SYMMETRY OF THE COULOMB FIELD

AND ITS APPLICATIONS

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PREFACE

In this thesis, the symmetries of the relativistic, non-relativistic and relativistic Symmetric Coulomb fields are studied. The symmetry properties are used to evaluate certain radial integrals involving multipole operators. The wavefunctions in Fock-Bargmann space and Momentum space are obtained. As an application of the Symmetric Hamiltonian to a problem of experimental interest, Stark effect was studied. The results show that for medium electric field strengths the agreement between the calculations and the experiment is good.

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CHAPTER I

INTRODUCTION

In the past few years dynamical groups and symmetries have played an increasing role in the understanding of quantum mechanical problems in atomic, nuclear and particle physics.[1] The investigation of the symmetries of simple exactly solvable quantum mechanical systems is necessary for the understanding of the appearance of these symmetries in elementary particle physics where the Hamiltonians are not too well known. Whereas the application of finite groups in molecular and solid state physics has long been known,[2] it is only in the past decade that the importance of continuous Lie groups, compact as well as non-compact, has been recognized. Apart from the three dimensional rotation group 0(3), the existence of 0(4) symmetry in the non-relativistic hydrogen atom was first pointed out by Fock[3] who studied the Schrodinger equation in momentum space. Fock and Pauli explained successfully the appearance of accidental degeneracy in terms of this bigger symmetry. The connection between this accidental degeneracy and the separability of the Schrodinger equation in two different coordinate systems, spherical and parabolic, has been shown by Bargmann to be a deep group theoretic relationship.

Jauch and Hill[4], as also Baker[5], pointed out the SU(3) symmetry of the isotropic three dimensional harmonic oscillator. They demonstrated the invariance of the non-relativistic Hamiltonian with respect to unitary unimodular transformations and later workers showed the explicit construction of the generators and the Lie algebra of the group of this Hamiltonian. Both of these simple atomic systems have the three dimensional rotation group O(3) as a subgroup which fact makes it possible to represent the respective solutions in terms of angular momentum states. These group structures were studied, however, only for understanding the bound state energy spectrum but their other applications of use in experimental physics was not recognized. Interest in these groups and symmetries was renewed[6] when the method of dynamical groups in understanding elementary particles and their interactions proved successful especially because in the latter case the interactions and the Hamiltonians are almost unknown. Furthermore a re-study of these simple atomic systems led to a deeper understanding of the group representations themselves.

On the other hand a more concrete use of these symmetries is being made. The O(4) symmetry of the coulomb field, in conjunction with the Green's function method, was exploited by Lieber[7] for the evaluation of the Bethe logarithm in Lamb shift and comparison with experiment. In nuclear structure calculations and the interpretation of the properties of excited states Elliott[8] used the SU(3) group extensively. It is a well known fact that the discovery of the Ω^- is mainly due to the Octet model of Gell Mann based on the SU(3) group. In all these cases even experimentally meaningful numerical results were obtained from group theory. It is for these reasons that a study of the group properties of the coulomb field and their applications have been taken up for study in this thesis.

The Hamiltonian introduced by Dirac to describe the relativistic motion of the electron in the hydrogen atom does not partake of the symmetry of the non-relativistic hydrogen atom. An approximate Hamiltonian was introduced by Biedenharn and Swamy[9] which removes this defect. This Symmetric Hamiltonian has even a higher symmetry than the Schrodinger Hamiltonian and the error involved in the use of this is rather small in most cases of interest. It has the added merit of simplicity in practical applications in preference to the Dirac equation. This thus opened up the possibility of the study of the symmetry of the relativistic coulomb field, and its practical applications.

In Chapter II a review of the symmetry of the non-relativistic hydrogen atom is presented especially because its non-invariance group has been fully understood only recently. The invariance and non-invariance groups of the Dirac Hamiltonian as well as the Symmetric Hamiltonian are discussed and their irreducible representations classified. The group structure of the continuum states is also discussed.

In Chapter III we discuss a special Hilbert Space introduced by Bargmann and transformations in this which make it convenient to study the group properties of simple quantum mechanical systems like the coulomb field and the harmonic oscillator. In the spirit of the Dirac quantum mechanical Transformation Theory Pauling and Podolsky calculated the solutions of the Schrodinger equation for the hydrogen atom in momentum space as early as 1928. Later Fock and Bargmann developed the connection between the solutions in momentum space and group theory. The Symmetric Hamiltonian has also been studied in momentum space in this chapter. Bargmann and Park established the group theoretic connection between the solutions of the hydrogen atom in spherical and parabolic coordinates. This is brought out even more elegantly in Fock-

Bargmann space.

In 1962 Pasternack and Sternheimer evaluated certain radial integrals of importance in connection with certain selection rules in electromagnetic transitions by direct computation. Biedenharn and others, in their coulomb excitation studies, calculated by extensive use of contour integration techniques similar radial matrix elements in the basis of continuum states. It transpires, however, that both these results can be derived elegantly by means of an operator calculus based on the symmetry of the coulomb field. A comprehensive discussion of this forms the content of Chapter IV.

A practical application of the Symmetric Hamiltonian has been made to study the relativistic Stark effect because in plasma physics the experimental Stark shifts are indirectly used for the measurement of the applied electric field and a quantum mechanical study of the relativistic Stark effect has not received much attention till now. For comparison use is also made of the exact Dirac Hamiltonian. Agreement of the theoretical calculations with experiment is discussed. This is done in Chapters V and VI.

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CHAPTER II

SYMMETRY OF THE COULOMB FIELD

In this chapter we will discuss the symmetry of the Coulomb field. The Kepler problem has been the most extensively investigated one in dynamics and it is, like the hormonic oscillator, an exactly solvable central force problem in classical as well as quantum mechanics. Both have accidental degeneracies, that is, they are more degenerate than implied by their obvious geometrical invariance under the three dimensional rotation group SO(3).

In Section I we will discuss the symmetry of the non-relativistic Coulomb field as described by time independent Schrodinger equation with the Coulomb potential. Here we will develop the O(4) (the four dimensional orthogonal group) symmetry of the problem, introduce Runge-Lentz-Pauli vector $\vec{A}$ and discuss the global method of Fock. Consequences of this symmetry will be reviewed.

In Section II a brief discussion of symmetry of the relativistic Kepler problem, as described by Dirac Coulomb Hamiltonian will be presented. Then we will investigate the symmetry and group structure of (approximate) relativistic Symmetric Hamiltonian introduced by Biedenharn and Swamy.

Section I

An explanation of the accidental degeneracy of the non-relativistic

Kepler problem was given as early as 1926 by Pauli[1] by pointing out the existence of a hermitian form of the classical Runge-Lentz[2] vector $\vec{A}$. Using the properties of $\vec{A}$ he was able to find the energy levels of the hydrogen atom within the frame work of Heisenberg's matrix mechanics. Later in 1935 Fock[3] showed that in momentum space one could project it steriographically on the surface of the unit sphere in a four dimensional space in such a way that the relevant integral equation becomes the eigenvalue equation for hyper spherical hormonics. We elaborate below this method which is some times referred to as the global method[4].

The non-relativistic quantum mechanical Kepler problem in coordinate space for an attractive Coulomb potential is

$$\left(-\frac{\hbar^2\nabla^2}{2m} - \frac{\alpha z\hbar c}{r}\right)\psi\,(r,\theta,\phi) = E\,\psi(r,\theta,\phi),\quad \alpha = \frac{e^2}{\hbar c} \tag{1}$$

According to Dirac's transformation theory, the three dimensional Fourier transform of the above equation gives the momentum space representation. The term $\frac{1}{r}\,\psi(\vec{r})$ gives rise to a convolution integral and we get

$$\left(\frac{P^2}{2m} - E\right)\phi(\vec{p}) = \frac{k}{2\pi^2\hbar}\int \frac{d^3p\ \psi(q)}{|q-p|^2} \tag{2}$$

Since in case of bound states E is negative and we introduce the quantity

$$P_o^2 = -2mE > 0 \tag{3}$$

and the energy dependent Fock variables

$$\xi_1 = \frac{2\, p_o\, p_x}{p_o^{\,2} + p^2} \qquad\qquad \xi_2 = \frac{2\, p_o\, p_y}{p_o^{\,2} + p^2}$$

$$= \sin\alpha \sin\theta \cos\phi \qquad\qquad = \sin\alpha \sin\theta \sin\phi$$

$$(4)$$

$$\xi_3 = \frac{2\, p_o\, p_z}{p_o^{\,2} + p^2} \qquad\qquad \xi_4 = \frac{p_o^{\,2} - p^2}{p_o^{\,2} + p^2} = \cos\alpha$$

$$= \sin\alpha \cos\phi$$

in polar form. With these coordinates $d\Omega = \sin^2\alpha\, d\alpha \sin\theta\, d\theta\, d\phi$ and

$d\vec{P} = dP_x dP_y dP_2 = P^2 dP \sin\theta\, d\theta\, d\phi = \frac{1}{8P_o^{\,3}} (P_o^{\,2} + P^2)^3\, d\Omega$ again changing the variables to

$$x_i = r\xi_i ; \left(\sum_{i=1}^{4} x_i^{\,2} = 1\right) \tag{5}$$

And using the Green's function approach Fock has shown that the appropriate integral equation is equivalent to a four dimensional Laplace equation

$$\frac{\partial^2 U_1}{\partial x_1^{\,2}} + \frac{\partial^2 U_2}{\partial x_2^{\,2}} + \frac{\partial^2 U_3}{\partial x_3^{\,2}} + \frac{\partial^2 U_4}{\partial x_4^{\,2}} = 0 \tag{6}$$

where

$$U = (\gamma^{n-1}\, \psi_n\, (\alpha,\theta,\phi))_{\gamma=1} \tag{7}$$

The hyperspherical hormonics are

$$\psi_{n\ell m}(\alpha,\theta,\phi) = \pi_\ell(n,\alpha)\, Y_{\ell m}\, (\theta,\phi) \tag{8}$$

where $\pi_\ell(n,\alpha)$ are the solutions of the differential equations

$$\frac{d^2\pi\ell}{d\alpha^2} + 2\cot\alpha\,\frac{d\pi\ell}{d\alpha} - \frac{\ell(\ell+1)}{\sin^2\alpha}\pi_\ell + (n^2-1)\,\pi_\ell = 0 \tag{9}$$

The π_ℓ functions also satisfy the ladder relations

$$-\frac{d\pi\ell}{d\alpha} + \ell\,\mathrm{ctg}\,\alpha\,\pi_\ell(n,\alpha) = \sqrt{n^2-(\ell+1)^2}\;\pi_{\ell+1}(n,\alpha). \tag{10.a}$$

$$\frac{d\pi\ell}{d\alpha} + (\ell+1)\,\mathrm{ctg}\,\alpha\,\pi_\ell(n,\alpha) = \sqrt{n^2-\ell^2}\;\pi_{\ell-1}(n,\alpha). \tag{10.b}$$

According to Malkin and Manko the invariant group signified by Eqn. (5) is 0(4)[5], whereas Equation (6) signifies that the non-invariance group is 0(4,2) non-compact group[7]. Next we briefly sketch the generators and Casimir invariants of the 0(4) group.

The 0(4) Group[8,9,10]

The generators of 0(4) group are well known[6], (L_1, L_2, L_3 and A_1, A_2, A_3). A commutes with H $\left(= -\frac{\hbar^2\nabla^2}{2m} - \frac{\alpha z\hbar c}{r}\right)$ and if we normalize $\vec{A}$ as

$$\vec{A} \rightarrow (1/\sqrt{-2m\underset{\sim}{H}})\;\vec{A} \tag{11}$$

the quantum mechanical commutation relations lead to the Lie algebra of the generators

$$[L_i, L_j] = i\hbar\, \varepsilon_{ijk}\, L_k \qquad \varepsilon_{ijk} \text{ is Levi chivitda tensor.}$$

$$[A_i, A_j] = i\hbar\, \varepsilon_{ijk}\, L_k \tag{12}$$

the six operators $\vec{L}$ and $\vec{A}$ are, therefore, the infinitesimal generators of the 0(4) group. The structure constants are simply $C^K_{ij} = i\varepsilon_{ijk}$ and form the condition for a semi-simple compact Lie group. We can use the prescription given by Carton(11) to get the invariants of the group. The two invariants are

$$A^2 + L^2 = N^2 - 1 \tag{13}$$

$$\vec{L}\cdot\vec{A} = \vec{A}\cdot\vec{L} = 0 \tag{14}$$

where N is the energy determining (principal) quantum number. The first invariant is called the Casimir invariant, because Casimir showed that $g^{\mu\nu} X_\mu X_\nu$ commutes with all X_μ, where

$$g^{\mu\nu} = \sum_{\beta\lambda} C^{\lambda}_{\mu\beta}\, C^{\beta}_{\nu\lambda}$$

and in our case $g^{\mu\nu} = \delta_{\mu\nu}$. The Equation (14) is the condition for a symmetric representation of the group.

Section II

This section deals with the symmetry of the relativistic Coulomb field. The Dirac Coulomb problem in general can be described by the time-dependent equation as

$$H\psi = (c\rho_1 \vec{\sigma}\cdot\vec{p} + \rho_3 m_o c^2 - \frac{\alpha z\hbar c}{r})\, \psi = i\hbar \frac{\partial\psi}{\partial t} \tag{15}$$

and for the stationary states by

$$H\psi = (c\rho_1\vec{\sigma}\cdot\vec{p} + \rho_3 m_o c^2 - \frac{\alpha Z\hbar c}{r})\ \psi = E\psi \tag{16}$$

where ρ and σ's are Dirac and Pauli 2 x 2 matrices[12,13]. The direct product of $\rho,\sigma_i = \alpha_i$, and of 1 and $\rho_3 = \beta$. In other words the above equation is written in ρ space. The bound state solutions of this problem are well known[14]. For example in coordinate space

$$\psi_{n\kappa\mu}(r,\theta,\varphi) = \begin{pmatrix} g_{n\kappa}(r) & \chi^{\mu}_{\kappa}(\theta,\varphi) \\ -if_{n\kappa}(r) & \chi^{\mu}_{-\kappa}(\theta,\varphi) \end{pmatrix} \tag{17}$$

where

$$\chi^{\mu}_{\kappa} = \sum_{\tau} C^{\,l(\kappa)\ \frac{1}{2}\ j(\kappa)}_{\mu-\tau,\ \tau,\ \mu}\ Y^{\mu-\tau}_{l}(\theta,\varphi)\ \chi^{\tau}_{1/2}$$

are the basis functions of the irreducible representations of the spin-orbit group SU(2) X 0(3) and

$$g_{n\kappa}(r) = -\sqrt{\frac{\Gamma(2\gamma_\kappa+n'+1)\,(1+\epsilon)}{n'!\,4N(N-\kappa)\{\Gamma(2\gamma_\kappa+1)\}^2}}\left(\frac{2Z}{Na_o}\right)^{3/2} e^{-\frac{Zr}{Na_o}}$$

$$\left(\frac{2Zr}{Na_o}\right)^{\gamma_\kappa-1}\left[-n'\,{}_1F_1\left({-n'+1 \atop 2\gamma_\kappa+1,}\ \frac{2Zr}{Na_o}\right) + (N-\kappa)\,{}_1F_1\left({-n' \atop 2\gamma_\kappa+1,}\ \frac{2Zr}{Na_o}\right)\right]$$

$$f_{n\kappa}(r) = -\frac{1}{\Gamma(2\gamma_\kappa+1)}\sqrt{\frac{\Gamma(2\gamma_\kappa+n'+1)\,(1-\epsilon)}{n'!\,4N(N-\kappa)}}\left(\frac{2Z}{Na_o}\right)^{3/2} e^{-\frac{Zr}{Na_o}} \tag{18}$$

(19)

$$\left(\frac{2Zr}{Na_o}\right)^{\gamma_\kappa-1}\left[n'\,{}_1F_1\left({-n'+1 \atop 2\gamma_\kappa+1,}\ \frac{2Zr}{Na_o}\right) + (N-\kappa)\,{}_1F_1\left({-n' \atop 2\gamma_\kappa+1,}\ \frac{2Zr}{Na_o}\right)\right]$$

The quantum numbers N, κ and μ take the following values

$$N = 1, 2, 3, -----,$$

$$\kappa = -N, -N+1, ---- -1, +1, ----, N-1,$$

$$\mu = -|\kappa| + \tfrac{1}{2}, -|\kappa| + 3/2, ---- |\kappa| + \tfrac{1}{2}.$$

Since Dirac equation is invariant under Lorentz transformation, we would expect that these solutions must form basis functions for some irreducible representations of the Lorentz group. Lorentz group can again be classified as homogeneous Lorentz group and inhomogeneous Lorentz group. A most general transformation in a Minkowsky 4 space is called proper orthochronous inhomogeneous Lorentz group of which homogeneous Lorentz group is a subgroup[15]. Here we will develop some of the basic material to show that $\psi_{n\kappa\mu}(\vec{r})$'s actually form the basis functions for the irreducible representation $\nu_{\frac{1}{2},\sigma}$ of the proper orthochronous inhomogeneous Lorentz group, which is also called as Poincare group P(3,1)[16]. This is, of course, an external symmetry of the Coulomb problem. Since Poincare group is neither a semisimple (because it has an invariant subgroup) nor a simple group[17,18,19], we will first construct the irreducible representations of a related simple noncompact group, and through contraction get the irreducible representations of P(3,1) group. The simple noncompact group under reference here is the De Sitter group 0(4,1).

