DEFORMING SO(4,2) GENERATORS

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ABSTRACT

DEFORMING SO(4,2) GENERATORS

The energy spectrum and degeneracy of a Hamiltonian can be studied using either the theory of special functions or spectrum generating algebras. In this thesis the second approach is used for the analysis of the H-atom Hamiltonian.

SO(2,1) provides the spectrum generating algebra for the H-atom problem. The geometrical symmetry group SO(3) was first generalized to SO(4), the *degeneracy group*, then merging it with SO(2,1), the *dynamical group* SO(4,2) was obtained. The ladder operators of SO(4,2) connect all the states of the H-atom. In the past, the generators of the SO(2,1) group were generalized by the point transformation $\vec{r} \to G(r)\hat{r}$ then these generators are deformed by the variation $G(r) \to G(r) + g(r)$. This formalism has led to a perturbation method. In this work the historical development of above formalism is traced and the 15 generators of the SO(4,2) group are deformed.

ÖZET

SO(4,2) JENERATÖRLERİNİN DEFORMASYONU

Verilen bir Hamilton operatörünün enerji spektrumu ve özdeğerlerinin çokkatlılığı özel fonksiyonlar teorisiyle ya da spektrum üretici cebirlerle incelenebilir. Bu tezde, ikinci yaklaşım benimsenerek hidrojen atomu Hamilton operatörünün analizinde kullanıldı.

İlk olarak, SO(2,1) grubunun hidrojen atomu problemi için spektrum üretici cebir olduğu gösterildi. Geometrik simetri grubu SO(3) önce *çokkatlılık* grubu SO(4)'e genelleştirildi. Daha sonra bu grup SO(2,1) grubu ile birleştirilerek *H-atomu dinamik grubu* SO(4,2) elde edildi. Geçmişte SO(2,1) grubu jeneratörleri $\vec{r} \to G(r)\hat{r}$ dönüşümü ile genelleştirilmişti. Daha sonra bu jeneratörler $G(r) \to G(r) + g(r)$ şeklinde deforme edilmiş ve bu bir pertürbasyon yöntemine yol açmıştı. Bu çalışmada aynı yol izlenip SO(4,2) grubunun jeneratörleri deforme edildi.

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LIST OF SYMBOLS/ABBREVIATIONS

CHGDE	Confluent Hypergeometric Differential Equation
CSCO	Complete Set of Commuting Observables
DE	Differential Equation
H-atom	Hydrogen Atom
LRL	Laplace-Runge-Lenz vector
N-D	N-dimensional
SGA	Spectrum Generating Algebra
so(n)	Lie Algebra of SO(n)
SO(n)	Lie Group SO(n)

1. INTRODUCTION

1.1. History and Formalism

Algebraic methods were first introduced to the study of quantum mechanical problems around 1925. Although the relationship between angular momentum and the Lie algebra so(3) was recognized before quantum mechanics, the significance of angular momentum in quantum mechanics in contrast to classical mechanics was noticed soon after the emergence of quantum mechanics and the necessary formalism was principally developed by Wigner, Weyl and Racah.

In the analysis of H-atom, both the algebraic approach due to Pauli (1926) and the DE approach due to Schrödinger (1926) were originated almost at the same time. Pauli was the first to obtain the quantum mechanical analog of the LRL vector and show that it is an invariant of motion for the H-atom (1926). However complete solution for the accidental degeneracy problem came with the realization that SO(4) is the symmetry group of the H-atom by Fock (1935) and the identification due to Bargmann of Fock's SO(4) generators with angular momentum and LRL vector came soon after (1936).

Since the DE approach was more accessible to the physicists of the time, the algebraic approach was largely forgotten. The revival of these techniques came with the development of quantum mechanics of elementary particles for which the explicit form of the Hamiltonian is unknown and therefore one can only make plausible assumptions about the symmetry. In the hope of finding a clue to the classification of elementary particles, the elementary particle physicists examined several non-compact Lie algebras in the mid-fifties. Although this hope did not materialize, these groups turned out to be relevant as the so-called dynamical groups for atomic physics. [1]

1.2. Generator of Radial Translations

The time independent Schrödinger Hamiltonian is

$$H = \frac{p^2}{2m} + V(\vec{r}) \tag{1.1}$$

For convenience the above Hamiltonian may be converted to dimensionless form using

$$\vec{p} \to \frac{\vec{p}}{mc} \qquad \vec{r} \to \frac{mc\vec{r}}{\hbar} \qquad V \to \frac{V}{mc^2} \qquad \textit{and} \qquad H \to \frac{H}{mc^2} \tag{1.2}$$

so that (1.1) becomes

$$H = \frac{p^2}{2} + V(\vec{r}) \tag{1.3}$$

The norm square of a vector $\vec{A}$ may be decomposed with respect to the unit vector $\hat{u}$ as follows

$$\vec{A} \cdot \vec{A} = A^2 = A^2(\cos\alpha)^2 + A^2(\sin\alpha)^2 = (\vec{A} \cdot \hat{u})^2 + |\vec{A} \times \hat{u}|^2 \tag{1.4}$$

Specifically decomposing p^2 with respect to the unit vector $\hat{r}$:

$$p^2 = (\hat{r} \cdot \vec{p})^2 + |\hat{r} \times \vec{p}|^2 \tag{1.5}$$

is obtained. Quantum mechanical operators corresponding to observables should be Hermitian. The second term is

$$\hat{r} \times \vec{p} = \frac{1}{r}\vec{L} = \vec{L}\frac{1}{r} \tag{1.6}$$

and therefore is already Hermitian. For the $\hat{r} \cdot \vec{p}$ term a symmetrization is necessary to make it Hermitian after which it may be identified as the *generator of radial translations* or simply *radial momentum*

$$K \equiv \frac{\hat{r} \cdot \vec{p} + \vec{p} \cdot \hat{r}}{2} \tag{1.7}$$

Using the commutation relation $[r_i, p_j] = i\delta_{ij}$ it is seen that

$$K = \hat{r} \cdot \vec{p} - \frac{i}{r} \quad ; \tag{1.8}$$

the representation $\vec{p} \to -i\vec{\nabla}$ yields $\hat{r} \cdot \vec{p} \to -i(\hat{r} \cdot \vec{\nabla}) = -i\frac{\partial}{\partial r}$. Hence the differential operator representation for K is :

$$K \to -i\left(\frac{\partial}{\partial r} + \frac{1}{r}\right) \tag{1.9}$$

and

$$[r, K] = i \quad , \tag{1.10}$$

that is, r and K form a conjugate pair as anticipated.

$$K^2 \to -\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)\left(\frac{\partial}{\partial r} + \frac{1}{r}\right) = -\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) = -\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} \tag{1.11}$$

In terms of K^2 and the well-known spectrum of L^2 the Hamiltonian becomes:

$$H = \frac{K^2}{2} + \frac{L^2}{2r^2} + V(\vec{r}) = \frac{K^2}{2} + \frac{l(l+1)}{2r^2} + V(\vec{r}) \tag{1.12}$$

where $l = 0, 1, 2, ...$

2. so(2,1)

2.1. The Lie Algebra so(2,1)

The commutation relations that define the Lie algebra so(2,1) are given by

$$[\Lambda_1, \Lambda_2] = -i\Lambda_3 \qquad [\Lambda_2, \Lambda_3] = i\Lambda_1 \qquad \textit{and} \qquad [\Lambda_3, \Lambda_1] = i\Lambda_2 \tag{2.1}$$

and the Casimir invariant is

$$\Lambda^2 = \Lambda_3^2 - \Lambda_1^2 - \Lambda_2^2 \tag{2.2}$$

Mutually commuting algebra elements together with the Casimir operators constitute the *complete set of commuting observables* (CSCO) and the states are labeled with the eigenvalues of CSCO. For the Lie algebras so(3) and so(2,1), the CSCO has two elements. The above algebra may be cast into the standard form by first choosing the operator to be diagonalized in the standard basis. Having made this selection , one may then construct the raising and lowering operators from the remaining two generators that will raise or lower the eigenvalues of the diagonalized operator by one unit. In the case of the compact Lie algebra so(3), the choice of the operator to be diagonalized is arbitrary, and each generator has a discrete eigenvalue spectrum. However, in the case of the noncompact Lie algebra so(2,1), only Λ_3 has a discrete spectrum; the other two generators Λ_1 and Λ_2 have continuous spectra. Therefore for bound state solutions one should choose Λ_3 to be diagonalized while for the continuum state solutions the remaining generators should be chosen.[2]

Choosing Λ_3 for diagonalization, the CSCO becomes $\{\Lambda^2, \Lambda_3\}$. It is well known that mutually commuting operators have common eigenvectors. Let $\mid \lambda, \mu \rangle$ be the simultaneous eigenvector of Λ^2 and Λ_3 with

$$\Lambda^2 \mid \lambda, \mu \rangle = \lambda \mid \lambda, \mu \rangle \qquad and \qquad \Lambda_3 \mid \lambda, \mu \rangle = \mu \mid \lambda, \mu \rangle \tag{2.3}$$

Forming the ladder operators $\Lambda_+ = \Lambda_1 + i\Lambda_2$ and $\Lambda_- = \Lambda_1 - i\Lambda_2$, the commutation relations (2.1) may alternatively be written as

$$[\Lambda_3, \Lambda_\pm] = \pm\Lambda_\pm \qquad and \qquad [\Lambda_+, \Lambda_-] = -2\Lambda_3 \tag{2.4}$$

These relations together with the identity

$$\Lambda_+\Lambda_- + \Lambda_-\Lambda_+ = 2(\Lambda_3^2 - \Lambda^2) \tag{2.5}$$

enables one to obtain the ladder relations

$$\Lambda_+ \mid \lambda, \mu \rangle = \sqrt{\mu^2 + \mu - \lambda} \mid \lambda, \mu + 1 \rangle \tag{2.6}$$

and

$$\Lambda_- \mid \lambda, \mu \rangle = \sqrt{\mu^2 - \mu - \lambda} \mid \lambda, \mu - 1 \rangle \tag{2.7}$$

From the relation $\Lambda^2 = \Lambda_3^2 - \Lambda_1^2 - \Lambda_2^2$ it follows that $\lambda \leq \mu^2$ which implies that μ is bounded from above or below, leading to two disjoint spectra with infinite levels.

