalent to the substitution

$$\nu \longrightarrow \nu + \delta \nu. \quad (43)$$

In other words, the eccentricity of the orbit, and therefore A and L are all changed in such a way that the energy, a and r_c (length of the semi-major axis) remain constant. In our example, both L and A are changed in length but not direction, so the plane and orientation of the orbit are unchanged. The general transformation $A \cdot \delta \mu$ will also rotate the plane of the orbit or the semi-major axis.

Figure 2 shows a set of orbits in configuration space with different values of the eccentricity $e = \sin \nu$, but the same total energy and the same semimajor axis r_c , which is the bold hypotenuse. The bold vertical and horizontal legs are A/a and L/a and they are related to the hypotenuse r_c by Pythagoras's theorem. The generator $A_2 \nu$ produces a deformation of the circular orbit into the various elliptical orbits shown. This classical degeneracy corresponds to the quantum mechanical degeneracy in energy levels that occurs for different eigenvalues of the angular momentum with a fixed principal quantum number.

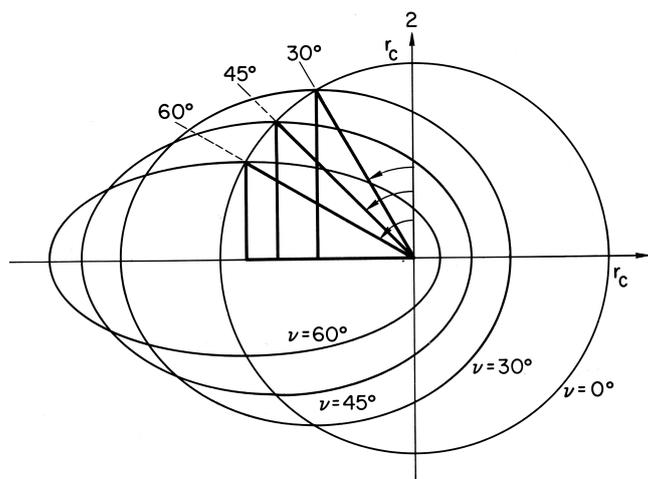


Figure 2. Kepler bound state orbits in configuration space for a fixed energy and different values of the eccentricity $e = \sin \nu$. The bold hypotenuse is the semi-major axis r_c , which makes an angle ν with the vertical 2-axis.

We can visualize all possible elliptical orbits for a fixed total energy or semi-major axis through a simple device. It is possible to produce an elliptical orbit with eccentricity $\sin \nu$ as the shadow of a circle of radius r_c which is rotated an amount ν about an axis perpendicular to the illuminating light. With a complete rotation of the circle, we will see all possible classical elliptical orbits corresponding to a given total energy. In quantum mechanics only certain angles of rotation would be possible corresponding to the quantized values of L . As the circle is rotated, we must imagine that the force center shifts as the sine of the angle of rotation, so that it always remains at the focus [101].

3.4. The Classical Hydrogen Atom in Momentum Space

We can derive the equation for the classical orbit in momentum space of a particle bound in a Coulomb potential using the conserved operators L and A . For convenience, we assume that we have rotated our axes, so that L lies along the 3-axis and A the 1-axis, as shown in Figure 1. We compute

$$\mathbf{p} \cdot \mathbf{A} = p_1 A = \frac{-mZ\alpha}{a} \mathbf{p} \cdot \frac{\mathbf{r}}{r} \equiv \frac{-mZ\alpha}{a} p_r \tag{44}$$

and we employ Equations (28) and (30) to show $A = \frac{mZ\alpha}{a} \sin \nu$, to obtain [102]

$$p_r = -\sin \nu p_1 \tag{45}$$

which we substitute into the identity

$$p_r^2 + \frac{L^2}{r^2} = p^2 = p_1^2 + p_2^2 \tag{46}$$

Using Equations (30) and (32) we find

$$1 = \left(\frac{2ap_1}{p^2 + a^2} \right)^2 + \left(\frac{2ap_2}{p^2 + a^2} \right)^2 \frac{1}{\cos^2 \nu} \tag{47}$$

and

$$p^2 - a^2 = 2ap_2 \tan \nu \tag{48}$$

which may also be written as

$$p_1^2 + (p_2 - a \tan \nu)^2 = \frac{a^2}{\cos^2 \nu}. \tag{49}$$

From Equation (49), we see the orbit in momentum space is a circle of radius $a/\cos \nu$ with its center displaced from the origin a distance $a \tan \nu$ along the 2-axis. Figure 3 shows the momentum space orbit that corresponds to the configuration space orbit in Figure 1.

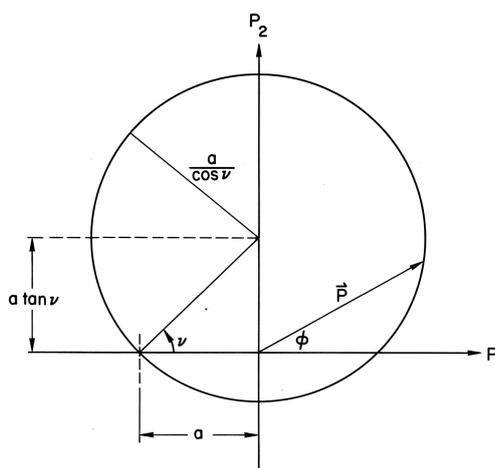


Figure 3. Kepler orbit in momentum space of radius $a/\cos \nu$, with its center at $p_2 = a \tan \nu$, corresponding to the orbit in configuration space shown in Figure 1. A circular orbit in configuration space corresponds to a circular orbit in momentum space centered on the origin with radius a .

As an alternative method of showing the momentum space orbits are circular, we can compute [103]

$$\left(\mathbf{p} - a \frac{\mathbf{L} \times \mathbf{A}}{L^2} \right)^2 = C^2. \tag{50}$$

Using the lemma

$$\mathbf{p} \times \mathbf{A} = -\frac{\mathbf{L}}{2a}(p^2 - a^2), \tag{51}$$

the fact that $\mathbf{L} \cdot \mathbf{A} = 0$, and Equation (30), we find $C = \frac{a}{\cos \nu}$. The orbit is a circle of radius $\frac{a}{\cos \nu}$ whose center lies at $a \frac{\mathbf{L} \times \mathbf{A}}{L^2}$, in agreement with the previous result.

We now consider what the generators A_i and L_i do to the orbit in momentum space. Clearly, L generates a rotation of the axes. For an A_i transformation, consider the same situation that we considered in our discussion of the configuration space orbit (see Figures 1 and 3). Because the generator $A_2 \delta \nu$ changes ν to $\nu + \delta \nu$, we conclude that in momentum space this shifts the center of the orbit along the 2-axis and changes the radius of the circle. However, the distance a from the 2-axis to the intersection of the orbit with the 1-axis remains unchanged. Figure 4 shows a set of momentum space orbits for a fixed energy that correspond to the set of orbits in configuration space shown in Figure 2.

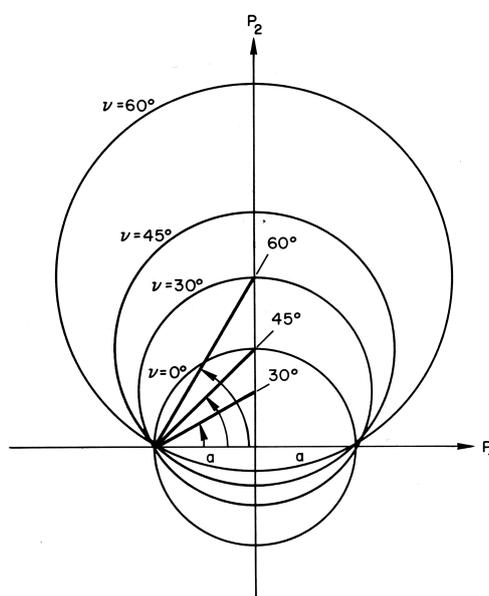


Figure 4. Kepler orbits in momentum space for a fixed energy and RMS momentum a with different values of the eccentricity $e = \sin \nu$ corresponding to the orbits in configuration space shown in Figure 2.

3.5. Four-Dimensional Stereographic Projection in Momentum Space

It is interesting that in classical mechanics the bound state orbits in a Coulomb potential are simpler in momentum space than in configuration space. In quantum mechanics the momentum space wave functions become simply four-dimensional spherical harmonics if one normalizes the momentum \mathbf{p} by dividing by the RMS momentum $a = \sqrt{-2mE}$ and performs a stereographic projection onto a unit hyper-sphere in a four-dimensional space [18,35]. We will do the analogous projection procedure for the classical orbits. The three-dimensional momentum space hyperplane passes through the center of the four-dimensional hypersphere, as shown in Figure 5. The unit vector in the fourth direction is $\hat{n} = (1, 0, 0, 0)$. The unit vector \hat{U} goes from the center of the sphere to the surface of the hypersphere, where it is intersected by the line connecting the vector \mathbf{p}/a to the north pole of the sphere.

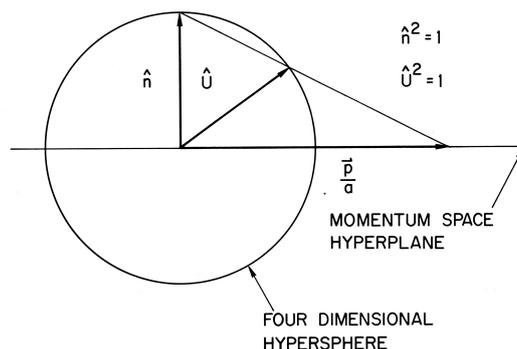


Figure 5. Stereographic projection in momentum space for a fixed energy, mapping p/a into \hat{U} . The unit vector in the four direction is \hat{n} and $\hat{n} \cdot \hat{U} = \cos \Theta_4$.

We find

$$U_i = \frac{2ap_i}{p^2 + a^2} \quad i = 1, 2, 3. \quad U_4 = \frac{p^2 - a^2}{p^2 + a^2} \tag{52}$$

or inverting,

$$p_i = \frac{aU_i}{1 - U_4} \quad p^2 = a^2 \frac{1 + U_4}{1 - U_4}. \tag{53}$$

Momentum space vectors for which $p/a < 1$ are mapped onto the lower hyperhemisphere. The advantage of this projection over one in which the hypersphere is tangent to the hyperplane is that we may have $|\hat{n}| = |\hat{U}| = 1$. At times it is convenient to describe \hat{U} in terms of spherical polar coordinates in four dimensions. Because \hat{U} is a unit vector we define

$$\begin{aligned} U_4 &= \cos \theta_4 \\ U_3 &= \sin \theta_4 \cos \theta \\ U_2 &= \sin \theta_4 \sin \theta \sin \phi \\ U_1 &= \sin \theta_4 \sin \theta \cos \phi \end{aligned} \tag{54}$$

where θ and ϕ are the usual coordinates in three dimensions. By comparison to Equation (52), we have

$$\theta_4 = 2 \cot^{-1} \frac{p}{a} \quad \theta = \cos^{-1} \frac{p_3}{p} \quad \phi = \tan^{-1} \frac{p_2}{p_1} \tag{55}$$

3.6. Orbit in U space

We want to find the trajectory of the particle on the surface of the hypersphere corresponding to the Kepler orbits in configuration space or the displaced circles in momentum space. We assume we have rotated the axes in configuration space so that L is along the 3-axis and A is along the 1-axis, as shown in Figure 1. The equation for the orbit in three-dimensional momentum space is given by Equations (48) or (50). Dividing Equation (48) by $p^2 + a^2$ immediately gives a parametric equation for the projected orbit in U space:

$$U_4 = U_2 \tan \nu. \tag{56}$$

Because the orbit is in the 1–2 plane in configurations space, $U_3 = 0$. The orbit lies in a hyperplane perpendicular to the 2–4 plane that goes through the origin and makes an angle $\pi/2 - \nu$ with the 4-axis, as shown in Figure 6 [104]. The orbit is the intersection of this plane with the hypersphere and it is therefore a great circle. To derive the exact equation for the projected orbit we express p in Cartesian components p_1 and p_2 in Equation (48) and substitute Equation (52) obtaining

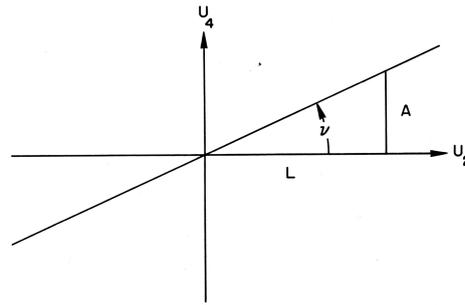


Figure 6. Showing the hyperplane containing the orbit making an angle ν with the U_2 plane. Notice $\tan \nu = A/L$ as required by Equation (30).

$$U_1^2 + U_2^2 - 2 \tan \nu U_2(l - U_4) = (1 - U_4)^2. \tag{57}$$

To interpret this equation, we consider it in a rotated coordinate system. If we perform a rotation by an amount $\delta\nu$ about the 1–3 plane ($A_2\delta\nu$ is the generator of this rotation), the equations of transformation may be written [105]

$$\begin{aligned} U_2 &= U_2' \cos \delta\nu + U_4' \sin \delta\nu, & U_3 &= U_3' \\ U_4 &= U_4' \cos \delta\nu - U_2' \sin \delta\nu, & U_1 &= U_1'. \end{aligned} \tag{58}$$

This transformation is equivalent to making the substitution $\nu \rightarrow \nu + \delta\nu$ in the equations relating to the orbit. For example, Equation (56) becomes

$$U_4' = U_2' \tan(\nu + \delta\nu). \tag{59}$$

We choose $\delta\nu = -\nu$, which means the orbital plane becomes $U_4' = 0$. Writing Equation (57) in terms of the primed coordinates, we find

$$U_1'^2 + U_2'^2 = 1 \tag{60}$$

which in the original system is

$$U_1^2 + (U_2 \cos \nu + U_4 \sin \nu)^2 = 1. \tag{61}$$

This is the equation of a great hypercircle $(\nu, 0)$ centered at the origin and lying in a hyperplane making an angle $\pi/2 - \nu$ with the 4-axis and an angle $\pi/2 - 0$ with the 3-axis. If L did not lie along the 3-axis, but, for example, was in the 1–3 plane, at an angle Θ from the 3-axis, then Equation (61) would be modified by the substitution

$$U_1 \rightarrow U_1 \cos \Theta + U_3 \sin \Theta \tag{62}$$

which follows, since U_i transforms as a three-vector. The corresponding great circle (ν, Θ) lies in a hyperplane making an angle $\pi/2 - \nu$ with the 4-axis and $\pi/2 - \Theta$ with the 3-axis.

The motion of the orbiting particle corresponds to a dot moving along the great circle $(\nu, 0$ or $\Theta)$ with a period T given by the classical period Equation (37). The velocity in configuration space can be expressed in terms of U_4 by using its definition in terms of p^2 Equation (53) or in terms of θ_4 Equation (55). The particle is moving at maximum velocity when θ_4 is a minimum, which occurs at the perihelion when $\theta_4 = \pi/2 - \nu$:

$$\max\left(\frac{p}{a}\right) = \sqrt{\frac{1+e}{1-e}} = \sqrt{\frac{r_2}{r_1}} \tag{63}$$

and at a minimum velocity when $\theta_4 = \pi/2 + v$:

$$\min\left(\frac{p}{a}\right) = \sqrt{\frac{1-e}{1+e}}. \tag{64}$$

These values of θ_4 correspond to turning points, at which r and p have extreme values. This is apparent when we use Equation (32) for the total energy to show

$$U_4 = \frac{r_c - r}{r_c}. \tag{65}$$

When $r > r_c$ then $p^2 < a^2$, so the particle is moving more slowly than the RMS velocity. Applying the virial theorem to any orbit we find $\langle p^2 \rangle = a^2$ so as expected a is the RMS momentum and $\langle \frac{1}{1-U_4} \rangle = 1 = \langle r_c/r \rangle$.

Figure 7 is a picture of a simple device illustrating the stereographic projection of the orbit in p/a -space onto the four-dimensional hypersphere in U -space. We assume that the orbit is in the 1–2 plane and that A lies along the 1-axis, so $p_3 = 0, U_3 = 0$. Because of this trivial dependence on p_3 , we have omitted the 3-axis. The vertical pin or rod represents the unit vector \hat{n} lying along the 4-axis. The circumference of the larger circle perpendicular to the 4-axis represents the orbit in p/a -space. One can see that it is displaced from the origin along the 2-axis. Centered at the origin, we must imagine a hypersphere of unit radius $\hat{U}^2 = 1$. The stereographic projection \hat{U} of the vector p/a is obtained by placing the string coming from the top of n directly at the head of the vector p/a . The intersection of the string with the unit hypersphere defines \hat{U} . As the string is moved along the orbit in p/a -space, it intersects the hypersphere along a great circle shown by the circumference of the unit circle making an angle v with the 1–2 plane. We can see for example, that at the closest approach, θ_4 is a minimum and U_4 is a maximum, $\hat{U} \cdot A = U_1$ is a minimum, and p/a is a maximum.

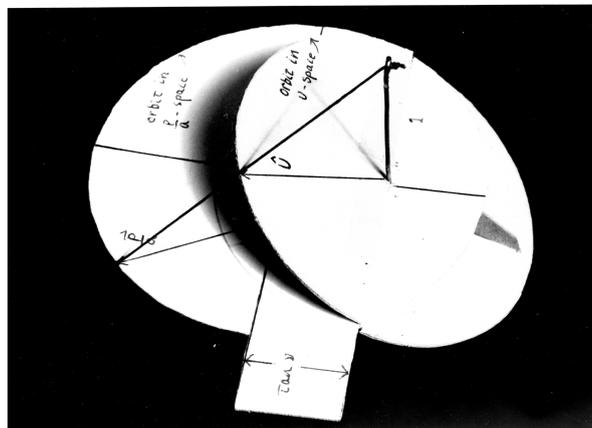


Figure 7. Model illustrating the stereographic projection from the 1–2 plane to a 4-d hypersphere. The pin represents the unit vector \hat{n} along the 4-axis, normal to the 1–2 plane.

3.7. Classical Time Dependence of Orbital Motion

We can determine the time dependence of the orbital motion by integrating the expression for the angular momentum $L = mr^2 d\phi_r / dt$

$$\int dt = \int \frac{mr^2}{L} d\phi_r \tag{66}$$

where r is given by the orbit equation Equation (33) and we are assuming the orbit is in the 1–2 plane. After integrating, we can use the equations relating the momentum space and configuration space variables to obtain the time dependence in p-space and U-space. We obtain

$$\frac{1}{r_c^2} \frac{1}{\cos \nu} \frac{L}{m} \int_0^t dt = \cos^3 \nu \int_0^{\phi_r(t)} \frac{d\phi_r}{(1 + \sin \nu \cos \phi_r)^2}. \quad (67)$$

The left-hand side of this equation is equal $\omega_{cl}t$, where ω_{cl} is the classical frequency. This follows by substituting Equations (30) and (38)

$$L = ar_c \cos \nu \quad \omega_{cl} = \frac{a}{mr_c}. \quad (68)$$

The integral on the right side gives [106]

$$\omega_{cl}t = -\frac{\sin \nu \cos \nu \sin \phi_r}{1 + \sin \nu \cos \phi_r} - \tan^{-1} \frac{\cos \nu \sin \phi_r}{\sin \nu + \cos \phi_r} \quad (69)$$

which may be simplified as

$$\omega_{cl}t = -\frac{A}{L} \frac{y}{r_c} - \tan^{-1} \frac{A}{L} \frac{y}{r_c - r} \quad (70)$$

where $y = r \sin \phi_r$.