The gist as stated by Inonu and Wigner is the following: From a physical point of view we are primarily interested in the relations between the unitary irreducible representations of two groups which are related to each other through a contraction. One way (the one which we will follow) of obtaining representations of the group obtained by contraction, from the representations of the contracted group, is to consider, together with the process of contraction, the limit of special sets of representations.

The De Sitter Group and its Unitary Representations

The group of real homogeneous linear transformation of w, x, y, z, and t that leaves

$$-t^2 + \omega^2 + x^2 + y^2 + z^2 = \text{invariant}$$

is the De Sitter group O(4,1). The Lie algebra of O(4,1) has ten basis elements which may be chosen as $\vec{M} = (M_1, M_2, M_3)$ $\vec{N} = (N_1, N_2, N_3)$ $\vec{P} = (P_1, P_2, P_3)$ and P_o. These satisfy the commutation relations

$$\begin{aligned}
[M_k, M_\ell] &= i\, \varepsilon_{k\ell m}\, M_m \\
[N_k, N_\ell] &= -i\, \varepsilon_{k\ell m}\, N_m \\
[P_k, P_\ell] &= i\, \varepsilon_{k\ell m}\, M_m \\
[M_k, N_\ell] &= [N_k, M_\ell] = i\, \varepsilon_{k\ell m}\, N_m \\
[M_k, P_\ell] &= [P_k, M_\ell] = i\, \varepsilon_{k\ell m}\, P_m \\
[P_o, N_k] &= i\, P_k \;;\; [P_o, P_k] = i\, N_k \\
[P_k, N_\ell] &= i\, \delta_{k\ell}\, P_o
\end{aligned} \tag{20}$$

All the generators are assumed to be hermitian. Here we can distinctly recognize two sub-algebras. If we just choose $\vec{M}$ and $\vec{P}$, then we have

$$[M_k, M_\ell] = i\, \varepsilon_{k\ell m}\, M_m = [P_k, P_\ell]$$

$$[M_k, P_\ell] = [P_k, M_\ell] = i\, \varepsilon_{k\ell m}\, P_m$$

We readily see that this is the Lie algebra of a four dimensional orthogonal semi-simple compact Lie group 0(4), whereas $\vec{M}$ and $\vec{N}$ form a subalgebra, the Lie algebra of homogeneous Lorentz group $L(3,1) \simeq 0(3,1)$. It is well known that representation spaces $H_{jj'}$ of 0(4) are $(2j + 1)(2j' + 1)$ dimensional and one can construct the unitary representation space of 0(4,1) by the direct sum of all representation spaces $H_{jj'}$ [20].

$$H = \sum_{jj'} \oplus H_{jj'} \tag{21}$$

In $H_{jj'}$ one can choose a basis $|j,\mu,j',\mu'\rangle$ where $(\vec{M} + \vec{P})^2$, $(\vec{M} - \vec{P})^2$, $(M_3 + P_3)$ and $(M_3 - P_3)$ are diagonal. The matrix elements of various operators are given by Dixmier[21] and are reviewed by Strom[22].

0(4,1) has two independent invariants, which are

$$G = P_o^{\,2} - P^2 - (M^2 - N^2) \tag{22}$$

$$F = (\vec{M}\cdot\vec{P}) - (P_o\vec{M} - \vec{P}x\vec{N})^2 - (\vec{M}\cdot\vec{N})^2 \tag{23}$$

The eigenvalues of these two operators can be used to lable the irreducible representations of the De Sitter group. There are two distinct classes of unitary representations of 0(4,1). They are continuous and discrete classes.

The Continuous Class

Let $\nu_{r\sigma}$ designate an irreducible representation, where r and σ are connected to the eigenvalues of the invariant operator. The three subclasses are

(1) The irreducible representation $\Upsilon_{r\sigma}$ with r = 1,2,3, ... and

$\sigma > 0$ where $r = \min(j + j')$.

(2) The irreducible representation with $r = 1/2, 3/2, \ldots., \sigma > \frac{1}{4}$.

(3) For $r = 0$, with $\sigma > -2$ the representation $\nu_{o\sigma}$.

To see how these come about we need the complete matrix elements of all the generators. Rather than writing the matrix elements, we have more explicitly

$$\frac{1}{2}(M_3 - P_3)|j\mu j'\mu'\rangle = \mu|j\mu j'\mu'\rangle$$
$$\frac{1}{2}(M_3 + P_3)|j\mu j'\mu'\rangle = \mu'|j\mu j'\mu'\rangle$$
$$\frac{1}{2}(M_\pm - P_\pm)|j\mu j'\mu'\rangle = \sqrt{(j\mp\mu)(j\pm\mu+1)}\,|j\,\mu\pm1,j'\mu'\rangle$$
$$\frac{1}{2}(M_\pm + P_\pm)|j\mu j'\mu'\rangle = \sqrt{(j'\mp\mu')(j'\pm\mu'+1)}\,|j\mu j'\mu'\pm1\rangle$$

where

$$M_\pm = (M_1 \pm iM_2);\ N_\pm = (N_1 \pm iN_2),\ P_\pm = (P_1 \pm iP_2) \tag{24}$$

Those given above have the step up and step down operator structure similar to SU(2), on the other hand N_+, N_-, N_3 and P_o give a complicated mixture of bases.

$$\begin{aligned} N_+|j\mu j'\mu'\rangle = i\Big\{&\sqrt{(j+\mu+1)(j'+\mu'+1)}\,A_{jj'}|j+\tfrac{1}{2},\mu+\tfrac{1}{2},j'+\tfrac{1}{2},\mu'+\tfrac{1}{2}\rangle \\ &+\sqrt{(j-\mu)(j'+\mu'+1)}\,B_{jj'}|j-\tfrac{1}{2},\mu+\tfrac{1}{2},j'+\tfrac{1}{2},\mu'+\tfrac{1}{2}\rangle \\ &+\sqrt{(j+\mu+1)(j'-\mu')}\,C_{jj'}|j+\tfrac{1}{2},\mu+\tfrac{1}{2},j'-\tfrac{1}{2},\mu'+\tfrac{1}{2}\rangle \\ &+\sqrt{(j-\mu)(j'-\mu')}\,D_{jj'}|j-\tfrac{1}{2},\mu+\tfrac{1}{2},j'-\tfrac{1}{2},\mu'+\tfrac{1}{2}\rangle\Big\} \end{aligned} \tag{25}$$

$$
\begin{aligned}
& N_- \, | j \mu j' \mu' \rangle \\
&= i \Big\{ -\sqrt{(j-\mu+1)(j'-\mu'+1)}\, A_{jj'} \\
&\qquad\qquad | j+\tfrac{1}{2}, \mu-\tfrac{1}{2}, j'+\tfrac{1}{2}, \mu'-\tfrac{1}{2} \rangle \\
&\quad + \sqrt{(j+\mu)(j'-\mu'+1)}\, B_{jj'} \\
&\qquad\qquad | j-\tfrac{1}{2}, \mu-\tfrac{1}{2}, j'+\tfrac{1}{2}, \mu'-\tfrac{1}{2} \rangle \\
&\quad + \sqrt{(j-\mu+1)(j'+\mu')}\, C_{jj'} \\
&\qquad\qquad | j+\tfrac{1}{2}, \mu-\tfrac{1}{2}, j'-\tfrac{1}{2}, \mu'-\tfrac{1}{2} \rangle \\
&\quad + \sqrt{(j+\mu)(j'+\mu')}\, D_{jj'} \\
&\qquad\qquad | j-\tfrac{1}{2}, \mu-\tfrac{1}{2}, j'-\tfrac{1}{2}, \mu'-\tfrac{1}{2} \rangle
\end{aligned}
\qquad (26)
$$

$$
\begin{aligned}
&N_3 \, | j \mu j' \mu' \rangle \\
&= \frac{i}{2} \Big\{ - A_{jj'} \Big[\sqrt{(j+\mu+1)(j'-\mu'+1)} \, | j+\tfrac{1}{2}, \mu+\tfrac{1}{2}, j'+\tfrac{1}{2}, \mu'-\tfrac{1}{2} \rangle \\
&\quad + \sqrt{(j-\mu+1)(j'+\mu'+1)} \, | j+\tfrac{1}{2}, \mu-\tfrac{1}{2}, j'+\tfrac{1}{2}, \mu'+\tfrac{1}{2} \rangle \Big] \\
&\quad + B_{jj'} \Big[- \sqrt{(j-\mu)(j'-\mu'+1)} \, | j-\tfrac{1}{2}, \mu+\tfrac{1}{2}, j'+\tfrac{1}{2}, \mu'-\tfrac{1}{2} \rangle \\
&\qquad + \sqrt{(j+\mu)(j'+\mu'+1)} \, | j-\tfrac{1}{2}, \mu-\tfrac{1}{2}, j'+\tfrac{1}{2}, \mu'+\tfrac{1}{2} \rangle \Big] \\
&\quad + C_{jj'} \Big[\sqrt{(j+\mu+1)(j'+\mu')} \, | j+\tfrac{1}{2}, \mu+\tfrac{1}{2}, j'-\tfrac{1}{2}, \mu'-\tfrac{1}{2} \rangle \\
&\qquad + \sqrt{(j-\mu+1)(j'-\mu')} \, | j+\tfrac{1}{2}, \mu-\tfrac{1}{2}, j'-\tfrac{1}{2}, \mu'+\tfrac{1}{2} \rangle \Big] \\
&\quad + D_{jj'} \Big[- \sqrt{(j-\mu)(j'-\mu')} \, | j-\tfrac{1}{2}, \mu+\tfrac{1}{2}, j'-\tfrac{1}{2}, \mu'+\tfrac{1}{2} \rangle \\
&\qquad + \sqrt{(j+\mu)(j'-\mu')} \, | j-\tfrac{1}{2}, \mu+\tfrac{1}{2}, j'-\tfrac{1}{2}, \mu'+\tfrac{1}{2} \rangle \Big]
\end{aligned}
\tag{27}
$$

and finally

$$
\begin{aligned}
&P_0 |j \mu j' \mu'\rangle \\
&= \frac{i}{2} \Big\{ A_{jj'} \Big[\sqrt{(j+\mu+1)(j'+\mu'+1)}\, |j+\tfrac{1}{2}, \mu+\tfrac{1}{2}, j'+\tfrac{1}{2}, \mu'+\tfrac{1}{2}\rangle \\
&\quad - \sqrt{(j-\mu+1)(j'+\mu'+1)}\, |j+\tfrac{1}{2}, \mu-\tfrac{1}{2}, j'+\tfrac{1}{2}, \mu'+\tfrac{1}{2}\rangle \Big] \\
&\quad + B_{jj'} \Big[\sqrt{(j-\mu)(j'-\mu+1)}\, |j-\tfrac{1}{2}, \mu+\tfrac{1}{2}, j'+\tfrac{1}{2}, \mu'-\tfrac{1}{2}\rangle \\
&\quad + \sqrt{(j+\mu)(j'+\mu'+1)}\, |j-\tfrac{1}{2}, \mu-\tfrac{1}{2}, j'+\tfrac{1}{2}, \mu'+\tfrac{1}{2}\rangle \Big] \\
&\quad + C_{jj'} \Big[\sqrt{(j+\mu+1)(j'+\mu')}\, |j+\tfrac{1}{2}, \mu+\tfrac{1}{2}, j'-\tfrac{1}{2}, \mu'-\tfrac{1}{2}\rangle \\
&\quad + \sqrt{(j-\mu+1)(j'-\mu')}\, |j+\tfrac{1}{2}, \mu-\tfrac{1}{2}, j'-\tfrac{1}{2}, \mu'-\tfrac{1}{2}\rangle \Big] \\
&\quad + D_{jj'} \Big[-\sqrt{(j-\mu)(j'-\mu')}\, |j-\tfrac{1}{2}, \mu+\tfrac{1}{2}, j'-\tfrac{1}{2}, \mu'+\tfrac{1}{2}\rangle \\
&\quad + \sqrt{(j+\mu)(j'-\mu')}\, |j-\tfrac{1}{2}, \mu-\tfrac{1}{2}, j'-\tfrac{1}{2}, \mu'+\tfrac{1}{2}\rangle \Big] \Big\}
\end{aligned}
\tag{28}
$$

The constants $A_{jj'}$, $B_{jj'}$, $C_{jj'}$, and $D_{jj'}$ are determined by commutation relations, unitarity and irreducibility conditions. They can be chosen as real and it turns out that[23]

$$D_{jj'} = A_{j-\frac{1}{2}, j'-\frac{1}{2}}, \text{ And } C_{jj'} = - B_{j+\frac{1}{2}, j'-\frac{1}{2}} \tag{29}$$

In terms of new parameters ℓ and n where $\ell = j + j' + 1$ and $n = j' - j$ we can rewrite A, B, C and D as $A_{jj'} = a_{\ell n}$, $B_{jj'} = b_{\ell n}$, $C_{jj'} = c_{\ell n}$ and $D_{jj'} = d_{\ell n}$. For continuous class that we gave above, these $a_{\ell n}$ and $b_{\ell n}$

are

$$a_{\ell n} = \sqrt{\frac{(\ell-r)(\ell+r+1)(\ell(\ell+1)+\sigma)}{(\ell-n)(\ell-n+1)(\ell+n)(\ell+n+1)}} \tag{30}$$

$$b_{\ell n} = \sqrt{\frac{(r-n)(r+n+1)(n(n+1)+\sigma)}{(\ell-n-1)(\ell-n)(\ell+n)(\ell+n+1)}} \tag{31}$$

and the values of invariants are given by for $\nu_{r\sigma}$

$$\langle G\rangle = -r(r+1) + 2 + \sigma \tag{32}$$

$$\langle F\rangle = -r(r+1)\sigma \tag{33}$$

Figure 1 gives the domain of ν.