For the case of upper limit $\Lambda_+ \mid \lambda \,, \mu_T \rangle = \mid \emptyset \rangle$ and therefore $\mu_T^2 + \mu_T - \lambda = 0$. $\lambda \leq \mu_T^2$ implies that $\mu_T \leq 0$. Hence $\mu_T = -\frac{1}{2} - \sqrt{\frac{1}{4} + \lambda}$ is an obvious solution whereas $\mu_T = -\frac{1}{2} + \sqrt{\frac{1}{4} + \lambda}$ is also valid if $-\frac{1}{4} \leq \lambda \leq 0$.

For the case of lower limit $\Lambda_- \mid \lambda \,, \mu_B \rangle = \mid \emptyset \rangle$ and therefore $\mu_B^2 - \mu_B - \lambda = 0$. $\lambda \leq \mu_B^2$ implies that $\mu_B \geq 0$. Hence $\mu_B = \frac{1}{2} + \sqrt{\frac{1}{4} + \lambda}$ is an obvious solution whereas $\mu_B = \frac{1}{2} - \sqrt{\frac{1}{4} + \lambda}$ is also valid if $-\frac{1}{4} \leq \lambda \leq 0$.

Choosing the set bounded from below, the spectrum of Λ_3 is obtained as

$$Spectrum(\Lambda_3) = \nu + \frac{1}{2} \pm \sqrt{\frac{1}{4} + \lambda} \qquad ; \qquad (\nu = 0, 1, 2, ...) \tag{2.8}$$

where the minus sign is valid only if : $\quad -\frac{1}{4} \leq \lambda \leq 0$

2.2. so(2,1) and bound states

For a bound state there should be no explosion or implosion of probability density function. Therefore the expectation value of radial momentum is zero : $\langle K \rangle = 0$. The radial wavefunction of a pure state can always be chosen as real since if R is a solution of the radial Schrödinger equation so is R^* and therefore their sum which is real. Then the expectation value

$$\langle K \rangle = -i \int_0^\infty 4\pi r^2 dr \, R \, (\frac{d}{dr} + \frac{1}{r}) \, R \tag{2.9}$$

may be shown to be zero, provided that rR vanishes ar $r = 0$ and $r = \infty$. The relation $\langle K \rangle = 0$ can be generalized to $\langle \sqrt{r} \; \mathrm{K} \sqrt{r} \rangle = 0$ as long as $\frac{1}{\sqrt{r}} R$ is also square integrable. The underlying reason is the dynamical symmetry of bound state systems, namely SO(2,1) algebra. This operator must be a linear combination of the step up and step down operators of the algebra , namely Λ_+ and Λ_-. Since these ladder operators themselves are linear combinations of Λ_1 and Λ_2 one may as well say that $\sqrt{r} \; \mathrm{K} \sqrt{r}$ is a linear combination of Λ_1 and Λ_2. Furthermore rK which is only a similarity transformation away from $\sqrt{r} \; \mathrm{K} \sqrt{r}$ may be set equal to Λ_2, without loss of generality, since group generators may be transformed into each other by an automorphism. Once Λ_2 is determined within a similarity transform , the SO(2,1) generators may be obtained by requiring :

- The generators are at most quadratic in K,
- so(2,1) commutation relations are satisfied,
- Λ_3 does not contain a K term,
- The Casimir operator is constant.

Then the remaining generators are found to be [6]

$$\Lambda_1 = \frac{rK^2}{2} + \frac{l(l+1)}{2r} - \frac{r}{2} \tag{2.10}$$

$$\Lambda_3 = \frac{rK^2}{2} + \frac{l(l+1)}{2r} + \frac{r}{2} \tag{2.11}$$

Actually this realization, which is appropriate for the H-atom Hamiltonian, is a special case of a more general form which will be obtained in chapter 6. For the given form, the Casimir invariant becomes:

$$Spectrum(\Lambda^2) = \lambda = l(l+1) \geq 0 \tag{2.12}$$

Therefore the spectrum of Λ_3 becomes:

$$Spectrum(\Lambda_3) = \nu + l + 1 \equiv n \qquad n = 1, 2, 3, ... \tag{2.13}$$

With the new labels n and l the simultaneous eigenkets of Λ^2 and Λ_3 may be represented by $\mid n, l \rangle$ or, more conveniently by the hydrogenic states $\mid n, l, m \rangle$ and the equations (2.3), (2.6), (2.7) become

$$\begin{gathered} \Lambda^2 \mid n, l, m \rangle = l(l+1) \mid n, l, m \rangle \qquad \Lambda_3 \mid n, l, m \rangle = n \mid n, l, m \rangle \\ \Lambda_\pm \mid n, l, m \rangle = \sqrt{n(n \pm 1) - l(l+1)} \mid n \pm 1, l, m \rangle \end{gathered} \tag{2.14}$$

for the H-atom.

2.3. Energy Spectrum of Hydrogen Atom

Energy spectrum of the H-atom may be found either using the theory of special functions or the spectrum generating algebras. In this section so(2,1) will be shown to be the energy spectrum generating algebra of the H-atom.

The potential energy term of the hydrogen Hamiltonian is

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r} = -\frac{\alpha\hbar c}{r} \tag{2.15}$$

Inserting this into (1.12), one obtain the following for the dimensionless Hamiltonian

$$H = \frac{K^2}{2} + \frac{l(l+1)}{2r^2} - \frac{\alpha}{r} \tag{2.16}$$

Consider the eigenvalue equation $H\psi = E\psi$. This implies that $(H - E)\,\psi = 0$ and multiplying both sides by r one obtains $(rH - rE)\,\psi = 0$. Writing the Hamiltonian explicitly, multiplying by two and considering the spectrum one obtains

$$\mathit{Spectrum}\left(rK^2 + \frac{L^2}{r} - 2\alpha - 2Er\right) = 0 \tag{2.17}$$

Notice that $rK^2 + \frac{L^2}{r} = (\Lambda_1 + \Lambda_3)$ and $-2Er = 2E(\Lambda_1 - \Lambda_3)$. Therefore above equation may be written as :

$$\mathit{Spectrum}\,[\,(\Lambda_1 + \Lambda_3) - 2\alpha + 2E(\Lambda_1 - \Lambda_3)\,] = 0 \tag{2.18}$$

or equivalently as

$$\mathit{Spectrum}\,[\,(1 + 2E)\,\Lambda_1 + (1 - 2E)\,\Lambda_3\,] = 2\alpha \tag{2.19}$$

Transforming this equation using the identities (A.12) and (A.13) one ends up with

$$\begin{aligned} \mathit{Spectrum}\,[\,\{(1 + 2E)\cosh\beta - (1 - 2E)\sinh\beta\}\Lambda_1 \\ + \{(1 - 2E)\cosh\beta - (1 + 2E)\sinh\beta\}\,\Lambda_3\,] = 2\alpha \end{aligned} \tag{2.20}$$

The tilting angle β may be chosen to diagonalize either the compact generator Λ_3 or the noncompact generator Λ_1. In the latter case the continuous part of the spectrum is obtained whereas in the former the discrete part. [2]

For $\tanh\beta = \left(\frac{1+2E}{1-2E}\right)$ the coefficient of Λ_1 vanishes and the discrete spectrum is obtained. Inserting the specific value for β and rearranging (2.20) become

$$Spectrum\left[\frac{(1-2E)^2-(1+2E)^2}{\sqrt{(1-2E)^2-(1+2E)^2}}\right]\Lambda_3 = 2\alpha \tag{2.21}$$

which reduces to

$$Spectrum\,[\,\sqrt{-8E}\,\Lambda_3\,] \;= 2\alpha \tag{2.22}$$

In other words

$$\sqrt{-8E}\,n = 2\alpha \tag{2.23}$$

Solving for E, the energy spectrum of H-atom is found to be:

$$E_n = -\frac{\alpha^2}{2n^2} \tag{2.24}$$

Multiplying by mc^2 one obtains the dimensionally correct energy spectrum.

$$E_n = -\frac{\alpha^2 mc^2}{2n^2} \tag{2.25}$$

where $n = 1, 2, 3....$ This result is identical to the famous Bohr energy formula of the H-atom.