The relationship between the angle $\phi \equiv \phi_p$ in momentum space and ϕ_r in configuration space follows by either differentiating the orbit equation Equation (33) with respect to time and using $L = mr^2\dot{\phi}_r$ or by simultaneously solving the configuration space orbit, the momentum space orbit equation Equation (48) and the energy equation Equation (32). We find

$$\sin \phi_r = -p \cos \phi \frac{\cos \nu}{a} \quad \cos \phi_r = p \sin \phi \frac{\cos \nu}{a} - \sin \nu. \quad (71)$$

From these equations, the definitions of the U_i , Equation (52), and the orbit and energy equations, it follows that for the classical orbit in the 1–2 plane

$$\begin{aligned} U_1 &= -\frac{r \sin \phi_r}{r_c \cos \nu} \\ U_2 &= \frac{r \sin \nu + \cos \phi_r}{r_c \cos \nu} = U_4 \cot \nu \\ U_3 &= 0 \\ U_4 &= \frac{r_c - r}{r_c}. \end{aligned} \quad (72)$$

Using these results in Equation (69) gives

$$\omega_{cl}t = U_1 \sin \nu + \tan^{-1} \left(\frac{U_2}{U_1 \cos \nu} \right) \quad (73)$$

which gives the time dependence in U space, and it agrees with the results of [97,107]. We could do rotations to generalize this result [102]. We can also rewrite the inverse tangent as $\cos^{-1} U_1$ using

$$U_1^2 + \frac{U_2^2}{\cos^2 \nu} = 1. \quad (74)$$

If we consider the last two equation for circular orbits with $e = \sin \nu = 0$ we obtain $\tan^{-1}(U_2/U_1) = \phi(t) = \omega_{cl}t = \phi_r(t) + \pi/2$, and our familiar circle $U_1^2 + U_2^2 = 1$.

Remark on Harmonic Oscillator

We can find a conserved Runge–Lenz vector for the non-relativistic hydrogen atom because the elliptical orbit does not precess, as it does for the relativistic atom. The only central force laws that yield classical elliptical orbits that do not precess are the inverse Kepler force and the linear harmonic oscillator force [108]. Thus, it seems reasonable that one could construct a constant vector similar to A for the oscillator, although the force center for the atom is at a focus and for the oscillator it is at the center of the ellipse. However, it is not readily possible [109]. Instead, one can construct a constant Hermitian second rank tensor T_{ij} :

$$T_{ij} = \frac{1}{m\omega_0} p_i p_j + m\omega_0 x_i x_j. \quad (75)$$

This constant tensor is analogous to the moment of inertia tensor for rigid body motion. The eigenvectors of the tensor will be constant vectors along the principal axes for the particular orbit being considered. The existence of the conserved tensor leads to the $U(3)$ symmetry algebra of the oscillator. The generators are $\lambda_{ij}^a T_{ij}$, where the λ 's are the usual $U(3)$ matrices [22]. The spectrum generating algebra is $SU(3,1)$.

In another approach, the Schrodinger equation for the hydrogen atom has been transformed into an equation for a four dimensional harmonic oscillator or two two dimensional harmonic oscillators. This approach which fits well with parabolic coordinates was used especially in the 1980's to analyze the group structure of the atom and relate it to $SU(3)$ [110–119]. We will not discuss this approach further.

4. The Hydrogenlike Atom in Quantum Mechanics; Eigenstates of the Inverse of the Coupling Constant

In this section we switch from classical dynamics to quantum mechanics and discuss the group structure and exploit it to determine the bound state energy spectrum directly, as Pauli and followers did almost a century ago [14,16]. In Section 4.3 we introduce a new set of basis states for the hydrogenlike atom, eigenstates of the coupling constant. Using these states allows us to display the symmetries in the most convenient manner and to treat bound and scattering states uniformly.

4.1. The Degeneracy Group $SO(4)$

The quantum mechanical Hamiltonian is

$$H = \frac{p^2}{2m} - \frac{Z\alpha}{r} = E. \quad (76)$$

The classical expression for the Runge–Lenz vector needs to be symmetrized to insure the corresponding quantum mechanical operator A is Hermitian:

$$A = \frac{1}{\sqrt{-2mH}} \left(\frac{\mathbf{p} \times \mathbf{L} - \mathbf{L} \times \mathbf{p}}{2} - mZ\alpha \frac{\mathbf{r}}{r} \right). \quad (77)$$

We may verify that A and $L = \mathbf{r} \times \mathbf{p}$ both commute with the Hamiltonian H . The commutation relations of L_i and A_i are the same as the corresponding classical Poisson bracket relations for bound states:

$$[L_i, L_j] = i\epsilon_{ijk} L_k, \quad [L_i, A_j] = i\epsilon_{ijk} A_k, \quad [A_i, A_j] = i\epsilon_{ijk} L_k \quad (78)$$

and form the algebra of $O(4)$ [35]. We can write the commutation relations in a single equation which makes the $O(4)$ symmetry explicit. If we define

$$S_{ij} = \epsilon_{ijk} L_k \quad S_{i4} = A_i \quad (79)$$

then

$$[S_{ab}, S_{cd}] = i(\delta_{ac}S_{bd} + \delta_{bd}S_{ac} - \delta_{ad}S_{bc} - \delta_{bc}S_{ad}) \quad a, b = 1, 2, 3, 4. \quad (80)$$

The Kronecker delta function δ_{ab} acts like a metric tensor.

4.2. Derivation of the Energy Levels

We can obtain the energy levels by determining which representations of the group SO(4) are realized by the degenerate eigenstates of the hydrogenlike atom [12,14,35]. The representations of SO(4) may be characterized by the numerical values of the two Casimir operators for SO(4):

$$C_1 = \mathbf{L} \cdot \mathbf{A} \quad C_2 = \mathbf{L}^2 + \mathbf{A}^2 \quad (81)$$

Once we know the value of C_2 , then the eigenvalues of H follow from the quantum mechanical form of Equation (31), namely

$$\mathbf{L}^2 + \mathbf{A}^2 + 1 = \frac{(mZ\alpha)^2}{-2mH}. \quad (82)$$

In order to determine the possible values of C_2 , we factor the $o(4)$ algebra into two disjoint SU(2) algebras [120], each of which has the same commutation relations as the ordinary angular momentum operators,

$$\mathbf{N} = \frac{1}{2}(\mathbf{L} + \mathbf{A}) \quad \mathbf{M} = \frac{1}{2}(\mathbf{L} - \mathbf{A}). \quad (83)$$

The commutation relations are

$$[M_i, N_j] = 0 \quad [M_i, M_j] = i\epsilon_{ijk}M_k \quad [N_i, N_j] = i\epsilon_{ijk}N_k. \quad (84)$$

In analogy with the results for the ordinary angular momentum operators, the Casimir operators are

$$\begin{aligned} M^2 &= j_1(j_1 + 1), \quad j_1 = 0, \frac{1}{2}, 1, \dots \\ N^2 &= j_2(j_2 + 1), \quad j_2 = 0, \frac{1}{2}, 1, \dots \end{aligned} \quad (85)$$

The numbers j_1 and j_2 , which may have half-integral values for SU(2) but not O(3), define the (j_1, j_2) representation of SO(4). From the definitions of \mathbf{A} and \mathbf{L} in terms of the canonical variables, it follows that $C_1 = \mathbf{L} \cdot \mathbf{A} = 0$ which means $j_1 = j_2 = j$, as in the classical case. For our representations, we find

$$M^2 = N^2 = \frac{1}{4}(\mathbf{L}^2 + \mathbf{A}^2) = j(j + 1), \quad j = 0, \frac{1}{2}, 1, \dots \quad (86)$$

and therefore

$$\mathbf{L}^2 + \mathbf{A}^2 + 1 = (2j + 1)^2. \quad (87)$$

Substituting this result into Equation (82) gives the usual formula for the bound state energy levels of the hydrogen atom:

$$H' = -\frac{m(Z\alpha)^2}{2n^2} = E_n \quad (88)$$

where the principal quantum number $n = 2j + 1 = 1, 2, \dots$ and the prime on H signifies an eigenvalue of the operator H .

Within a subspace of energy E_n , the Runge–Lenz vector is

$$\mathbf{A} = \frac{1}{a_n} \left(\frac{\mathbf{p} \times \mathbf{L} - \mathbf{L} \times \mathbf{p}}{2} - mZ\alpha \frac{\mathbf{r}}{r} \right). \quad (89)$$

where $a_n = \sqrt{-2mE_n} = \frac{mZ\alpha}{n}$.

Our considerations of the Casimir operators have shown that the hydrogen atom provides completely symmetrical tensor representations of SO(4), namely, $(j, j) = (\frac{n-1}{2}, \frac{n-1}{2})$, $n = 1, 2, \dots$. The dimensionality is n^2 , corresponding to the n^2 degenerate states. The appearance of only

symmetrical tensor representations ($j_1 = j_2$) may be traced to $L \cdot A$ vanishing, which is a consequence of the structure of L and A in terms of the dynamical variables for the hydrogenlike atom. For systems other than the hydrogenlike atom, it is not generally possible to find the expression for the energy levels in terms of all the different quantum numbers alone. It worked here, since we could express the Hamiltonian as a function of the Casimir operators that contained all quantum numbers explicitly.

There are a variety of possible basis states. We could choose basis states for the $SO(4)$ representation that reflect the $SU(2)$ decomposition, namely eigenstates of M^2 , N^2 , M_3 and N_3 [120]. Another possibility is to have a basis with eigenstates of the Casimir operator C_2 , and A_3 , and M_3 . This choice fits well with the use of parabolic coordinates [60]. A more physically understandable choice is to choose the common basis states $|nlm\rangle$ that are eigenstates of C_2 , L^2 , and L_3 . For this set of basis states, we have

$$\sqrt{(L^2 + A^2 + 1)}|nlm\rangle = n|nlm\rangle \quad L^2|nlm\rangle = l(l+1)|nlm\rangle \quad L_3|nlm\rangle = m|nlm\rangle \quad (90)$$

We can define raising and lowering operators for m :

$$L_{\pm} = L_1 \pm iL_2 \quad (91)$$

which obeys the commutation relations

$$[L^2, L_{\pm}] = 0 \quad [L_3, L_{\pm}] = \pm L_{\pm}. \quad (92)$$

Therefore, we can use L_{\pm} to change the value of m for the basis states

$$L_{\pm}|nlm\rangle = \sqrt{l(l+1) - m(m \pm 1)}|nl, m \pm 1\rangle \quad (93)$$

for $l \geq 1$. We can also use the generators A to change the angular momentum. A general $SO(4)$ transformation can be expressed as a rotation induced by L , followed by a rotation induced by A_3 , followed by another rotation generated by L [121]. Our interest is primarily in changing the angular momentum l , which is most directly done while using A_3 , which commutes with L_3 and C_2 , and so only changes l :

$$A_3|nlm\rangle = \left(\frac{(n^2 - (l+1)^2)((l+1)^2 - m^2)}{4(l+1)^2 - 1} \right)^{\frac{1}{2}} |nl+1, m\rangle + \left(\frac{(n^2 - l^2)(l^2 - m^2)}{4l^2 - 1} \right)^{\frac{1}{2}} |nl-1, m\rangle. \quad (94)$$

for $l \geq 1$.

4.3. Relativistic and Semi-Relativistic Spinless Particles in the Coulomb Potential and Klein–Gordon Equation

The Klein–Gordon equation

$$\left(p^2 - (\tilde{E} - V)^2 + m^2 \right) \tilde{\psi} = 0$$

where \tilde{E} is the relativistic total energy, may be solved exactly for a Coulomb potential, $V = -(Z\alpha)/r$ [122]. The energy levels depend on a principal quantum number and on the magnitude of the angular momentum but not its direction. The only degeneracy present is associated with the $O(3)$ symmetry of the Hamilton. For a relativistic scalar particle, there is no degeneracy to be lifted by a Lamb shift.

If we neglect the V^2 term the resulting equation can be written in the form

$$\left(\frac{p^2}{2\tilde{E}} + V - \frac{\tilde{E}^2 - m^2}{2\tilde{E}} \right) \tilde{\psi} = 0$$

This is exactly the same as the nonrelativistic Schrodinger equation with the substitutions

$$m \rightarrow \tilde{E} \quad E \rightarrow \frac{\tilde{E}^2 - m^2}{2\tilde{E}}.$$

Thus, we regain the O(4) symmetry of the nonrelativistic hydrogen atom, and can define two conserved vectors, as indicated in Table 1. It is possible to take the “square root” of this approximate Klein-Gordon equation (in the same sense that the Dirac equation is the square root of the Klein-Gordon equation) and get an approximate Dirac equation whose energy eigenvalues are independent of the orbital angular momentum [123].

4.4. Eigenstates of the Inverse Coupling Constant $(Z\alpha)^{-1}$

Solutions to Schrodinger’s equation for a particle of energy $E = -\frac{a^2}{2m}$ in a Coulomb potential

$$\left[p^2 + a^2 - \frac{2mZ\alpha}{r} \right] |a\rangle = 0 \quad (95)$$

may be found for certain critical values of the energy $E_n = -\frac{a_n^2}{2m}$ where $a_n = \frac{mZ\alpha}{n}$. The corresponding eigenstates of the Hamiltonian are $|nlm\rangle$ which satisfy Equation (95) with a replaced by a_n . In addition to the bound states, because there is no upper bound on p^2 in the Hamiltonian, we also have the continuum of scattering states that have $E > 0$.

Because the quantity that must have discrete values for a solution to exist is actually $\frac{a}{mZ\alpha}$, as noted in Section 2.3, we might ask if eigensolutions to Equation (95) exist for certain critical values of $Z\alpha$ while keeping a and the energy fixed [1]. To investigate such solutions it is convenient to algebraically transform Equation (95):

$$\left[\frac{1}{\sqrt{\rho(a)}} \left(\frac{p^2 + a^2}{a} \right) \frac{1}{\sqrt{\rho(a)}} - \frac{1}{\sqrt{\rho(a)}} \left(\frac{2mZ\alpha}{ar} \right) \frac{1}{\sqrt{\rho(a)}} \right] \sqrt{\rho(a)} |a\rangle = 0$$

where

$$\rho(a) = \frac{p^2 + a^2}{2a^2}. \quad (96)$$

Because $\rho(a)$ commutes with p^2 , we obtain the eigenvalue equation

$$\left[\left(\frac{a}{mZ\alpha} \right) - K(a) \right] |a\rangle = 0 \quad (97)$$

where the totally symmetric and real kernel is

$$K(a) = \sqrt{\frac{2a^2}{p^2 + a^2}} \frac{1}{ar} \sqrt{\frac{2a^2}{p^2 + a^2}} \quad (98)$$

and

$$|a\rangle = (\rho(a))^{\frac{1}{2}} |a\rangle. \quad (99)$$

As before, solutions to this transformed equation may found for the eigenvalues

$$K'(a) = \left(\frac{a}{mZ\alpha} \right)' = \frac{1}{n}. \quad (100)$$

If we hold $Z\alpha$ constant and let a vary, we obtain the usual spectrum $a_n = \sqrt{-2mE_n} = \frac{mZ\alpha}{n}$. For $a = a_n$, Equation (99) reduces to the equation for the eigenstates

$$\sqrt{\rho(a_n)} |nlm\rangle = |nlm; a_n\rangle. \quad (101)$$

Alternatively, if we hold a constant, then $Z\alpha$ has the spectrum

$$(Z\alpha)_n = \frac{na}{m} \quad (102)$$

with the corresponding eigenstates of $(Z\alpha)^{-1}$ being

$$|nlm; a\rangle. \quad (103)$$

The relationship between the usual energy eigenstates of the energy $|nlm\rangle$ and the eigenstates $|nlm; a\rangle$ of $(Z\alpha)^{-1}$ is

$$|nlm\rangle = \frac{1}{\sqrt{\rho(a_n)}} |nlm; a_n\rangle, \quad (104)$$

which requires that both sets of states have the same quantum numbers. Note that the magnitude $\langle a|K(a)|a\rangle$ is proportional to $\langle 1/ar\rangle_n = (1/a_n)(1/n^2a_0)$ where a_0 is the Bohr radius for the ground state, and so is positive and bounded. The kernel $K(a)$ is real and symmetric in p and r and manifestly Hermitian. Because the kernel K in Equation (98) is bounded, definite, and Hermitian with respect to the eigenstates $|nlm; a_n\rangle$ [124] the set of normalized eigenstates

$$|nlm; a\rangle \quad n = 0, 1, 2, \dots; \quad l = 0, 1, \dots, n-2, n-1; \quad m = -l, -l+1, \dots, l-1, l. \quad (105)$$

where

$$\left(\frac{1}{n} - K(a)\right) |nlm; a\rangle = 0 \quad (106)$$

is a complete orthonormal basis for the hydrogenlike atom:

$$(nlm; a|n'l'm'; a) = \delta_{nn'}\delta_{ll'}\delta_{mm'} \quad (107)$$

$$\sum_{nlm} |nlm; a\rangle\langle nlm; a| = 1. \quad (108)$$

There are several important points to notice with regard to these eigenstates of the inverse of the coupling constant:

(1) **Because of the boundedness of K , there is no continuum portion in the eigenvalue spectrum of $(Z\alpha)^{-1}$, the eigenvalues are discrete.** Because K is a positive definite Hermitian operator, all eigenvalues are positive, real numbers. This feature leads to a unified treatment of all states of the hydrogenlike atom as opposed to the treatment in terms of energy eigenstates in which we must consider separately the bound states and the continuum of scattering states.

(2) It follows from Equation (104) that **the quantum numbers, multiplicities, and degeneracies of these states $|nlm; a\rangle$ are precisely the same as those of the usual bound energy eigenstates.** For example, there are n^2 eigenstates of $(Z\alpha)^{-1}$ that have the principal quantum number equal to n or $(Z\alpha)$ equal to $\frac{na}{m}$.

(3) **A single value of the RMS momentum a or the energy $E = \frac{-a^2}{2m}$ applies to all the states in our complete basis,** as opposed to the usual energy eigenstates where each nondegenerate state has a different value of a . We have made this explicit by including a in the notation for the states: $|nlm; a\rangle$. Sometimes we will write the states as $|nlm\rangle$, provided the value of a has been specified. This behavior in which a single value of a applies to all states will prove to be very useful. In essence, it permits us to generalize from statements applicable in a subspace of Hilbert space with energy E_n or energy parameter a_n to the entire Hilbert space.