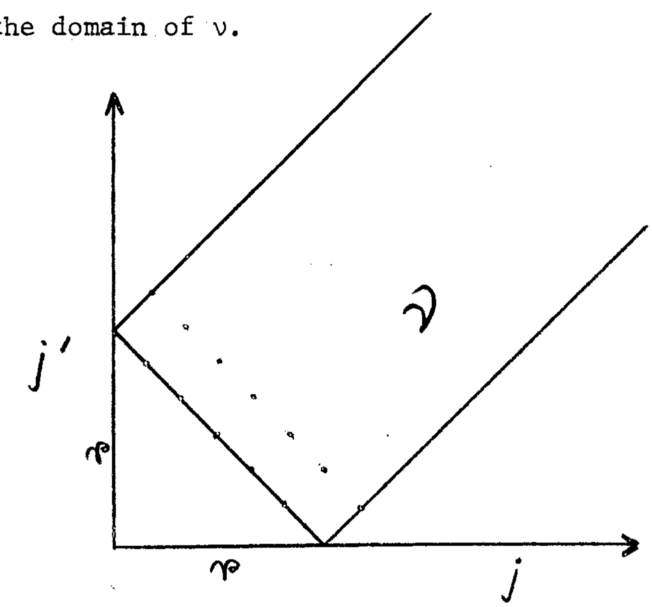

Figure 1

Now we can consider the connection between 0(4,1) and the Poincare group P(3,1). We consider the contraction by putting

$$\vec{P} = \lambda\,\vec{P} \qquad p_o = \lambda\,p_p \tag{34}$$

where now small p's are the operators. With this substitution the commutation relations become

$$[p_o,\vec{p}] = i\,\lambda^2\,\vec{N} \quad \text{And} \quad [p_k,p_\ell] = i\,\lambda^2\,M_m\,\varepsilon_{k\ell m} \tag{35}$$

whereas all other commutation relations remain the same except that we have to replace p_o for P_o and p for P in Equation (20). In the limit $\lambda \to o$, $\vec{M}$, $\vec{N}$, $\vec{p}$ and p_o have the Lie algebra

$$\begin{aligned} &[p_o,\vec{p}] = 0 = [p_k,p_\ell] = [M_k,p_o], \ [p_o,N_k] = i\,p_k \\ &[M_k,M_\ell] = i\,\varepsilon_{k\ell m}\,M_m, \ [N_k,N_\ell] = i\,\varepsilon_{k\ell m}\,N_m; [p_k,N_\ell] = i\,\delta_{k\ell}\,p_o \\ &[M_k,p_\ell] = [p_k,M_\ell] = i\,\varepsilon_{k\ell m}\,p_m \end{aligned} \tag{36}$$

This is nothing but the Lie algebra of Poincare group P(3,1) or O(3,1). The invariants are

$$G' = p_o^{\,2} - \vec{p}^{\,2} \tag{37}$$

$$F' = \vec{M}\cdot\vec{p} - (p_o\vec{M} - \vec{p} \times \vec{N})^2 \tag{38}$$

The physical meaning of these two invariants was discussed by Wigner[19] and Pauli[15]. They show that G' corresponds to the rest mass of the particle whereas F' corresponds to the spin of the particle times the rest mass.

The relation between the quantum numbers for a particle in Dirac Coulomb field N, κ, and μ, and the eigenvalues of the operators given above are worked out by Fradkin[17] and we will not repeat them here, because the dialation operator which he and (independently) Barut, introduce, is a very complicated thing and in deriving its relationships to the operators we might lose the insight and elegance that the group theoretic approach is suppose to give.

Relativistic Symmetric Hamiltonian

It was pointed out in Section 1 that even though the dynamical symmetry group of Schrodinger Coulomb Hamiltonian and Dirac Coulomb Hamiltonian is the same, their invariant symmetry groups are different and that the basis functions that span the complete Hilbert space of Schrodinger Coulomb Hamiltonian correspond to the irreducible representation $\gamma_{0\sigma}$ while that for Dirac Coulomb Hamiltonian correspond to the irreducible representation $\gamma_{\frac{1}{2}\sigma}$. It also should be noted that Dirac Coulomb problem does not belong to the invariant group O(4), to which Schrodinger problem belongs. Beidenharn and Swamy introduced an approximate relativistic Hamiltonian[24] in 1964. It was shown by Russians Mulkin and Manko[25] and Fradkin and Kiefer[17] in 1967 that this Hamiltonian has an advantage over both Dirac and Schrodinger representations in the sense the wavefunctions of this Symmetric Hamiltonian form the bases functions of irreducible representation $\gamma_{\frac{1}{2}\sigma}$ but unlike Dirac, its invariant subgroup is still the compact semi-simple Lie group O(4). This added advantage should clarify many of the symmetry effects and separate distinctly in to relativistic effects and spin effects. This point will be elaborated through out this thesis, whenever need arises. Following is a brief review of relativistic Symmetric Hamiltonian.

The Symmetric Hamiltonian approximates Dirac Hamiltonian with Coulomb with an error of the order of $(\alpha Z)^2/\chi$, where α is Sommerfeld fine structure constant and κ is Dirac angular momentum quantum number.

The behaviour of an electron in an attractive Coulomb field is described by the Hamiltonian

$$H_D = \rho_1 \vec{\sigma}\cdot\vec{p} + \rho_3 m_o - \frac{\alpha Z}{r} \qquad \hbar = c = 1 \tag{39}$$

where ρ and σ's are Dirac and Pauli 2 x 2 matrices with ρ_3 diagonal. Biedenharn and Swamy introduced the Symmetric Hamiltonian[24]

$$H_{SB} = \rho_1 \sigma\circ\vec{p} + \rho_3 m_o - \frac{\alpha Z}{r} + \rho_2 \frac{\vec{\sigma}\cdot\vec{r}}{r} \underset{\sim}{K} \{[1+(\frac{\alpha Z}{\underset{\sim}{K}})^2]^{\frac{1}{2}} - 1]\} \tag{40}$$

where $\underset{\sim}{\kappa} = \rho_3(\vec{\sigma}\cdot\vec{L} + 1)$ is the Dirac operator. $H_D = H_{s\beta} + H_{sf}$ where H_{fs} is responsible for the fine structure of the energy levels of hydrogen atom. The states of the discrete spectrum of the symmetric Hamiltonian are characterized by the principle quantum number N, have the energy $E = M_o |\sqrt{1 + (\frac{\alpha Z}{N})^2}$ and are $2N^2$ fold degenerate: The energy levels incidentally go over into the non-relativistic Bohr levels in the first approximation when a binomial expansion is made of the denominator. With $S_1 = \mathrm{Exp}[-\frac{1}{2}\, \rho_2\, \vec{\sigma}\cdot\hat{r} \sin h^{-1} \frac{\alpha Z}{\underset{\sim}{\kappa}}]$, the Hamiltonian $H_{s\beta}$ can be obtained as the transformation

$$H_{SB} = S_1^2\, H_p = S_1^2\, (\rho_1 \vec{\sigma}\circ\vec{p} - \rho_3 m_o) \tag{41}$$

where H_p is the Dirac plane wave equation. Let us put $\tilde{H} = S_1^2\, H_p = S_1\, H_{sym}\, S_1^{-1}$. Then we get the bound state eigenvalue problem as

$$\tilde{H}\, \psi_{n\kappa\mu} = E_N\, \psi_{N\kappa\mu} \tag{42}$$

The solutions of the Equation (42) are worked out in reference (24) and for continuous state by Chatterji[27], and more accurately by Fradkin[28]. The normalized bound state wavefunction in spherical coordinates are

$$\psi_{N\kappa\mu}(r,\theta,\phi) = \begin{pmatrix} \left\{\frac{(\zeta+1)\ \varepsilon_N}{2(2\zeta^2-1)}\right\}^{\frac{1}{2}} & F_{N\ell}\ (kr)\ \chi^{\mu}_{\kappa} \\ \left\{\frac{(\zeta-1)\ \varepsilon_N}{2(2\zeta^2-1)}\right\}^{\frac{1}{2}} & F_{N\bar{\ell}}(kr)\ i\ S_{\kappa}\ \chi^{\mu}_{-\kappa} \end{pmatrix} \tag{43}$$

These $\psi_{N\kappa\mu}$'s are normalized such that

$$(\psi_{N\kappa\mu},\ S_1^{-2}\ \psi_{N\kappa\mu}) = 1 \tag{44}$$

here

$$\varepsilon_N = \frac{E_N}{m_o} = \frac{1}{\sqrt{1+(\frac{\alpha Z}{N})^2}} \qquad G = \varepsilon_N \sqrt{1+(\frac{\alpha Z}{\kappa})^2}$$

$$F_{N\ell}(k_b r) = C_{N\ell}\ e^{-k_b r}\ (2k_b r)^{\ell}\ {}_1F_1(-N+\ell+1,\ 2\ell+2,\ 2k_b r)$$

where $k_b = \frac{Z}{Na_o}$, a_o is the first Bohr radius.

$$C_{N\ell} = \sqrt{\frac{\Gamma(N+\ell+1)}{2N\ \Gamma(N-\ell)[\Gamma(2\ell+2)]^2}}\ \left(\frac{2Z}{Na_o}\right)^{3/2} \quad \text{and} \quad \int F_{N\ell}^{\ 2}(k_b r)\ r^2 dr = 1$$

Symmetry and Invariant Properties of B.S. Hamiltonian

The total angular momentum operator $\vec{J}$ and the Dirac operator $\vec{K}$ commute with the Symmetric Hamiltonian.

$$[\vec{J},\tilde{H}] = 0 = [\vec{K},\tilde{H}] \tag{45}$$

A generalized Coulomb helicity Lippman-Johnson[29] operator in this case is given by

$$\tilde{\Lambda} = [m_o^2 - \tilde{H}^2]^{-\frac{1}{2}} \{\rho_3 \alpha Z \vec{\sigma}\cdot\hat{r} \tilde{H} - i \vec{K} \vec{\sigma}\cdot\vec{p}\} \tag{46}$$

The commutation relations are

$$[\tilde{H},\tilde{\Lambda}] = 0 = [\vec{J},\tilde{\Lambda}] = [\vec{K},\tilde{\Lambda}]_+ \tag{47}$$

and $\tilde{\Lambda}^2 + \vec{K}^2 \rightarrow \vec{N}^2$ where N^2 is the operator given by

$$\vec{N}^2 \rightarrow (\alpha Z)^2 \tilde{H}^2/(m_o^2 - \tilde{H}^2) \tag{48}$$

Hence here we have an operator which explains the degeneracy w.r.t. sign of κ, and operator $\vec{J}$ which is generalization of $\vec{L}$. The operator which corresponds to non-relativistic Runge-Lentz vector though complicated, is constructed by Swamy[24]. For q^{th} component

$$(\vec{\Omega})_q \psi_{N\kappa\mu} = \rho_1 S_1^{-2} [(\frac{\vec{\sigma}x\vec{L}}{2})_q (\frac{1+\rho_3}{2}), \tilde{H}] \psi_{N\kappa\mu} \tag{49}$$

An operator $\vec{B}$ (K in their notation) can be defined as

$$\vec{B} = \vec{B}^+ + \vec{B}^- + \vec{B}\,\Pi \tag{50}$$

where $(\vec{B})_q \psi_{N\kappa\mu}$ can be defined in terms of $(\Omega)_q \psi_{N\kappa\mu}$. So the Lie algebra for bound states is,

$$[J_i,J_j] = i \varepsilon_{ijk}J_k, [\vec{B}_i,\vec{B}_j] = i \varepsilon_{ijk}J_k \tag{51}$$

the invariant relations happen to be

$$2 \vec{J}\cdot\vec{B} = (\tilde{N} - \tfrac{1}{2}) \tag{52}$$

$$(\vec{J} + \vec{B})^2 = \tilde{N}^2 - 1 \tag{53}$$

Equations (51) to (53) show that the invariant group to which Symmetric Hamiltonian belongs is O(4) but Equation (52) shows that the irreducible representation now is not $\nu_{o,\sigma}$ of O(4,1) but that it is $\nu_{\frac{1}{2}\sigma}$. That is the basis functions do not belong to symmetric representation as is the case with non-relativistic Coulomb problem. This is, of course, the first order equation, but when we go to the quadrated equation then it should be O(4) x SU(2,2), because SU(2,2) is the symmetry of the Dirac 15 operators.

Continuum State Wavefunction

It has been shown by Malkin and Manko, that for the positive energy states the symmetry of the Schrodinger equation in terms of generators

$$\vec{A} = (\sqrt{E^2 - m_o^2 - \tilde{H}^2})\ \tfrac{1}{2}[(\vec{L}x\vec{p} - \vec{p}x\vec{L}) + \alpha ZE\hat{r}]$$

and $\vec{L}$ is SL(2,C). This is because of the commutation relations

$$[L_i, L_j] = i\ \varepsilon_{ijk}\ L_k \qquad [L_i, A_k] = i\ \varepsilon_{ik\ell}\ A_\ell \tag{56}$$

and most important

$$[A_i, A_j] = -i\ \varepsilon_{ijk}\ L_k \tag{57}$$

an important - sign in Equation (57) distinguishes this Lie algebra from the Lie algebra of the bound state generators (Equation 12). The above algebra belongs to SL(2,C) generators. It should be noted that this group is isomorphic to the homogeneous orthochronous Lorentz group[30].

The Casimir invariants are

$$C_1 = \sum_i (\vec{L}_i + i\vec{A}_i)^2 = -1 - \frac{\alpha^2 Z^2 E^2}{E^2 - m_o^2} \tag{58}$$

$$C_2 = \sum_i (\vec{L}_i - i\vec{A}_i)^2 = -1 - \frac{\alpha^2 Z^2 E^2}{E^2 - m_o^2} \tag{59}$$

with

$$\rho = \frac{2\alpha ZE}{\sqrt{E^2 - m_o^2}} \qquad 2\alpha Z < \rho < \infty$$

we can write C_1 and C_2 as

$$\begin{aligned} C_1 &= \left(\frac{m}{2} - 1 - \frac{i\rho}{2}\right)\left(\frac{m}{2} + 1 - \frac{i\rho}{2}\right) \\ C_2 &= \left(\frac{m}{2} - 1 + \frac{i\rho}{2}\right)\left(\frac{m}{2} + 1 + \frac{i\rho}{2}\right) \quad \text{and} \quad E > m_o \,. \end{aligned} \tag{60}$$

Since the Dirac matrices γ_i commute with the Schrodinger Hamiltonian, the full symmetry of the equation is SL(2,C) X SU(2,2) for continuum wavefunctions for $E > m_o$. Since in case of Symmetric Hamiltonian the second invariant $\vec{J}\cdot\vec{B} \neq 0$, as opposed to Schrodinger case, C_1 and C_2 here are slightly different. They are

$$C_1 = \sum_i (\vec{J}_i + i\vec{B}_i)^2 = -1 - \frac{\alpha^2 Z^2 E^2}{E^2 - m_o^2} \tag{61}$$

$$C_2 = \sum_i (\vec{J}_i - i\vec{B}_i)^2 = -2i\tilde{N} - \frac{\alpha^2 Z^2 E^2}{E^2 - m_o^2} \tag{62}$$

Using the same ρ as above we can say that the whole space of the states with energy E is decomposed in to two spaces H_+ and H_-. Here H_+ and H_- form the spaces of irreducible representations corresponding to the invariant operators

$$m_o = -1,\ \rho = i + \frac{2\alpha ZE}{\sqrt{E^2-m_o^2}} \quad \text{and} \quad m = 1,\ \rho = -i + \frac{2\alpha ZE}{\sqrt{E^2-m_o^2}} \qquad (63)$$

Thus we see that in case of Symmetric Hamiltonian in case of bound states the invariant group is O(4) and the dynamical group is O(4,1). The wavefunctions form the basis for irreducible representation. The continuum state wavefunctions, with proper choice of generators and their normalization, form irreducible representation of $SL_j(2,C)$. The dynamical group is at least as large as $SL_j(2,C) \times SU(2,2)$.

In the subsequent chapters the discussion of momentum space wavefunctions, Fock-Bargmann representation is given. The importance of generating function will be discussed.

Some important consequences of the symmetry relations are discussed in a different chapter.

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CHAPTER III

FOCK BARGMANN SPACE, MOMENTUM REPRESENTATION OF SYMMETRIC HAMILTONIAN AND COEFFICIENTS CONNECTING FREE FIELD AND STARK WAVEFUNCTIONS OF HYDROGEN ATOM

In the first section we will discuss the vectors in Fock Bargmann space, the integral kernel and its connection to the generating function of various spacial functions arising in quantum mechanics. We will distinguish between Green's functions arising in the Extended Hilbert space of ordinary quantum mechanics and the integral kernels in the Fock Bargmann space which is also a vector in Hilbert space.

In second section we will discuss momentum wavefunctions of the Symmetric Hamiltonian.

At the end of the chapter we will derive coefficients connecting free field and Stark wavefunctions of the hydrogen atom from the group theoretical points of view and compare it with recent published work. This will prove that the powerful techniques of group theory can also give quantitative results and a better understanding of the processes involved.