2.4. Relation to CHGDE

Consider the CHGDE with $G = G(r)$ as its independent variable instead of r

$$[G, \gamma - G, -\alpha]\ {}_1F_1(\alpha, \gamma; G) = 0 \tag{2.26}$$

For square integrable solutions, the choice $\alpha = -\nu$, with $(\nu = 0, 1, 2, ...)$ is necessary. Using equations (A.4), (A.5) and (A.6) one obtains the invariant form of the above DE as

$$\left[1\,,\,0\,,\frac{\frac{\gamma}{2}-\frac{\gamma^2}{4}}{G^2}+\frac{\nu+\frac{\gamma}{2}}{G}-\frac{1}{4}\right]\;e^{-\frac{G}{2}}\;G^{\frac{\gamma}{2}}\;{}_1F_1(-\nu,\gamma;G)=0 \tag{2.27}$$

Converting the independent variable to r using

$$\frac{d}{dG}=\frac{1}{G'}\frac{d}{dr} \qquad and \qquad \frac{d^2}{dG^2}=\frac{1}{G'^2}\frac{d^2}{dr^2}-\frac{G''}{G'^3}\frac{d}{dr} \tag{2.28}$$

one obtains

$$\left[\frac{1}{G'^2}\,,\,-\frac{G''}{G'^3}\,,\,\frac{\frac{\gamma}{2}-\frac{\gamma^2}{4}}{G^2}+\frac{\nu+\frac{\gamma}{2}}{G}-\frac{1}{4}\right]\;e^{-\frac{G}{2}}\,G^{\frac{\gamma}{2}}\;{}_1F_1(-\nu,\gamma;G)=0 \tag{2.29}$$

Once more going through the procedure of putting a DE into invariant form, one ends up with

$$\left[1\,,\,0\,,\,\frac{G'''}{2G'}-\frac{3G''^2}{4G'^2}+\left(\frac{\gamma}{2}-\frac{\gamma^2}{4}\right)\frac{G'^2}{G^2}+\left(\nu+\frac{\gamma}{2}\right)\frac{G'^2}{G}-\frac{G'^2}{4}\right] \\ \frac{e^{-\frac{G}{2}}G^{\frac{\gamma}{2}}}{\sqrt{G'}}\quad {}_1F_1(-\nu,\gamma;G)=0 \tag{2.30}$$

Remembering $K \to -i\left(\frac{\partial}{\partial r}+\frac{1}{r}\right)$ and $K^2 \to -\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}$ and using the identity

$$-rK\frac{f}{r} \;\to\; \frac{1}{r}\frac{d}{dr}r^2\frac{d}{dr}\frac{f}{r} \;=\; \frac{d^2}{dr^2} \tag{2.31}$$

the above DE may be converted to the operator equation

$$\left[K^2-\frac{G'''}{2G'}+\frac{3G''^2}{4G'^2}-\left(\frac{\gamma}{2}-\frac{\gamma^2}{4}\right)\frac{G'^2}{G^2}-\left(\nu+\frac{\gamma}{2}\right)\frac{G'^2}{G}+\frac{G'^2}{4}\right] \\ \frac{e^{-\frac{G}{2}}G^{\frac{\gamma}{2}}}{r\sqrt{G'}}\quad {}_1F_1(-\nu,\gamma;G)=0 \tag{2.32}$$

Rearranged , it becomes [6]

$$\left[\frac{G}{G'^2}K^2 + \frac{\frac{\gamma}{2} - \frac{\gamma^2}{4}}{G} - \frac{GG'''}{2G'^3} + \frac{3GG''^2}{4G'^4} + \frac{G}{4}\right] R = \left(\nu + \frac{\gamma}{2}\right) R \tag{2.33}$$

where

$$R = \frac{e^{-\frac{G}{2}}\, G^{\frac{\gamma}{2}}}{r\,\sqrt{G'}}\ {}_1F_1(-\nu, \gamma; G) \tag{2.34}$$

For $G(r) = r$ and $\frac{\gamma^2}{4} - \frac{\gamma}{2} = l(l+1)$ the operator in brackets given by (2.33) becomes

$$rK^2 + \frac{l(l+1)}{r} + \frac{r}{4} \tag{2.35}$$

Applying the scaling transformation (A.8) such that $\vec{r} \to 2\vec{r}$ and $\vec{p} \to \frac{\vec{p}}{2}$ one obtain

$$\frac{rK^2}{2} + \frac{l(l+1)}{2r} + \frac{r}{2} \tag{2.36}$$

which is nothing but the realization of Λ_3 given by (2.11)

3. so(3)

3.1. Infinitesimal Generators of Rotation and Rotational Invariance

In 2-D a rotation by an angle γ around the z-axis has the following effect on the coordinates and momenta

$$\begin{pmatrix} x \\ y \end{pmatrix} \rightarrow \begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\gamma & -\sin\gamma \\ \sin\gamma & \cos\gamma \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \tag{3.1}$$

and

$$\begin{pmatrix} p_x \\ p_y \end{pmatrix} \rightarrow \begin{pmatrix} p'_x \\ p'_y \end{pmatrix} = \begin{pmatrix} \cos\gamma & -\sin\gamma \\ \sin\gamma & \cos\gamma \end{pmatrix} \begin{pmatrix} p_x \\ p_y \end{pmatrix} \tag{3.2}$$

Denoting the operator that rotates the 2-D vectors by $R_z(\gamma)$ the above equations may be cast into the form $\vec{v'} = R_z(\gamma)\,\vec{v}$. Let $U[R_z(\gamma)]$ be the operator in the Hilbert space that corresponds to $R_z(\gamma)$. Then $|\,\psi\,\rangle \rightarrow |\,\psi'\,\rangle = U[R_z(\gamma)]\,|\,\psi\,\rangle$. Since in the quantum formulation the expectation values play the role of the classical variables, it may be claimed that the transformed state $|\,\psi'\,\rangle$ should satisfy the following:

$$\langle x' \rangle = \langle x \rangle \cos\gamma - \langle y \rangle \sin\gamma \tag{3.3}$$

$$\langle y' \rangle = \langle x \rangle \sin\gamma + \langle x \rangle \cos\gamma \tag{3.4}$$

$$\langle p'_x \rangle = \langle p_x \rangle \cos\gamma - \langle p_y \rangle \sin\gamma \tag{3.5}$$

$$\langle p'_y \rangle = \langle p_x \rangle \sin\gamma + \langle p_y \rangle \cos\gamma \tag{3.6}$$

where

$$\langle x' \rangle = \langle \psi' \mid x \mid \psi' \rangle = \langle \psi \mid U^\dagger \, x \, U \mid \psi \rangle = \langle U^\dagger \, x \, U \rangle \tag{3.7}$$

and

$$\langle x \rangle = \langle \psi \mid x \mid \psi \rangle \tag{3.8}$$

In the case of an infinitesimal rotation $\epsilon_z \hat{z}$, U becomes :

$$U[R_z(\epsilon_z)] = I - \frac{i\epsilon_z L_z}{\hbar} \tag{3.9}$$

where L_z is called the *generator of infinitesimal rotations about z-axis*. Since U is unitary, it satisfies $UU^\dagger = I$. Putting (3.9) into this, one may show that $L_z = L_z^\dagger$ i.e. L_z is Hermitian. Then putting (3.9) also into (3.7), the following is obtained:

$$\langle x' \rangle = \langle x \rangle + \frac{i\epsilon_z}{\hbar} \langle [L_z, x] \rangle \tag{3.10}$$

Putting (3.10) into (3.3) , with $\cos \epsilon_z = 1$, $\sin \epsilon_z = \epsilon_z$ the following is obtained:

$$\langle \frac{i}{\hbar} [L_z, x] + y \rangle = 0 \tag{3.11}$$

Since $\mid \psi \rangle$ is arbitrary, one may choose it to be any of the eigenvectors of the operator in the paranthesis. Then all the eigenvalues vanishes, implying that the operator itself vanishes. That is :

$$[L_z, x] = i\hbar y \tag{3.12}$$

If the same procedure is followed for y' , p'_x and p'_y one further obtains:

$$[L_z, y] = -i\hbar x \tag{3.13}$$

$$[L_z, p_x] = i\hbar p_y \tag{3.14}$$

$$[L_z, p_y] = -i\hbar p_x \tag{3.15}$$

Using the commutation relations $[r_i, p_j] = i\delta_{ij}$, $[r_i, r_j] = 0$ and $[p_i, p_j] = 0$ it may be shown that the equations (3.12) to (3.15) imply the identification

$$L_z = xp_y - yp_x \tag{3.16}$$

Finite rotations about z-axis are generated by L_z as follows

$$U[R_z(\gamma)] = \lim_{N\to\infty} \left(I - \frac{i\gamma}{N\hbar} L_z\right)^N = exp(-\frac{i\gamma}{\hbar} L_z) \tag{3.17}$$

Invariance under rotations about the z-axis is defined as:

$$U^\dagger \, H \, U = H \tag{3.18}$$

For an infinitesimal rotation this equation reduces to:

$$\left(I + \frac{i\epsilon_z}{\hbar} L_z\right) H \left(I - \frac{i\epsilon_z}{\hbar} L_z\right) = H \tag{3.19}$$

from which one obtains the simple equation

$$[L_z, H] = 0 \tag{3.20}$$

for invariance under rotations about the z-axis.

Repeating the whole procedure for rotations about x-axis and y-axis, respectively, yields the generators of infinitesimal rotations about x and y axes

$$L_x = yp_z - p_z y \tag{3.21}$$

and

$$L_y = zp_x - p_x z \tag{3.22}$$

and invariance under rotations about x and y axes, respectively, may be expressed as:

$$[L_x, H] = 0 \tag{3.23}$$

and

$$[L_y, H] = 0 \tag{3.24}$$

Unifying the results, rotational invariance expressed as

$$U^\dagger \, H \, U = H \tag{3.25}$$

reduces to

$$[L_i, H] = 0 \qquad for \qquad i = 1, 2, 3 \qquad (or \qquad x, y, z) \tag{3.26}$$

considering infinitesimal rotations.