(4) **By a suitable scale change or dilation, we may give the quantity a any positive value we desire.** This is affected by the unitary operator

$$D(\lambda) = e^{i\frac{1}{2}(\mathbf{p}\cdot\mathbf{r}+\mathbf{r}\cdot\mathbf{p})\lambda} \quad (109)$$

which transforms the canonical variables

$$D(\lambda)\mathbf{p}D^{-1}(\lambda) = e^{-\lambda}\mathbf{p} \quad D(\lambda)\mathbf{r}D^{-1}(\lambda) = e^{\lambda}\mathbf{r} \quad (110)$$

and the kernel $K(a)$

$$D(\lambda)K(a)D^{-1}(\lambda) = K(ae^{\lambda}). \quad (111)$$

and the eigenvalue equation

$$\left(\frac{1}{n} - K(ae^{\lambda})\right) D(\lambda)|nlm;a\rangle = 0. \quad (112)$$

Therefore the states transform as

$$D(\lambda)|nlm;a\rangle = |nlm;ae^{\lambda}\rangle. \quad (113)$$

These transformed states form a new basis corresponding to the new value $e^{\lambda}a$ of the RMS momentum.

The relationship between the energy eigenstates and the $(Z\alpha)^{-1}$ eigenstates can be written while using the dilation operator:

$$|nlm\rangle = \frac{1}{\sqrt{\rho(a_n)}} D(\lambda_n) |nlm;a\rangle \quad \text{where } e^{\lambda_n} = \frac{a_n}{a}. \quad (114)$$

The usual energy eigenstates $|nlm\rangle$ are obtained from the eigenstates of $(Z\alpha)^{-1}$ by first performing a scale change to ensure that the energy parameter a has the value a_n and then multiplying by a factor $\rho^{-1/2}$. The need for the scale change is apparent from dimensional considerations: from the $(Z\alpha)^{-1}$ eigenvalue equation, we see that the eigenfunctions are functions of p/a or ar while from the energy eigenvalue equation the eigenfunctions are functions of p/a_n and $a_n r$. The factor $\rho^{-1/2}$ was required in order to convert Schrodinger's equation to one involving a bounded Hermitean operator.

Using the eigenstates of $(Z\alpha)^{-1}$ as our basis allows for us to analyze the mathematical and physical structure of the hydrogenlike atom in the easiest and clearest way.

4.5. Another Set of Eigenstates of $(Z\alpha)^{-1}$

We may transform Schrodinger's equation Equation (95) to an eigenvalue equation for $(Z\alpha)^{-1}$ that differs from Equation (96) by similar methods:

$$\left(\frac{1}{n} - K_1(a)\right) |nlm;a\rangle = 0 \quad (115)$$

where

$$K_1(a) = \frac{1}{\sqrt{ar}} \frac{2a^2}{p^2 + a^2} \frac{1}{\sqrt{ar}} \quad \rho(a) = n/ar \quad \sqrt{\rho(a_n)}|nlm\rangle = |nlm;a_n\rangle \quad (116)$$

This kernel, like $K(a)$, is a bounded, positive definite, Hermitian operator so the eigenstates form a complete basis. The relationship of these basis states to the energy eigenstates is the same as that of the previously discussed eigenstates of $(Z\alpha)^{-1}$ Equation (114) but with $\rho(a) = n/ar$. The n insures that the two sets of eigenstates have consistent normalization, which may be checked by means of the virial theorem. The n cancels out when similarity transforming from the basis of energy eigenstates to the basis of $(Z\alpha)^{-1}$. Note that, classically, both kernels equal $1/ar_c$.

The first set of basis states of $(Z\alpha)^{-1}$ with $\rho(a) = \frac{p^2+a^2}{2a^2}$ is more convenient to use when working in momentum space and the second set with $\rho(a) = n/ar$ is more convenient in configuration space.

Other researchers have used other approaches to secure a bounded kernel for the Schrodinger hydrogen atom, for example, by multiplying the equation from the left by r to regularize it [82].

However, the methods used have not symmetrized the kernels to make them Hermitian, nor are all the generators of the corresponding groups Hermitian, and they have to redefine the inner product [38,82].

4.6. Transformation of A and L to the New Basis States

We must transform A as given in Equation (89) and $L = \mathbf{r} \times \mathbf{p}$ when we change our basis states from eigenstates of the energy to eigenstates of the inverse coupling constant. The correct transformation may be derived by requiring that the transformed generators produce the same linear combination of new states as the original generators produced of the old states. Thus, because

$$A|nlm\rangle = \sum_{l',m'} |nl'm'\rangle A_{l'm'}^{lm} \quad (117)$$

where the coefficients $A_{l'm'}^{lm}$ are the matrix elements of A , we require that the transformed generator \mathbf{a} satisfies the equation

$$\mathbf{a}|nlm\rangle = \sum_{l'm'} |nl'm'\rangle A_{l'm'}^{lm}. \quad (118)$$

In other words, since the Runge–Lenz vector A is a symmetry operator of the original energy eigenstates, \mathbf{a} will be a symmetry operator of the new states with precisely the same properties and matrix elements. Because A is Hermitian, \mathbf{a} is Hermitian.

To obtain a differential expression for \mathbf{a} acting on the new states, we need to transform the generator using Equation (114):

$$\mathbf{a} = D^{-1}(\lambda_n) \left(\sqrt{\rho(a_n)} A \frac{1}{\sqrt{\rho(a_n)}} \right) D(\lambda_n). \quad (119)$$

The effect of the scale change on the quantity in large parenthesis is to replace a_n everywhere by a . By explicit calculation, we find

$$\mathbf{a} = \frac{1}{2a} \left(\frac{\mathbf{r}p^2 + p^2\mathbf{r}}{2} - \mathbf{r} \cdot \mathbf{p}\mathbf{p} - \mathbf{p}\mathbf{p} \cdot \mathbf{r} \right) - \frac{a\mathbf{r}}{2} \quad (120)$$

for $\rho(a) = (p^2 + a^2)/2a^2$. And we obtain

$$\mathbf{a} = \frac{1}{2a} \left(\frac{\mathbf{r}p^2 + p^2\mathbf{r}}{2} - \mathbf{r} \cdot \mathbf{p}\mathbf{p} - \mathbf{p}\mathbf{p} \cdot \mathbf{r} - \frac{\mathbf{r}}{4r^2} \right) - \frac{a\mathbf{r}}{2} \quad (121)$$

for $\rho(a) = n/ar$.

Both of these expressions for \mathbf{a} are manifestly Hermitian. In addition, since there is no dependence on the principal quantum number these expressions are valid in the entire Hilbert space, and not just in a subspace spanned by the degenerate states, as was the case when we used the energy eigenstates as a basis (Equation (89)).

The angular momentum operator is invariant under scale changes and it commutes with scalar operators. Therefore L is invariant under the similarity transformation $\frac{1}{\sqrt{\rho(a_n)}} D(\lambda_n)$ and the expression for the angular momentum operator with respect to the eigenstates of $(Z\alpha)^{-1}$ is the same as the expression with respect to the eigenstates of the energy.

4.7. The $\langle U' |$ Representation

The U' coordinates provide the natural representation for the investigation of the symmetries of the hydrogenlike atom in quantum mechanics, as in classical mechanics [125]. Therefore, we briefly

consider the relevant features of this representation and, in particular, its relationship to the momentum representation. The eigenstate $\langle U' |$ of U_b , $b = 1, 2, 3, 4$, is defined by

$$\langle U' | U_b = U'_b \langle U' | \quad (122)$$

These states are complete on the unit hypersphere in four dimensions:

$$\int |U'\rangle \langle U'| d^3\Omega' = 1 \quad (123)$$

where Ω refers to the angles (θ_4, θ, ϕ) defined in Equation (54). The U variables are defined in terms of the momentum variables and the quantity a in Equation (52). Therefore, the momentum and the U operators commute

$$[p_i, U_b] = 0 \quad (124)$$

and the state $\langle U' |$ is proportional to a momentum eigenstate $\langle p' |$:

$$\langle U' | = \langle p' | \sqrt{J(p)} \quad (125)$$

where the momentum eigenstate is defined by $\langle p' | p = p' \langle p' |$ and

$$\int d^3 p' |p'\rangle \langle p'| = 1. \quad (126)$$

The function $J(p')$ may be determined by equating the completeness conditions and substituting Equation (125):

$$1 = \int d^3 p' |p'\rangle \langle p'| = \int d^3 \Omega' |U'\rangle \langle U'| = \int d^3 \Omega' J(p') |p'\rangle \langle p'| \quad (127)$$

which leads to the identification of the differential quantities

$$d^3 p' = d^3 \Omega' J(p') \quad (128)$$

demonstrating that $J(p')$ is the Jacobian of the transformation from the p - to the U - space. Noting that on the unit sphere

$$U_4^2 = 1 - U_i U_i \quad (129)$$

we can compute the Jacobian

$$J(p') = \left[\frac{p'^2 + a^2}{2a} \right]^3. \quad (130)$$

Therefore from Equation (125) we have the important result

$$\langle U' | = \langle p' | \left[\frac{p'^2 + a^2}{2a} \right]^{3/2}. \quad (131)$$

We can use this result to compute the action of \mathbf{r} on $\langle U' |$ in terms of the differential operators. Using the equation

$$\langle p' | \mathbf{r} = i \nabla_{p'} \langle p' | \quad (132)$$

we obtain

$$\langle U' | \mathbf{r} = \left(i \nabla_{p'} - \frac{3i p'}{p'^2 + a^2} \right) \langle U' |. \quad (133)$$

Action of \mathbf{a} and \mathbf{L} on $\langle U' |$

Using Equation (133) for the action of \mathbf{r} on $\langle U' |$ and using the expression Equation (120) for \mathbf{a} since $\langle U' |$ is proportional to $\langle p' |$, we immediately find that when acting on $\langle U' |$, \mathbf{a} has the differential representation

$$\mathbf{a}' = \frac{i}{2a} \left((p'^2 - a^2) \nabla_{p'} - 2\mathbf{p}' \cdot \nabla_{p'} \right) \quad (134)$$

where

$$\langle U' | \mathbf{a} = \mathbf{a}' \langle U' |. \quad (135)$$

We can also write \mathbf{a}' in terms of the U' variables by using the relationship Equation (52) between the p and U variables:

$$\mathbf{a}' = U'_4 i \nabla_{U'} - \mathbf{U}' i \partial / \partial U'_4 \quad (136)$$

where the spatial part of the four vector U' is $\mathbf{U} = (U_1, U_2, U_3)$ and U_4 is the fourth component. This is the differential representation of a rotation operator mixing the spatial and the fourth components of U'_a . When acting on the state $\langle U' |$, clearly $e^{i\mathbf{a}' \cdot \mathbf{v}}$ generates a four-dimensional rotation that produces a new eigenstate $\langle U'' |$. To explicitly derive the form of the finite transformation, we compute

$$[a'_j, U'_j] = iU'_4 \delta_{ij} \quad [a'_j, U'_4] = -iU'_i. \quad (137)$$

For a finite transformation $a^{i\mathbf{a}' \cdot \mathbf{nv}}$ with $\mathbf{n}^2 = 1$, we have

$$\begin{aligned} \mathbf{U}'' &= e^{i\mathbf{a}' \cdot \mathbf{nv}} \mathbf{U}' e^{-i\mathbf{a}' \cdot \mathbf{nv}} \\ &= \mathbf{U}' - \mathbf{nn} \cdot \mathbf{U}' + \mathbf{nn} \cdot \mathbf{U}' \cos \nu - nU'_4 \sin \nu \end{aligned} \quad (138)$$

and

$$\begin{aligned} U_4'' &= e^{i\mathbf{a}' \cdot \mathbf{nv}} U'_4 e^{-i\mathbf{a}' \cdot \mathbf{nv}} \\ &= U'_4 \cos \nu + \mathbf{n} \cdot \mathbf{U}' \sin \nu \end{aligned} \quad (139)$$

These equations of transformation are like those for a Lorentz transformation of a four-vector (\mathbf{r} , it). We can illustrate the equations for $e^{i\mathbf{a}' \cdot \mathbf{nv}}$ (cf Equation (58)), which mixes the two and four components of U' :

$$\begin{aligned} U_1'' &= U'_1 & U_3'' &= U'_3 \\ U_2'' &= U'_2 \cos \nu - U'_4 \sin \nu & U_4'' &= U'_2 \sin \nu + U'_4 \cos \nu \end{aligned} \quad (140)$$

When \mathbf{L} acts on $\langle U' |$, it has the differential representation

$$\mathbf{L}' = \mathbf{U}' \times i \nabla_{U'} \quad (141)$$

This result follows directly, since U'_i equals p'_i times a factor that is a scalar under rotations in three dimensions. When $e^{i\mathbf{L}' \cdot \boldsymbol{\omega}}$ acts on $\langle U' |$ it produces a new state $\langle U'' |$, where the spatial components of U' have been rotated to produce U'' .

In summary, we see that U' is a four-vector under rotations generated by \mathbf{a}' and \mathbf{L}' . Therefore the states $\langle U' |$ provide a vector representation of the group of rotations in four dimensions $SO(4)$, with the generators \mathbf{a} and \mathbf{L} .

5. Wave Functions for the Hydrogenlike Atom

In this section, we analyze the wave functions of the hydrogenlike atom, working primarily in the $\langle U' |$ representation and using eigenstates of the inverse of the coupling constant $(Z\alpha)^{-1}$ for the basis states. In this representation the wave functions are spherical harmonics in four dimensions. We derive the relationship of the usual energy eigenfunctions in momentum space to the spherical harmonics and discuss the classical limits in momentum and configuration space.

5.1. Transformation Properties of the Wave Functions under the Symmetry Operations

We can show that the wave functions $Y_{nlm}(U')$ in the $\langle U' |$ representation with respect to the eigenstates of $(Z\alpha)^{-1}$

$$Y_{nlm}(U') \equiv \langle U' | nlm \rangle \quad (142)$$

transform as four-dimensional spherical harmonics under the four-dimensional rotations generated by the Runge-Lenz vector \mathbf{a} and the angular momentum \mathbf{L} . We note that the quantity a is implicit in both the bra and the ket in Equation (142). For our basis states we employ the set of $(Z\alpha)^{-1}$ eigenstates $|nlm\rangle$ of the inverse coupling constant that are convenient for momentum space calculations ($\rho = \frac{p^2+a^2}{2a^2}$). We choose these states rather than those convenient for configuration space calculations, because the $\langle U' |$ eigenstates are proportional to the $\langle p' |$ eigenstates.

If we transform our system by the unitary operator $e^{i\theta}$ where $\theta = \mathbf{L} \cdot \boldsymbol{\omega} + \mathbf{a} \cdot \mathbf{v}$, then the wave function in the new system is

$$Y'_{nlm}(U') = \langle U' | e^{i\theta} | nlm \rangle. \quad (143)$$

There are two ways in which we may interpret this transformation, corresponding to what have been called the active and the passive interpretations. In the passive interpretation we let $e^{i\theta}$ act on the coordinate eigenstate $\langle U' |$. As we have seen in Section 3.6, this produces a new eigenstate $\langle U'' |$, where the four-vector U'' is obtained by a four-dimensional rotation of U' (Equations (138) and (139)). Thus, we have

$$Y'_{nlm}(U') = \langle U'' | nlm \rangle = Y_{nlm}(U''). \quad (144)$$

In the active interpretation, we let $e^{i\theta}$ act on the basis state $|nlm\rangle$. Because \mathbf{L} and \mathbf{a} are symmetry operators of the system, transforming degenerate states into each other, it follows that $e^{i\theta}|nlm\rangle$ must be a linear combination of states with principal quantum number equal to n . Therefore, we have

$$Y'_{nlm}(U') = \sum_{l'm'} \langle U' | R_{nl'm'}^{nlm} | nl'm' \rangle = \sum_{l'm'} R_{nl'm'}^{nlm} Y_{nl'm'}(U'). \quad (145)$$

The wave functions for degenerate states with a given n transform irreducibly among themselves under the four-dimensional rotations, forming a basis for an irreducible representation of $SO(4)$ of dimensions n^2 . Equating the results of the two different interpretations gives

$$Y_{nlm}(U'') = \sum_{l'm'} R_{nl'm'}^{nlm} Y_{nl'm'}(U'). \quad (146)$$

The transformation properties Equation (146) of Y_{nlm} are precisely analogous to those of the three-dimensional spherical harmonic functions. It follows that the Y_{nlm} are four-dimensional spherical harmonics [35,124].

5.2. Differential Equation for the Four Dimensional Spherical Harmonics $Y_{nlm}(U')$

The differential equation for the $Y_{nlm}(U')$ may be obtained from the equation

$$(\mathbf{L}'^2 + \mathbf{a}'^2)Y_{nlm}(U') = (n^2 - 1)Y_{nlm}(U') \quad (147)$$

which follows from $C_2 = n^2 - 1$ and the definition of C_2 , Equation (81). Substituting in the differential expressions Equations (134) and (141) for \mathbf{a}' and \mathbf{L}' we find that $\mathbf{L}'^2 + \mathbf{a}'^2$ equals $\nabla_{U'}^2 - (\mathbf{U}' \cdot \nabla_{U'})^2$, which is the angular part of the Laplacian operator in four dimensions (cf in three dimensions, $\mathbf{L}^2/r^2 = p^2 - p_r^2$). Thus, Equation (147) is the differential equation for four-dimensional spherical harmonics with the degree of homogeneity equal to $n - 1$, which means n^2 such functions exist, in agreement with the known degree of degeneracy.

5.3. Energy Eigenfunctions in Momentum Space

We want to determine the relationship between the usual energy eigenfunctions in momentum space $\psi_{nlm}(p') \equiv \langle p' | nlm \rangle$ (with $a = a_n$) and the four-dimensional spherical harmonic eigenfunctions $Y_{nlm}(U'; a) = \langle U' | nlm; a \rangle$.

We choose the RMS momentum a to have the value a_n . If we use the expression Equation (131) for $\langle U' |$ in terms of $\langle p' |$

$$\langle U' | = \langle p' | \left(\frac{p^2 + a_n^2}{2a_n} \right)^{3/2} \quad (148)$$

and the expression Equation (104) for the eigenstates of $(Z\alpha)^{-1}$ in terms of the energy eigenstates

$$|nlm; a_n\rangle = \sqrt{\frac{p^2 + a_n^2}{2a_n^2}} |nlm\rangle \quad (149)$$

we find the desired result

$$Y_{nlm}(U'; a_n) = \left(\frac{p^2 + a_n^2}{2a_n} \right)^2 \frac{1}{\sqrt{a_n}} \psi_{nlm}(p'). \quad (150)$$

The usual method of deriving this relationship between the wave function in momentum space and the corresponding spherical harmonics in four dimensions involves transforming the Schrodinger wave equation to an integral equation in momentum space [18,35]. As in the classical case, to do this we first replace p by p/a and perform a stereographic projection from the hyperplane corresponding to the three-dimensional momentum space to a unit hypersphere in a four-dimensional space. The resulting integral equation manifests a four-dimensional invariance. When the wave functions are normalized as in Equation (150), the solutions are spherical harmonics in four dimensions. As another alternative to this procedure, we can Fourier transform the configuration space wave functions directly [126].