Section I

The states of a quantum mechanical system of n degrees of freedom are usually described by functions either in coordinate real space

(q_1---q_n) or momentum space (p_1---p_n). But the complex coordinates $\xi_k = \frac{1}{\sqrt{2}}(q_k + ip_k)$ and $\eta_k = \frac{1}{\sqrt{2}}(q_k - ip_k)$ play an important role not only in quantum field theory but also in classical mechanics.[1-2] We can easily see that

$$\xi_K = \eta_K^* \text{ and } \eta_k = \xi_k^* \, ; \, [\xi_k, \xi_l] = 0 = [\eta_k, \eta_l] \quad (1)$$

and

$$[\xi_K, \eta_L] = \delta_{KL}$$

Fock[3] was the first to realize the importance of this combination coordinate system and as early as 1928, he introduced the operator solution for commutation relation $[\xi_k, \eta_k] = 1$ as $\xi_k = \frac{\partial}{\partial \eta_K}$ in analogy with the Schrodinger operator solution $p_K = -i\frac{\partial}{\partial q_K}$ of the commutation relation $[q_k, p_k] = i$ where k refers to a cartesian index. Bargmann[2] studied the function space on which the Fock solutions are realized. We call this Hilbert space (F_n) as Fock-Bargmann space. He also discussed the connection between this Hilbert space and ordinary Hilbert space (H_n) of square integrable functions $\psi_n(q)$ or $\psi_n(p)$.

We summarize below some of the results peculiar to this Hilbert space F_n.

The complex variables Z_i and let $Z = (Z_1$---$Z_n)$ stand for a point in a coplex n dimensional space C_n. Let $Z = x + iy$ where x and y ε R_n the real n dimensional space. There exists a function $\rho_n(x,y)$ which is real and defines inner product in Fock-Bargmann Hilbert space F_n, that is

$$(f, g) = \int f(z)^* g(z) \rho_n(x,y) d^n z \quad (2)$$

The connection between two Hilbert spaces is given by

$$f(z) = \int A_n(z,q)\,\Psi(q)\,d^n q \qquad d^n q = dq_1\, dq_2 \cdots dq_n \tag{3}$$

Which is a unitary mapping of H_n on to F_n, which properly relates the operators ξ, η of H_n to Z, $\frac{\partial}{\partial Z}$ of F_n. So for any given Hamiltonian if we determine $\rho_n(x,y)$ and $A_n(z,q)$ then we have a complete knowledge of Hilbert space F_n in terms of Hilbert space H_n. The volume element $d\mu_n(Z)$ in F_n is connected to $\rho_n(x,y)$ by relation

$$d\mu_n(z) = \rho_n(x,y)\, d^n x\, d^n y \tag{4}$$

The most important feature of the Fock-Bargmann space is in the fact that the basis vectors in this space are simplest orthonormal set of vectors.

$$u_{m_1} = \frac{Z^{m_1}}{\sqrt{m_1!}} \quad \text{for one dimensional space} \tag{5}$$

If f is an entire function in the n dimensional Fock-Bargmann space then f has the form

$$f(z) = f(z_1, \cdots, z_n) = \frac{z_1^{m_1} z_2^{m_2} \cdots z_n^{m_n}}{\sqrt{m_1!\, m_2! \cdots m_n!}} = \prod_k \frac{z_k^{m_k}}{\sqrt{m_k!}} \tag{6}$$

where m_k's are integers.

Similar to closure property in the ordinary Hilbert space(4)

$$\sum_n \Psi_n(q)\, \Psi_n(q') = \delta(q - q') \tag{7}$$

here we have

$$\int A_n(z,q)\, A_n^*(\omega,q)\, d^n q = e^{z\cdot\omega^*}$$

(8)

Which is also a vector in the Fock-Bargmann space. All other details of inequality, normalization, etc., are given in Bargmann's article and we will not repeat them here, with the exception of the linear harmonic oscillator which is here discussed to illustrate Bargmann's ideas. In Section IV of this chapter we will make use of the wave functions in Fock-Bargmann space corresponding to hydrogen atom in the spherical and parabolic coordinates and show how clearly one can bring out the hidden Clebch-Gordon connection between these two types of wave functions.

Fock-Bargmann Space Wave Functions

for Harmonic Oscillator

The Hamiltonian for n identical uncoupled linear Harmonic oscillators after subtracting the zero point energy, is given by

$$\underset{\sim}{H} = \frac{1}{2} \sum_{k=1}^{n} \left(p_k^2 + q_k^2 - 1\right) = \sum_{k=1}^{n} \eta_k \xi_k \tag{9}$$

The wavefunctions in q space (coordinate space) are expressed in terms of Hermite polynomials

$$\phi_m(q_k) = \left(2^m m! \sqrt{\pi}\right)^{-1/2} e^{-q_k^2/2} H_m(q_k) \tag{10}$$

$\tilde{H} = A_n H A_n^{-1}$ is the Hamiltonian in Z space and is equal to $\sum_K Z_K \frac{\partial}{\partial Z_K}$. (11)

This latter expression is in fact part of the underlying philosophy of the Bargmann approach. So the eigenvalue equation in Z space for the uncoupled Harmonic oscillators becomes

$$\tilde{H} f(z) = E f(z) = \sum_{k=1}^{n} z_k \frac{\partial f(z_k)}{\partial z_k} \qquad (12)$$

This reduces the analysis of $\tilde{H}$ to a triviality. The eigenfunctions are

$$f_{m_1}(z_{k_1}) = \alpha_{m_1} z_1^{m} \;;\; f = \sum_{m_1 m_2 \cdots} \alpha_{m_1} \cdots \alpha_{m_n} z_1^{m_1} \cdots z_n^{m_n} \qquad (13)$$

And
$$H f(z) = \sum_{m_1 m_2 \cdots} |m| \alpha_{m_1} \cdots \alpha_{m_n} z_1^{m_1} \cdots z_n^{m_n}$$

So eigenvalue
$$= l = |m| = m_1 + m_2 + \cdots + m_n$$

Here
$$A_n(z, q) = \sum_m \psi_m^*(q) f_m(z)$$
$$= C' \exp\left\{ -\frac{1}{2} \left(\sum_{k=1}^{n} z_k^2 + q_k^2 \right) + \sqrt{2} \sum_k z_k q_k \right\} \qquad (14)$$

with $C' = 1 / \pi^{n/4}$

It can be shown by straight forward integration that

$$f(z) = \int A_n(z, q) \psi(q)\, dq \qquad (15a)$$

and
$$\psi(q) = \int A_n^*(z, q) f(z)\, dz \qquad (15b)$$

Furthermore, the appropriate volume element is

$$d\mu_n(z) = \rho_n(x_i, y_i)\, dx_i\, dy_i$$
$$= C e^{-\sum_i z_k^* \cdot z_k} dx_1 \cdots dx_n\, dy_1 \cdots dy_n$$

Then

$$f(z) = \int \sum_m \psi_m^*(q) f_m(z) \psi_n(q)\, dq$$

$$= \sum_m \int \psi_m^*(q) \psi_n(q) f_m(z)\, dq$$

$$= f_m(z) \sum_m \int \psi_m^*(q) \psi_n(q)\, dq = f_m(z)\, \delta_{mn}$$

$$= f_m(z) = \sum_{m_1 \cdots m_n} \alpha_{m_1} \cdots \alpha_{m_n} z_1^{m_1} \cdots z_n^{m_n} \tag{16}$$

Similarly

$$\psi(q) = \int \sum_m \psi_m(q) f_m^*(z) f_n(z)\, d\mu_\nu(z)$$

$$= \sum_m \psi_m(q) \int f_m^*(z) f_n(z)\, d\mu_\nu(z) \tag{17}$$

$$= \sum_m \psi_m(q)\, \delta_{mn} = \psi_m(q)$$

Also

$$\int A_n(z, q)\, A_n^*(\omega, q)\, d^n q$$

$$= \int C' C'' e^{-1/2 \sum_k \{(z_k^2 + q_k^2) + 2\sqrt{2}\, z_k q_k\}}$$

$$e^{-1/2 \sum_k \{-(\omega_k^{*2} + q_k^2) - 2\sqrt{2}\, \omega_k^* q_k\}}$$

$$dq_k$$

For $n=1$

$$= \int c' c'' e^{-\frac{1}{2}(z_k^2+q_k^2)+\sqrt{2}z_k q_k-\frac{1}{2}(\omega_k^{*2}+q_k^2)} e^{-\sqrt{2}\,\omega_k^* q_k}\, dq_k$$

$$= \frac{1}{\sqrt{\pi}}\int e^{-\left(q_k-\frac{1}{\sqrt{2}}(z_k+\omega_k^*)\right)^2} e^{z_k\cdot\omega_k^*} dq_k = e^{z_k\cdot\omega_k^*} \qquad (18)$$

The merit of the Bargmann transformation is then that because of the simplicity of the structure of the Hamiltonian in this space, study of its symmetry properties becomes easy.

Section II

While discussing the symmetry of the coulomb field in Chapter II, we have indicated the importance of momentum space representation obtained by Fock to bring out the O(4) symmetry of non-relativistic Coulomb problem. The wavefunctions obtained in this manner by Fock[5] agree with those evaluated directly using the Fourier Transform of hydrogenic wavefunctions in coordinate space by Pauling and Podolsky[6] in the spirit of Dirac's transformation theory. A transformation of Schrödinger differential equation has been made by Hylleraas[7]. The result being

$$(p^2-2mE)^2\left[\frac{\partial^2}{\partial p_x^2}+\frac{\partial^2}{\partial p_y^2}+\frac{\partial^2}{\partial p_z^2}\right]+(p^2-2mE)\left[6\left(p_x\frac{\partial}{\partial p_x}+p_y\frac{\partial}{\partial p_y}+p_z\frac{\partial}{\partial p_z}\right)+12\right]+2m\left(E+4R_h\right)=0 \qquad (19)$$

The complexity arises from the fact that x's & p's do not commute. The transformation of Symmetric Hamiltonian and its solutions in momentum space have been done by Swamy and Biedenharn[8].

The momentum space equation in its complexity is in sharp contrast to the integral relationship of Fock, the essential difficulty in such transformations being the fact that the Coulomb potential is prescribed in coordinate space. The attempts at transforming the relativistic Dirac-Coulomb Hamiltonian and its solutions in momentum space have not met with as much success as the non-relativistic case. While Levy[9] has shown how the Dirac Hamiltonian for arbitrary potentials can be transformed into a momentum space integral equation, the solutions[10] even for the Coulomb potential cannot be obtained in closed form. In contrast to this situation, however, it turns out that the relativistic (approximate) Symmetric Dirac-Coulomb Hamiltonian[11] can be transformed into momentum space straightforwardly and that this Hamiltonian has solutions in momentum space as simple as those in position space.

Representation of the Symmetric Hamiltonian in Momentum Space

In order to derive the momentum space Hamiltonian it is convenient to start from an inspection of the non-relativistic system. If we write the non-relativistic Schrodinger equation with the Coulomb potential as

$$\left(-\frac{1}{2m}\vec{p}^{\,2}-\frac{\alpha Z}{r}\right)|N\kappa\mu\rangle = E_{NR}\,|N\kappa\mu\rangle = \frac{m}{2}\left(\frac{\alpha Z}{N}\right)^2|N\kappa\mu\rangle \tag{20}$$

the operator 1/r can be expressed as

$$\frac{1}{r}\,|N\kappa\mu\rangle = \left(\frac{1}{2\alpha Z m}\vec{p}^{\,2}+\frac{1}{2}\,\frac{m\alpha Z}{N^2}\right)|N\kappa\mu\rangle \tag{21}$$

and this essentially defines a way of handling 1/r in momentum space. From the Dirac rule[12]

$$(\vec{\sigma}\cdot\vec{p})(\vec{\sigma}\cdot\vec{r}) = \vec{p}\cdot\vec{r} - i\,\vec{\sigma}\cdot\vec{p}\times\vec{r} \tag{22}$$

and writing $\vec{p} \times \vec{r} = -\vec{L}$ it can simply be shown that $\vec{\sigma}\cdot\vec{r}$ in momentum space is given by

$$\vec{\sigma}\cdot\vec{r} = i\,\vec{\sigma}\cdot\hat{p}\left\{\frac{\partial}{\partial p} + \frac{1-(\vec{\sigma}\cdot\vec{L}+1)}{p}\right\} \tag{23}$$

where $\hat{p} = \frac{\vec{p}}{p}$, the unit vector. Equations (24) and (22) facilitate, writing $\vec{\sigma}\cdot\hat{r} = \vec{\sigma}\cdot\vec{r}\,\frac{1}{r}$, the expression of the "Coulomb Helicity Operator" in momentum space. We thus have

$$\begin{aligned}\vec{\sigma}\cdot\vec{A}\,|N\kappa\mu\rangle &= \frac{N}{\alpha Zm}\Big\{(\alpha Zm)\,i\,\vec{\sigma}\cdot\vec{p}\left(\frac{\partial}{\partial p} + \frac{1-(\vec{\sigma}\cdot\vec{L}+1)}{p}\right)\\ &\quad\left(\frac{\vec{p}^{\,2}}{2\alpha Zm} + \frac{\alpha Zm}{2N^2}\right) + i\,\vec{\sigma}\cdot\vec{p}\,(\vec{\sigma}\cdot\vec{L}+1)\Big\}\,|N\kappa\mu\rangle \\ &= i\,S_{(\kappa)}\sqrt{N^2-\kappa^2}\,|N\kappa\mu\rangle\end{aligned} \tag{24}$$

We also have the relation

$$\vec{\sigma}\cdot\hat{p}\;\bar{\chi}_{\kappa}^{\mu}(\hat{p}) = -\bar{\chi}_{-\kappa}^{\mu}(\hat{p}) \tag{25}$$

where the bar on the spherical spinors signifies their being expressed as functions of the polar angles of the momentum vector. With the help of Equations (24) and (25) and introducing the variable

$$\varpi = \left(\frac{N}{\alpha Zm}\right)p = \tan\alpha/2 \tag{26}$$

we get the 'recursion relation' connecting two radial momentum space wavefunctions belonging to $\ell_{(\kappa)}$ and $\ell_{(-\kappa)}$

$$\left\{ \frac{1}{2}\left(\frac{\partial}{\partial \varpi} + \frac{\kappa+1}{\varpi} \right)(1+\varpi^2) - \varpi\kappa \right\} P_{Nl(\kappa)}(p)$$
$$= S_{(-\kappa)} \sqrt{N^2-\kappa^2}\; P_{Nl(-\kappa)}(p) \qquad (27)$$

which is to be compared with

$$\left[\frac{d}{dr} + \frac{1+\kappa}{r} - \frac{\alpha Z \epsilon}{\kappa} \right] F_{Nl(\kappa)}(kr) = \frac{k}{\kappa} \left| \sqrt{N^2-\kappa^2} \right| F_{Nl(-\kappa)} \qquad (28)$$

for coordinate space radial wavefunctions.[13] With the substitutions (26 & 29) the recursion relation (27) agrees with Equation (27) of Fock within a phase factor.

$$P_{Nl}(p) = \cos^{-4}\alpha/2\ \Pi_l(n\alpha) \qquad (29)$$

In order now to go to the relativistic case we need to replace the non-relativistic operator Equation (22) by

$$\frac{1}{r} \longrightarrow \frac{1}{2\alpha Z}\left(\vec{p}^{\,2} - \tilde{H}^2 + m_0^2 \right) \tilde{H}^{-1} \qquad (30)$$

where $\tilde{H}$ is now the approximate relativistic Dirac-Coulomb Hamiltonian. Now (choosing $\hbar = c = 1$ as in RKP II.)

$$\tilde{H} = S_1^2 H_p$$
$$= e^{-\rho_2 \vec{\sigma}\cdot\hat{r}\, \sinh^{-1}\frac{\alpha Z}{k}} \left(\rho_1 \vec{\sigma}\cdot\vec{p} - \rho_3 m_0 \right) \qquad (31)$$

In $\tilde{H}$ the factor H_p is already in momentum space. The operator S_1^2 can be written

$$S_1^2 = e^{-\rho_2 \vec{\sigma}\cdot\hat{r}\, \sinh^{-1}\frac{\alpha Z}{k}}$$
$$= \sqrt{1 + \left(\frac{\alpha Z}{k}\right)^2} - \frac{\alpha Z}{k}\rho_2 \vec{\sigma}\cdot\hat{r} \qquad (32)$$

---

[13] A similar recursion relation existing between continuum state functions is given in Equation 25 of RKP I.