And the general form of the finite rotation operator becomes:

$$U[R(\vec{\theta})] = \lim_{N \to \infty} \left(I - \frac{i}{N\hbar} \, \vec{\theta} \cdot \vec{L} \right)^N = exp(-\frac{i}{\hbar} \, \vec{\theta} \cdot \vec{L}) \tag{3.27}$$

3.2. The Lie algebra so(3)

The generators introduced in the previous section define the Lie algebra so(3) with the following commutation relations

$$[L_1, L_2] = iL_3 \qquad [L_2, L_3] = iL_1 \qquad and \qquad [L_3, L_1] = iL_2 \tag{3.28}$$

or, more compactly, as:

$$[L_i, L_j] = i\,\epsilon_{ijk}\,L_k \tag{3.29}$$

Other basic commutators related with these generators are:

$$[L_i, r_j] = i\,\epsilon_{ijk}\,r_k \qquad and \qquad [L_i, p_j] = i\,\epsilon_{ijk}\,p_k \tag{3.30}$$

Generalizing above relations, *a vector operator* may be defined as the collection of three components satisfying:

$$[L_i, V_j] = i\,\epsilon_{ijk}\,V_k \tag{3.31}$$

A *scalar operator* (or *so(3) scalar*) , on the other hand, is defined as:

$$[L_i, Scalar] = 0 \tag{3.32}$$

It may be shown that if $\vec{A}$ and $\vec{B}$ are vector operators then their scalar product $\vec{A} \cdot \vec{B}$ is a scalar operator. $L^2 = \vec{L} \cdot \vec{L}$ is a scalar and commutes with each L_i, thereby being the Casimir operator for so(3). As stated before, any of the generators L_i may be chosen for diagonalization. L_3 is chosen, since it has the simplest expression in the spherical coordinates. . Therefore CSCO becomes $\{L^2, L_3\}$.

Let $\mid \lambda, m \rangle$ be the common eigenvectors of L^2 and L_3 with

$$L^2 \mid \lambda, m \rangle = \lambda \mid \lambda, m \rangle \qquad and \qquad L_3 \mid \lambda, m \rangle = m \mid \lambda, m \rangle \tag{3.33}$$

Consider a finite rotation about z-axis through an angle γ

$$U[R_z(\gamma)] \mid lm \rangle = e^{-iL_3\gamma} \mid lm \rangle \tag{3.34}$$

If $\gamma = 2\pi$ then the same eigenvector should be obtained, implying that $e^{-2\pi im} = 1$. Therefore m should be an integer. The ladder operators L_+ and L_- are defined as:

$$L_\pm = L_1 \pm L_2 \tag{3.35}$$

Then the commutation relations (3.28) are replaced by

$$[L_3, L_\pm] = \pm L_\pm \qquad [L_+, L_-] = 2L_3 \tag{3.36}$$

These commutators together with the identity

$$L_+L_- + L_-L_+ = 2(L^2 - L_3^2) \tag{3.37}$$

leads to

$$L_\pm \mid \lambda, m \rangle = \sqrt{\lambda - m^2 \mp m} \mid \lambda, m \pm 1\rangle \tag{3.38}$$

$L^2 = L_1^2 + L_2^2 + L_3^2$ implies that $\lambda \geq m^2$ therefore m is bounded from above and below. m_T denoting the top state and m_B the bottom state:

$$L_+ \mid \lambda, m_T \rangle = \mid \emptyset \rangle \qquad and \qquad L_- \mid \lambda, m_B \rangle = \mid \emptyset \rangle \tag{3.39}$$

Then $\lambda - m_T^2 - m_T = 0$ and $\lambda - m_B^2 + m_B = 0$ which leads to the results

$$m_T = -\frac{1}{2} + \sqrt{\frac{1}{4} + \lambda} \qquad \textit{and} \qquad m_B = -m_T \tag{3.40}$$

Therefore $m_T - m_B = 2m_T$ which is an even integer $2l$. With this definition $m_T = l$, $m_B = -l$ and $\lambda = l(l+1)$ follows. The states $\mid \lambda, m \rangle$ may be relabelled as $\mid l, m \rangle$ without ambiguity and equations (3.33), (3.38) may then be rewritten as

$$L^2 \mid l, m \rangle = l(l+1) \mid l, m \rangle \tag{3.41}$$

$$L_3 \mid l, m \rangle = m \mid l, m \rangle \tag{3.42}$$

$$L_\pm \mid l, m \rangle = \sqrt{(l \mp m)(l \pm m + 1)} \mid l, m \pm 1 \rangle \tag{3.43}$$

The differential representations in spherical coordinates for the operators L_3, L^2 and $L_\pm$ are:

$$L_3 \to -i \frac{\partial}{\partial \phi} \tag{3.44}$$

$$L^2 \to -\left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] \tag{3.45}$$

and

$$L_\pm \to e^{\pm i\phi} \left[\pm \frac{\partial}{\partial\theta} + i \cot\theta \frac{\partial}{\partial\phi} \right] \tag{3.46}$$

3.3. Degeneracy of the orbital angular momentum quantum number l

If the Hamiltonian is a scalar operator then it is rotationally invariant. Consider the equation (1.12). $\frac{K^2}{2}$ and $\frac{L^2}{2r^2}$ terms are already scalar. Therefore, if the term $V(\vec{r})$ is a scalar, then the Hamiltonian becomes scalar and hence rotationally invariant. Then $[H, L_i] = 0$, which implies that $[H, L_\pm] = 0$. Applying $L_\pm$ repeatedly to an eigenvector $|\, l, m\,\rangle$, one may go through $2l + 1$ values of m without changing the energy. That is, $|\, l, l\,\rangle$, $|\, l, l-1\,\rangle$, ...$|\, l, -l\,\rangle$ all have the same energy eigenvalue. A naive observation of this fact leads one to expect a $2l + 1$-fold degeneracy for the energy levels of H-atom.

4. so(4)

4.1. Accidental Degeneracy and Construction of SO(4)

The energy spectrum of the H-atom for the dimensionless Hamiltonian was found to be

$$E = -\frac{\alpha^2}{2n^2}, \qquad n = 1, 2, 3, ... \tag{4.1}$$

where $n = \nu + l + 1$. For each n, the allowed values of l are

$$l = n - \nu - 1 = n - 1, n - 2, ..., 1, 0 \tag{4.2}$$

For each l, there correspond "$2l + 1$" m values. Hence for a given principal quantum number n, degeneracy should be

$$\sum_{l=0}^{n-1} (2l + 1) = n^2 \tag{4.3}$$

From rotational symmetry the naive prediction of degeneracy of each level was $2l + 1$, whereas the correct value is n^2. This indicates that rotational symmetry is not the whole story, there must be another invariant of motion. This was called *accidental degeneracy* before mastering the complete symmetry structure of the H-atom. The resolution of the problem involves the LRL vector.

The classical LRL vector is defined as:

$$\vec{y} = (\vec{p} \times \vec{L}) - \alpha\hat{r} \tag{4.4}$$

Being an invariant of motion for the classical Kepler problem, classical LRL points in the direction of the major axis and its magnitude is proportional to the eccentricity of the orbit. With regard to the correspondence principle, it may be generalized to quantum mechanics. For it to be a quantum mechanical operator corresponding to an observable, it should be Hermitian. For it to be Hermitian, the first term needs a symmetrization. Then the quantum mechanical analog of the LRL vector becomes

$$\vec{Y} = \frac{1}{2}(\vec{p} \times \vec{L} - \vec{L} \times \vec{p}) - \alpha\hat{r} = \vec{Y}^{\dagger} \tag{4.5}$$

Using the commutation relations of $\vec{r}$, $\vec{p}$ and $\vec{L}$, one may write $\vec{Y}$ equivalently as:

$$\vec{Y} = \vec{r}p^2 - rK\vec{p} - \alpha\hat{r} \tag{4.6}$$

or as

$$\vec{Y} = \frac{\vec{r}p^2}{2} - rK\vec{p} + \vec{r}H \tag{4.7}$$

where $H = \frac{p^2}{2} - \frac{\alpha}{r}$. Components of $\vec{Y}$, like the components of $\vec{L}$, commute with the Hamiltonian,

$$[Y_i, H] = 0 \qquad i = 1, 2, 3 \tag{4.8}$$

therefore being three additional invariants of motion. $\vec{Y}$ and $\vec{L}$ satisfy the following commutation relations

$$[L_i, L_j] = i\,\epsilon_{ijk}\,L_k \qquad [L_i, Y_j] = i\,\epsilon_{ijk}\,Y_k \qquad \textit{and} \qquad [Y_i, Y_j] = (-2H)\,i\,\epsilon_{ijk}\,L_k \tag{4.9}$$

and the identities

$$\vec{L} \cdot \vec{Y} = \vec{Y} \cdot \vec{L} = 0 \qquad , \qquad Y^2 = 2H(L^2 + 1) + \alpha^2 \tag{4.10}$$

Except for the $-2H$ factor, the equations (4.9) are the defining commutation relations for the Lie algebra so(4). In order to obtain a realization of so(4), the factor $-2H$

must be removed from (4.9). The two possibilities are: replacing it by one of its continuum or bound state energy eigenvalues. The first choice leads to a realization of so(3,1), whereas the second chocie to a realization of so(4). With the second choice, the modified LRL vector is written as:

$$\vec{W} = \frac{1}{\sqrt{-2E_n}}\vec{Y} \tag{4.11}$$

Then the components of $\vec{W}$ and $\vec{L}$ satisfy the commutation relations of so(4):

$$[L_i, L_j] = i\,\epsilon_{ijk}\,L_k \qquad [L_i, W_j] = i\,\epsilon_{ijk}\,W_k \qquad and \qquad [W_i, W_j] = i\,\epsilon_{ijk}\,L_k \tag{4.12}$$