5.4. Explicit Form for the Spherical Harmonics

The spherical harmonics in four dimensions can be expressed as [127]:

$$Y_{nlm}(\Omega) = N_1(n, l) (\sin \theta_4)^l C_{n-1-l}^{l+1}(\cos \theta_4) \cdot \left[N_2(l, m) (\sin \theta)^m C_{l-m}^{m+1/2}(\cos \theta) \frac{e^{im\phi}}{\sqrt{2\pi}} \right]. \quad (151)$$

The factor in brackets is equal to $Y_l^m(\theta, \phi)$, the usual spherical harmonic in three-dimensions [127]. The Gegenbauer polynomials C_n^λ of degree n and order λ are defined in terms of a generating function:

$$\frac{1}{(1 - 2tx + t^2)^\lambda} = \sum_{n=0}^{\infty} t^n C_n^\lambda. \quad (152)$$

$N_1(n, l)$ and $N_2(l, m)$ are chosen to normalize the Y_{nlm} on the surface of the unit sphere:

$$\int |Y_{nlm}(\Omega)|^2 d^3\Omega_U = 1 \quad (153)$$

where $d^3\Omega_U = \sin^2 \theta_4 \sin \theta d\theta d\phi$. We find

$$N_1(n, l) = \sqrt{\frac{2^{2l+1}}{\pi} \frac{n(n-l-1)!(l!)^2}{(n+l)!}} \quad (154)$$

$$N_2(l, M) = \sqrt{\frac{2^{2m}}{\pi} \left(l + \frac{1}{2}\right) \frac{(l-m)!}{(l+m)!} \left[\Gamma\left(m + \frac{1}{2}\right)\right]^2}. \quad (155)$$

In the next section, we discuss the asymptotic behavior of Y_{nlm} for large quantum numbers and compare it to the classical results of Section 3.

5.5. Wave Functions in the Classical Limit

5.5.1. Rydberg Atoms

Advances in quantum optics, such as the development of ultra short laser pulses, microwave spectroscopy, and atom interferometry, have opened new possibilities for experiments with atoms and Rydberg states, meaning hydrogenlike atoms in states with very large principal quantum numbers and correspondingly large diameter electron orbits. The pulsed electromagnetic fields can be used to modify the behavior of the orbital electrons. Semi-classical electron wave packets in hydrogenlike atoms were first generated in 1988 by ultrashort laser pulses, and today are often generated by unipolar terahertz pulses [128–130]. Over the last few decades, there has been interest in the classical limit of the hydrogenlike atom for n very large, Rydberg states, for a number of reasons [131]: 1. Rydberg states are at the border between bound states and the continuum, and any process which leads to excited bound states, ions or free electrons usually leads to the production of Rydberg states. This includes, for example, photo-ionization or the application of microwave fields. The very large cross section for scattering is unique. 2. Rydberg states can be used to model atoms with a higher atomic number that have an excited valence electron that orbits beyond the core. 3. In Rydberg states, the application of electric and magnetic fields breaks the symmetry of the atom and allows for the study of different phenomena, including the transition from classical to quantum chaos [132]. 4. Rydberg atoms can be used to study coherent transient excitation and relaxation, for example, the response to short laser pulses creating coherent quantum wave packets that behave like a classical particle.

The square of the wave function for a given quantum state gives a probability distribution for the electron that is independent of time. If we want to describe the movement of an electron in a semiclassical state, with a large radius, going around the nucleus with a classical time dependence, then we need to form a wave packet. The wave packet is built as a superposition of many wave functions with a band of principal quantum numbers.

A variety of theoretical methods have been used to derive expressions for the hydrogen atom wave functions and wave packets for highly excited states. There is general agreement on the wave functions for large n , and that the wave functions display the expected classical behavior, elliptical orbits in configuration space, and great circles in the four dimensional momentum space [133–136].

Researchers have proposed a variety of wave packets to describe Rydberg states. There are general similarities in the wave packets that describe electrons going in circular or elliptical orbits with a classical time dependence for some characteristic number of orbits, and it is maintained that the quantum mechanical wave packets provide results that agree with the classical results [129,130,133–139]. Most of the approaches exploit the $SO(4)$ or $SO(4,2)$ symmetry of the hydrogen atom which is used to rotate a circular orbital to an elliptical orbit. The starting orbital is often taken as a coherent state, which is usually considered a classical like state with minimum uncertainty. The most familiar example of a coherent state is for a one dimensional harmonic oscillator characterized by creation and annihilation operators a^\dagger and a . The coherent state $|\alpha\rangle$ is a superposition of energy eigenstates that is an eigenstate of a where $a|\alpha\rangle = \alpha|\alpha\rangle$ for a complex α . This coherent state will execute harmonic motion like a classical particle [140]. To obtain a coherent state for the hydrogenlike atom, eigenstates of the operator that lowers the principal quantum number n (which will be discussed in Section 7.4) have been used [141], as well as lowering operators based on the equivalence of the four dimensional harmonic oscillator representation of the hydrogen atom [134,135,142].

In either case, this coherent eigenstate is characterized by a complex eigenvalue, which needs to be specified. Several constraints have been used to obtain the classical wave packet that presumably obeys Kepler's Laws, such as requiring that the orbit lie in a plane so $\langle z \rangle = 0$ for the orbital, or that $\langle r - r_{classical} \rangle$ be a minimum, or that some minimum uncertainty relationship is obtained. In addition, there are issues regarding the approximations used, in particular, those that relate to time. For times

characteristic of the classical hydrogen atom, the wavepackets act like a classical system. For longer times, the wavepacket spreads in the azimuthal direction and after some number of classical revolutions of order 10 to 100 the spread is 2π , so the electron is uniformly spread over the entire orbit. The spread arises because the component wave functions forming the wavepacket have different momenta. In two derivations, still longer times were considered, and recoherence was predicted to occur after about $n/3$ (where n is the approximate principal quantum number) revolutions, although there is some difference in the predicted amount of recoherence [131,136]. Because of the conservation of L and A , the spread of the wave packets is inhibited, except in the azimuthal direction.

This is a system with very interesting physics. For example, one can view the transition from a well defined wave packet representing the electron to a 2π spread and back again as a dynamical illustration of the wave-particle duality.

Brown took a different approach to develop a wavepacket for a circular orbit [139]. He first developed the asymptotic wave function for large n and then optimized the coefficients in a Gaussian superposition to minimize the spread in ϕ , obtaining a predicted characteristic decoherence time of about 10 minutes, considerable longer than any other predicted decoherence time.

Other authors have explored the problem from the perspective of classical physics and the correspondence principle [133,137,143,144]. The results from the different methods are similar with the basic conclusion that the wave functions are peaked on the corresponding classical Kepler trajectories: “atomic elliptic states sew the wave flesh on the classical bones” [129].

With the variety of experimental methods used to generate Rydberg states, a variety of Rydberg wave packets are created, and it is not clear which theoretical model, if any, is preferred [131]. We take a very simple approach to forming a wavepacket and simply use a Gaussian weight for the different frequency components. This does not give an intentionally optimized wave packet, but it is a much simpler approach and the result has all of the expected classical behavior that is very similar to that obtained from much more complicated derivations. We start with a circular orbit and then do a SO(4) rotation to secure an elliptical orbit. We show that it has the classical period of rotation.

5.5.2. Wave Functions in the Semi-Classical Limit

We need to derive the semiclassical limit of the wave functions that correspond to circular orbits in configuration space. For this case, $\sin \nu$, which we interpret as the expectation value of the eccentricity, vanishes. We derive expressions for the wave functions in momentum space and then form a wavepacket. To obtain corresponding expressions for elliptical orbits, we perform a rotation by $e^{ia \cdot \nu}$, which does not alter the energy but changes the eccentricity and the angular momentum.

Case 1: Circular orbits, $\sin \nu = e = 0$

We derive the asymptotic form of Y_{nlm} for large quantum numbers, where for simplicity we choose the quantum numbers $n - 1 = l = m$ corresponding to a circular orbit in the 1–2 plane. From Equation (151) we see we encounter Gegenbauer polynomials of the form C_0^λ , which, by Equation (152), are unity. For a very large l , $\sin^l \theta$ will have a very strong peak at $\theta = \pi/2$, so we make the expansion [103]

$$\sin \theta = \sin \left(\frac{\pi}{2} + \left(\theta - \frac{\pi}{2} \right) \right) = 1 - \frac{1}{2} \left(\theta - \frac{\pi}{2} \right)^2 + \dots \approx e^{-(1/2)(\theta - \pi/2)^2} \quad (156)$$

to obtain

$$\sin^l \theta \approx e^{-(1/2)l(\theta - \pi/2)^2}. \quad (157)$$

The asymptotic forms for N_1 and N_2 can be computed using the properties of Γ functions:

$$\begin{aligned} \Gamma(2z) &= \left(\frac{1}{\sqrt{2\pi}} \right) 2^{2z-1/2} \Gamma(z) \Gamma \left(z - \frac{1}{2} \right) \\ \lim_{z \rightarrow \infty} \Gamma(az + b) &\simeq \sqrt{2\pi} e^{-az} (az)^{az+b-1/2}. \end{aligned} \quad (158)$$

We finally obtain [145]

$$Y_{n,n-1,n-1}(\Omega) = \sqrt{\frac{n}{2\pi^2}} e^{-\frac{1}{2}n(\theta_4 - \frac{\pi}{2})^2} \cdot e^{-\frac{1}{2}n(\theta - \frac{\pi}{2})^2} e^{i(n-1)\phi}, \quad (159)$$

which gives the probability density

$$|Y_{n,n-1,n-1}(\Omega)|^2 = \frac{n}{(2\pi^2)} e^{-n(\theta_4 - \frac{\pi}{2})^2} \cdot e^{-n(\theta - \frac{\pi}{2})^2}. \quad (160)$$

We have Gaussian probability distributions in θ_4 and θ about the value $\pi/2$. The distributions are quite narrow with widths $\Delta\theta_4 \approx \Delta\theta \approx 1/\sqrt{n}$ and the spherical harmonic essentially describes a circle ($\theta_4 = \theta = \pi/2$) on the unit sphere in the 1–2 plane. As n becomes very large, $U_4 = \cos\theta_4 \approx (r - r_c)/r$ (Equations (54) and (72)) and $U_3 = \sin\theta_4 \cos\theta$, which is proportional to p_3 , both go to zero as $1/\sqrt{n}$. The distribution approaches the great circle $U_1^2 + U_2^2 = 1$ that we found in Section 3.6 for a classical particle moving in a circular orbit in the 1–2 plane in configuration space. Note that this state is a stationary state with a constant probability density. To get the classical time dependence we need to form a wavepacket.

Forming a Wavepacket

We form a time dependent wavepacket for circular orbits by superposing circular energy eigenstates:

$$\chi(\Omega, t) = \sum_n e^{itE_n} Y_{n,n-1,n-1} A_{n-N} \quad (161)$$

where A_{n-N} is an amplitude peaked about $n = N \gg 1$. For $n \gg 1$ we expand E_n about E_N :

$$E_n = E_N + \left. \frac{\partial E}{\partial n} \right|_N s + \left. \frac{\partial^2 E}{\partial n^2} \right|_N s^2 + \dots \quad (162)$$

where $s = n - N$. From the equation for the energy levels, $E = -m(Z\alpha)^2/(2n^2)$ we compute

$$\left. \frac{\partial E_n}{\partial n} \right|_N = \frac{m(Z\alpha)^2}{N^3} = \sqrt{\frac{-8E_N^3}{m(Z\alpha)^2}}. \quad (163)$$

In agreement with the Bohr Correspondence Principle, the right-hand side of this equation is just the classical frequency ω_{cl} as given in Equation (38). For the second order derivative, we have

$$\left. \frac{\partial^2 E}{\partial n^2} \right|_N = -\frac{3}{N} \omega_{cl} \equiv \beta \quad (164)$$

which gives

$$\chi(\Omega, t) = e^{-itE_N} e^{i\phi(N-1)} \sum_{s=-N+1}^{\infty} e^{-i(\omega_{cl}st - (\frac{\beta}{2})s^2t - s\phi)} \cdot A_s |Y_{N+s, N+s-1, N+s-1}|. \quad (165)$$

We choose a Gaussian form for A_s

$$A_s = \frac{1}{\sqrt{2\pi N}} e^{-s^2/(2N)}. \quad (166)$$

Brown used $A_s = Ce^{-s^2 3\omega_{cl}t/N}$ which minimizes the diffusion in ϕ at time t [139]. Since $|Y_{N+s, N+s-1, N+s-1}|$ varies slowly with s for $N \gg 1$ we can take it outside the summation in Equation (165). We now replace the sum by an integral over s . Because A_s is peaked about N

we can integrate from $s = -\infty$ to $s = +\infty$. We perform the integral by completing the square in the usual way. The final result for the probability amplitude for a circular orbital wave packet is

$$|x(\Omega, t)|^2 = |Y_{N,N-1,N-1}|^2 \left(1 + \beta^2 t^2 N^2\right)^{-1} \cdot \exp \left[-(\phi - \omega_{cl} t)^2 \frac{N}{1 + (\beta t N)^2} \right]. \quad (167)$$

This represents a Gaussian distribution in ϕ that is centered about the classical value $\phi = \omega_{cl} t$, meaning that the wavepacket is traveling in the classical trajectory with the classical time dependence. The width of the ϕ distribution is

$$\Delta\phi = (N)^{(-1/2)}(1 + \beta^2 t^2 N^2)^{1/2} = (N)^{(-1/2)}(1 + 9\omega_{cl}^2 t^2)^{1/2}. \quad (168)$$

The distribution in ϕ at $t = 0$ is very narrow, proportional to $1/\sqrt{N}$, but after several orbits $\Delta\phi$ is increasing linearly with time.

The distributions in θ_4 and θ are Gaussian and centered about $\pi/2$ in each case as for the circular wave function (cf. Equation (160)) with widths equal to $(N)^{-1/2}$. The spreading of these distributions in time is inhibited because of the conservation of angular momentum and energy. The detailed behavior of the widths depend on our use of the Gaussian distribution. Other distributions will give different widths, although the general behavior is expected to be similar.

As a numerical example, consider a hydrogen atom that is in the semiclassical region when the orbital diameter is about 1 cm. The corresponding principal quantum number is about 10^4 , the mean velocity is about 2.2×10^4 cm/s and the period about 1.5×10^{-4} s. After about 34 revolutions or 5×10^{-3} s, the spread in ϕ is about 2π , meaning the electron is spread uniformly about the entire circular orbit. This characteristic spreading time can be compared to 1.6×10^{-3} s for a fully optimized wave packets formed from coherent SO(4,2) states [136,146]. In order to make predictions about significantly longer times, we would need to retain more terms in the expansion Equation (162) of E_n .

Case 2: Elliptical orbits $\sin \nu = e \neq 0$

We can obtain the classical limit of the wave function for elliptical orbits by first writing our asymptotic form Equation (159) for $Y_{n,n-1,n-1}$ in terms of the U variables instead of the angular variables by using definitions Equation (52), and setting $a = a_n$. Retaining only the lowest order terms in $(\theta_4 - \pi/2)$ and $(\theta - \pi/2)$, we find

$$Y_{n,n-1,n-1}(U) = \left(\frac{n}{2\pi^2}\right)^{1/2} e^{i(n-1)\tan^{-1}\left(\frac{U_2}{U_1}\right)} \cdot e^{-\frac{1}{2}n(U_4)^2} e^{-\frac{1}{2}n(U_3)^2} \quad (169)$$

For large n , this represents a circular orbit in the 1–2 plane. We now perform a rotation by $A_2\nu$, which will change the eccentricity to $\sin \nu$, and change the angular momentum, but will not change the energy or the orbital plane. Using Equation (140) to express the old coordinates in terms of the new coordinates, we find to lowest order

$$Y'_{n,n-1,n-1}(U) = \left(\frac{n}{2\pi^2}\right)^{1/2} e^{i(n-1)\tan^{-1}\left(\frac{U_2}{U_1 \cos \nu}\right)} \cdot e^{-\frac{1}{2}n\{U_2 \sin \nu - U_4 \cos \nu\}^2} \cdot e^{-\frac{1}{2}n(U_3)^2}. \quad (170)$$

In Section 3.6, we found that the vanishing of the term in braces $0 = U_2 \sin \nu - U_4 \cos \nu$ specifies the classical great hypercircle orbit (Equation (56)) corresponding to an ellipse in configuration space with eccentricity $e = \sin \nu$ and lying in the 1–2 plane. The probability density $|Y'_{n,n-1,n-1}(U)|^2$ vanishes except within a hypertorus with a narrow cross section of radius approximately $\frac{1}{\sqrt{n}}$, which is centered about the classical distribution. Because the width $\frac{1}{\sqrt{n}}$ of the distribution is constant in U space, it will not be constant when projected onto p space.

In terms of the original momentum space variables, the asymptotic spherical harmonic is

$$\begin{aligned}
 Y_{n,n-1,n-1}(\mathbf{p}) &= \left(\frac{n}{2\pi^2}\right)^{\frac{1}{2}} e^{i(n-1)\tan^{-1}\left(\frac{p_2}{p_1 \cos \nu}\right)} \\
 &\cdot \exp\left\{-\left(\frac{n}{2}\right)\left[p_1^2 + (p_2 - a \tan \nu)^2 - \frac{a^2}{\cos^2 \nu}\right]^2 \left(\frac{\cos \nu}{p^2 + a^2}\right)\right\}^2 \\
 &\cdot \exp\left\{-\left(\frac{n}{2}\right)\left(\frac{2p_3 a}{p^2 + a^2}\right)\right\}^2 \Big|_{a = a_n}
 \end{aligned} \tag{171}$$

The expression in brackets corresponds to the momentum space classical orbit equation we found previously (Equation (49)). As we expect, p_3 is Gaussian about zero since the classical orbit is in the 1–2 plane. We can simplify the expressions for the widths by observing that to lowest order we can use Equation (48), which implies $p^2 + a^2 = 2a^2 + 2ap_2 \tan \nu$ in the exponentials. The widths of both distributions therefore increase linearly with p_2 . We also note that, since classically there exists a one-to-one correspondence between each point of the trajectory in momentum space and each point in configuration space, we may interpret the widths of the distributions using Equation (32) $\frac{p^2 + a^2}{a^2} = \frac{2r_c}{r}$. Accordingly, the widths increase as the momentum increases or as the distance to the force center decreases (Figure 8).

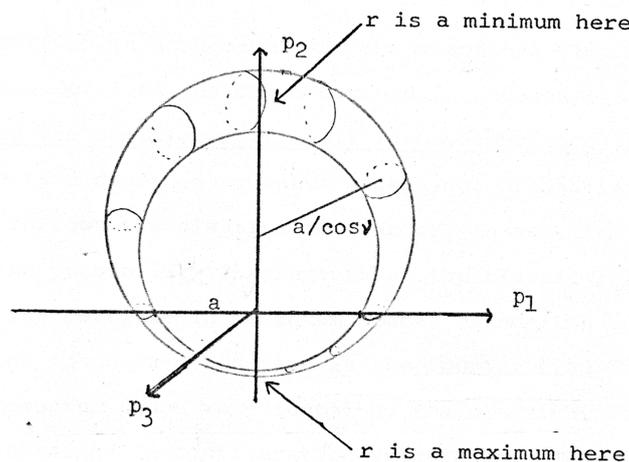


Figure 8. Wave function probability distribution $|Y'_{n,n-1,n-1}(\mathbf{p})|^2$ in momentum space for large n , showing the variation in the width of the momentum distribution about the classical circular orbit. The center of the distribution is at $p_2 = a \tan \nu$. The classical orbit is in the 1–2 plane.