Now introducing the operator relation in Equation (30) and with the help of Equation (22) this can be transcribed into momentum space as

$$S_1^2 = \sqrt{1+\left(\frac{\alpha Z}{\underset{\sim}{k}}\right)^2} - \frac{\alpha Z}{\underset{\sim}{k}}\rho_2\left[\vec{\sigma}\cdot\hat{p}\left(\frac{\partial}{\partial p}+\frac{1-\rho_3\underset{\sim}{k}}{p}\right)\right]\frac{1}{2\alpha Z}\left(p^2-\tilde{H}^2+m_0^2\right)\tilde{H}^{-1} \tag{33}$$

and we thus have the integral equation for the Symmetric Hamiltonian in momentum space

$$\tilde{H} = \sqrt{1+\left(\frac{\alpha Z}{\underset{\sim}{k}}\right)^2} - \frac{\alpha Z}{\underset{\sim}{k}}\rho_2\left\{\vec{\sigma}\cdot\hat{p}\left(\frac{\partial}{\partial p}+\frac{1-\rho_3\underset{\sim}{k}}{p}\right)\right\} \times \frac{1}{2\alpha Z}\left(\vec{p}^2-\tilde{H}^2+m_0^2\right)\tilde{H}^{-1}\left(\rho_1\vec{\sigma}\cdot\vec{p}-\rho_3 m_0\right) \tag{34}$$

Using the commutation relation

$$\begin{aligned}\left[\vec{\sigma}\cdot\vec{p}, S_1^2\right] &= \frac{\alpha Z}{\underset{\sim}{k}}\rho_2\left[\vec{\sigma}\cdot\vec{p}, \vec{\sigma}\cdot\hat{r}\right]_+ \\ &= -2\alpha Z\rho_1\frac{1}{r}+2\alpha Z\frac{1}{\underset{\sim}{k}}\rho_2\vec{\sigma}\cdot\hat{r}\;\vec{\sigma}\cdot\vec{p}\end{aligned} \tag{35}$$

the integral equation can be written, after some operator-algebraic manipulations, as

$$\begin{aligned}&\left(\rho_1\vec{\sigma}\cdot\vec{p}-\rho_3 m_0\right)\sqrt{1+\left(\frac{\alpha Z}{\underset{\sim}{k}}\right)^2}\,\tilde{H} \\ &= \vec{p}^2+m_0^2+\left\{\left(\rho_1\vec{\sigma}\cdot\vec{p}+\rho_3 m_0\right)\left(\frac{2}{\underset{\sim}{k}}\rho_2\vec{\sigma}\cdot\hat{p}\right) - ip\frac{1}{\underset{\sim}{k}}\rho_3\right\} \times\left(\frac{\partial}{\partial p}+\frac{1-\rho_3\underset{\sim}{k}}{p}\right)\left(\vec{p}^2-\tilde{H}^2+m_0^2\right)\end{aligned} \tag{36}$$

It is easy to see that this goes over into a free-field Dirac Hamiltonian in the limit $(\alpha z) \to 0$ if we remember that in this case $\vec{p}^2 + m_o^2 \to \tilde{H}^2$. In view of Hylleraas' equation for the non-relativistic case, this complicated Hamiltonian is not a surprising result.

Transformation of the Wavefunctions

An even simpler task than the transformation of the Hamiltonian happens to be the evaluation of the momentum space wavefunctions. The transformation of the solutions of the Dirac-Coulomb Hamiltonian has been attempted by Rubinowicz who only succeeded in expressing the momentum space radial functions in numerical form. The momentum space solution of the Symmetric Hamiltonian is given by the Fourier transform of the coordinate space solution

$$\Psi_{N+\varkappa\mu}(\vec{p}) = \frac{1}{(2\pi)^{3/2}} \int e^{-i\vec{p}\cdot\vec{r}}\, \Psi_{N+\varkappa\mu}(\vec{r}) \tag{37}$$

$\Psi_{N\kappa\mu}(\vec{r})$ satisfies the eigenvalue equation

$$\begin{aligned} \tilde{H}\,\Psi_{N+\varkappa\mu} &= \left\{ e^{-\rho_2 \vec{\sigma}\cdot\hat{r}\,\sin^{-1}\frac{\alpha Z}{\tilde{\varkappa}}} \left(\rho_1 \vec{\sigma}\cdot\vec{p} - \rho_3 m_o \right) \right\} \Psi_{N+\varkappa\mu}(\vec{r}) \\ &= E_N\, \Psi_{N+\varkappa\mu} \end{aligned} \tag{38}$$

The coordinate solution is given explicitly by Equation (51) of RKP II

$$\Psi_{N\kappa\mu}(\vec{r}) = \begin{pmatrix} A\,\chi^{\mu}_{\kappa}\, F_{N\ell(\kappa)}(k\xi) \\ -\,iB\chi^{\mu}_{-\kappa}\, F_{N\bar{\ell}(\kappa)}(k\xi) \end{pmatrix} \tag{39}$$

A and B being numerical functions of N and κ. Since the Dirac operator $\underset{\sim}{\kappa} = \rho_3(\vec{\sigma}\cdot\vec{L} + 1)$ as well as the angular momentum operator have the same form in coordinate space and in momentum space (10) the spin angle functions in the two spherical spinors χ^{μ}_{κ} and $\chi^{\mu}_{-\kappa}$ are form-invariant and $\Psi^{(\vec{p})}_{N\kappa\mu}$ can be written, The χ^{μ}_{κ} now being functions of the polar angles of the momentum vector. The radial functions $M_{n\ell\bar{\ell}}$ and $M_{N\ell(-\kappa)\ell(\kappa)}$ are those evaluated by Podolsky and Pauling[7].

$$\Psi_{N\kappa\mu}(\vec{p}) = \begin{pmatrix} A\,\chi^{\mu}_{\kappa}\, M_{N\,\ell(\kappa)\bar{\ell}(\kappa)}(p) \\ -iB\,\chi^{\mu}_{-\kappa}\, M_{N\,\ell(-\kappa)\bar{\ell}(-\kappa)}(p) \end{pmatrix} \tag{40}$$

If one wishes to use the solutions of the Hermitian form of the Symmetric Hamiltonian in momentum space, however, more caution is needed. In the Fourier transformation, while the spin-angle part of the wavefunctions is carried over in a manner similar to the transformation of $\Psi_{N\kappa\mu}$ the radial integrals to be evaluated are of the more general type

$$M_{N\,\ell(\kappa)\,\ell(-\kappa)}(p) = (-1)^{3\frac{\ell+2}{2}} \int_0^{\infty} (pr)^{-\frac{1}{2}}\, J_{\ell+\frac{1}{2}}(pr)\, F_{N\ell(-\kappa)}(r)\, r^2\, d\xi \tag{41}$$

This is because in Ψ_s there is a mixing of $\ell_{(\kappa)}$ and $\ell_{(-\kappa)}$ in each component of the column vector. We now proceed to evaluate this integral. Introducing the variables $\xi = 2\frac{\gamma}{N}r \equiv 2\,\frac{Z}{N}\,r$ and $\zeta = \frac{2pr}{\xi}$ we have

$$F_{N\ell(-\kappa)}(r) = a_{N\ell(-\kappa)}\, e^{-\xi/2}\, \xi^{\ell(-\kappa)}\, L^{2\ell(-\kappa)+1}_{N+\ell(-\kappa)}(\xi)$$
$$\int_0^{\infty} F^2_{N\ell(-\kappa)}(r)\, r^2\, dr = 1 \tag{42}$$

L_a^b is the associated Laguerre polynomial (7). Equation (42) now becomes

$$M_{N\ell\ell(-\kappa)} = \frac{(-1)^{\frac{3\ell+2}{2}}\, a_{N\ell(-\kappa)}}{2^{\ell(-\kappa)+5/2}\,\gamma_N^3\,\varphi^{\frac{1}{2}}} \int_0^\infty \xi^{\ell(-\kappa)+3/2}\, e^{-\xi/2} \cdot \tag{43}$$

$$\cdot\, J_{\ell+\frac{1}{2}}\left(\tfrac{1}{2}\varphi\xi\right) L_{N+\ell(-\kappa)}^{2\ell(\kappa)+1}(\xi)\, d\xi$$

In order to evaluate the Hankel Transform, consider the infinite series

$$U = \int_0^\infty \left\{ \sum_{N=\ell(-\kappa)+1}^{\infty} \frac{1}{(N+\ell(\kappa))} L_{N+\ell(-\kappa)}^{2\ell(\kappa)+1}(\xi)\, t^{N-\ell(-\kappa)-1} \right\} \tag{44}$$

$$e^{-\xi/2}(\xi)^{\ell(-\kappa)+3/2}\, J_{\ell+\frac{1}{2}}\left(\tfrac{1}{2}\varphi\xi\right) d\xi$$

which can be summed as[14]

$$U = (-1)^{\ell(-\kappa)+\frac{3}{2}\ell(\kappa)} \left\{ \frac{a_{N\ell(-\kappa)}}{\gamma_N^3} \frac{2^{\ell(-\kappa)-\ell(\kappa)-\frac{1}{2}}}{\Gamma(\ell+3/2)} \right.$$

$$\left. \frac{\Gamma(\ell(\kappa)+\ell(\kappa)+3)\, \varphi^{\ell}\, (1-t)^{\ell(\kappa)-\ell(-\kappa)+1}}{(1+t)^{\bar{\ell}+\ell+3}} \right\} \cdot {}_2F_1 .$$

where ${}_2F_1$ is given by

---

[14] This is given explicitly in reference 2. In their derivation, however, there appears to be a difference in phase of between their Equation (22) and the step preceding it.

$$
{}_2F_1 =
$$

$$
{}_2F_1\left(\begin{matrix}\frac{\ell(\kappa)+\ell(-\kappa)+3}{2}, & \frac{\ell(\kappa)+\ell(-\kappa)+4}{2} \\ \ell+3/2 & ; -\varphi^2\left(\frac{1-t^2}{1+t^2}\right)\end{matrix}\right)
$$

$$
\therefore U \equiv
$$

$$
B_{N\ell\,\ell(-\kappa)} \frac{(1-t)^{\ell(\kappa)+\ell(-\kappa)+1}}{(1+t)^{\ell(\kappa)+\ell(-\kappa)+3}} \; {}_2F_1 \tag{44a}
$$

There are three cases to be considered now.

(a) $\ell_{(-\kappa)} = \ell + 1$ (κ negative). By making use of the following relation between contiguous hypergeometric functions[15]

$$
(b-a)\,{}_2F_1\left(\begin{matrix}a, b; \\ c; z\end{matrix}\right) + a\,{}_2F_1\left(\begin{matrix}a+1, b \\ c; z\end{matrix}\right) = b\,{}_2F_1\left(\begin{matrix}a, b+1 \\ c; z\end{matrix}\right)
$$

Equation (44) reduces to

$$
U = B_{N\ell(\kappa)\,\ell+1}\left\{\left(\frac{2\ell+4}{2\ell+3}\right)\frac{(1+t)^2}{(\varphi^2+1)^{\ell+3}\left[1-2Xt+t^2\right]^{\ell+3}} - \left(\frac{1}{2\ell+3}\right)\frac{1}{\left[1-2Xt+t^2\right]^{\ell+2}}\right\}
$$

where $X = \dfrac{\zeta^2-1}{\zeta^2+1}$

(b) $\ell_{(-\kappa)} = \ell$ (non-relativistic). This case has been treated by Podolsky and Pauling[6] and we get

$$U = B_{N\ell\ell} \frac{1-t^2}{(\varphi^2+1)^{\ell+2}(1-2xt+t^2)^{\ell+2}} \tag{44b}$$

(c) $\ell_{(-\kappa)} = (\ell-1)$ (κ positive). The hypergeometric function ${}_2F_1$ in Equation (44a) is degenerate and gets summed as

$$U = B_{N\ell,\ell-1} \frac{(1-t)^2}{(\varphi^2+1)^{\ell+1}\left[1-2xt+t^2\right]^{\ell+1}} \tag{44c}$$

Now with the help of following contiguous relations existing between the gegenbauer function

$$C_{k-2}^{\gamma+1}(x) = C_k^{\gamma+1}(x) - \frac{(\gamma+k)}{\gamma} C_k^{\gamma}(x)$$

$$\times \quad C_{k-1}^{\gamma+1}(x) = C_k^{\gamma+1}(x) - \left(\frac{2\gamma+k}{2k}\right) C_k^{\gamma}(x)$$

we obtain after some manipulation[6]

$$M_{N\ell,\ell+1} = (-1)^{\frac{\ell}{2}+1} \sqrt{\frac{8(N-\ell-2)}{N(N+\ell+1)\gamma_N^3}} \; \frac{(2\ell+3)!}{\Gamma(\ell+3/2)} \; .$$

$$\times \frac{\varphi^{\ell}}{(\varphi^2+1)^{\ell+3}} \Big\{ \left(\frac{2\ell+4}{2\ell+3}\right)\left(2+\frac{2}{x}\right) C_{N-\ell-2}^{\ell+3}(x)$$

$$-\left(\frac{-1}{2\ell+3}\right)\left(\frac{2}{1-x}\right) C_{N-\ell-2}^{\ell+2}(x)$$

$$-\left(\frac{2\ell+4}{2\ell+3}\right)\left(\frac{N}{\ell+2}+\frac{N+\ell+2}{(\ell+2)N}\right) C_{N-\ell-2}^{\ell+2}(x) \Big\}$$

(45a)

$$M_{N\ell\ell} = (-1)^{\ell/2} \sqrt{\frac{2(N-\ell-1)!}{N(N+\ell)!\,\gamma_N^3}} \; \frac{(2\ell+2)!}{\Gamma(\ell+3/2)}$$

$$\cdot \frac{\varphi^{\ell}}{(\varphi^2+1)^{\ell+2}} \left(\frac{N}{\ell+1}\right) C_{N-\ell-1}^{\ell+1}(x)$$

$$M_{N,\ell,\ell-1}(x)$$

(45b)

$$= (-1)^{\frac{\ell}{2}-1} \sqrt{\frac{(N-\ell)!}{2N(N+\ell-1)!\,\gamma_N^3}} \; \frac{(2\ell+1)!}{\Gamma(\ell+3/2)} \; \frac{\varphi^{\ell}}{(\varphi^2+1)^{\ell+1}}$$

$$\cdot \Big\{ \left(2-\frac{2}{x}\right) C_{N-\ell}^{\ell+1}(x) + \left(\frac{N+\ell}{\ell x}-\frac{N}{\ell}\right) C_{N-\ell}^{\ell}(x) \Big\}$$

(45c)

Because of 'Parseval's Theorem' in Hankel Transforms[16] we have

$$\int_0^\infty F_{N\ell}(r)\, F_{N\ell(-x)}(r)\, r^2\, dr = \delta_{\ell\,\ell(x)}$$

$$= \int_0^\infty M_{N\ell\,\ell(-x)}(p)\, M_{N\ell\,\ell(x)}(p)\, p^2\, dp$$

$$= -\sqrt{\frac{N^2-x^2}{N^2}} \quad \text{for } \ell \neq \ell(-x) \tag{46}$$

Section III

Discussion of the Connection Between Field Free Wave Function and the Stark Wave Functions of the Hydrogen Atom*

In a recent paper Tarter derived an expression for the coefficients connecting the non-relativistic wavefunctions of hydrogen atom in spherical and parabolic coordinates. Tarter's derivation is a mathematical expression of one set wavefunctions in terms of the other, or stated more precisely, an evaluation of the transformation coefficients connecting the representation of the state vector in Hilbert space in two different representations, in accordance with Dirac's transformation theory[18-19] although this was done in slightly different form by Rojansky[19] several years before Tarter's work. It is the purpose of this section to bring out group theoretical meaning of this mathematical connection which has to do with the peculiar symmetry of the Coulomb field.