The identities (4.9) become:

$$\vec{L}\cdot\vec{W} = \vec{W}\cdot\vec{L} = 0 \qquad , \qquad W^2 = -(L^2+1) - \frac{\alpha^2}{2E_n} \tag{4.13}$$

The commutation relations given in (4.12) may be simplified if one introduces two new vector operators:

$$\vec{J} = \frac{1}{2}(\vec{L}+\vec{W}) \qquad and \qquad \vec{J'} = \frac{1}{2}(\vec{L}-\vec{W}) \tag{4.14}$$

to give

$$[J_i, J_j] = i\,\epsilon_{ijk}\,J_k \qquad [J'_i, J'_j] = i\,\epsilon_{ijk}\,J'_k \qquad and \qquad [J_i, J'_j] = 0 \tag{4.15}$$

It is seen that the six components $J_i\,,J'_j$ generate the Lie algebra of the product group $SU(2)\times SU(2)$ which is locally isomorphic to SO(4). The operators J^2 and J'^2 are the Casimir operators of the two su(2) algebras with the eigenvalues

$$J^2 = j(j+1) \qquad and \qquad J'^2 = j'(j'+1) \qquad with \qquad j, j' = 0, \frac{1}{2}, 1, ... \tag{4.16}$$

One may form two Casimir operators for so(4)

$$C_1 = J^2 + J'^2 = \frac{1}{2}(L^2 + W^2) \qquad and \qquad C_2 = J^2 - J'^2 = \vec{L} \cdot \vec{W} \quad , \tag{4.17}$$

but one has from (4.13) that $C_1 = -1 - \frac{\alpha^2}{2E_n}$ and $C_2 = 0$. Hence $j = j'$ and

$$C_1 = -1 - \frac{\alpha^2}{2E_n} = 2j(j+1) \qquad with \qquad j = 0, \frac{1}{2}, 1, ... \tag{4.18}$$

Identifying $2j+1$ as n, the energy spectrum is obtained

$$E_n = -\frac{\alpha^2}{2n^2} \tag{4.19}$$

The representations of $SU(2)\times SU(2)$ are of degree $(2j+1)\times(2j'+1) = (2j+1)^2 = n^2$. Therefore SO(4) explains the degeneracy and is hence the *degeneracy group* of the hydrogen atom.

The so(4) generalization that is constructed is not suitable for merging with so(2,1). The difficulty arises from the energy dependence of the realization of $\vec{W}$ given by (4.11). In chapter 2, it was shown that the so(2,1) generator Λ_3 is related to the hydrogen atom Hamiltonian via a scaling transformation and this suggests that the same scaling transformation should be applied to the so(4) generators $\vec{L}$ and $\vec{W}$ to obtain a scaled realization of so(4). The scaling transformation angle of Λ_1 and Λ_3 satisfied $\tanh\beta = \left(\frac{1+2E}{1-2E}\right)$ which leads to $e^{\beta} = \frac{1}{\sqrt{-2E}}$.

$$\vec{W} = \frac{1}{\sqrt{-2E_n}}\left(\frac{\vec{r}\,p^2}{2} - rK\vec{p} + \vec{r}\,H\right) \tag{4.20}$$

If one applies the scaling transformation (A.8) with

$$e^{\beta} = \frac{1}{\sqrt{-2E_n}} \tag{4.21}$$

then $\tilde{\vec{r}} = e^{\beta}\,\vec{r}$ and $\tilde{\vec{p}} = e^{-\beta}\,\vec{p}$, and one ends up with

$$\vec{A} \equiv \tilde{\vec{W}} = \frac{\vec{r}\,p^2}{2} - rK\vec{p} - \frac{\vec{r}}{2} \tag{4.22}$$

which is *the scaled LRL vector*. Since $\vec{r}$ and $\vec{p}$ transform inversely $\vec{L} = \vec{r} \times \vec{p}$ is invariant under scaling. Thus, one obtains the energy independent realization of the so(4) Lie algebra with the defining commutation relations:

$$[L_i, L_j] = i\,\epsilon_{ijk}\,L_k \qquad [L_i, A_j] = i\,\epsilon_{ijk}\,A_k \qquad \textit{and} \qquad [A_i, A_j] = i\,\epsilon_{ijk}\,L_k \tag{4.23}$$

There is a close connection between the set $\{H, \vec{L}, \vec{W}\}$ and the set $\{\Lambda_3, \vec{L}, \vec{A}\}$ obtained from it via the scaling transformation. The so(4) Lie algebra generated by $\{\vec{L}, \vec{W}\}$ is the dynamical invariance algebra for the hydrogenic Hamiltonian, whereas $\{\vec{L}, \vec{A}\}$ plays the same role for the Λ_3 operator.

4.2. Hydrogenic Tower of States

The action of L_3, $L_\pm$, and L^2 on the eigenkets were expressed in (3.41),(3.42) and (3.43). The corresponding formulae for the remaining generators may be found using the commutation relations of SO(4) generators and a number of useful identities between the SO(3) vector operators and SO(3) generators to be

$$\begin{aligned} A_3 \mid n, l, m\,\rangle = {} & \sqrt{(l-m)(l+m)} \quad a_l^n \quad \mid n, l-1, m\,\rangle \\ & + \sqrt{(l-m+1)(l+m+1)} \quad a_{l+1}^n \quad \mid n, l+1, m+1\,\rangle \end{aligned} \tag{4.24}$$

$$\begin{aligned} A_\pm \mid n, l, m\,\rangle = {} & \pm\sqrt{(l \mp m)(l \mp -1)} \quad a_l^n \quad \mid n, l-1, m \pm 1\,\rangle \\ & \mp\sqrt{(l \pm m+1)(l \pm m+2)} \quad a_{l+1}^n \quad \mid n, l+1, m \pm 1\,\rangle \end{aligned} \tag{4.25}$$

where

$$a_l^n = \sqrt{(n^2 - l^2)/(4l^2 - 1)} \tag{4.26}$$

It follows from (4.25) that

$$A_+ \mid n, l-1, l-1 \,\rangle = b_l^n \mid n, l, l \,\rangle \tag{4.27}$$

where

$$b_l^n = -\sqrt{2l(n^2 - l^2)/(2l+1)} \tag{4.28}$$

Therefore, A_+ is a raising operator that connects the states with $m = l$. All such states can be generated from $\mid n, 0, 0 \,\rangle$ with the formula

$$\mid n, l, l \,\rangle = (\Pi_{i=1}^{l} b_i^n)^{-1} (A_+)^l \mid n, 0, 0 \,\rangle \tag{4.29}$$

Moreover applying L_- to the states with $m = l$ one may move down to the state with any alowed m. It follows from (3.43) that

$$\mid n, l, m \,\rangle = (\Pi_{i=m}^{l-1} c_i^n)^{-1} (L_-)^{l-m} \mid n, l, l \,\rangle \tag{4.30}$$

where

$$c_l^n = \sqrt{(l+m+1)(l-m)} \tag{4.31}$$

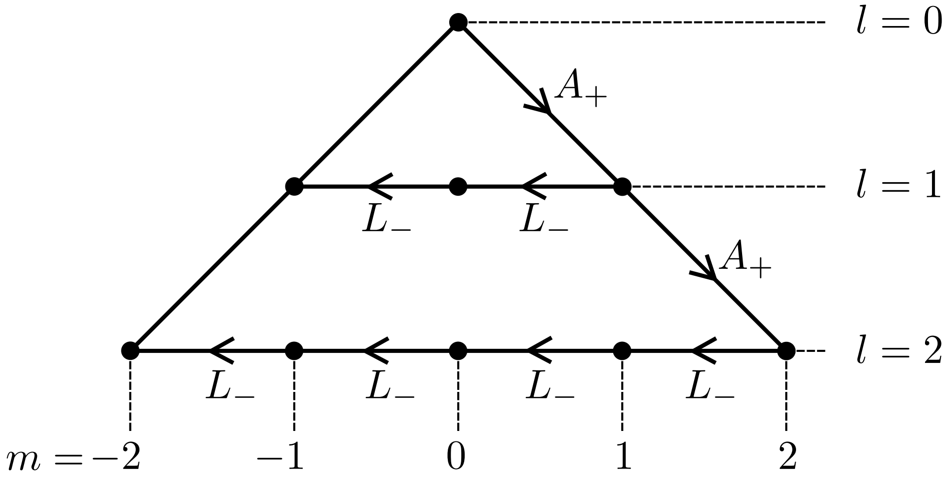

Figure 4.1. An so(4) subtower representing the n^2 eigenstates obtained from the top by the appropriate application of the A_+ and L_- operators.