Forming a Wave packet for Elliptical Motion

We may form a time dependent wavepacket superposing the wave functions of Equation (170). Care must be taken to include the first order dependence (through a_n) of $\tan^{-1}(U_2/U_1 \cos \nu)$ on the principal quantum number when integrating over the Gaussian weight function. The result for the probability density is the same as before (Equation (167)), except $|Y'_{N,N-1,N-1}|^2$ (given in Equation (170)) replaces $|Y_{N,N-1,N-1}|^2$ and

$$\omega_{cl}t = \tan^{-1}\left(\frac{U_2}{U_1 \cos \nu}\right) + \sin \nu (U_1) \tag{172}$$

where replaces $\omega_{cl}t = \phi$. The result is exactly the same as the classical time dependence Equation (73). The spreading of the wave packet will be controlled by the same factor as for the circular wave packet.

Remark on the Semiclassical Limit in Configuration Space

The time dependent quantum mechanical probability density follows the classical trajectory in momentum space meaning that the probability is greatest at the classical location of the particle in momentum space. Because the configuration space wave function is the Fourier transform of the momentum space wave function, the classical limit must also be obtained in configuration space. That this limit is obtained is made explicit by observing that the momentum space probability density is large when

$$(U_2 \sin \nu - U_4 \cos \nu)^2 \approx 0. \quad (173)$$

However from Section 3 we can show that

$$U_2 \sin \nu - U_4 \cos \nu = \cos \nu \left(\frac{r - r_{\text{classical}}}{r_{\text{classical}}} \right) \quad (174)$$

where $r_{\text{classical}}$ is given by the classical orbit Equation (33). Accordingly, we see that the configurations space probability will be large when

$$\left[\frac{r - r_{\text{classical}}}{r_{\text{classical}}} \right]^2 \approx 0. \quad (175)$$

5.6. Quantized Semiclassical Orbits

It is convenient at times to have a semiclassical model for the orbitals of the hydrogenlike atom. Historically this was first done by Pauling and Wilson [147]. We can obtain a model by interpreting the classical formulae for the geometrical properties of the orbits as corresponding to the expectation values of the appropriate quantum mechanical expressions. Thus, when the energy $E = -a^2/2m$ appears in a classical formula, we employ the expression for a for the quantized energy levels $a = \frac{1}{m r_0}$ where $r_0 = (mZ\alpha)^{-1}$, which is the radius 0.53 Angstrom of the ground state. Similarly if L^2 appears in a classical formula, we substitute $l(l+1)$, where l is quantized $l = 0, 1, 2, \dots, n-2, n-1$; and m , the component of L along the 3-axis is quantized: $m = -l, -l+1, -l+2, \dots, l$.

Orbits in Configuration Space

Recalling Equation (28) $r_c = \frac{mZ\alpha}{a^2}$, we see $ar_c = n$, which gives a semimajor axis of length $r_c = n^2 r_0$, where r_0 is the radius for the circular orbit of the ground state and r_c is for a circular orbit for a state with principal quantum number n . The equations for the magnitude of L and A are

$$L = r_c a \cos \nu = n \cos \nu = \sqrt{l(l+1)} \quad (176)$$

$$A = r_c a \sin \nu = n \sin \nu = \sqrt{n^2 - l(l+1)} \quad (177)$$

This gives an eccentricity $\sin \nu$ equal to

$$e = \sin \nu = \sqrt{1 - \frac{l(l+1)}{n^2}} \quad (178)$$

and a semi-major axis equal to

$$b = r_c \sin \nu = n \sqrt{l(l+1)}. \quad (179)$$

Note that the expression for e is limited in its meaning. For an s state, it always gives $e = 1$, and for states with $l = n - 1$ it give $e = \sqrt{1/n}$, not the classically expected 0 for a circular orbit.

Orbits in U-Space

The corresponding great hypercircle orbits (ν, Θ) in U-space are described by giving the quantized angle ν , between the three-dimensional hyperplane of the orbit and the 4-axis, and the quantized angle Θ , between the hyperplane of the orbit and the 3-axis:

$$\cos \nu = \sqrt{\frac{l(l+1)}{n^2}} \quad (180)$$

$$\cos \Theta = \sqrt{\frac{m^2}{l(l+1)}}. \quad (181)$$

Note the similarity in these two equations, suggesting that m relates to l the same way that l relates to n , which suggests a generalization of the usual vector model of the atom which only describes the precession of L about the z axis.

The results for orbits in configuration and momentum space illustrate some interesting features:

1. The equation $ar = n$ illustrates that the characteristic dimensions of an orbit in configuration space and the corresponding orbit in momentum space are inversely proportional, as expected, since they are related by a Fourier transform, consistent with the Heisenberg Uncertainty Principle.

2. If $l = 0$, then no classical state exists. The orbit in configuration space degenerates into a line passing through the origin while the corresponding circular orbit in momentum space attains an infinite radius and an infinite displacement from the origin. Although this seems peculiar from the pure classical viewpoint, quantum mechanically it follows, since for S states there is a nonvanishing probability of finding the electron within the nucleus.

In order to interpret these statements about quantized semiclassical elliptical orbits we observe that for quantum mechanical state of the hydrogenlike atom with definite n, l, m , the probability density is (1) independent of ϕ_r or ϕ_p and (2) it does not confine the electron to some orbital plane. Because the quantum mechanical distribution for such a state specifies no preferred direction in the 1–2 plane, we must imagine this distribution as corresponding in some way to an average over all possible orientations of the semiclassical elliptical orbit. This interpretation is supported by the fact that the region within which the quantum mechanical radial distribution function differs largely from zero is included between the values of r corresponding to the semiclassical turning points $r_c(1 \pm \sin \nu)$.

5.7. Four-Dimensional Vector Model of the Atom

In configuration space or momentum space, the angle between the classical plane of the orbit and the 3-axis is Θ , which is usually interpreted in terms of the vector model of the atom in which we imagine L to be a vector of magnitude $\sqrt{l(l+1)}$ precessing about the 3-axis, with m as the component along the 3-axis. This precession may be linked to the ϕ_r independence of the probability and the absence of an orbital plane as mentioned at the end of the preceding section. The precession constitutes a classical mechanism which yields the desired average over all possible orientations of the semiclassical elliptical orbit. Because the angle Θ is restricted to have only certain discrete values one can say that there is a quantization of space.

The expression for $\cos \nu = \sqrt{l(l+1)}/n^2$ is quite analogous to that for Θ and so suggests a generalization of the vector model of the atom to four dimensions. The projection of the four-dimensional vector model onto the physical three-dimensional subspace must give the usual vector model. We can achieve this by imagining that a four-dimensional vector of length n , where n is the principal quantum number, is precessing in such a way that its three and four components are constants, while the one and two components vary periodically. The projection onto the 1–2–3 hyperplane is a vector of constant magnitude $\sqrt{l(l+1)}$ precessing about the 3-axis. The component along the 3-axis is m . The component along the 4-axis is $A = \sqrt{n^2 - l(l+1)}$ the magnitude of the vector A . The vectors L and A are perpendicular to each other. Thus, the precessing n vector makes a

constant angle Θ with the 3-axis and a constant angle $\pi/2 - \nu$ with the 4-axis. Because both angles are restricted to certain values, we may say that we have a quantization of four-dimensional space.

6. The Spectrum Generating Group SO(4,1) for the Hydrogenlike Atom

We consider the Schrodinger hydrogen atom and its unitary “noninvariance” or spectrum generating operators $e^{iD_i\beta_i}$ where D_i is a generator and β_i is a real parameter, using eigenstates of $(Z\alpha)^{-1}$ for our basis of our representation. These operators transform an eigenstate of the kernel K with a definite value of the coupling constant (or principal quantum number) into a linear combination of eigenstates with different values of the coupling constant (or different principal quantum numbers), and different l and m . Unlike the invariance generators L and A , the noninvariance generators clearly do not generally commute with the kernel K , $[D_i, K] \neq 0$, so they change the principal quantum number.

The set of all invariance and noninvariance operators forms a group with which we may generate all eigenstates in our complete set from a given eigenstate. We show that this group, called the Spectrum Generating Group of the hydrogenlike atom, is SO(4,1), the group of orthogonal transformations in a 5-dimensional space with a metric $g_{AB} = (-1, 1, 1, 1, 1)$, where $A, B = 0, 1, 2, 3, 4$. The complete set of eigenstates of $(Z\alpha)^{-1}$ for the hydrogenlike atom forms a unitary, irreducible, infinite-dimensional representation of SO(4,1) which, we shall find, can be decomposed into an infinite sum of irreducible representations of SO(4), each corresponding to the degeneracy group for a particular principal quantum number. A unitary representation means all generators are unitary operators. An irreducible representation does not contain lower dimensional representations of the same group. In Section 6.3, we discuss the isomorphism between the spectrum generating group SO(4,1) and the group of conformal transformations in momentum space. An isomorphism means the groups have the same structure and can be mapped into each other.

6.1. Motivation for Introducing the Spectrum Generating Group Group SO(4,1)

We have examined the group structure for the degenerate eigenstates of $(Z\alpha)^{-1}$ for the Schrodinger hydrogenlike atom: the n^2 degenerate states form an irreducible representation of SO(4). The next question we might ask is: Do all or some of the states with different principal quantum numbers form an irreducible representation of some larger group which is reducible into SO(4) subgroups? If such a group exists then it clearly is not an invariance group of the kernel K (Equation (106)). If we want our noninvariance group to include just some of the states then it will be a compact group, since unitary representations of compact groups can be finite dimensional. If we want to include all states then it will be a noncompact group since there are an infinite number of eigenstates of $(Z\alpha)^{-1}$ and all unitary representations of noncompact groups are infinite dimensional [9].

We can find a compact noninvariance group for the first N levels of the coupling constant, $n = 1, 2, \dots, N$. The dimensionality of our representation is

$$\sum_{n=1}^N n^2 = \frac{N(N+1)(2N+1)}{6}. \quad (182)$$

Mathematical analysis of the group SO(5) shows that this is the dimensionality of the irreducible symmetrical tensor representation of SO(5), given by the tensor with five upper indices $T^{abc\dots}$, where $a, b, \dots = 1, 2, 3, 4$ or 5 [11]. Reducing this representation of SO(5) into its SO(4) components gives

$$\begin{aligned} (\text{symm} \cdot \text{tensor } N)_{SO(5)} &= (0, 0) \oplus \left(\frac{1}{2}, \frac{1}{2}\right) \oplus \dots \oplus \left(\frac{N-1}{2}, \frac{N-1}{2}\right) \\ &= (\text{symm} \cdot \text{tensor } n = 1)_{SO(4)} \oplus \\ &\quad (\text{symm} \cdot \text{tensor } n = 2)_{SO(4)} \oplus \\ &\quad \dots \oplus (\text{symm} \cdot \text{tensor } n = N)_{SO(4)} \end{aligned} \quad (183)$$

which is precisely the structure of the first N levels of a hydrogenlike atom. If we want to include all levels then we guess that the appropriate noncompact group is $SO(4,1)$, whose maximal compact subgroup is $SO(4)$. Thus, we conjecture that all states form a representation of $SO(4,1)$.

Consider the Lie algebra of $O(4,1)$ and the general structure of its generators in terms of the canonical variables. The algebra of $O(n)$ has $\frac{n(n-1)}{2}$ generators so to extend the algebra of $O(n)$ to $O(n+1)$ takes n generators, which can be taken as the components of a n -vector. To extend the Lie algebra from $O(4)$ to $O(5)$ or $O(4,1)$ we can choose the additional generators G_a to be components of a four-vector G under $O(4)$:

$$[S_{ab}, G_c] = i(G_b\delta_{ac} - G_a\delta_{bc}) \quad a, b, c = 1, 2, 3, 4. \tag{184}$$

If we apply Jacobi's identity to S_{ab} , G_a , and G_b and use Equation (184) we find

$$[S_{ab}, [G_a, G_b]] = 0. \tag{185}$$

We require that the Lie algebra closes, so $[G_a, G_b]$ must be a linear combination of the generators, clearly proportional to S_{ab} and we choose the normalization, such that

$$[G_a, G_b] = -iS_{ab}. \tag{186}$$

If we define

$$G_4 = S_{40} = S; \quad G_i = S_{i0} = B_i \tag{187}$$

and recall Equation (79)

$$L_i = \epsilon_{ijk}S_{jk} \quad A_i = S_{i4}$$

then the additional commutation relations that realize $SO(4,1)$ may be written in terms of L, A, B , and S :

$$\begin{aligned} [L_i, B_j] &= i\epsilon_{ijk}B_k & [L_i, S] &= 0 \\ [S, A_j] &= iB_j & [S, B_j] &= iA_j \\ [A_j, B_k] &= i\delta_{jk}S & [B_i, B_j] &= -i\epsilon_{ijk}L_k. \end{aligned} \tag{188}$$

The top two commutators show that B transforms as a three-vector under $O(3)$ rotations and that S is a scalar under rotations. Alternatively, we can write the commutation relations in terms of the generators S_{AB} , $A, B = 0, 1, 2, 3, 4$:

$$[S_{AB}, S_{CD}] = i(g_{AC}S_{BD} + g_{BD}S_{AC} - g_{AD}S_{BC} - g_{BC}S_{AD}) \tag{189}$$

where $g_{00} = -1, g_{aa} = 1$.

The commutators above follow directly from the mathematical theory of $SO(4,1)$, but the theory does not tell us what these generators represent, just their commutation properties. We now investigate the general features of the representations of $SO(4,1)$ provided by the hydrogenlike atom and how to represent the generators in terms of the canonical variables.

6.2. Casimir Operators

The two Casimir operators of $SO(4,1)$ are [120]

$$Q_2 = -\frac{1}{2}S_{AB}S^{AB} = S^2 + B^2 - A^2 - L^2 \tag{190}$$

and

$$Q_4 = -w_A w^A = (SL - AxB)^2 - \frac{1}{4}[L \cdot (A + B) - (A + B) \cdot L]^2 \tag{191}$$

where $w_A = \frac{1}{8}\epsilon_{ABCDE}S^{BC}S^{DE}$.

For SO(4), we recall that for the SO(4) representations the structure of the generators in terms of the canonical variables led to the vanishing of one Casimir operator $C_1 = L \cdot A$ and, consequently, the appearance of only symmetrical tensor representations. We will find Q_4 vanishes for analogous reasons.

If B is a pseudovector, it is proportional to L , which is the only independent pseudovector that can be constructed from the dynamical variables. The coefficient of proportionality, a scalar, X need not commute with H :

$$B = XL \quad [X, L] = 0 \quad [X, H] \neq 0 \quad (192)$$

Because $[B_i, B_j] = -ie_{ijk}L_k$ it follows that $X^2 = -1$ and B would therefore be a constant multiple of L and not an independent generator. Thus B must be a vector and expressible as

$$B = fr + hp \quad (193)$$

where f and h are scalar functions of r, p^2 , and $r \cdot p$. Accordingly we find

$$B \cdot L = L \cdot B = 0 \quad (194)$$

Further, since B is a vector and A is a vector, $A \times B$ is a pseudovector and therefore is proportional to L :

$$A \times B = YL, \quad [Y, L] = 0 \quad (195)$$

For this equation to be consistent with the SO(4,1) commutation relations we find $Y = S$ and, therefore

$$A \times B = SL. \quad (196)$$

It follows from substituting $L \cdot A = 0$ and Equations (194) and (196) into Equation (191) that for the SO(4,1) representations realized by the hydrogenlike atom

$$Q_4 = 0. \quad (197)$$

As with the SO(4) symmetry, the dynamics of the hydrogen atom require that only certain representations of SO(4,1) appear. From the mathematical theory of irreducible infinite dimensional unitary representations of SO(4,1), we have the following results:

$$\begin{aligned} \text{Class I: } Q_4 = 0; \quad Q_2 \text{ real, } > 0 \\ \text{SU(2) } \times \text{SU(2) content:} \\ (Q)^I = (0,0) \oplus \left(\frac{1}{2}, \frac{1}{2}\right) \oplus (1,1) \oplus \dots \end{aligned} \quad (198)$$

$$\begin{aligned} \text{Class II: } Q_4 = 0, Q_2 = -(s-1)(s+2), s = \text{integer } > 0 \\ \text{SU(2) } \times \text{SU(2) content:} \\ (Q)^{II} = \left(\frac{s}{2}, \frac{s}{2}\right) \oplus \left(\frac{s+1}{2}, \frac{s+1}{2}\right) \oplus \dots \end{aligned} \quad (199)$$

The class I representations are realized by the complete set of eigenstates of $(Z\alpha)^{-1}$ for the hydrogenlike atom. Note, however, that we have an infinite number of such class I representations since Q_2 may have any positive real value. We shall find that for $Q_2 = 2$ we may extend our group from SO(4,1) to SO(4,2). The class II representations are realized by the eigenstates of $(Z\alpha)^{-1}$ with principal quantum numbers from $n = s + 1$ to n becomes infinite. The first s levels could, if we desire, be described by SO(5).

In this section, we have analyzed the group structure and the representations using the complete set of eigenstates of $(Z\alpha)^{-1}$ for our basis. We might ask: what if we used energy eigenstates instead as a basis for the representations? From Section 4.3 we know that the quantum numbers and multiplicities

of the $(Z\alpha)^{-1}$ eigenstates are precisely the same as those of the bound energy eigenstates. Thus, with the energy eigenstates as our basis, we would reach the same conclusions about the group structure as before but we would be including only the bound states in our representations and we would be ignoring all scattering states.

6.3. Relationship of the Dynamical Group $SO(4,1)$ to the Conformal Group in Momentum Space

We can give a more complete analysis of the hydrogenlike atom in terms of $SO(4,1)$ by considering the relationship between the four-dimensional rotations of the four-vector U'_a , with $a = 1, 2, 3, 4$, which we discussed in Section 4.6, and the group of conformal transformations in momentum space. Conformal transformations preserve the angles between directed curves, but not necessarily lengths. The rotations generated by the Runge-Lenz vector \mathbf{a} and the angular momentum \mathbf{L} leave the scalar product $U_a V^a$ of four-vectors invariant and, therefore, are conformal transformations. The stereographic projection we employed is also a conformal transformation. Since the product of two conformal transformations is itself a conformal transformation, we must conclude that \mathbf{a} generates a conformal transformation of the momentum three-vector \mathbf{p} .

We must introduce two additional operators that correspond to the operators \mathbf{B} and S introduced in Section 6.1 in order to express the most general conformal transformation. By employing the isomorphism between the generators \mathbf{L} , \mathbf{a} , \mathbf{B} , and S of $SO(4,1)$ and the generators of conformal transformations in momentum space we can immediately obtain expressions for the additional generators \mathbf{B} and S in terms of the canonical variables, which is our objective. We need these additional generators to complete our $SO(4,1)$ group for the hydrogen atom.