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*A paper with this title has been submitted for publication

In Chapter II we have discussed, in detail, the 0(4) symmetry of the non-relativistic Coulomb field. Let $\vec{A}$ be Runge Lentz vector and $\vec{L}$ the angular momentum operator obeying the commutation relations given in Equations (12) of Chapter II. From the viewpoint of the 0(4) group these commutation relations are the Lie algebra satisfying the six generators of the group L_i and A_i. Then we can define two generators $\vec{L}_1$ and $\vec{L}_2$ by

$$\vec{L}_1 = \tfrac{1}{2}(\vec{L}+\vec{A}) \quad \text{and} \quad \vec{L}_2 = \tfrac{1}{2}(\vec{L}-\vec{A})$$

Where L_i are the required elements of the Lie algebra of 0(3) and

$$[L_{1i}, L_{1j}] = i\epsilon_{ijk}L_{1k} \qquad [L_{2i}, L_{2j}] = i\epsilon_{ijk}L_{2k}$$
$$[L_{1i}, L_{2j}] = 0 \tag{47}$$

Equations (47) mean that the decomposition of the symmetry group[20,21] $0(4) \rightarrow 0(3) \otimes 0(3)$ is possible. The eigenvalues of L_{iz} and L_i^2 are

$$l_1(l_1+1) = l_2(l_2+1) \rightarrow \frac{N-1}{2}\left(\frac{N-1}{2}+1\right)$$

$$L_{1z} \rightarrow \frac{n_1-n_2+m}{2} \qquad L_{2z} \rightarrow \frac{n_2-n_1+m}{2}$$

Where N is the energy determining principal quantum number. The wave-functions of the Schrodinger equation for Coulomb field in spherical coordinates are simultaneous eigenfunctions of L^2, $\underline{H}$ and L_z. Whereas those in parabolic coordinates diagonalize $\underline{H}$, A_z and L_z. Furthermore,

$$\vec{L}_1 + \vec{L}_2 = \vec{L}$$

and because of this we get the result that the connection is just a quantum mechanical vector addition and, therefore, transformation coefficients are essentially Clebsch-Gordan coefficients. Let $\phi_{n\ell m}(r,\theta,\phi)$ be the wavefunctions in spherical coordinates and $\phi_{n_1 n_2 m}(\xi,\eta,\phi)$ be those in parabolic coordinates, then

$$\phi_{n\ell m}(r,\theta,\varphi) = \sum_{\mu_1\mu_2} C^{\ell_1 \ell_2 \ell}_{\mu_1 \mu_2 m}\, \phi_{n_1 n_2 m}(\xi,\eta,\varphi)$$

The different quantum numbers are explicitly given below

$$\ell_1 = \ell_2 = \frac{1}{2}(n-1) = \frac{n_1+n_2+|m|}{2}$$

$$\mu_1 = \frac{n_1-n_2+m}{2} \qquad \mu_2 = \frac{n_2-n_1+m}{2}$$

Hence, $\mu_1 + \mu_2 = m$. The Clebsch-Gordan coefficients can be expressed in terms of a hypergeometric function[22]

$$C^{\ell_1 \ell_2 \ell}_{\mu_1 \mu_2 m} = (-1)^{\ell_2+\mu_2}\left[\frac{(\ell+\ell_1-\ell_2)!}{(\ell-\ell_1+\ell_2)!}\,\frac{(\ell_1+\ell_2-\ell)!}{(\ell_1+\ell_2+\ell+1)!}\,\frac{(\ell-m)!}{(\ell+m)!}\,\frac{(\ell_2-\mu_2)!}{(\ell_1+\mu_1)!}\,\frac{(2\ell+1)}{(\ell_2+\mu_2)!}\right]^{\frac{1}{2}} \frac{1}{\sqrt{(\ell_2-\mu_2)!}}\,\frac{(\ell+\ell_2+\mu_1)!}{(\ell_1-\ell_2-\mu_2)!}\,.$$

$$\cdot\ {}_3F_2\left(\begin{matrix} -\ell+\ell_1+\ell_2, & \ell_1-\mu_1+1, & -\ell-m\,;\ 1 \\ \ell_1-\ell_2-m+1, & -\ell-\ell_2-\mu_1 & \end{matrix}\right) \tag{48}$$

If we use the recursion relation[23]

$${}_3F_2\left(\begin{matrix} a, & a', & -N\,; & 1 \\ c', & 1-N-c, & & \end{matrix}\right) = \frac{(c+a)_N}{(c)_N}\ {}_3F_2\left(\begin{matrix} a, & c'-a', & -N\,;\ 1 \\ c', & c+a, & \end{matrix}\right)$$

and apply it twice it is easy to arrive at the result (49)

$$
{}_3F_2\left(\begin{matrix} -\ell, & n_2+|m|+1, & -\ell+m; & 1 \\ m+1, & -\ell-n_2 & & \end{matrix}\right)
$$

$$
= \frac{n_1!}{(n_1+m+1)!}\,\frac{(m+n_1)!}{n_1!}\,\frac{(n_1+n_2)!}{(n_1+\ell)!}\,\frac{(n_1-\ell+m)!}{(n_1+n_2-\ell-m)!}
$$

$$
\cdot\,{}_3F_2\left(\begin{matrix} \ell+m+1, & -n_2, & -\ell+m; & 1 \\ m+1, & -n_1-n_2; & & \end{matrix}\right) \tag{50}
$$

A comparison with the Tarter's Equation (22) establishes the equivalence

$$
C^{\ell_1\ell_2\ell}_{\mu_1\mu_2 m} = (-1)^{\ell-m-n_2}\, A^{n_1 n_2}_{n\ell m} \tag{51}
$$

Where $A^{n_1n_2}_{n\ell m}$ are the expansion coefficients evaluated by Tarter. The following few useful relations follow readily from the well known symmetry properties of the Clebsch-Gordan coefficients.

$$
A^{n_1 n_2}_{n\ell m} = (-1)^{\ell-m} A^{n_2 n_1}_{n\ell m}
$$

$$
A^{n_1 n_2}_{n\ell m} = (-1)^{-(\ell+m)} A^{n_2 n_1}_{n\ell -m}
$$

$$
\begin{aligned}
C^{\ell_1\ \ell_2\ \ell}_{\mu_1, -m, -\mu_2} &= (-1)^{\ell-m}\left(\frac{n}{2\ell+1}\right)^{\frac{1}{2}} A^{n_1 n_2}_{n\ell m} \\
&= \left(\frac{n}{2\ell+1}\right)^{\frac{1}{2}} A^{n_2 n_1}_{n\ell m}
\end{aligned} \tag{52}
$$

In the next section we will show that wavefunctions have the simplest possible form in the Fock-Bargmann space. This is because in the latter mapping the complicated mathematical solutions for the hydrogen atom can be written as simple polynomial in the Z variables.

Section IV

In this section we apply the results derived in Section I to non-relativistic Coulomb problem. We have shown in Section I that in Z space $U_m = N_m Z^m$ form a complete orthonormal set. N_m the normalization factor depends upon the domain of Z and the choice of appropriate volume element $d\mu_\nu(Z)$. If $|Z| < 1$ the disk, then $d\mu_\nu(Z)$ can be chosen as

$$d\mu_\gamma(z) = \frac{\gamma}{\pi}\left(1 - z^*.z\right)^{\gamma-1} dz \qquad \gamma \neq 0 \tag{53}$$

This choice shows that (with $Z = r\,e^{i\theta}$)

$$\int d\mu_\gamma(z) = \frac{\gamma}{\pi}\int_0^{2\pi}\int_0^1 (1-r^2)^{\gamma-1}\, r\,dr\,d\theta = 1 \tag{54}$$

And

$$\begin{aligned} \langle u_m | u_n \rangle &= \int N_m^*(z^m)^* N_n(z^n)\, d\mu_\gamma(z) \\ &= \delta_{mn}\frac{\Gamma(m+1)\,\Gamma(\gamma+1)}{\Gamma(\gamma+m+1)} N_m^* N_n \end{aligned} \tag{55}$$

$$\therefore \quad N_m = \binom{\gamma+m}{m}^{\frac{1}{2}} = \left\{\frac{\Gamma(\gamma+m+1)}{\Gamma(\gamma+1)\,\Gamma(m+1)}\right\}^{\frac{1}{2}}$$

Then we have an orthonormal set in Fock-Bargmann space as

$$u_m(z) = \binom{\gamma+m}{m}^{\frac{1}{2}} z^m \qquad \text{with } |z| < 1$$

The corresponding q space wavefunctions are

$$\phi_m(q) = \frac{1}{\sqrt{\gamma!}} \sqrt{\frac{(\gamma+m)!}{m!\,\gamma!}}\; e^{-q/2}\, q^{\gamma/2}\, L_m^{\gamma}(q) \tag{56}$$

where $L_m^{\gamma}(q)$ is the associated Laugerre polynomial. So

$$A(z,q) = \sum_m \phi_m(q)\, u_m(z) = \frac{e^{-\frac{q}{2}\left(\frac{1+z}{1-z}\right)}}{(1-z)^{\gamma+1}} \tag{57}$$

is the transformation kernel. The hydrogenic wavefunctions in parabolic coordinates are given by

$$\begin{aligned}\psi_{n_1 n_2 m}(\xi,\eta,\phi) &= \frac{\sqrt{2}}{n^2}\,\frac{1}{(|m|)!}\sqrt{\frac{(n_1+|m|)!}{n_1!}}\,(n_1+1)! \\ &\cdot L_{n_1}^{|m|}(\alpha\xi)\, e^{-\frac{1}{2}\alpha\xi}\,(\alpha\xi)^{\frac{|m|}{2}} \cdot \frac{1}{(|m|)!}\sqrt{\frac{(n_2+|m|)!}{n_2!}} \\ &\cdot (n_2+1)!\, L_{n_2}^{|m|}(\alpha\eta)\, e^{-\frac{1}{2}\alpha\eta}\,(\alpha\eta)^{\frac{|m|}{2}}\,\frac{1}{\sqrt{2\pi}}\, e^{im\phi}\end{aligned} \tag{58}$$

with $q_1 = \alpha\xi$ and $q_2 = \alpha\eta$ we get

$$\psi_{n_1 n_2 m}(\xi,\eta,\phi) = \frac{1}{\sqrt{\pi}\, n^2}(n_1+1)!\,(n_2+1)!\, e^{im\phi}\, \phi_{n_1 n_2}(q_1,q_2) \tag{59}$$

The corresponding Fock-Bargmann wavefunctions are

$$\begin{aligned}&u_{n_1 n_2}(z_1, z_2) \\ &= \sqrt{\frac{(n_1+|m|)!}{n_1!\,(|m|)!}}\sqrt{\frac{(n_2+|m|)!}{n_2!\,(|m|)!}}\; z_1^{n_1}\, z_2^{n_2}\end{aligned} \tag{60}$$

and

$$d\mu_m(z_1 z_2) = \left(\frac{|m|}{\pi}\right)^2 \left[(1-z_1^* \cdot z_1)(1-z_2^* \cdot z_2)\right]^{|m|-1} dz_1 dz_2 \tag{61}$$

The above Equation (60) shows the simplicity of wavefunctions in Fock-Bargmann space.

The hydrogenic wavefunctions in the spherical coordinates are

$$\psi_{n\ell m}(\rho, \theta, \varphi) = \left\{\left(\frac{2Z}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n((n+\ell)!)^3}\right\}^{\frac{1}{2}} \cdot e^{-\frac{1}{2}\rho} \rho^\ell L_{n-\ell-1}^{2\ell+1}(\rho) \, Y_\ell^m(\theta,\varphi) \tag{62}$$

The corresponding Fock-Bargmann wavefunctions in this case are

$$V_{n\ell m}(t_1, t_2) = \sqrt{\frac{(n+\ell)!}{(2\ell+1)!\,(n-\ell-1)!}}\; t_1^{\,n-\ell-1} \sqrt{\frac{(2\ell)!}{(\ell+m)!\,(\ell-m)!}}\; t_2^{\,\ell+m} \tag{63}$$

$$|t_1| < 1 \qquad |t_2| < \infty$$

$$= \sqrt{\frac{(n+\ell)!\;(2\ell)!}{(2\ell+1)!\,(n-\ell-1)!\,(\ell+m)!\,(\ell-m)!}} \left\{\frac{t_2}{\sqrt{1-t_2^2}}\right\}^{\ell+m} t_1^{\,n-\ell-1}$$

$$|t_1| < 1 \qquad |t_2| < 1$$

$$= \sqrt{\frac{(n+\ell)!}{(2\ell+1)\;(n-\ell-1)!\,(\ell+m)!\,(\ell-m)!}} \cdot \sum_{k=0}^{\ell+m} (-1)^k \frac{\left(\frac{\ell+m}{2}\right)_k}{k!}\; t_1^{\,n-\ell-1}\; t_2^{\,\ell+m+2k} \tag{64}$$

Which are also polynomials in a complex space of t_1 and t_2. The Clebsch-Gordan theorem is a connection between the wavefunctions $U_{n_1 n_2}(Z_1 Z_2)$ and $V_{n\ell m}(t_1 t_2)$

$$\upsilon_{n\ell m}(t_1 t_2) = \sum_{\mu_1 \mu_2} C^{\frac{n-1}{2}, \frac{n-1}{2}, \ell}_{\mu_1\ \mu_2\ m}\ U_{n_1 n_2}(Z_1 Z_2) \tag{65}$$

To prove this we use the inductive method. First we assume Equation (65) holds good. Then we derive relation between t_1, t_2 and Z_1, Z_2, and show that they must be linear combinations $t_1 = f(Z_1 - Z_2)$ and $t_2 = f(Z_1 + Z_2)$, let

$$\upsilon_{n\ell m}(t_1, t_2) = \sum_{\mu_1 \mu_2} C^{\frac{n-1}{2}\ \frac{n-1}{2}\ \ell}_{\mu_1\ \mu_2\ m}\ U_{n_1 n_2}(Z_1 Z_2)$$

we can expand $C^{\frac{n-\ell}{2}\ \frac{n-\ell}{2}\ \ell}_{\mu_1, \mu_2, m}$ in terms of $3F_2$ function, then

$$C^{\frac{n-1}{2}, \frac{n-1}{2}, \ell}_{\mu_1\ \ \mu_2, m} = (-1)^{\frac{n-1}{2}+\mu_2}\left[\frac{(n-\ell-1)!\,(\ell-m)!\,(\frac{n-1}{2}-\mu_2)!}{(n+\ell)!\,(\ell+m)!\,(\frac{n-1}{2}+\mu_1)!}\right.$$

$$\left.\frac{(2\ell+1)}{(\frac{n-1}{2}+\mu_2)!\,(\frac{n-1}{2}-\mu_2)!}\right]^{\frac{1}{2}} \frac{(\ell+\frac{n-1}{2}+\mu_1)!}{(n-m-1)!}\ 3F_2\begin{pmatrix}-\ell, n_2+1, -\ell-m; 1\\ -m+1, -n_1-m;\end{pmatrix} \tag{66}$$

$$\therefore \upsilon_{n\ell m}(t_1, t_2) = \sum_{\mu_1 \mu_2} (-1)^{n_2+m} \frac{(\ell+n_2+m)!}{(n-1-m)!}$$

$$\left[\frac{(n-1-\ell)!\,(\ell-m)!\,(2\ell+1)}{(n+\ell)!\,(\ell+m)!\,(n_1+m)!\,(n_2+m)!}\right]^{\frac{1}{2}}$$

$$\sqrt{\frac{(n_1+m)!\,(n_2+m)!}{n_1!\,n_2!\,m!\,m!}}\ 3F_2\begin{pmatrix}-\ell, n_2+1, -\ell-m, 1\\ -m+1, -n_1-m;\end{pmatrix}.$$

$$Z_1^{n_1} Z_2^{n_2}$$

Expanding $3F_2$ and interchanging summations and summing over n_1 and n_2. It can be shown that

$$
\begin{aligned}
\upsilon_{n\ell m}(t_1,t_2) &= \sum_{k=0} \sqrt{\frac{(n-\ell-1)!\,(\ell+m)!}{(\ell-m)!\,(2\ell+1)!\,(n+\ell)!\,(2m)!}} \\
&\quad (-1)^k \frac{\left(\frac{1}{2}(\ell+m)\right)!}{\left(\frac{\ell+m}{2}-k\right)!\;k!} (Z_1-Z_2)^{n-\ell-1} (Z_1+Z_2)^{\ell+m+k} \\
&= \sqrt{\frac{(n-\ell-1)!\,(\ell+m)!}{(n+\ell)!\,(2\ell+1)!\,(2m)!}} (Z_1+Z_2)^{\ell+m} (Z_1-Z_2)^{n-\ell-1} \\
&\quad \cdot \sum_{k=0}^{(\ell+m)/2} \left(\frac{\ell-m}{2}\right)! \left[\frac{1}{\left(\frac{\ell+m}{2}-k\right)!\,k!}\right] (Z_1+Z_2)^k
\end{aligned} \tag{67}
$$

Which are again vectors in Fock-Bargmann space, but the variables here are the linear combinations of Z_1 and Z_2. Thus, the theorem is established. Papov and Peremolov extended this to continuous solutions and established a connection between Coulomb scattering phase shifts and complex Clebsch-Gordan coefficients. Here we should note that the domain of their variables is entirely different than the one given in Section IV of this chapter.[24]

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CHAPTER IV

EVALUATION OF CERTAIN RADIAL INTEGRALS USING SYMMETRY PROPERTIES OF THE COULOMB FIELD*

In this chapter we discuss some physical applications of the symmetry properties of the Coulomb field by evaluating certain radial integrals which are of importance in determining selection rules in Coulomb excited transitions. In Section I we derive some of the very often used relations between certain basic sets of operators like $\underset{\sim}{K}$, $\hat{Z}\cdot(\vec{\sigma}\times\vec{L})$, $\vec{\sigma}\cdot\vec{a}$, $\vec{\sigma}\cdot\hat{r}$ $\frac{1}{rq}$ ip_r, and $2m\underset{\sim}{H}$.