Combining these results

$$| \, n, l, m \, \rangle = (\Pi_{i=1}^{l} \, b_i^n)^{-1} (\Pi_{j=m}^{l-1} \, c_j^n)^{-1} (L_-)^{l-m} (A_+)^l \, | \, n, 0, 0 \, \rangle \tag{4.32}$$

This may be represented by a graph called *triangular so(4) subtower* which is shown in Figure (4.1). Finally using equations (2.14), one may move from the ground state $| \, 1, 0, 0 \, \rangle$ to $| \, n, 0, 0 \, \rangle$

$$| \, n, 0, 0 \, \rangle = (\Pi_{i=0}^{n-1} d_0^i)^{-1} \Lambda_+^{n-1} \, | \, 1, 0, 0 \, \rangle \tag{4.33}$$

where

$$d_0^n = \sqrt{n(n+1)} \tag{4.34}$$

Thus one may express all bound states in terms of the ground state as the follows

$$\begin{aligned} | \, n, l, m \, \rangle = (\Pi_{i=1}^{l} \, b_i^n)^{-1} \, (\Pi_{i=m}^{l-1} \, c_i^n)^{-1} \, (\Pi_{i=0}^{n-1} \, d_0^i)^{-1} & \\ (L_-)^{l-m} \, (A_+)^l \quad (\Lambda_+)^{n-1} \, | \, 1, 0, 0 \, \rangle & \end{aligned} \tag{4.35}$$

This leads to the pictorial representation of all bound hydrogenic states which is given in Figure (4.2).

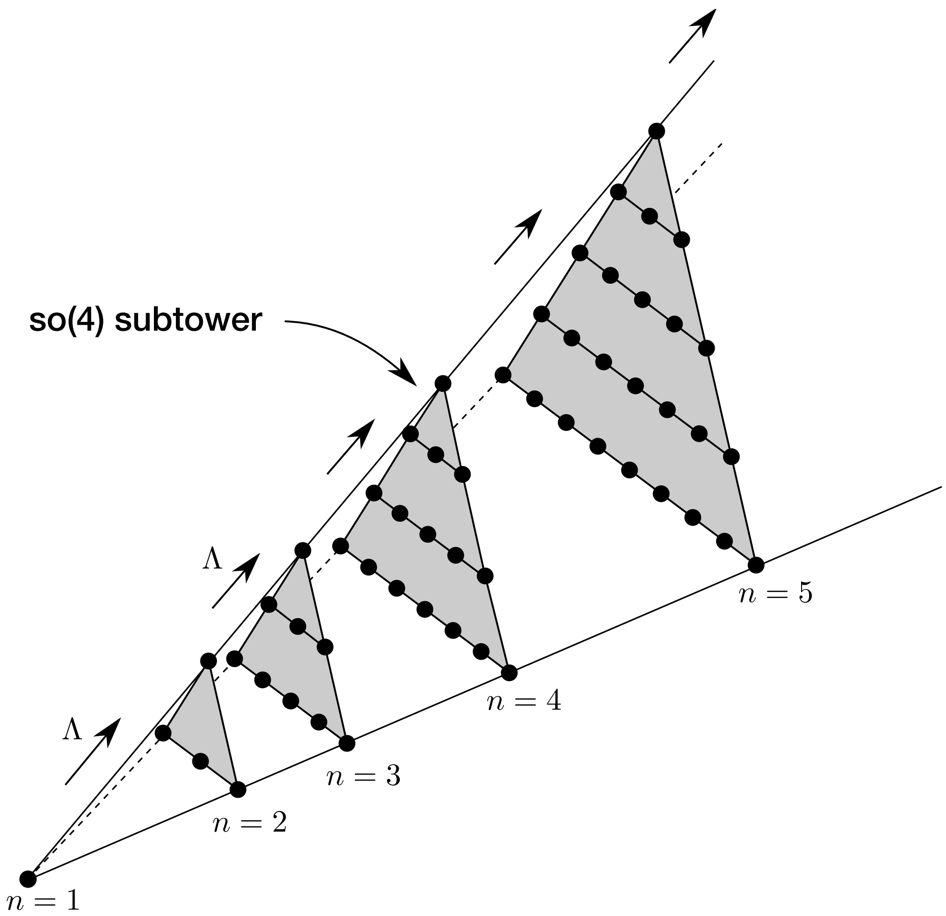

Figure 4.2. The collection of so(4) subtowers for n=1,2,3... form an so(4,2) tower linking all hydrogenic states. The top states in so(4) subtowers are linked by the so(2,1) operator Λ_3.

5. so(4,2)

It was seen that so(2,1) and so(4) provide the ladder operators for the quantum numbers $n\,,l$ and $m\,.$ In order to provide a complete algebraic framework for the analysis of H-atom problem one has to merge so(2,1) and so(4) into a bigger Lie algebra which we call the *dynamical group* of the H-atom. It is also desirable to obtain simple expressions for coordinates and momenta in terms of these generators, since the most general type of perturbations are functions of them and therefore the dynamical group should contain these generators.

One may start with, combining the generators of so(4) and the so(2,1) generator Λ_2. To close out all commutation relations among the operators $\vec{L}\,,\vec{A}$ and Λ_2 it is necessary to introduce an additional vector operator whose realization is

$$\vec{M} = \frac{\vec{r}\,p^2}{2} - rK\vec{p} + \frac{\vec{r}}{2} \tag{5.1}$$

since

$$[\vec{L}, \Lambda_2] = 0 \qquad but \qquad [\vec{A}, \Lambda_2] = \vec{M} \tag{5.2}$$

The result is the Lie algebra so(4,1) having ten generators $\vec{L}$, $\vec{A}$, $\vec{M}$ and Λ_2. Moreover one has the simple expression $\vec{r} = \vec{M} - \vec{A}$. Next trying to combine Λ_1 and Λ_3 with the so(4,1) generators, to close out the commutation table, one requires another vector operator $\vec{\Gamma}$ whose realization is

$$\vec{\Gamma} = r\,\vec{p} \tag{5.3}$$

since

$$[L_i, \Lambda_1] = [L_i, \Lambda_3] = 0 \tag{5.4}$$

$$[A_i, \Lambda_1] = \Gamma_i \qquad [A_i, \Lambda_3] = 0 \tag{5.5}$$

$$[M_i, \Lambda_1] = 0 \qquad [M_i, \Lambda_3] = \Gamma_i \tag{5.6}$$

where i=1,2,3. Thus one finally obtains the Lie algebra so(4,2) and its realization defined by the 15 generators $\vec{L}$, $\vec{A}$, $\vec{M}$, $\vec{\Gamma}$, Λ_1 , Λ_2 and Λ_3.

Using either so(4,1) or so(4,2) one can find infinite dimensional unitary irreducible representations. The so(4,2) is more suitable for purposes related to perturbations since it includes Λ_1 and Λ_3 which provide the simple expressions such as $r = \Lambda_3 - \Lambda_1$.

The defining commutation relations of so(4,2) may be expressed in a compact form. Let X_{ab} be an antisymmetric set of operators, i.e.

$$X_{ab} = -X_{ba} \qquad ; \qquad a, b = 1, 2, ...6 \tag{5.7}$$

such that

$$X_{12} = L_3 \quad , \quad X_{23} = L_1 \quad , \quad X_{31} = L_2 \tag{5.8}$$

$$X_{i4} = A_i \quad , \quad X_{i5} = M_i \quad , \quad X_{i6} = \Gamma_i \qquad where \quad i = 1, 2, 3 \tag{5.9}$$

$$X_{45} = \Lambda_2 \quad X_{46} = \Lambda_1 \quad X_{56} = \Lambda_3 \tag{5.10}$$

Then the defining commutation relations of so(4,2) can be expressed as

$$[X_{ab}, X_{cd}] = i\,(g_{ac}X_{bd} + g_{bd}X_{ac} - g_{bc}X_{ad} - g_{ad}X_{bc}] \tag{5.11}$$

Table 5.1. Subgroups of $SO(4,2)$

$SO(2)\times SO(4)$	(Λ_3) $(\vec{L},\, \vec{A})$
$SO(4,1)$	$\vec{L}$ $\vec{A}$ $\vec{M}$ Λ_2
$SO(4,1)^*$	$\vec{L}$ $\vec{A}$ $\vec{\Gamma}$ Λ_1
$SO(3,2)$	$\vec{L}$ $\vec{M}$ $\vec{\Gamma}$ Λ_3
$SO(3,1)$	$\vec{L}$ $\vec{\Gamma}$
$SO(3,1)^*$	$\vec{L}$ $\vec{M}$
$SO(4)$	$\vec{L}$ $\vec{A}$
$SO(2,1)\times SO(3)$	$(\Lambda_1,\, \Lambda_2,\, \Lambda_3)$ $(\vec{L})$
$SO(2,1)^*\times SO(2,1)^{**}$	$(N^1_\pm, N^1_3)$ $(N^2_\pm, N^2_3)$

where g_{ab} is associated with the diagonal metric (–,–,–,–,+,+). The noncompact group SO(4,2) has three simultaneously diagonalizable operators and therefore three Casimir operators. The first two Casimir operators may be expressed as

$$C_1 = L^2 + A^2 - M^2 - \Gamma^2 + \Lambda_3^2 - \Lambda_1^2 - \Lambda_2^2 \tag{5.12}$$

and

$$C_2 = -\Lambda_1(\vec{M}\cdot\vec{L}) + \Lambda_2(\vec{\Gamma}\cdot\vec{L}) + \Lambda_3(\vec{A}\cdot\vec{L}) + \vec{A}\cdot(\vec{M}\times\vec{\Gamma}) \tag{5.13}$$

whereas C_3 has an even more complicated expression. It turns out that

$$C_1 = -3 \quad C_2 = 0 \quad and \quad C_3 = 0 \tag{5.14}$$

The subgroups of SO(4,2) are summarized in Table 5.1. The elements of the product group $SO(2,1)^*\times SO(2,1)^{**}$ that are denoted by N are given by

$$N^1_1 = \frac{1}{2}(\Lambda_1 + M_3) \qquad N^1_2 = \frac{1}{2}(\Lambda_2 - \Gamma_3) \qquad N^1_3 = \frac{1}{2}(\Lambda_3 + A_3) \tag{5.15}$$

and

$$N_1^2 = \frac{1}{2}(\Lambda_1 - M_3) \qquad N_2^2 = \frac{1}{2}(\Lambda_2 + \Gamma_3) \qquad N_3^2 = \frac{1}{2}(\Lambda_3 - A_3) \tag{5.16}$$

whereas the ladder operators are

$$N_\pm^1 = N_1^1 \pm iN_2^1 \qquad \textit{and} \qquad N_\pm^2 = N_1^2 \pm iN_1^2 \tag{5.17}$$

as usual. These operators have significance in the analysis of parabolic states $\mid n_1, n_2, m\,\rangle$ which provide a natural basis for the treatment of the Stark effect. The operators N_3^1, N_3^2 and L_3 are diagonalized in the parabolic states whereas the operators $N_\pm^1$ are the ladder operators for n_1 and $N_\pm^2$ are ladder operators for n_2.[2]