To derive the isomorphism we use the most convenient representation, namely that based on eigenstates of $(Z\alpha)^{-1}$ convenient for momentum space calculations ($\rho = \frac{p^2+a^2}{2a^2}$). Once established, the isomorphism becomes a group theoretical statement and it is independent of the particular representation.

The Conformal Group in Momentum Space

An arbitrary infinitesimal conformal transformation in momentum three-space may be written as

$$\delta p_j = \delta a_j + \delta \omega_{jk} p_k + \delta \rho p_j + \left(p^2 \delta c_j - 2 p_j \mathbf{p} \cdot \delta \mathbf{c} \right) \quad (200)$$

where $\delta \omega_{jk} = -\delta \omega_{kj}$.

The terms in δp_j arise as follows:

$$\begin{aligned} \delta a_j & \text{ translation generated by } \mathbf{R} \cdot \delta \mathbf{a} \\ \delta \omega_{jk} & \text{ rotation generated by } \mathbf{J} \cdot \delta \boldsymbol{\omega}, J_{ij} = \epsilon_{ijk} J_k \\ \delta \rho & \text{ dilation generated by } D \delta \rho \\ \delta c_j & \text{ special conformal transformation generated by } \mathbf{K} \cdot \delta \mathbf{c} \end{aligned} \quad (201)$$

This is a ten parameter group with the generators $(\mathbf{R}, \mathbf{J}, D, \mathbf{K})$ which obey the following commutation relations:

$$\begin{aligned} [D, R_j] &= i R_j & [D, J_i] &= 0 \\ [D, K_j] &= -i K_j & [R_i, J_k] &= i \epsilon_{ijk} R_k \\ [K_n, R_m] &= 2i \epsilon_{nmr} J_r - 2i \delta_{mn} D & [J_i, J_k] &= i \epsilon_{ikm} J_m \\ [R_i, R_j] &= 0 & [K_i, J_k] &= i \epsilon_{ikm} K_m \\ [K_j, K_j] &= 0 & & \end{aligned} \quad (202)$$

There is an isomorphism between the algebra of the generators of conformal transformations and the dynamical noninvariance algebra of $SO(4,1)$ of the hydrogen atom. Because J_i is the generator

of spatial rotations we make the association $L_i = J_i$. Comparing the differential change in p_i from a transformation generated by $\mathbf{a} \cdot \delta \mathbf{v}$ (in the representation with $\rho = \frac{(p^2 + A^2)}{2a^2}$)

$$\begin{aligned} \delta p_i &= i[\mathbf{a} \cdot \delta \mathbf{v}, p_i] \\ &= -\frac{1}{2a} \left[(p^2 - a^2) \delta v_i - 2\mathbf{p} \cdot \delta \mathbf{v} p_i \right] \end{aligned} \quad (203)$$

to the differential change in p_i from a conformal transformation leads to the association

$$a_i = \frac{1}{2} \left(\frac{K_i}{a} - aR_i \right). \quad (204)$$

To confirm the identification we can use the commutation relations of the conformal group to show that the $O(4)$ algebra of L and \mathbf{a} corresponds precisely to that of J and $\frac{1}{2}(\frac{K}{a} - aR)$. This result alone suggests that our $SO(4)$ degeneracy group should be considered as a subgroup of the larger group $SO(4,1)$. It suggests introducing the operators

$$\mathbf{B} = \frac{1}{2} \left(\frac{\mathbf{K}}{a} + a\mathbf{R} \right) \quad S = D. \quad (205)$$

The commutation relations of S and \mathbf{B} which follow from Equations (205) and the commutation relations Equation (202) are identical to the commutation relations given for S and \mathbf{B} in Section 6.1. Thus, by considering the \mathbf{a} and L transformations in momentum space as conformal transformations, we were led to introduce the generators \mathbf{B} and S and obtain the dynamical algebra $SO(4,1)$. Further, we are led to the expressions for these generators in terms of the canonical variables.

By comparing the expression for \mathbf{a} in terms of the conformal generators with our known expressions for \mathbf{a} , Equation (120) or Equation (121), we obtain expressions for K_i and R_i in terms of the canonical variables. If we use the eigenstates convenient for configuration space calculations ($\rho = n/ar$) we make the identifications

$$\begin{aligned} \mathbf{K} &= \frac{1}{2}(r\mathbf{p}^2 + p^2\mathbf{r}) - r \cdot \mathbf{p}\mathbf{p} - \mathbf{p}\mathbf{p} \cdot r - r \frac{1}{4r^2} \\ \mathbf{R} &= r. \end{aligned} \quad (206)$$

Substituting these results in the equation for \mathbf{B} we find

$$\mathbf{B} = \frac{1}{2a} \left(\frac{p^2\mathbf{r} + r\mathbf{p}^2}{2} - r \cdot \mathbf{p}\mathbf{p} - \mathbf{p}\mathbf{p} \cdot r - \frac{r}{4r^2} \right) + \frac{ar}{2} \quad (207)$$

which is a manifestly Hermitean operator valid throughout Hilbert space. From Equations (204) and (205) we note that

$$\mathbf{B} - \mathbf{a} = ar. \quad (208)$$

To compute D , we substitute the expressions for \mathbf{K} and \mathbf{R} into the commutation relation

$$D = \frac{i}{2} [K_i, R_i]$$

obtaining the result

$$S = \frac{1}{2} (\mathbf{p} \cdot r + r \cdot \mathbf{p}) = D \quad (209)$$

which is identical to the generator of the scale change transformation $D(\lambda)$ defined in Equation (109) in Section 4.3.

The significance of the generator $D = S$ of the scale change in terms of $SO(4,1)$ is apparent if we compute

$$e^{i\lambda D} \left(\frac{\mathbf{K}}{a} \pm a\mathbf{R} \right) e^{-i\lambda D} = \frac{\mathbf{K}}{a'} \pm a'\mathbf{R} \tag{210}$$

where $a' = e^\lambda a$.

The unitary transformation $e^{i\lambda D}$ may be viewed as generating an inner automorphism of $SO(4,1)$ which is an equivalent representation of $SO(4)$ that is characterized by a different value of the quantity a or the energy. In other words, under the scale change $e^{i\lambda D}$, the basis states for our representation of $SO(4,1)$, $|nlm; a\rangle$, transform to a new set, $|nlm; e^\lambda a\rangle$ in agreement with our discussion in Section 4.3.

Because the algebra of our generators closes, we may also view $e^{i\lambda D}$ as transforming a given generator into a linear combination of the generators. With the definitions of \mathbf{a} and \mathbf{B} (Equation (204) and (205)), we can easily show that Equation (210), with the upper sign, may also be written

$$e^{i\lambda D} \mathbf{B} e^{-i\lambda D} = \mathbf{B} \cosh \lambda + \mathbf{a} \sinh \lambda. \tag{211}$$

7. The Group $SO(4,2)$

7.1. Motivation for Introducing $SO(4,2)$

We would like to express Schrodinger’s equation as an algebraic equation in the generators of some group [37,38]. As we are unable to do this with our $SO(4,1)$ generators S_{AB} we again expand the group. To guide us, we recall that to expand $SO(3)$ to $SO(4)$ we added a three-vector of generators \mathbf{A} , and to expand $SO(4)$ to $SO(4,1)$, we added a four-vector of generators (S, \mathbf{B}) . In both cases, this type of expansion produced a set of generators convenient for the study of the hydrogenlike atom. We guess that the appropriate expansion of $SO(4,1)$ is obtained by adding a five-vector (under $SO(4,1)$) of generators Γ_A to obtain $SO(4,2)$ [37,38]. We can provide additional motivation for this choice by considering Schrodinger’s equation. The generators in terms of which we want to express this equation must be scalars under L_i rotations. Additionally we know $S = S_{40}$ (Equation (187)) generates scale changes of Schrodinger’s equation. The fact that S_{40} mixes the zero and four components of a five-vector suggests that Schrodinger’s equation may be expressed in terms of the components Γ_0 and Γ_4 which are scalars under L_i , of the five vector Γ_A . Since Γ_A is a five-vector under $SO(4,1)$, it must satisfy the equation

$$[S_{AB}, \Gamma_C] = i(\Gamma_B g_{AC} - \Gamma_A g_{BC}). \tag{212}$$

The spatial components of Γ_A which are $(\Gamma_1, \Gamma_2, \Gamma_3) = \mathbf{\Gamma}$ transform as a vector under rotations generated by L .

To construct the Lie algebra of $SO(4,2)$ we require that the set of operators $\{\Gamma_A, S_{AB}; A, B = 0, 1, 2, 3, 4\}$ must close under the operations of commutation. By applying Jacobi’s identity to Γ_A, Γ_B , and S_{AB} , and requiring that Γ_A and Γ_B do not commute, we find

$$[S_{AB}, [\Gamma_A, \Gamma_B]] = 0 \quad A, B = 0, 1, 2, 3, 4.$$

Because we require that our Lie algebra closes, the commutator of Γ_A and Γ_B must be proportional to S_{AB} . We normalize Γ , so

$$[\Gamma_A, \Gamma_B] = -iS_{AB} \quad A, B = 0, 1, 2, 3, 4. \tag{213}$$

If we define

$$S_{A5} = \Gamma_A = -S_{5A} \quad A = 0, 1, 2, 3, 4. \tag{214}$$

and recall

$$A_i = S_{i4} \quad B_i = S_{i0} \quad L_i = e_{ijk} S_{jk} \quad S = S_{40}$$

then we may unite all the commutations relations of Γ_A and S_{AB} in the single equation :

$$[S_{AB}, S_{CD}] = i(g_{AC}S_{BD} + g_{BD}S_{AC} - g_{AD}S_{BC} - g_{BC}S_{AD}) \quad (215)$$

where $A, B, \dots = 0, 1, 2, 3, 4, 5$ and $g_{00} = g_{55} = -1$; $g_{aa} = 1, a = 1, 2, 3, 4$.

These are the commutation relation for the Lie algebra of $SO(4,2)$. In terms of A, B, L, S and Γ_A the additional commutation relations for the noncommuting generators are [53]:

$$\begin{aligned} [B_i, \Gamma_j] &= i\Gamma_0\delta_{ij} & [\Gamma_i, \Gamma_j] &= -i\epsilon_{ijk}L_k \\ [A_i, \Gamma_j] &= i\Gamma_4\delta_{ij} & [\Gamma_i, \Gamma_0] &= -iB_i \\ [L_i, \Gamma_j] &= i\epsilon_{ijk}\Gamma_k & [\Gamma_i, \Gamma_4] &= -iA_i \\ & & [\Gamma_4, \Gamma_0] &= -iS \\ [B_i, \Gamma_0] &= i\Gamma_i & [A_i, \Gamma_4] &= -i\Gamma_i \\ [S, \Gamma_0] &= i\Gamma_4 & [S, \Gamma_4] &= i\Gamma_0 \end{aligned} \quad (216)$$

7.2. Casimir Operators

The Lie algebra of $SO(4,2)$ is rank three, so it has three Casimir operators W_2, W_3 , and W_4 [43]:

$$W_2 = -\frac{1}{2}S_{AB}S^{AB} = Q_2 + \Gamma_A\Gamma^A \quad (217)$$

where Q_2 is the nonvanishing $SO(4,1)$ Casimir operator Equation (190) and

$$W_3 = \epsilon^{ABCDE\mathcal{F}}S_{AB}S_{CD}S_{\mathcal{E}\mathcal{F}} \quad (218)$$

$$W_4 = S_{AB}S^{BC}S_{CD}S^{DA}. \quad (219)$$

Computation of W_3

We can show that $W_3 = 0$ from dynamical considerations similar to those used in the discussion of $SO(4,1)$ Casimir operators. The only terms that can be included in W_3 are scalars that are formed from products of three generators with different indices

$$\begin{aligned} \mathbf{B} \cdot \mathbf{A} \times \boldsymbol{\Gamma}, \quad \mathbf{A} \cdot \boldsymbol{\Gamma} \times \mathbf{B}, \quad \boldsymbol{\Gamma} \cdot \mathbf{B} \times \mathbf{A} \\ \Gamma_4 \mathbf{L} \cdot \mathbf{B}, \quad \Gamma_0 \mathbf{L} \cdot \mathbf{A}, \quad S \boldsymbol{\Gamma} \cdot \mathbf{L} \end{aligned} \quad (220)$$

It is interesting that these terms are actually all pseudoscalars. Terms like $\mathbf{B} \cdot \mathbf{A} \times \mathbf{L}$ are simply not possible because of the structure of W_3 . We know that $\boldsymbol{\Gamma} = (\Gamma_1, \Gamma_2, \Gamma_3)$ must not be pseudovector, otherwise it would be proportional to \mathbf{L} . Since it is a vector, it must equal a linear combination of \mathbf{r} and \mathbf{p} . Therefore, we conclude

$$\boldsymbol{\Gamma} \cdot \mathbf{L} = \mathbf{L} \cdot \boldsymbol{\Gamma} = 0. \quad (221)$$

Because $\boldsymbol{\Gamma}$ and \mathbf{B} are both vectors and \mathbf{L} is the only pseudovector we have $\boldsymbol{\Gamma} \times \mathbf{B} = \Lambda \mathbf{L}$. In order to determine the scalar Λ we evaluate the commutators

$$[B_k, (\boldsymbol{\Gamma} \times \mathbf{B})_k], \quad \text{and} \quad [\Gamma_k, (\boldsymbol{\Gamma} \times \mathbf{B})_k] \quad (222)$$

and find

$$\boldsymbol{\Gamma} \times \mathbf{B} = \Gamma_0 \mathbf{L} = -\mathbf{B} \times \mathbf{L}. \quad (223)$$

The analogous equations for \mathbf{A} and $\boldsymbol{\Gamma}$, and for \mathbf{A} and \mathbf{B} , are

$$\begin{aligned} \boldsymbol{\Gamma} \times \mathbf{A} &= -\Gamma_4 \mathbf{L} = -\mathbf{A} \times \boldsymbol{\Gamma} \\ \mathbf{A} \times \mathbf{B} &= S \mathbf{L} = -\mathbf{B} \times \mathbf{A}. \end{aligned} \quad (224)$$

From Equations (223) and (224), we see that because of the dynamical structure of the generators each of the quantities in the first line of Equation (220) is proportional to the quantity directly below in the second line. We also have shown that (Equations (194) and (221))

$$L \cdot B = L \cdot A = \Gamma \cdot L = 0. \tag{225}$$

Accordingly, each scalar in our list vanishes and

$$W_3 = 0. \tag{226}$$

Computation of W_2

In order to compute W_2 we need to evaluate

$$\Gamma^2 \equiv \Gamma_A \Gamma^A = \Gamma_4^2 + \Gamma_i \Gamma^i - \Gamma_0^2. \tag{227}$$

From the structure of W_2 as shown in Equation (217), we see that Γ^2 must be a number since W_2 and Q_2 are both Casimir operators and therefore equal numbers for a particular representation. Accordingly, we have

$$[\Gamma^2, \Gamma_A] = 0. \tag{228}$$

From this equation, we can deduce a lemma allowing us to easily evaluate W_2 and W_4 in terms of the number Γ^2 . Using Equation (227) and the definition of S_{AB} Equation (213) we find

$$\Gamma^A S_{AB} + S_{AB} \Gamma^A = 0.$$

Contracting Equation (212) with g_{AC} gives

$$S_{AB} \Gamma^A - \Gamma^A S_{AB} = 4i \Gamma_B.$$

Consequently, it must follow that

$$S_{AB} \Gamma^A = 2i \Gamma_B = -\Gamma^A S_{AB}. \tag{229}$$

We are now able to evaluate the quantity

$$S_{AB} S_C^B = i S_{AB} [\Gamma^B, \Gamma_C] = i (S_{AB} \Gamma^B \Gamma_C - S_{AB} \Gamma_C \Gamma^B).$$

Using Equation (212) for the commutator of S_{AB} with Γ_C and Equation (229) for the contraction $S_{AB} \Gamma^B$ we prove the lemma

$$S_{AB} S_C^B = 2i S_{CA} - \Gamma_A \Gamma_C + \Gamma^2 g_{AC}. \tag{230}$$

The value of the SO(4,1) Casimir operator $Q_2 = \frac{1}{2} g^{AC} S_{AB} S_C^B$ follows directly from the lemma:

$$Q_2 = 2\Gamma^2. \tag{231}$$

Accordingly, we have from Equation (217)

$$W_2 = 3\Gamma^2. \tag{232}$$

Computation of W_4

The Casimir operator W_4 can be written as

$$W_4 = S_{AB} S^{BC} S_{CD} S^{DA} + S_{AB} S^{B5} S_{5D} S^{DA} + S_{5B} S^{BC} S_{CD} S^{D5} + S_{5B} S^{B5} S_{5D} S^{D5}. \tag{233}$$

where $B, D = 0, 1, 2, 3, 4, 5$ and $A, C = 0, 1, 2, 3, 4$.

In order to evaluate W_4 in terms of Γ^2 we compute $S_{AB}S^{BC}$. Recalling $\Gamma_A = S_{A5}$ we see

$$S_{AB}S^{BC} = \Gamma_A\Gamma^C + S_{AB}S^{BC}. \quad (234)$$

Substituting the lemma Equation (230), we find

$$S_{AB}S^{BC} = 2iS_A^C - \Gamma^2g_A^C. \quad (235)$$

From Equation (229), it follows that

$$S_{5B}S^{BC} = 2i\Gamma^C. \quad (236)$$

Substituting Equations (231), (232), (235), and (236) into Equation (233) for W_4 we find

$$W_4 = 6(\Gamma^2)^2 - 24\Gamma^2. \quad (237)$$

The fact that the nonvanishing Casimir operators (Q_2 , W_2 , and W_4) for $SO(4,1)$ and $SO(4,2)$ are given in terms of Γ^2 implies that the representation of $SO(4,2)$ determines the particular representation of $SO(4,1)$ appropriate to the hydrogenlike atom. In turn the value of Γ^2 is determined by the structure of the Γ s in terms of the canonical variables. In Section 7.4, we derive these structures and find that

$$\Gamma^2 = 1.$$

Therefore, the quadratic $SO(4,1)$ Casimir operator Q_2 has the value

$$Q_2 = 2$$

and the $SO(4,2)$ Casimir operators have the values:

$$W_2 = 3 \quad W_3 = 0 \quad W_4 = -18.$$

The researchers that have published different representations of $SO(4,2)$ based on the hydrogen atom that give their Casimir operators all have $W_2 = 3$ (or its equivalent) and $W_3=0$ [34,79,82], however, two authors have representations with $W_4 = 0$ [34,82] and one [79] has $W_4 = -12$, as compared to our value of -18.

From the mathematical theory of representations, it follows that our representations of $SO(4,1)$ and $SO(4,2)$ are both unitary and irreducible. This means there is no subset of basis vectors that transform among themselves as either $SO(4,1)$ or as $SO(4,2)$.