In Section II we discuss the radial matrix elements involving the bound state wave functions. Here we give a group theoretic derivation of Pasternack Sternheimer[1] result along with certain recusion relations between the expectation values of various multipole operators[2].

In Section III we discuss the radial integrals involving continuous state wave functions and establish certain difference equations between the various matrix elements of multipole operators. A possible extention to higher multipoles and the Symmetric Hamiltonian is suggested at the end of the chapter.

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Section I

The Derivation of the Set of Useful Operator Relations

Here we will derive nearly all operator relations between the primary operators

$$\underset{\sim}{K}_1 = \vec{\sigma}\cdot\vec{L} + 1,\ \Omega_o = \hat{z}\cdot(\vec{\sigma}\mathrm{x}\vec{L}),\ \vec{\sigma}\cdot\vec{a},\ \vec{\sigma}\cdot\hat{r},\ \text{etc.}$$

To prove $[\kappa_1, \Omega_o] = \Omega_o$ we consider $[\vec{\sigma}\cdot\vec{L}, \hat{z}\cdot(\vec{\sigma}\mathrm{x}\vec{L})]_+$. And noting that for all i and j, $[\sigma_i, L_j] = 0$ and $[\sigma_x, \sigma_y] = i\sigma_z$ we get $[\vec{\sigma}\cdot\vec{L}, \Omega_o]_+ = -\Omega_o$
$[\vec{\sigma}\cdot\vec{L} + 1, \Omega_o]_+ = +\Omega_o$ where $\Omega_o = \hat{z}\cdot(\vec{\sigma}\times\vec{L})$

To prove

$$[\Omega_o, 1-2\underset{\sim}{K}]_+ = 0 \tag{2}$$

From 1 we have $2[\Omega_o, \underset{\sim}{K}]_+ = 2\Omega_o$ and $[\Omega_o, 1]_+ = 2\Omega_o$ $[\Omega_o, 1 - 2\underset{\sim}{K}]_+ = 0.$

$$\left[\frac{1}{r^\nu}, ip_r\right] = \nu/r^{\nu+1} = \left[\frac{1}{r^\nu}, \left[r, m\underset{\sim}{H}\right]\right] \tag{3}$$

$$\left[\frac{1}{r^\nu}, p_r^2\right] = -\frac{2\nu}{r^{\nu+1}}\, ip_r + \nu(\nu+1)\frac{1}{r^{\nu+2}} = \left[\frac{1}{r^\nu}, 2m\underset{\sim}{H}\right] \tag{4}$$

$$\begin{aligned}\left[ip_r, 2m\underset{\sim}{H}\right] &= \left[ip_r, \left(p_r^2 + \frac{K_1^2 - K_1}{r^2} - \frac{2\alpha Z m}{r}\right)\right] \\ &= \frac{2\alpha Z m}{r^2} + \frac{2\left(K_1 - K_1^2\right)}{r^3} \\ &= \left[\left[r, m\underset{\sim}{H}\right], 2m\underset{\sim}{H}\right]\end{aligned} \tag{5}$$

This is because ip_r commutes with p_r^2 and the angular operators K_1 and K_1^2. It does not commute with r and functions of r. Let us consider

$$\frac{1}{2}\left[\frac{1}{r^q}ip_r, 2m\underset{\sim}{H}\right] = \frac{1}{2}\frac{1}{r^q}\left[ip_r, 2m\underset{\sim}{H}\right] + \frac{1}{2}\left[\frac{1}{r^q}, 2m\underset{\sim}{H}\right]ip_r$$

and substituting the values we get,

$$= \frac{\alpha Zm}{r^{q+2}} + \frac{q}{r^{q+1}}p_r^{\,2} + \frac{q(q+1)}{2}\frac{1}{r^{q+2}}ip_r + \frac{K_1-K_1^{\,2}}{r^{q+3}} \quad (6)$$

But we know that

$$p_r^{\,2} = 2m\underset{\sim}{H} + \frac{K_1-K_1^{\,2}}{r^2} + \frac{2\alpha Zm}{r}$$

and

$$\frac{1}{r^{q+2}}ip_r = \frac{q+2}{2}\frac{1}{r^{q+3}} + \frac{1}{2(q+1)}\left[2m\underset{\sim}{H}, \frac{1}{r^{q+1}}\right]$$

substituting these it leads to

$$\frac{1}{2}\left[\frac{1}{r^q}\left[r, m\underset{\sim}{H}\right], 2m\underset{\sim}{H}\right] + \frac{q}{4}\left[\frac{1}{r^{q+1}}, 2m\underset{\sim}{H}\right]$$

$$= \frac{q}{r^{q+1}}\left(2m\underset{\sim}{H}\right) + \frac{2q+1}{r^{q+2}}\alpha Zm + (q+1)\left\{\frac{q(q+2)}{4} + (K_1-K_1^{\,2})\right\}\frac{1}{r^{q+3}}$$

Since $\vec{\sigma}\cdot\hat{r}$ and K_1 anticommute we get

$$\left[\vec{\sigma}\cdot\hat{r}, (K_1-K_1^2)\right] = \left[\vec{\sigma}\cdot\hat{r}, \underset{\sim}{K_1}\right] - \left[\vec{\sigma}\cdot r, K_1^2\right] = 2\vec{\sigma}\cdot\hat{r}K_1 \quad (7)$$

and hence we get

$$\left[\vec{\sigma}\cdot\hat{r}, 2m\underset{\sim}{H}\right] = -2\vec{\sigma}\cdot\hat{r}K_1\frac{1}{r^2}$$

Now

$$\left[\vec{\sigma}\cdot\hat{r}\frac{1}{r^{q-1}}, 2m\underset{\sim}{H}\right]$$

$$= -2\vec{\sigma}\cdot\hat{r}K_1\frac{1}{r^{q+1}} + \vec{\sigma}\cdot\hat{r}\left\{-2(q-1)\frac{1}{r^q}ip_r + \frac{q(q-1)}{r^{q+1}}\right\} \quad (8)$$

or multiplying through out from left by $\frac{\vec{\sigma}\cdot\hat{r}}{2(q-1)}$ we get

$$\frac{\vec{\sigma}\cdot\hat{r}}{2(q-1)}\left[2m\underset{\sim}{H}, \frac{\vec{\sigma}\cdot\hat{r}}{r^{q-1}}\right] = \frac{1}{r^q}ip_r + \left\{\frac{K_1}{q-1} - \frac{q}{2}\right\}\frac{1}{r^{q+1}}$$

And multiplying with $\frac{\vec{\sigma}\cdot\hat{r}}{2(q-1)}$ from right we get

$$\frac{1}{2(q-1)}\left[2m\underset{\sim}{H}\,\frac{\vec{\sigma}\cdot\hat{r}}{r^{q-1}}\right]\vec{\sigma}\cdot\hat{r} = \frac{1}{r^{q}}ip_r - \left\{\frac{k_1}{q-1}+\frac{q}{2}\right\}\frac{1}{r^{q+1}} \quad (9)$$

or we can use this relation to replace $\frac{1}{r^q}ip_r$ by (a commutator with Hamilton) $x\vec{\sigma}\cdot\hat{r}$ and a power of r.

Now we consider

$$\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^{q-1}}ip_r, 2m\underset{\sim}{H}\right] = \vec{\sigma}\cdot\hat{r}\left[\frac{1}{r^{q-1}}ip_r, 2m\underset{\sim}{H}\right] + \left[\vec{\sigma}\cdot\hat{r}, 2m\underset{\sim}{H}\right]\frac{1}{r^{q-1}}ip_r$$

$$= \frac{2(q-1)}{r^q}\vec{\sigma}\cdot\hat{r}\,p_r^2 + \frac{2\alpha Zm}{r^{q+1}}\vec{\sigma}\cdot\hat{r} + \left\{q(q-1)-2k_1\right\}\frac{1}{r^{q+1}}ip_r + \frac{2\vec{\sigma}\cdot\hat{r}}{r^{q+2}}(k_1-k_1^2)$$

and using the similar techniques we get

$$\vec{\sigma}\cdot\hat{r}\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^{q-1}}ip_r, 2m\underset{\sim}{H}\right]$$
$$= \vec{\sigma}\cdot\hat{r}\left\{q(q-1)+2k_1\right\}\frac{1}{2q}\left[2m\underset{\sim}{H}, \frac{\vec{\sigma}\cdot\hat{r}}{r^q}\right] + \frac{2(q-1)}{r^q}2m\underset{\sim}{H}$$
$$+ 2\alpha Zm(2q-1)\frac{1}{r^{q+1}} + \frac{1}{2q}(q-1)(q+1)(q-2k_1)(q+2k_1)\frac{1}{r^{q+2}} \quad (10)$$

Similarly

$$\left[2m\underset{\sim}{H}, \vec{\sigma}\cdot\hat{r}\frac{1}{r^q}ip_r\right]\vec{\sigma}\cdot\hat{r}$$
$$= \frac{2\alpha Zm}{r^{q+2}} + \frac{2q}{r^{q+1}}p_r^2 + \left\{q(q+1)+2k_1\right\}\frac{1}{r^{q+2}}ip_r - \frac{2k_1}{r^{q+3}}(k_1+1)$$

$$= \left\{ q(q-1) - 2K_1 \right\} \frac{1}{2q} \left[2m\underset{\sim}{H}, \frac{\vec{\sigma}\cdot\vec{r}}{r^q} \right] \vec{\sigma}\cdot\hat{r}$$

$$+ 2(q-1)\frac{1}{r^q} 2m\underset{\sim}{H} + 2\alpha Z m (2q-1)\frac{1}{r^{q+1}}$$

$$+ \frac{1}{2q}(q-1)(q+1)(q-2K_1)(q+2K_1)\frac{1}{r^{q+2}} \qquad (11)$$

$$\left[\vec{\sigma}\cdot\vec{a}, \frac{1}{r^q}\right] = \left[\frac{\vec{\sigma}\cdot\hat{r}}{K^2}\left(2Zm + ip_r K_1 - \frac{K_1^2}{r}\right), \frac{1}{r^q}\right] \qquad (12)$$

$$= -\frac{q}{K^2}\,\vec{\sigma}\cdot\hat{r}\,K_1\,\frac{1}{r^{q+1}}$$

$$\left[\vec{\sigma}\cdot\vec{a}, \vec{\sigma}\cdot\hat{r}\frac{1}{r^q}\right] = \vec{\sigma}\cdot\vec{a}\;\vec{\sigma}\cdot\hat{r}\frac{1}{r^q} - \vec{\sigma}\cdot\hat{r}\frac{1}{r^q}\vec{\sigma}\cdot\vec{a}$$

Since $$\vec{\sigma}\cdot\vec{a} = \frac{\vec{\sigma}\cdot\hat{r}}{K^2}\left(2Zm + ip_r K_1 - \frac{1}{r}K_1^2\right)$$

we get

$$\left[\vec{\sigma}\cdot\vec{a}, \vec{\sigma}\cdot\hat{r}\frac{1}{r^q}\right] = \frac{1}{K^2(q-1)}\left[\frac{1}{r^{q-1}}, 2m\underset{\sim}{H}\right] \qquad (13)$$

We now derive the commutation relation which we used very often in our analysis of operator technique for radial matrix elements. By these relations we can bring Ω_o to the extreme right or extreme left of the given operator.

Consider

$$\left[\vec{\sigma}\cdot\vec{a}\;\;\vec{\sigma}\cdot\hat{r}\;\frac{1}{r^q}, r_o\right]$$

$$= \left[\frac{1}{K^2}\left(\alpha Z m - \frac{1}{r^q} ip_r K_1 - \frac{1}{r^{q+1}}K_1^2\right), r_o\right]$$

using the relation $[K_1, \Omega_0]$ and $[K_1^2, \Omega_0]$ we get

$$\left[\vec{\sigma}\cdot\vec{a}\ \vec{\sigma}\cdot\hat{r}\ \frac{1}{r^q}, r_0\right]$$

$$= \frac{1}{K^2}\left\{\frac{q-1}{r^{q+1}} - \frac{1}{r^q} i p_r\right\}\Omega_0 (1-2K_1) \qquad (14)$$

$$= \frac{1}{2K^2(q-1)}\left[\frac{1}{r^{q-1}}, 2m\underset{\sim}{H}\right]\Omega_0(1-2K_1) + \frac{q-2}{2K^2}\frac{1}{r^{q+1}}\Omega_0(1-2K_1)$$

where in the second step we have replaced $\frac{1}{r^q} ip_r$ by the appropriate Hamiltonian commutator with $1/r^{q-1}$ and a power of r.

Many times we need the commutator with $\vec{\sigma}\cdot r$ out side the bracket. So we derive that result also i.e.,

$$\left[\vec{\sigma}\cdot\vec{a}\ \vec{\sigma}\cdot\hat{r}\ \frac{1}{r^q}, \Omega_0\right]$$

$$= \frac{1}{K^2}\Omega_0(1-2K_1)\left\{\frac{1}{2(q-1)}\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^{q-1}}, 2m\underset{\sim}{H}\right]\vec{\sigma}\cdot\hat{r} - \left(\frac{K_1}{q-1} + \frac{2-q}{2}\right)\frac{1}{r^{q+1}}\right\} \qquad (15)$$

$$= \frac{1}{K^2}\Omega_0(1-2K_1)\left\{\frac{\vec{\sigma}\cdot\hat{r}}{2(q-1)}\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^{q-1}}, 2m\underset{\sim}{H}\right] + \left(\frac{K_1}{q-1} + \frac{q-2}{2}\right)\frac{1}{r^{q+1}}\right\}$$

The other relation similar to 14 and 15 is 16.

$$\left[\Omega_0, \frac{1}{r^q}\vec{\sigma}\cdot\hat{r}\ \vec{\sigma}\cdot\vec{a}\right] = \frac{1}{K^2}\left\{\frac{1}{r^q} i p_r - \frac{1}{r^{q+1}}\right\}(1-2K_1)\Omega_0 \qquad (16)$$

And here too $\frac{1}{r^q} ip_r$ or $\vec{\sigma}\cdot\hat{r}\ \frac{1}{r^q} ip_r$ can be replaced by appropriate commutator bracket and a power of r.