6. Generalized Forms

In quantum mechanics one should obtain different realizations of generators for different problems. For this, one approach is forming ad hoc realizations for each problem. Another approach, which will be employed here, is first obtaining a more general form and then studying the special cases to obtain different realizations. One should first transform the building blocks so that it is easy to check the fundamental commutation relations. The building blocks for most of the quantum mechanical operators are $\vec{r}$, $\vec{p}$ and the scalars $r^2 = \vec{r}\cdot\vec{r}$, $p^2 = \vec{p}\cdot\vec{p}$, $K = \frac{1}{r}(\vec{r}\cdot\vec{p} - i)$.

Starting with the point transformation

$$\vec{r} \to G(r)\,\hat{r} \tag{6.1}$$

one may look for the new forms for $\vec{p}$ and K, keeping the commutation relations $[r_i, p_j] = i\delta_{ij}$ and $[r, K] = i$ invariant. Then $\vec{p}$ becomes

$$\vec{p} \to \frac{r}{G}\,\vec{p} + \left(\frac{1}{G'} - \frac{r}{G}\right)\hat{r}\,K + h(r)\,\hat{r} \tag{6.2}$$

where h(r) is arbitrary since it does not affect the commutator $[r_i, p_j] = i\delta_{ij}$. If h(r) is chosen to be $\frac{i}{2}\frac{G''}{G'^2}$ then the generalized $\vec{p}$ becomes Hermitian. But then the generalized p^2 involves a K term :

$$p^2 \to \frac{1}{G'^2}K^2 + 2i\frac{G''}{G'^3}K + \frac{L^2}{G^2} + \frac{1}{2}\frac{G'''}{G'^3} - \frac{5}{4}\frac{G''^2}{G'^4} \tag{6.3}$$

To avoid K term in the generalized p^2 thereby sacrificing Hermitian property in favor of calculational simplicity, one sees that h(r) should be $-\frac{i}{2}\frac{G''}{G'^2}$. Moreover the two forms are just similarity transformations of each other:

$$G'\left[\frac{r}{G}\vec{p} + \left(\frac{1}{G'} - \frac{r}{G}\right)\hat{r}\,K - \frac{i\,G''}{2\,G'^2}\,\hat{r}\right]\frac{1}{G'} = \left[\frac{r}{G}\vec{p} + \left(\frac{1}{G'} - \frac{r}{G}\right)\hat{r}\,K + \frac{i\,G''}{2\,G'^2}\,\hat{r}\right] \tag{6.4}$$

that is

$$G' \, (\, \vec{p}_{simple} \,) \, \frac{1}{G'} \; = \; \vec{p}_{Hermitian} \tag{6.5}$$

For $\vec{p}_{simple}$, p^2 becomes

$$p^2 \to \frac{1}{G'^2} K^2 + \frac{L^2}{G^2} - \frac{1}{2} \frac{G'''}{G'^3} + \frac{3}{4} \frac{G''^2}{G'^4} \tag{6.6}$$

Next step is determining the generalization of K, that holds $[r, K] = i$ invariant. K may be shown to be

$$K \to \frac{1}{G'} K + h(r) \tag{6.7}$$

where again the choice $h(r) = -\frac{i}{2} \frac{G''}{G'^2}$ is made for calculational simplicity. Then

$$K^2 \to \frac{1}{G'^2} K^2 - \frac{1}{2} \frac{G'''}{G'^3} + \frac{3}{4} \frac{G''^2}{G'^4} \tag{6.8}$$

Each form may equivalently be written as

$$K_{Hermitian} \to \frac{1}{\sqrt{G'}} \, K \, \frac{1}{\sqrt{G'}} \tag{6.9}$$

$$K_{simple} \to \frac{1}{G'^{3/2}} \, K \, \sqrt{G'} \tag{6.10}$$

so that one encounters the same similarity transformation

$$K_s \; = \; \frac{1}{G'} \, K_H \, G' \qquad and \qquad K_H \; = \; G' \, K_s \, \frac{1}{G'} \tag{6.11}$$

That is, if one transforms $\vec{p}$, then K is automatically transformed.

Let us look for other operators that stay invariant under this transformation. Invariant operators are very useful in the generalization of complicated operators such as $\vec{A}, \vec{M}$ and $\vec{Y}$. Expressing them in terms of the invariant operators decreases the number of operations. The most trivial invariant vector is

$$\hat{r} \to \hat{r} \tag{6.12}$$

Secondly, angular momentum operator is invariant under this transformation

$$L_i = \epsilon_{ijk}\, r_j\, p_k \to \epsilon_{ijk} \left(G\, \frac{r_j}{r} \right) \left(\frac{r}{G}\, p_k + (\frac{1}{G'} - \frac{r}{G})\, \frac{r_k}{r}\, K + \frac{i}{2}\, \frac{G''}{G'^2}\, \frac{r_k}{r} \right) \tag{6.13}$$

which reduces back to $\epsilon_{ijk}\, r_j\, p_k$.

Finally, $\vec{\mu} \equiv \vec{r}K - r\vec{p}$ is also invariant

$$\vec{\mu} = \vec{r}K - r\vec{p} \to (G\,\hat{r}) \left(\frac{1}{G'}\, K + \frac{i}{2}\, \frac{G''}{G'^2} \right) - G \left(\frac{r}{G}\, \vec{p} + \left(\frac{1}{G'} - \frac{r}{G} \right) \frac{\vec{r}}{r}\, K + \frac{i}{2}\, \frac{G''}{G'^2}\, \frac{\vec{r}}{r} \right) \tag{6.14}$$

which reduces back to the original form $\vec{r}K - r\vec{p}$.

Having constructed the building blocks, one is now ready to generalize the so(4,2) generators. The generalized forms of so(2,1) subalgebra $\{\Lambda_1, \Lambda_2, \Lambda_3\}$ become

$$\Lambda_1 = \frac{G}{2G'^2} K^2 + \frac{L^2}{2G} - \frac{GG'''}{4G'^3} + \frac{3GG''^2}{8G'^4} - \frac{G}{2} \tag{6.15}$$

$$\Lambda_2 = \frac{G}{G'} K - \frac{i}{2} \frac{GG''}{G'^2} \tag{6.16}$$

$$\Lambda_3 = \frac{G}{2G'^2} K^2 + \frac{L^2}{2G} - \frac{GG'''}{4G'^3} + \frac{3GG''^2}{8G'^4} + \frac{G}{2} \tag{6.17}$$

In section 2.2, the expectation value $\langle K\rangle$ was generalized to $\langle\sqrt{r}\,K\sqrt{r}\rangle$ in obtaining the realization of so(2,1) generators. If instead, it was generalized to $\langle\sqrt{G(r)}\,K\sqrt{G(r)}\rangle$ then the above form may have been directly obtained. In Table (6.1) $G(r)$ for a number of problems is listed. [3],[4],[5]

Table 6.1. G(r) for Various Problems

$G\rightarrow r$	Hydrogen Atom
$G\rightarrow r^2$	3-D Simple Harmonic Oscillator
$G\rightarrow e^{\alpha r}$	$l=0$ Morse potential problem

Before generalizing the remaining generators which are vectors, one should first express them in $\{\hat{r},\vec{L},\vec{\mu}\}$ notation for convenience:

$$\vec{\Gamma}=r\vec{p}=rK\hat{r}-\vec{\mu} \tag{6.18}$$

$$\vec{A}=\frac{\vec{r}p^2}{2}-rK\vec{p}-\frac{\vec{r}}{2}=\left(-\frac{rK^2}{2}+\frac{L^2}{2r}-\frac{r}{2}\right)\hat{r}+K\vec{\mu} \tag{6.19}$$

$$\vec{M}=\frac{\vec{r}p^2}{2}-rK\vec{p}+\frac{\vec{r}}{2}=\left(-\frac{rK^2}{2}+\frac{L^2}{2r}+\frac{r}{2}\right)\hat{r}+K\vec{\mu} \tag{6.20}$$

and finally the LRL vector become

$$\vec{Y}=\vec{r}p^2-rK\vec{p}-\alpha\hat{r}=\left(\frac{L^2}{r}-\alpha\right)\hat{r}+\left(K-\frac{i}{r}\right)\vec{\mu} \tag{6.21}$$