7.3. Some Group Theoretical Results

In this section, we derive the transformation properties of the generators of $SO(4,2)$ and then a novel contraction formula that will prove useful for situations in which we want to employ perturbation theory, for example, in our calculation of the radiative shift for the hydrogen atom in Section 8. We will work primarily with the $SO(4,2)$ generators expressed as the combination of the $SO(4,1)$ generators S_{AB} and the five-vector Γ , with $g_{AB} = (-1, 1, 1, 1, 1)$ where $A, B = 0, 1, 2, 3, 4$.

Transformation Properties of the Generators

We can evaluate quantities like

$${}^{AB}\Gamma_B(\theta) \equiv e^{iS_{AB}\theta}\Gamma_B e^{-iS_{AB}\theta} \quad \text{no sum over A or B} \quad (238)$$

by expanding the exponentials in an infinite series and then using the commutation relations Equations (212) and (213) of the generators S_{AB} and Γ_A, Γ_B repeatedly. However, it is easier to

solve the differential equations satisfied by ${}^{AB}\Gamma_B$ and to use the appropriate boundary conditions. Differentiating Equation (238) and using the commutation relations, we obtain the equations

$$\frac{d}{d\theta} {}^{AB}\Gamma_B = -g_{BB} {}^{AB}\Gamma_A \quad \frac{d^2}{d\theta^2} {}^{AB}\Gamma_B = -g_{AA}g_{BB} {}^{AB}\Gamma_B \quad (239)$$

which have the solution

$${}^{AB}\Gamma_B = \Gamma_B \cos \sqrt{g_{AA}g_{BB}}\theta + \frac{g_{BB}}{\sqrt{g_{AA}g_{BB}}}\Gamma_A \sin \sqrt{g_{AA}g_{BB}}\theta. \quad (240)$$

Using a similar procedure we find

$$e^{i\Gamma_A\theta} S_{AB} e^{-i\Gamma_A\theta} = S_{AB} \cosh \sqrt{g_{AA}}\theta + \sqrt{g_{AA}}\Gamma_B \sinh \sqrt{g_{AA}}\theta \quad (241)$$

$$e^{i\Gamma_A\theta} \Gamma_B e^{-i\Gamma_A\theta} = \Gamma_B \cosh \sqrt{g_{AA}}\theta + \frac{1}{\sqrt{g_{AA}}} S_{AB} \sinh \sqrt{g_{AA}}\theta \quad (242)$$

where no summation over A or B is implied.

These formulae, Equation (240)–(242), give the $SO(4,2)$ transformation properties of the $SO(4,2)$ generators.

The Contraction Formula

If we multiply Equation (241) from the right by $e^{i\Gamma_A\theta}$ and then contract from the left with Γ_B , we obtain

$$\sum_B \Gamma^B e^{i\Gamma_A\theta} \Gamma_B = \left[(1 - g_{AA}\Gamma_A^2) \cosh \sqrt{g_{AA}}\theta + \frac{2i\Gamma_A}{\sqrt{g_{AA}}} \sinh \sqrt{g_{AA}}\theta \right] e^{i\Gamma_A\theta} + g_{AA}\Gamma_A^2 e^{i\Gamma_A\theta} \quad (243)$$

where we have used $\Gamma^2 = 1$ and Equation (229). Expanding the hyperbolic functions in terms of exponentials and collecting terms gives

$$\sum_B \Gamma^B e^{i\Gamma_A\theta} \Gamma_B = \frac{1}{2} \left(1 + \frac{i\Gamma_A}{\sqrt{g_{AA}}} \right)^2 e^{i(\Gamma_A - i\sqrt{g_{AA}})\theta} + \frac{1}{2} \left(1 - \frac{i\Gamma_A}{\sqrt{g_{AA}}} \right)^2 e^{i(\Gamma_A + i\sqrt{g_{AA}})\theta} + g_{AA}\Gamma_A^2 e^{i\Gamma_A\theta}. \quad (244)$$

A Fourier decomposition of a function Γ_A may be written

$$f(\Gamma_A) = \frac{1}{2\pi} \int d\theta h(\theta) e^{i\Gamma_A\theta}. \quad (245)$$

Consequently we have

$$\sum_B \Gamma^B f(\Gamma_A) \Gamma_B = \frac{1}{2} \left(1 + \frac{i\Gamma_A}{\sqrt{g_{AA}}} \right)^2 f(\Gamma_A - i\sqrt{g_{AA}}) + \frac{1}{2} \left(1 - \frac{i\Gamma_A}{\sqrt{g_{AA}}} \right)^2 f(\Gamma_A + i\sqrt{g_{AA}}) + g_{AA}\Gamma_A^2 f(\Gamma_A). \quad (246)$$

By performing a suitable rotation we can generalize this formula from functions of Γ_A to functions of $\Gamma_A n^A$ where $n_A n^A = \pm 1$. For $n^2 = -1$ we start with $\Gamma_A = \Gamma_0$ and rotate to obtain a very general result

$$\sum_B \Gamma_B f(n\Gamma) \Gamma^B = \frac{1}{2} (n\Gamma + 1)^2 f(n\Gamma + 1) + \frac{1}{2} (n\Gamma - 1)^2 f(n\Gamma - 1) - (n\Gamma)^2 f(n\Gamma). \quad (247)$$

We will have occasion to apply this formula for the special case

$$f(n\Gamma) = \frac{1}{\Gamma n - \nu}. \quad (248)$$

Using the representation

$$\frac{1}{\Gamma n - \nu} = \int_0^\infty ds e^{\nu s} e^{-\Gamma n s} \tag{249}$$

we obtain the result

$$\Gamma_A \frac{1}{\Gamma n - \nu} \Gamma^A = -2\nu \int_0^\infty ds e^{\nu s} \frac{d}{ds} \left(\sinh^2 \frac{s}{2} e^{-\Gamma n s} \right) \tag{250}$$

which is in a form convenient for perturbation calculations.

Derivation of the Γ_A in terms of the Canonical Variables

For our basis states, we shall use eigenstates of $(Z\alpha)^{-1}$ convenient for configuration space calculations ($\rho = na/r$). We choose these states rather than those convenient for momentum space calculations because they lead to simpler expressions for the Γ_A in terms of the canonical variables, although the expression for a is slightly more complicated. Thus, our states obey the equation

$$\left[\frac{1}{K_1(a)} - n \right] |nlm\rangle = 0 \tag{251}$$

where $K_1(a)$ is given by Equation (116). We know that K_1^{-1} must commute with the generators of the SO(4) symmetry group $(a)_i = S_{i4}$ and $S_{ij} = \epsilon_{ijk} L_k$. This suggests that we choose

$$\Gamma_0 = [K_1(a)]^{-1} = \sqrt{ar} \frac{p^2 + a^2}{2a^2} \sqrt{ar} = \frac{1}{2} \left(\frac{\sqrt{r} p^2 \sqrt{r}}{a} + ar \right) \tag{252}$$

so that

$$(\Gamma_0 - n) |nlm\rangle = 0. \tag{253}$$

This last equation is the Schrodinger equation expressed in our language of SO(4,2): our states $|nlm\rangle$ are eigenstates of Γ_0 with eigenvalue n .

To find Γ_4 , we calculate $\Gamma_4 = -i[S, \Gamma_0]$, using Equation (209) for S ,

$$\Gamma_4 = \sqrt{ar} \frac{p^2 - a^2}{2a^2} \sqrt{ar} = \frac{1}{2} \left(\frac{\sqrt{r} p^2 \sqrt{r}}{a} - ar \right). \tag{254}$$

Sometimes it is convenient to use the linear combinations

$$\Gamma_0 - \Gamma_4 = ar \quad \Gamma_0 + \Gamma_4 = \frac{\sqrt{r} p^2 \sqrt{r}}{a} \tag{255}$$

which can be used to express the dipole transition operator [33]. We can find Γ_i from Equation (216), $\Gamma_i = -i[B_i, \Gamma_0]$

$$\Gamma_i = \sqrt{r} p_i \sqrt{r} \tag{256}$$

which we might have guessed initially since $[rp_i, rp_j] \sim L_k$. Every component of Γ_A is Hermitean, consequently the generators S_{AB} given by the commutators Equation (213) are also Hermitian. We may explicitly verify that these expressions for Γ_A lead to a consistent representation of all generators in the SO(4,2) Lie algebra.

Under a scale change generated by S , Γ_i is invariant and Γ_4 and Γ_0 transform in the same manner as a and B (Equation (210)): they retain their form but a is transformed into $e^\lambda a$:

$$e^{i\lambda S} \left\{ \begin{matrix} \Gamma_0 \\ \Gamma_4 \end{matrix} \right\} e^{-i\lambda S} = \frac{1}{2} \left(\frac{\sqrt{r} p^2 \sqrt{r}}{e^\lambda a} \pm e^\lambda ar \right) \tag{257}$$

The scale change generates an inner automorphism of SO(4,2) characterized by a different value of the parameter a .

7.4. Subgroups of SO(4,2)

The two most significant subgroups are [53]:

1. L_i, a_i or S_{jk}, S_{i4} , forming an SO(4) subgroup. These generators commute with Γ_0 and therefore constitute the degeneracy group for states of energy $-a^2/(2m)$ and fixed principal quantum number n (or fixed coupling constant na/m). The Casimir operator for this subgroup is

$$a^2 + L^2 = n^2 - 1 = \Gamma_0^2 - 1. \tag{258}$$

We discussed this subgroup in Section 4.2 in terms of L and A and the states $|nlm\rangle$. The same results are obtained with the generators L and a with the states $|nlm\rangle$. For example, we have the raising and lowering operators for m and l (Equations (93) and (94)). With the definition

$$L_{\pm} = L_1 \pm iL_2 \tag{259}$$

it follows that

$$[L_3, L_{\pm}] = \pm L_{\pm} \tag{260}$$

which gives

$$L_{\pm}|nlm\rangle = \sqrt{(l(l+1) - m(m\pm 1))}|nl, m\pm 1\rangle \quad L_3|nlm\rangle = m|nlm\rangle. \tag{261}$$

for $l \geq 1$. In analogy to L_{\pm} one can define

$$a_{\pm} = a_1 \pm ia_2 \tag{262}$$

which obey the relations

$$[a_3, a_{\pm}] = \pm L_3 \quad [L_3, a_{\pm}] = \pm a_{\pm} \tag{263}$$

and

$$a_{\pm}|nlm\rangle = \mp \left(\frac{(n^2 - (l+1)^2)(l+2\pm m)(l+1\pm m)}{4(l+1)^2 - 1} \right)^{\frac{1}{2}} |nl+1, m\pm 1\rangle \tag{264}$$

$$\pm \left(\frac{(n^2 - l^2)(l\mp m)(l-1\mp m)}{4l^2 - 1} \right)^{\frac{1}{2}} |nl-1, m\pm 1\rangle$$

for $l \geq 1$. The action of a_{\pm} is not directly analogous to that of L_{\pm} , because we are using $|nlm\rangle$ as basis states. If we used $|na_3l_3 = m\rangle$ as basis states, the action would be similar. An operator that only changes the angular momentum is a_3

$$a_3|nlm\rangle = \left(\frac{(n^2 - (l+1)^2)((l+1)^2 - m^2)}{4(l+1)^2 - 1} \right)^{\frac{1}{2}} |nl+1, m\rangle + \left(\frac{(n^2 - l^2)(l^2 - m^2)}{4l^2 - 1} \right)^{\frac{1}{2}} |nl-1, m\rangle. \tag{265}$$

for $l \geq 1$. Since a_3 commutes with L_3 and Γ_0 , it does not change n or m .

2. $\Gamma_4, S = S_{40}, \Gamma_0$, forming a SO(2,1) subgroup. These operators commute with L but not with Γ_0 , hence then can change n but not L or m . The Casimir operator for this subgroup is

$$\Gamma_0^2 - \Gamma_4^2 - S^2 = L^2 = l(l+1). \tag{266}$$

We can define the operators [53]

$$j_1 = \Gamma_4 \quad j_2 = S \quad j_3 = \Gamma_0 \tag{267}$$

with commutators

$$[j_1, j_2] = -ij_3 \quad [j_2, j_3] = ij_1 \quad [j_3, j_1] = ij_2 \tag{268}$$

We can define the raising and lowering operators

$$j_{\pm} = j_1 \pm ij_2 = \Gamma_4 \pm iS \tag{269}$$

which obey the commutation relations

$$[j_{\pm}, j_3] = \mp j_{\pm}. \tag{270}$$

We find (in analogy to Equation (261))

$$\Gamma_0|nlm\rangle = n|nlm\rangle \quad (\Gamma_4 \pm iS)|nlm\rangle = \sqrt{n(n \pm 1) - l(l + 1)}|n \pm 1 lm\rangle \tag{271}$$

We can express the action of $\Gamma_0 - \Gamma_4 = ar$ on our states

$$ar|nlm\rangle = \frac{1}{2} \left((n)(n - l) - l(l + 1) \right)^{\frac{1}{2}} |n - 1 lm\rangle + n|nlm\rangle + \frac{1}{2} \left((n)(n + l) - l(l + 1) \right)^{\frac{1}{2}} |n + 1 lm\rangle \tag{272}$$

As previously mentioned, the operator S generates scale changes as shown in Equation (257), where the value of a is changed. We can also express the action of S equivalently as transforming Γ_0 into Γ_4

$$e^{iS\lambda}\Gamma_0e^{-iS\lambda} = \Gamma_0 \cosh \lambda - \Gamma_4 \sinh \lambda \quad e^{iS\lambda}\Gamma_4e^{-iS\lambda} = \Gamma_4 \cosh \lambda - \Gamma_0 \sinh \lambda. \tag{273}$$

7.5. Time Dependence of SO(4,2) Generators

For a generator to be a constant it must commute with the Hamiltonian as discussed in Section 2.1. Because the SO(4,2) group is the non-invariance or spectrum generating group, the additional generators do not all commute with the Hamiltonian and may have a harmonic time dependence as discussed in Section 2.2. It is notable that as far as we know only one paper considers the time dependence of the generators of non-invariance groups in general and one considers SO(4,2) specifically [97,136]. Our results certainly clarify and make explicit the time dependence, and show that it is just a particular aspect of the SO(4,2) transformations. In our representation with basis states $|nlm; a\rangle$, the Hamiltonian, which is the generator of translations in time, has been transformed into Γ_0 and the Schrodinger energy eigenvalue equation has become $\Gamma_0|nlm\rangle = n|nlm\rangle$. Accordingly, all of the generators that commute with Γ_0 are constants of the motion, which includes a, L . The other operators, B, Γ, S, Γ_4 have a time dependence given by Equations (241) and (242), for example

$$S(t) = e^{iHt}S(0)E^{-iHt} = e^{i\Gamma_0t}S_0e^{-i\Gamma_0t} = S \cos t + \Gamma_4 \sin t. \tag{274}$$

$$\Gamma_4(t) = e^{iHt}\Gamma_4(0)E^{-iHt} = e^{i\Gamma_0t}\Gamma_4_0e^{-i\Gamma_0t} = \Gamma_4 \cos t - S \sin t. \tag{275}$$

Consequently, terms like j_{\pm} have a simple exponential time dependence

$$j_{\pm}(t) = j_{\pm}(0)e^{\pm it}. \tag{276}$$

Similarly $\Gamma \pm iB$ has an exponential time dependence.

7.6. Expressing the Schrodinger Equation in Terms of the Generators of SO(4,2)

We can write the Schrodinger equation for the energy eigenstate $E_n = -a_n^2/2m$ of a particle in a Coulomb potential in terms of the SO(4,2) generators, which are expressed in terms of the energy $-a^2/2m$, by making a scale change. From Section 4.3, Equation (114), the relationship between the Schrodinger energy eigenstate $|nlm\rangle$ and the eigenstate of $(Z\alpha)^{-1}$ is:

$$|nlm; a\rangle = e^{-iS\lambda_n} \sqrt{\rho(a_n)} |nlm\rangle \tag{277}$$

where

$$e^{\lambda_n} = \frac{a_n}{a} \quad \rho(a_n) = \frac{n}{a_n r}. \quad (278)$$

Substituting Equation (277) into the eigenvalue equation Equation (253) for $|nlm; a\rangle$ and employing the transformation Equation (273), we find the usual Schrodinger equation can be expressed in SO(4,2) terms as

$$(\Gamma n - n) \sqrt{\rho(a_n)} |nlm\rangle = 0 \quad (279)$$

where

$$\Gamma n \equiv \Gamma_A n^A = \Gamma_0 n^0 + \Gamma_i n^i + \Gamma_4 n^4 \quad (280)$$

$$n^0 = \cosh \lambda_n = \frac{a^2 + a_n^2}{2aa_n}, \quad n^i = 0, \quad n^4 = -\sinh \lambda_n = \frac{a^2 - a_n^2}{2aa_n} \quad (281)$$

and $n_A n^A = n_4^2 - n_0^2 = -1$.

Equation (279) expresses Schrodinger's equation for an ordinary energy eigenstate $|nlm\rangle$ with energy $E_N = -a_n^2/2m$ in the language of SO(4,2). It shows the relationship between these energy eigenstates and the basis states of $(Z\alpha)^{-1}$ used for the SO(4,2) representation,

8. SO(4,2) Calculation of the Radiative Shift for the Schrodinger Hydrogen Atom

In the 1930's, it was generally believed that the Dirac equation predicted the energy levels of the hydrogen atom with excellent accuracy, but there were some questions about the prediction that the energy levels for a given principal quantum number and given total angular momentum were independent of the orbital angular momentum. To finally resolve this issue, in 1947, Willis Lamb and his student Robert Retherford at Columbia University in New York City employed rf spectroscopy and exploited the metastability of the hydrogen $2s_{1/2}$ level in a beautiful experiment and determined that the $2s_{1/2}$ and $2p_{1/2}$ levels were not degenerate and that the energy difference between the levels was about 1050 MHz, or 1 part in 10^6 of the $2s_{1/2}$ level [5,148]. Shortly thereafter Hans Bethe [6] published a ground breaking nonrelativistic quantum theoretical calculation of the shift assuming it was due to the interaction of the electron with the ground state electromagnetic field of the quantum vacuum field. This radiative shift accounted for about 96% of the measured shift. The insight that one needed to include the interaction of the atom with the vacuum fluctuations and how one could actually do it ushered in the modern world of quantum electrodynamics [7]. Here, we compute in the non-relativistic dipole approximation and to first order in the radiation field, as did Bethe, the radiative shift, but we use group theoretical methods based on the SO(4,2) symmetry of the non-relativistic hydrogen atom as developed in this paper. Bethe's calculation required the numerical sum over intermediate states to obtain the average value of the energy of the states contributing to the shift. In our calculation, we do not use intermediate states, and we derive an integral equivalent to Bethe's log, and more generally derive the shift for all levels in terms of a double integral.

An expression for the radiative shift Δ_{NL} for energy level E_N of a hydrogen atom in a state $|NL\rangle$ can be readily obtained using second order perturbation theory (to first order in α the radiation field) [6,149–151]

$$\Delta_{NL} = \frac{2\alpha c}{3\pi m^2} \sum_n^s \int_0^{\omega_c} d\omega \frac{(E_n - E_N) \langle NL | p_i | n \rangle \langle n | p_i | NL \rangle}{E_n - E_N + \omega - i\epsilon}, \quad (282)$$

where ω_c is a cutoff frequency for the integration that we will take as $\omega_c = m$.