Now the remaining operators may easily be generalized

$$\vec{\Gamma}\rightarrow\left(\frac{G}{G'}K-\frac{iGG''}{2G'^2}\right)\hat{r}-\vec{\mu} \tag{6.22}$$

$$\vec{A} \to \left(-\frac{G}{2G'^2}K^2 + \frac{GG'''}{4G'^3} - \frac{3GG''^2}{8G'^4} + \frac{L^2}{2G} - \frac{G}{2}\right)\hat{r} + \left(\frac{1}{G'}K - \frac{iG''}{2G'^2}\right)\vec{\mu} \tag{6.23}$$

$$\vec{M} \to \left(-\frac{G}{2G'^2}K^2 + \frac{GG'''}{4G'^3} - \frac{3GG''^2}{8G'^4} + \frac{L^2}{2G} + \frac{G}{2}\right)\hat{r} + \left(\frac{1}{G'}K - \frac{iG''}{2G'^2}\right)\vec{\mu} \tag{6.24}$$

$$\vec{Y} \to \left(\frac{L^2}{G} - \alpha\right)\hat{r} + \left(\frac{1}{G'}K - \frac{iG''}{2G'^2} - \frac{i}{G}\right)\vec{\mu} \tag{6.25}$$

And finally the Hamiltonian is generalized to

$$H \to \frac{1}{2G'}K^2 - \frac{G'''}{4G'^3} + \frac{3G''^2}{8G'^4} + \frac{L^2}{2G^2} - \frac{\alpha}{G} \tag{6.26}$$

7. Perturbations

Having obtained the generalized forms of the generators, one is now ready for perturbations. The most natural way of perturbing the generators is perturbing the function G. Introducing the perturbation $g(r)$

$$G(r) \to G(r) + g(r) \tag{7.1}$$

one obtain the following variations for the generators

$$\delta\vec{L} = 0 \tag{7.2}$$

$$\delta\vec{\Gamma} = g\left[\left(\frac{1}{G'}K - \frac{iG''}{2G'^2}\right)\hat{r}\right] + g'\left[\left(-\frac{G}{G'^2}K + \frac{iGG''}{G'^3}\right)\hat{r}\right] + g''\left[\left(-\frac{iG}{2G'^2}\right)\hat{r}\right] \tag{7.3}$$

$$\begin{aligned} \delta\vec{A} &= g\left[\left(-\tfrac{1}{2G'^2}K^2 + \tfrac{G'''}{4G'^3} - \tfrac{3G''^2}{8G'^4} - \tfrac{L^2}{2G^2} - \tfrac{1}{2}\right)\hat{r}\right] \\ &+g'\left[\left(\tfrac{G}{G'^3}K^2 - \tfrac{3GG'''}{4G'^4} + \tfrac{3GG''}{2G'^5}\right)\hat{r} + \left(-\tfrac{1}{G'^2}K + \tfrac{iG''}{G'^3}\right)\vec{\mu}\right] \\ &+g''\left[\left(-\tfrac{3GG''}{4G'^4}\right)\hat{r} + \left(-\tfrac{i}{2G'^2}\right)\vec{\mu}\right] + g'''\left[\left(\tfrac{G}{4G'^3}\right)\hat{r}\right] \end{aligned} \tag{7.4}$$

$$\begin{aligned} \delta\vec{M} &= g\left[\left(-\tfrac{1}{2G'^2}K^2 + \tfrac{G'''}{4G'^3} - \tfrac{3G''^2}{8G'^4} - \tfrac{L^2}{2G^2} + \tfrac{1}{2}\right)\hat{r}\right] \\ &+g'\left[\left(\tfrac{G}{G'^3}K^2 - \tfrac{3GG'''}{4G'^4} + \tfrac{3GG''}{2G'^5}\right)\hat{r} + \left(-\tfrac{1}{G'^2}K + \tfrac{iG''}{G'^3}\right)\vec{\mu}\right] \\ &+g''\left[\left(-\tfrac{3GG''}{4G'^4}\right)\hat{r} + \left(-\tfrac{i}{2G'^2}\right)\vec{\mu}\right] + g'''\left[\left(\tfrac{G}{4G'^3}\right)\hat{r}\right] \end{aligned} \tag{7.5}$$

$$\delta\Lambda_1 = g\left[\tfrac{1}{2G'^2}K^2 - \tfrac{L^2}{2G^2} - \tfrac{G'''}{4G'^3} + \tfrac{3G''^2}{8G'^4} - \tfrac{1}{2}\right]$$
$$+g'\left[-\tfrac{G}{G'^3}K^2 + \tfrac{3GG'''}{4G'^4} - \tfrac{3GG''^2}{2G'^5}\right] + g''\left[\tfrac{3GG''}{4G'^4}\right] + g'''\left[-\tfrac{G}{4G'^3}\right] \tag{7.6}$$

$$\delta\Lambda_2 = g\left[\frac{1}{G'}K - \frac{iG''}{2G'^2}\right] + g'\left[-\frac{G}{G'^2}K + \frac{iGG''}{G'^3}\right] + g''\left[-\frac{iG}{2G'^2}\right] \tag{7.7}$$

$$\delta\Lambda_3 = g\left[\tfrac{1}{2G'^2}K^2 - \tfrac{L^2}{2G^2} - \tfrac{G'''}{4G'^3} + \tfrac{3G''^2}{8G'^4} + \tfrac{1}{2}\right]$$
$$+g'\left[-\tfrac{G}{G'^3}K^2 + \tfrac{3GG'''}{4G'^4} - \tfrac{3GG''^2}{2G'^5}\right] + g''\left[\tfrac{3GG''}{4G'^4}\right] + g'''\left[-\tfrac{G}{4G'^3}\right] \tag{7.8}$$

and finally

$$\delta\vec{Y} = g\left[\left(-\frac{L^2}{G^2}\right)\hat{r} + \left(\frac{i}{G^2}\right)\vec{\mu}\right] + g'\left[\left(-\frac{1}{G'^2}K + \frac{iG''}{G'^3}\right)\vec{\mu}\right] + g''\left[-\frac{G}{4G'^3}\right] \tag{7.9}$$

8. CONCLUSIONS

In this thesis the usefulness of Lie groups in the analysis of quantum mechanical systems is demonstrated.

The physics of bound states led to the use of the Lie algebra so(2,1) as a SGA. H-atom Hamiltonian is written in terms of these generators. After a scaling transformation and a few algebraic manipulations the correct enegy spectrum is obtained. Without direct referrence to the explicit form of the Hamiltonian but using its symmetry properties, the degeneracy group SO(4) which together with SO(2,1) explains the general structure of the framework of states is obtained. The Lie algebra so(4,2) that contains both so(4) and so(2,1) as subalgebras, is formed which has a single irreducible representation covering hydrogenic states. It is shown that all the states are connected to each other by the application of the ladder operators of the algebra. The generators of so(4,2) are generalized by a simple point transformation for the analysis of further problems. And finally perturbations of these generators are expressed in a simple form.

APPENDIX A:

A.1. Invariant Form of a DE

The most general second order, homogeneous DE

$$F_2(x)\frac{d^2y}{dx^2} + F_1(x)\frac{dy}{dx} + F_0(x)y = 0 \tag{A.1}$$

in the standard form, i.e. $F_2(x) = 1$ may be represented alternatively as

$$[1, F_1, F_0]y = 0 \tag{A.2}$$

By transforming the dependent variable as

$$y(x) = \phi(x)\psi(x) \tag{A.3}$$

the DE is put into invariant form

$$[1, 0, I]\psi = 0 \tag{A.4}$$

for $\phi(x) = exp\left(\int \frac{F_1}{2}\, dx\right)$ so that the new dependent variable ψ become

$$\psi = \left[exp\left(\int \frac{F_1}{2}\, dx\right)\right] y \tag{A.5}$$

and $I = I(x)$ is given by

$$I = F_0 - \left(\frac{F_1}{2}\right)' - \left(\frac{F_1}{2}\right)^2 \tag{A.6}$$

A.2. Scaling Transformations

Let an operator S be given such that

$$\tilde{f}(r) = Sf(r) = f(\lambda r) \qquad \lambda \geq 0 \tag{A.7}$$

and let $\lambda = e^{\beta}$ so that β can be any real number. Corresponding to these scaling transformations, the scaling transformations of operators X is defined by:

$$\tilde{X} = SXS^{-1} \tag{A.8}$$

These scaling transformations may be identified with the so(2,1) generator Λ_2. Expanding $f(e^{\beta}r)$ in a Taylor series in β about $\beta = 0$ and using $\frac{d}{d\beta} = r\frac{d}{dr}$, it can be shown that

$$e^{\beta r \frac{d}{dr}} f(r) = f(e^{\beta} r) \tag{A.9}$$

Since $\Lambda_2 = rK = ir\frac{d}{dr}$, then (A.7) and (A.8) becomes:

$$e^{i\beta\Lambda_2} f(r) = f(e^{\beta} r) \qquad \textit{and} \qquad \tilde{X} = e^{i\beta\Lambda_2} X e^{-i\beta\Lambda_2} \tag{A.10}$$

where $\tilde{r} = e^{\beta} r$, $\tilde{K} = e^{-\beta} K$. To find the transformed operators, one may use *Baker-Hausdorff Lemma*

$$e^{-B} A e^{B} = A + [A, B] + \frac{1}{2!}[[A, B], B] + ... \tag{A.11}$$

Using the commutation relations that define so(2,1) one may show that:

$$\tilde{\Lambda}_3 = e^{i\beta\Lambda_2} \Lambda_3 e^{-i\beta\Lambda_2} = \Lambda_3 \cosh\beta - \Lambda_1 \sinh\beta \tag{A.12}$$

and

$$\tilde{\Lambda}_1 = e^{i\beta\Lambda_2}\Lambda_3 e^{-i\beta\Lambda_2} = \Lambda_1 \cosh\beta - \Lambda_3 \sinh\beta \tag{A.13}$$

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