This expression, which is the same as Bethe's, has been derived by inserting a complete set of states $|n\rangle\langle n|$, a step that we eliminate with our group theoretical approach:

$$\Delta_{NL} = \frac{2\alpha}{3\pi m^2} \int_0^{\omega_c} d\omega \langle NL | p_i \frac{H - E}{H - (E - \omega) - i\epsilon} p_i | NL \rangle \quad (283)$$

If we add and subtract ω from the numerator, we find the real part of the shift is

$$Re\Delta_{NL} = \frac{2\alpha}{3\pi m^2} Re \int_0^{\omega_c} d\omega [\langle NL|p^2|NL\rangle - \omega\Omega_{NL}] \tag{284}$$

where

$$\Omega_{NL} = \langle NL|p_i \frac{1}{H - E_N + \omega - i\epsilon} p_i|NL\rangle \tag{285}$$

and

$$H = \frac{p^2}{2m} - \frac{Z\alpha}{r}. \tag{286}$$

The imaginary part of the shift gives the width of the level [7].

The matrix element Ω_{NL} can be converted to a matrix element of a function of the generators Γ_A taken between eigenstates $|nlm\rangle$ of $(Z\alpha)^{-1}$. To do this we insert factors of $1 = \sqrt{r} \frac{1}{\sqrt{r}}$ and use the definitions of the Γ_A in terms of the canonical variables, Equations (254)–(256). Letting the parameter a take the value a_N , we obtain the result

$$\Omega_{NL} = \frac{mv}{N^2} (NL|\Gamma_i \frac{1}{\Gamma n(\xi) - \nu} \Gamma_i|NL) \tag{287}$$

where

$$n^0(\xi) = \frac{2 + \xi}{2\sqrt{1 + \xi}} = \cosh \phi \quad n^i = 0 \quad n^4(\xi) = -\frac{\xi}{2\sqrt{1 + \xi}} = -\sinh \phi \tag{288}$$

and

$$\xi = \frac{\omega}{|E_N|} \quad \nu = \frac{N}{\sqrt{1 + \xi}} = Ne^{-\phi}. \tag{289}$$

From the definitions we see $\phi = \frac{1}{2} \ln(1 + \xi) > 0$ and $n_A(\xi)n^A(\xi) = -1$. The quantity

$$\nu = \frac{mZ\alpha}{\sqrt{-2m(E_N - \omega)}}$$

may be considered the effective principal quantum number for a state of energy $E_N - \omega$. The contraction over i in Ω_{NL} may be evaluated using the group theoretical formula Equation (250):

$$\begin{aligned} \Omega_{NL} = & -2 \frac{mv^2}{N^2} \int_0^\infty ds e^{\nu s} \frac{d}{ds} \left(\sinh^2 \frac{s}{2} M_{NL}(s) \right) \\ & - m \frac{\nu}{N^2} (NL|\Gamma_4 \frac{1}{\Gamma n(\xi) - \nu} \Gamma_4|NL) + m \frac{\nu}{N^2} (NL|\Gamma_0 \frac{1}{\Gamma n(\xi) - \nu} \Gamma_0|NL) \end{aligned} \tag{290}$$

where

$$M_{NL}(s) = (NL|e^{-\Gamma n(\xi)s}|NL). \tag{291}$$

In order to evaluate the last-two terms in Ω_{NL} , we can express the action of Γ_4 on our states in terms of $\Gamma n(\xi) - \nu$. Substituting the equation

$$\Gamma_0|NL) = N|NL) \tag{292}$$

into the expression for $\Gamma n(\xi) - \nu$, with $n(\xi)$ given by Equation (288), gives

$$\Gamma_4 = N - \left(\frac{1}{\sinh \phi} \right) (\Gamma n(\xi) - \nu) \tag{293}$$

when acting on the state $|NL\rangle$. If we substitute Equation (293) into the expression for the $Re\Delta E_{NL}$ Equation (284) and simplify using the virial theorem

$$(NL|p^2|NL) = a_N^2$$

we find that the term in p^2 exactly cancels the last two terms in Ω_{NL} , yielding the result

$$Re\Delta E_{NL} = \frac{4m\alpha(Z\alpha)^4}{3\pi N^4} \int_0^{\phi_c} d\phi \sinh \phi e^\phi \int_0^\infty ds e^{vs} \frac{d}{ds} \left(\sinh^2 \frac{s}{2} M_{NL}(s) \right) \tag{294}$$

where

$$\phi_c = \frac{1}{2} \ln \left(1 + \frac{\omega_c}{|E_N|} \right) = \frac{1}{2} \ln \left(1 + \frac{2N^2}{(Z\alpha)^2} \right) \tag{295}$$

and $\omega_c = m$.

Comparison to the Bethe Logarithm

The first order non-relativistic radiative shift is commonly given in terms of the Bethe logarithm $\gamma(N, L)$, which is interpreted as the average over all states, including scattering states, of $\ln \frac{|E_n - E_N|}{\frac{1}{2}m(Z\alpha)^2}$ [149]:

$$\begin{aligned} \gamma(N, L) &= \sum_n^S (E_n - E_N) \langle N0 | p_i | n \rangle \langle n | p_i | N0 \rangle \\ &= \sum_n^S (E_n - E_N) \langle NL | p_i | n \rangle \langle n | p_i | NL \rangle \ln \frac{|E_n - E_N|}{\frac{1}{2}m(Z\alpha)^2} \end{aligned} \tag{296}$$

We use the dipole sum rule [150]

$$2 \sum_n^S (E_n - E_N) \langle N | p_i | n \rangle \langle n | p_i | N \rangle = - \langle N | \nabla^2 V | N \rangle \tag{297}$$

and apply it for the Coulomb potential $\nabla^2 V(r) = 4\pi Z\alpha\delta(r)$. The use of the Bethe log allowed Bethe to take the logarithmic expression obtained from the frequency integration outside the summation over the states, and replace it with the average value. Only the S states contribute to the expectation value in Equation (297), giving, from Equation (282), an expression for the shift

$$Re \Delta E_{NL} = \left[\frac{4m}{3\pi} \alpha(Z\alpha)^4 \right] \frac{1}{N^3} \left\{ \delta_{L0} \ln \frac{2}{(Z\alpha)^2} - \gamma(N, L) \right\}. \tag{298}$$

Comparing the shift in terms of M_{NL} Equation (294) to the shift in terms of $\gamma(N, L)$ we find that the Bethe log is

$$\gamma(N, L) = \int_0^{\phi_c} d\phi \sinh \phi e^\phi \int_0^\infty ds e^{vs} \frac{d}{ds} \left(\sinh^2 \frac{s}{2} M_{NL}(s) \right) - \delta_{L0} \ln \frac{1}{(Z\alpha)^2} \tag{299}$$

8.1. Generating Function for the Shifts

We can derive a generating function for the shifts for any eigenstate characterized by N and L if we multiply Equation (291) by $N^4 e^{\beta N}$ and sum over all $N, N \geq L + 1$. To simplify the right side of the resulting equation, we use the fact that the $O(2,1)$ algebra of Γ_0, Γ_4 , and S closes. We can compute the sum on the right hand side:

$$\sum_{N=L+1}^\infty e^{-\beta N} M_{NL} = \sum_{N=L+1}^\infty (NL | e^{-j\psi} | NL). \tag{300}$$

where

$$e^{-j\psi} \equiv e^{-\beta\Gamma_0} e^{-s\Gamma_n(\xi)}. \tag{301}$$

We perform a j transformation, such that

$$e^{-j \cdot \psi} \rightarrow e^{-j_3 \psi} = e^{-\Gamma_0 \psi} \quad (302)$$

so

$$\sum_{N=L+1}^{\infty} e^{-\beta N} M_{NL} = \sum_{N=L+1}^{\infty} (NL | e^{-j_3 \psi} | NL) = \sum_{N=L+1}^{\infty} e^{-N \psi} \quad (303)$$

$$= \frac{e^{-\psi(L+1)}}{1 - e^{-\psi}}. \quad (304)$$

In order to find a particular M_{NL} , we must expand the right hand side of the equation in powers of $e^{-\beta}$ and equate the coefficients to those on the left hand side. First, we need an equation for $e^{-\psi}$. This can be obtained using the isomorphism between j and the Pauli σ matrices:

$$(\Gamma_4, S, \Gamma_0) \rightarrow (j_1, j_2, j_3) \rightarrow \left(\frac{i}{2} \sigma_1, \frac{i}{2} \sigma_2, \frac{1}{2} \sigma_3 \right) \quad (305)$$

Using the formula

$$e^{\frac{i}{2} \mathbf{s} \cdot \boldsymbol{\sigma}} = \cos \frac{s}{2} + i \mathbf{n} \cdot \boldsymbol{\sigma} \sin \frac{s}{2} \quad (306)$$

where $|\mathbf{n}| = 1$, we find

$$\cosh \frac{\psi}{2} = \cosh \frac{\beta}{2} \cosh \frac{s}{2} + \sinh \frac{\beta}{2} \sinh \frac{s}{2} \cosh \phi. \quad (307)$$

We can rewrite this equation in a form easier for expansion

$$e^{+\frac{1}{2}\psi} = d e^{\frac{1}{2}\beta} + b e^{-\frac{1}{2}\beta} - e^{-\frac{1}{2}\psi} \quad (308)$$

where

$$\begin{aligned} d &= \cosh \frac{s}{2} + \sinh \frac{s}{2} \cosh \phi \\ b &= \cosh \frac{s}{2} - \sinh \frac{s}{2} \cosh \phi \end{aligned} \quad (309)$$

Let β become very large and iterate the equation for $e^{-\frac{1}{2}\psi}$ to obtain the result

$$e^{-\psi} = A e^{-\beta} \left[1 + A_1 e^{-\beta} + A_2 e^{-2\beta} + \dots \right] \quad (310)$$

where

$$\begin{aligned} A &= A_0 = \frac{1}{d^2} \\ A_1 &= - \left(\frac{2}{d} \right) (b - d^{-1}) \\ A_2 &= 3d^{-2} (b - d^{-1})^2 - 2^{-2} (b - d^{-1}) \\ &\vdots \end{aligned} \quad (311)$$

Note $b - d^{-1} = -d^{-1} \sinh^2 \frac{s}{2} \sinh^2 \phi$.

8.2. The Shift between Degenerate Levels

Expressions for the energy shift between degenerate levels with the same value of N may be obtained directly from the generating function using Equations (294) and (304). We find

$$\sum_{N=L+1}^{\infty} e^{-\beta N} N^4 \operatorname{Re} \Delta E_{NL} - \sum_{N=L'+1}^{\infty} e^{-\beta N} N^4 \operatorname{Re} \Delta E_{NL'} =$$

$$\frac{4m\alpha(Z\alpha)^4}{3\pi} \int_0^{\phi_c} d\phi e^\phi \sinh \phi \int_0^\infty ds e^{vs} \frac{d}{ds} \left(\sinh^2 \frac{s}{2} \frac{e^{-\psi(L+1)} - e^{-\psi(L'+1)}}{1 - e^{-\psi}} \right). \tag{312}$$

For an example, consider $L = 1, L' = 0$. For the shifts between levels we obtain

$$\sum_{N=2}^\infty e^{-\beta N} N^4 \operatorname{Re} (\Delta E_{N0} - \Delta E_{N1}) + \operatorname{Re} \Delta E_{10} e^{-\beta} = \frac{4m\alpha(z\alpha)^4}{3\pi} \int_0^{\phi_c} d\phi e^\phi \sinh \phi \int_0^\infty ds e^{vs} \frac{d}{ds} \left(\sinh^2 \frac{s}{2} e^{-\psi} \right) \tag{313}$$

Substituting Equation (310) for $e^{-\psi}$, using the coefficient AA_{N-1} of $e^{-N\beta}$, gives

$$\operatorname{Re}(\Delta E_{N0} - \Delta E_{N1}) = \frac{4m\alpha(Z\alpha)^4}{3\pi N^4} \int_0^{\phi_c} d\phi e^\phi \sinh \phi \int_0^\infty ds e^{vs} \frac{d}{ds} \left(\sinh^2 \frac{s}{2} AA_{N-1} \right). \tag{314}$$

where A and A_{N-1} are given in Equation (311) in terms of the variables of integration s and ϕ .

General Expression for M_{NL}

Once we have a general expression for M_{NL} , we can use Equation (294) to calculate the shift for any level E_{NL} . We can obtain expressions for the values of M_{NL} by letting β become large, expanding the denominator in Equation (304) and equating coefficients of powers of $e^{-\beta}$. For large β , we have large ψ . We have

$$\frac{e^{-\psi(L+1)}}{1 - e^{-\psi}} = \sum_{m=1}^\infty e^{-\psi(m+L)}$$

and for large β it follows from Equation (310) that

$$\sum_{N=L+1}^\infty e^{-\beta N} M_{NL} = \sum_{m=1}^\infty \left[e^{-\beta A} \left(1 + A_1 e^{-\beta} + \dots \right) \right]^{m+L}. \tag{315}$$

Using the multinomial theorem [124], the right side of the equation becomes

$$\sum_{m=1}^\infty A^{m+L} \sum_{r,s,t,\dots} \frac{(m+L)!}{r!s!t!\dots} A_1^r A_2^t \dots e^{-\beta(m+L+s+2t+\dots)}. \tag{316}$$

where $r + s + t + \dots = m + L$.

To obtain the expression for M_{NL} , we note N is the coefficient of β so $N = m + L + s + 2t + \dots = r + 2s + 3t + \dots$. Accordingly we find

$$M_{NL} = \sum_{r,s,t,\dots} A^{(r+s+t+\dots)} \frac{(r+s+t+\dots)!}{r!s!t!\dots} A_1^r A_2^t \dots \tag{317}$$

where $r + 2s + 3t + \dots = N$ and $r + s + t + \dots > L$.

By applying this formula, we obtain the results:

$N = 1$:

$$M_{10} = A \tag{318}$$

$N = 2$:

$$\begin{aligned} M_{20} &= A^2 + AA_1 \\ M_{21} &= A^2 \end{aligned} \tag{319}$$

Shifts for $N = 1$ and $N = 2$

To illustrate these results, we can calculate the shift for a given energy level using Equation (294). For $N = 1$, we note from Equation (318) that $M_{10} = A$, and from Equation (311) that $A = 1/d^2$. We find that the real part of the radiative shift for the 1S ground state is

$$Re\Delta E_{10} = \frac{4m\alpha(Z\alpha)^4}{3\pi} \int_0^{\phi_c} d\phi e^\phi \sinh \phi \int_0^\infty ds e^{se^{-\phi}} \frac{d}{ds} \frac{1}{(\coth \frac{s}{2} + \cosh \phi)^2} \quad (320)$$

For the shift between two states Equation (314) can be used. For the $N = 2$ Lamb shift between 2S-2P states, the radiative shift to first order in α is

$$Re(\Delta E_{20} - \Delta E_{21}) = \frac{m\alpha(Z\alpha)^4}{6\pi} \int_0^{\phi_c} d\phi e^\phi \sinh^3 \phi \int_0^\infty ds e^{2se^{-\phi}} \frac{d}{ds} \frac{1}{(\coth \frac{s}{2} + \cosh \phi)^4} \quad (321)$$

The s integral can be computed in terms of a Jacobi function of the second kind [127].

As one check on our group theoretical methods, we can compare our matrix elements $\langle 10|e^{iS\phi}|n0\rangle$ with those of Huff [45]. To go from Equation (301) to Equation (302), we did a rotation $R(\phi) = e^{i\phi S}$ generated by S that transformed Γn into Γ_0 . For $N, L = 1, 0$ we have

$$M_{10} = \langle 10|e^{-\Gamma ns}|10\rangle = \langle 10|R(\phi)e^{-\Gamma_0 s}R^{-1}(\phi)|10\rangle = \frac{1}{(\cosh \frac{s}{2} + \sinh \frac{s}{2} \cosh \phi)^2} \quad (322)$$

Expanding the hyperbolic functions, we get

$$\begin{aligned} M_{10} &= \frac{4e^{-s}}{(1 + \cosh \phi)^2} \left[1 - e^{-s} \tanh^2 \frac{s}{2} \right]^{-2} \\ &= \frac{4}{(1 + \cosh \phi)^2} \sum_{n=1}^{\infty} n e^{-ns} \left(\tanh^2 \frac{\phi}{2} \right)^{n-1}. \end{aligned} \quad (323)$$

We can also compute M_{10} by inserting a complete set of states and using $\Gamma_0|n0\rangle = n|n0\rangle$ in Equation (322). Because the generator S is a scalar, only states with $L = 0, m = 0$ can contribute:

$$M_{10} = \sum_{nlm} e^{-ns} |n \langle 10|R(\phi)|n0\rangle|^2. \quad (324)$$

Comparing this to Equation (323), we make the identification

$$|\langle 10|R(\phi)|n0\rangle|^2 = \frac{4n}{(1 + \cosh \phi)^2} \left(\tanh^2 \frac{\phi}{2} \right)^{n-1}. \quad (325)$$

Huff computes this matrix element by analytically continuing the known $O(3)$ matrix element of $e^{iJ_y\phi}$ obtaining

$$|\langle 10|R(\phi)|n0\rangle|^2 = \frac{4n}{\cosh^2 \phi - 1} \left(\tanh^2 \frac{\phi}{2} \right)^n \cdot [{}_2F_1(0, -1; n; \frac{1}{2}(1 - \cosh \phi))]^2. \quad (326)$$

By algebraic manipulation and using ${}_2F_1 = 1$ for the arguments here, we see that this result agrees with our much more simply expressed result from group theory.

9. Conclusions and Future Research

Measuring and explaining the properties of the hydrogen atom has been central to the development of modern physics over the last century. One of the most useful and profound ways to understand its properties is through its symmetries, which we have explored in this paper, beginning with the symmetry of the Hamiltonian, which reflects the symmetry of the degenerate levels, then the larger non-invariance and spectrum-generating groups, which include all of the states. The successes in using symmetry to explore the hydrogen atom led to use of symmetry to understand and model other physical systems, particularly elementary particles.

The hydrogen atom will doubtless continue to be one of testing grounds for fundamental physics. Researchers are exploring the relationship between the hydrogen atom and quantum information [152], the effect of non-commuting canonical variables $[x_i, x_j] \neq 0$ on energy levels [153–155], muonic hydrogen spectra [156], and new physics using Rydberg states [157–162]. The ultra high precision of the measurement of the energy levels has led to new understanding of low Z two body systems, including muonium, positronium, and tritium [151]. As mentioned in the introduction, measurements of levels shifts are currently being used to measure the radius of the proton [2]. We can expect that further investigations of the hydrogen atom and hydrogenlike atoms will continue to reveal new vistas of physics and that symmetry considerations will play an important part.

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102. This equation and any other equation written in this specific coordinate system can be generalized to an arbitrary coordinate system by noting that the Cartesian unit vectors may be written in a manner that is independent of the coordinate system: $\hat{i} = \frac{A}{A}$, $\hat{j} = \frac{L \times A}{LA}$, $\hat{k} = \frac{L}{L}$.
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