By expansion of $\vec{\sigma}\cdot\vec{a}$ and using (4) we get,

$$\frac{K^2}{r^q}\vec{\sigma}\cdot\hat{r}\ \vec{\sigma}\cdot\vec{a} = \frac{\alpha Z m}{r^q} + \frac{1}{r^q} i p_r K_1 - \frac{1}{r^{q+1}} K_1^2$$

$$= \frac{\alpha Z m}{r^q} + \left(\frac{qK_1}{2} - K_1^2\right)\frac{1}{r^{q+1}} + \frac{K_1}{2(q-1)}\left[2m\underset{\sim}{H}, \frac{1}{r^{q-1}}\right] \quad (17)$$

And

$$K^2 \ \vec{\sigma}.\vec{a} \ \vec{\sigma}.\hat{r} \ \frac{1}{r^q}$$

$$= \frac{\alpha Z m}{r^q} + \left(\frac{qK_1}{2} - K_1^2\right)\frac{1}{r^{q+1}} + \frac{1}{2(q-1)}\left[\frac{1}{r^{q-1}}, 2m\underset{\sim}{H}\right]K_1 \quad (18)$$

Taking the matrix element of this operator between $\psi_{N\kappa\mu}$ and $\psi_{N\kappa\mu}$

and replacing $<\frac{1}{r^{q+1}}>$ using Pasternack result we get

$$K a_{l+1} < l+1 | \frac{1}{r^q} | l >$$

$$= \frac{2 Z m (q-2)}{(q-1)(l+q/2)}\left\{l - \frac{q}{2} + \frac{3}{2}\right\}\left<\frac{1}{r^q}\right> - \frac{K^2(q-2)(l+1)}{(q-1)(l+\frac{q}{2})}\left<\frac{1}{r^{q-1}}\right> \quad (19)$$

where

$$a_{l+1} = \sqrt{N^2 - (l+1)^2}$$

Expanding $\vec{\sigma}\cdot\vec{a}\,\frac{1}{r^q}$ and using (8) we get

$$\vec{\sigma}.\vec{a}\frac{1}{r^q} = \frac{\vec{\sigma}.\hat{r}}{K^2}\left\{\frac{\alpha Z m}{r^q} - \frac{qK_1}{2}\frac{1}{r^{q+1}} - \frac{q}{q-1}\frac{K_1^2}{r^{q+1}}\right\} + \left[1/2(q-1)K^2\right]\left[\frac{\vec{\sigma}.\hat{r}}{r^{q-2}}, 2m\underset{\sim}{H}\right]$$

Taking the matrix element between $\psi_{N-\kappa\mu}$ and $\psi_{N\kappa\mu}$ we get

$$\left(\frac{q}{q-1}\right)(l+1)\left(l+\frac{1}{2}+\frac{q}{2}\right)\left<l+1\right|\frac{1}{r^q}\left|l\right>$$
$$- \alpha Z m \left<l+1\right|\frac{1}{r^q}\left|l\right>$$
$$= K a_{l+1}\left<l\right|\frac{1}{r^q}\left|l\right> = K a_{l+1}\left<\frac{1}{r^q}\right> \quad (20)$$

$$\left[\vec{\sigma}.\vec{a} \ \vec{\sigma}.\vec{a}, \Omega_0\right] = \frac{1}{K^2}\Omega_0(1-2K_1) \quad (21)$$

$$[\vec{\sigma}\cdot\vec{a}, \Omega_0^2] = 2K_1\,\vec{\sigma}\cdot\vec{a} \tag{22}$$

By taking matrix element of few of the derived operators we get many relations between the matrix elements or expectation values to illustrate we give the following relations.

We have the operator

$$\vec{\sigma}\cdot\hat{r}\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^{q-1}}\,i p_r, 2m\underset{\sim}{H}\right]$$

$$= \vec{\sigma}\cdot\hat{r}\,\{q(q-1)+2K_1\}\frac{1}{2q}\left[2m\underset{\sim}{H}, \frac{\vec{\sigma}\cdot\hat{r}}{r^{q-1}}\right]$$

$$+ 2(q-1)\frac{1}{r^q}\,2m\underset{\sim}{H} + 2\alpha Z m\,(2q-1)\frac{1}{r^{q+1}}$$

$$+ \frac{(q-1)(q+1)}{2q}\,\frac{q^2-4K_1^2}{r^{q+2}} \equiv \underset{\sim}{Q}$$

letting $q \to q-1$ and taking the expectation values between

$$\langle \Psi_{N-K\mu} | \vec{\sigma}\cdot\hat{r}\,Q | \Psi_{NK\mu} \rangle$$

we get

$$q(q-2)\left(l+\frac{1}{2}+\frac{q}{2}\right)\left(l+\frac{3}{2}-\frac{q}{2}\right)\langle l+1|\frac{1}{r^{q+1}}|l\rangle$$

$$-(q-1)(2q-3)\alpha Z m\,\langle l+1|\frac{1}{r^q}|l\rangle \tag{23}$$

$$+K^2(q-2)(q-1)\langle l+1|\frac{1}{r^q}|l\rangle = 0$$

(where q = o, or any integer).

Pasternack[3] Result (1937)

$$q\left\langle\frac{1}{r^{q+2}}\right\rangle = -\frac{K^2(q-1)}{\left(l+\frac{1}{2}+\frac{q}{2}\right)\left(l+\frac{1}{2}-\frac{q}{2}\right)}\left\langle\frac{1}{r^q}\right\rangle \tag{24}$$

$$+\frac{\alpha Z m\,(2q-1)}{(l+1/2+q/2)(l+1/2-q/2)}\left\langle\frac{1}{r^{q+1}}\right\rangle$$

We have the operator

$$K^2 \vec{\sigma}_1 \vec{\alpha}\, \vec{\sigma}_1 \hat{r} \frac{1}{r^q} = \frac{\alpha Z m}{r^q} + \left(\frac{q}{2} K_1 - K_1^2\right) \frac{1}{r^{q+1}} + \frac{1}{2(q-1)}\left[\frac{1}{r^{q-1}}, \underset{\sim}{2mH} \cdot K_1\right] = Q'$$

so $<\psi_{N\kappa\mu}, \underset{\sim}{Q}\ \psi_{N\kappa\mu}>$ gives

$$K\, a_{L+1} \left< L+1 \left| \frac{1}{r^q} \right| L \right> = -\alpha Z m \left< \frac{1}{r^q} \right> + (L+1) \left\{ (L+1) - \frac{q}{2} \right\} \left< \frac{1}{r^{q+2}} \right> \tag{25}$$

To express $\vec{\sigma}\cdot\hat{r}$ (some powers of r) as the commutators of power of r with the Hamiltonians.

Putting $q = 1$ in the relation (10) we get

$$2 \vec{\sigma}\cdot\hat{r}\ \frac{\alpha Z m}{r^2} = \left[\vec{\sigma}\cdot\hat{r}\, i p_r,\ 2m\underset{\sim}{H}\right] + K_1 \left[\frac{\vec{\sigma}\cdot\hat{r}}{r},\ 2m\underset{\sim}{H}\right] \tag{26}$$

Thus we see that $2\vec{\sigma}\cdot\hat{r}\ \frac{\alpha Z m}{r^2}$ can be completely put as a $\vec{\sigma}\cdot\hat{r}\ \frac{1}{r^q}$ commutation with Hamiltonian.

Putting $q = 2$ we have

$$\vec{\sigma}\cdot\hat{r} \left\{ \frac{2}{r^2}\, 2m\underset{\sim}{H} + 6\alpha Z m \frac{1}{r^3} + 3(1-K_1)(1+K_1)\frac{1}{r^4} \right\} = \left[\vec{\sigma}\cdot\hat{r}\,\frac{1}{r}\, i p_r,\ 2m\underset{\sim}{H}\right] + \frac{1+K_1}{2}\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^2},\ 2m\underset{\sim}{H}\right] \tag{27a}$$

Combining this result appropriately with (26) we get

$$\vec{\sigma}\cdot\hat{r} \left\{ \frac{2\alpha Z m}{r^3} + \frac{(1-K_1)(1+K_1)}{r^4} \right\} = \frac{1}{3}\left[\vec{\sigma}\cdot\hat{r}\,\frac{1}{r}\, i p_r,\ 2m\underset{\sim}{H}\right] + \frac{1}{6}(1+K_1)\left[\frac{\vec{\sigma}\cdot\hat{r}}{r},\ 2m\underset{\sim}{H}\right]_{2m\underset{\sim}{H}} \tag{27b}$$

Taking the appropriate matrix element of (27b) we get

$$2\alpha Z m \left< L+1 \left| \frac{1}{r^3} \right| L \right> - L(L+2)\left< L+1 \left| \frac{1}{r^4} \right| L \right> = 0$$

Putting q = 3 in the Equation 10 and eliminating using the result 27 we get

$$-\frac{1}{3\alpha Z m^2}k_1\left[\frac{\vec{\sigma}\cdot\hat{r}'}{r}, 2m\underset{\sim}{H}\right]\left(2m\underset{\sim}{H}\right)^2 + \vec{\sigma}\cdot\hat{r}'\left\{5\alpha Z m\frac{1}{r^4} - \frac{1-k_1^2}{\alpha Z m}\frac{1}{r^4}2m\underset{\sim}{H} + \frac{2}{3}(3-2k_1)(3+2k_1)\frac{1}{r^5}\right\}$$

$$= \frac{1}{2}\left[\vec{\sigma}\cdot\hat{r}\frac{1}{r^2}ip_r, 2m\underset{\sim}{H}\right] + \left(\frac{3+k_1}{6}\right)\left[\frac{\vec{\sigma}\cdot\hat{r}'}{r^3}, 2m\underset{\sim}{H}\right] - \frac{1}{3\alpha Z m}\left[\vec{\sigma}\cdot\hat{r}\frac{1}{r}ip_r, 2m\underset{\sim}{H}\right]2m\underset{\sim}{H}$$

$$-\frac{1+k_1}{6\alpha Z m}\left[\frac{\vec{\sigma}\cdot\hat{r}'}{r^2}, 2m\underset{\sim}{H}\right]2m\underset{\sim}{H} + \frac{1}{3(\alpha Z m)^2}\left[\vec{\sigma}\cdot\hat{r}'ip_r, 2m\underset{\sim}{H}\right]\left(2m\underset{\sim}{H}\right)^2 \qquad (28)$$

And this leads to the relation between matrix elements as

$$\left\{5N^2 - l(l+2)\right\}\left\langle l+1\left|\frac{1}{r^4}\right|l\right\rangle - \frac{2}{3}\frac{\alpha Z m}{k^2}(2l-1)(2l+5)\left\langle l+1\left|\frac{1}{r^5}\right|l\right\rangle = 0 \qquad (29)$$

Following the same procedure as above one can build appropriate operators which will lead relations between the $\langle \ell+1|\frac{1}{r^q}|\ell\rangle$'s of higher values.

Section II

Bound States

As shown earlier the vector invariant characteristic of the O(4) group to which the non-relativistic Coulomb field belongs, is the Runge-Lentz-Pauli vector $\vec{a}$. Since the radial matrix element discussed here pertains to a particular subspace of Hilbert space corresponding to principal quantum number N we shall choose the invariant pseudo scalar

"Coulomb helicity operator" as[4]

$$\vec{\sigma}\cdot\vec{a} = \frac{1}{K_\beta^2}\,\vec{\sigma}\cdot\hat{r}\left\{\alpha Z m + i p_r \underset{\sim}{K_1} - \frac{1}{r} K_1^2\right\} \tag{30}$$

and

$$(\vec{\sigma}\cdot\vec{a})\,\Psi_{N\kappa\mu} = \frac{1}{K_\beta^2}\,\vec{\sigma}\cdot\hat{r}\left\{\alpha Z m + i p_r \underset{\sim}{K_1} - \frac{1}{r} K_1^2\right\} F_{NL}\,\chi_\kappa^\mu \tag{31}$$

or

$$(\vec{\sigma}\cdot\vec{a})\,\Psi_{N\kappa\mu} = \frac{1}{K_\beta^2}\left\{\alpha Z m - i p_r K_1 - \frac{K_1^2}{r}\right\} F_{NL}\,\chi_{-\kappa}^\mu$$

$$= -\frac{i}{K_\beta}\, a_\kappa\, F_{NL(-\kappa)}\, i\, \chi_{-\kappa}^\mu$$

$$= -\frac{i}{K_\beta}\, a_\kappa\, \Psi_{N-\kappa\mu} \tag{32}$$

Where we define

$$\Psi_{N-\kappa\mu}(r,\theta,\varphi) = F_{NL(-\kappa)}(r)\, i\, \chi_{-\kappa}^\mu(\theta,\varphi) \tag{33}$$

$$a_\kappa = \left|\sqrt{N^2-\kappa^2}\right| \quad ; \quad K_\beta = \frac{\alpha Z m}{N} \tag{34}$$

And the radial momentum operator

$$p_r = \frac{1}{2}\left(\vec{r}\cdot\vec{p} + \vec{p}\cdot\vec{r}\right) \longleftrightarrow -i\left(\frac{\partial}{\partial r} + \frac{1}{r}\right) \tag{35}$$

$$[\,r, p_r\,] = i \tag{36}$$

We write the non-relativistic Hamiltonian as

$$\underset{\sim}{H} = \frac{\vec{p}^{\,2}}{2m} - \frac{\alpha Z}{r} \tag{37}$$

$$= \frac{p_r^{\,2}}{2m} + \frac{K_1^{\,2} - K_1}{2mr^2} - \frac{\alpha Z}{r} \tag{38}$$

Where α is the Sommerfeld fine structure constant and we choose ($\hbar$ = c = 1).

As a preliminary to the understanding of the Pasternack result we shall give some important operator relationships which are built out of $\vec{\sigma}\cdot\vec{a}$, $\vec{\sigma}\cdot\hat{r}$, $\hat{z}\cdot(\vec{\sigma}\times\vec{L})$ and $\underset{\sim}{K}_1$.

We can easily see that

$$[ip_r, r^q] = q r^{q-1} \quad \text{for any integer q.} \tag{39}$$

And

$$[p_r^{\,2}, r^q] = -q(q-1) r^{q-2} - 2q r^{q-1} ip_r \tag{40}$$

Now we consider the commutation of r^{-q} with $2m\underset{\sim}{H}$,

$$[r^{-q}, 2m\underset{\sim}{H}] = [r^{-q}, p_r^{\,2} + \frac{\vec{L}^2}{r^2} - \frac{2\alpha Zm}{r^2}] \tag{41}$$

therefore we get

$$[r^{-q}, 2m\underset{\sim}{H}] = q(q+1) r^{-q-2} - 2q r^{-q-1} ip_r \tag{42}$$

Taking the expectation value of Equation (42) between the bound state eigenfunction $|N\ell m\rangle$ we get

$$\langle r^{-q} ip_r \rangle = \frac{q}{2} \langle r^{-q-1} \rangle \tag{42a}$$

Also consider

$$\left[i p_r , 2m\underset{\sim}{H} \right] = \left[i p_r , \left(p_r^2 + \frac{K_1^2 - K_1}{r^2} - \frac{2\alpha Z m}{r} \right) \right]$$

$$= \left[\left[r, m\underset{\sim}{H} \right], 2m\underset{\sim}{H} \right]$$

$$= \frac{2\alpha Z m}{r^2} + \frac{2\left(K_1 - K_1^2\right)}{r^3} \qquad (43)$$

So we get

$$\frac{1}{2}\left[\frac{1}{r^q}\left[r, m\underset{\sim}{H} \right], 2m\underset{\sim}{H} \right] = \frac{1}{2}\left[\frac{1}{r^q} i p_r , 2m\underset{\sim}{H} \right]$$

$$= \frac{\alpha Z m}{r^{q+2}} + \frac{q}{r^{q+1}} p_r^2 + \frac{q(q+1)}{2} \frac{1}{r^{q+2}} i p_r + \frac{K_1 - K_1^2}{r^{q+3}} \qquad (44)$$

and substituting

$$p_r^2 = 2m\underset{\sim}{H} + \frac{K_1 - K_1^2}{r^2} + \frac{2\alpha Z m}{r}$$

and

$$\frac{1}{r^{q+2}} i p_r = \frac{q+2}{2} \frac{1}{r^{q+3}} + \frac{1}{2(q+1)}\left[2m\underset{\sim}{H}, \frac{1}{r^{q+1}} \right]$$

we get

$$\frac{1}{2}\left[\frac{1}{r^q} i p_r , 2m\underset{\sim}{H} \right] = \frac{1}{2}\left[\frac{1}{r^q}\left[r, m\underset{\sim}{H} \right], 2m\underset{\sim}{H} \right]$$

$$= \frac{q}{4}\left[2m\underset{\sim}{H}, \frac{1}{r^{q+1}} \right] + \frac{(2q+1)\alpha Z m}{r^{q+2}}$$

$$+ (q+1)\left\{ \frac{q(q+2)}{4} + K_1 - K_1^2 \right\} \frac{1}{r^{q+3}} + \frac{q}{r^{q+1}} 2m\underset{\sim}{H} \qquad (45)$$

or more importantly

$$\frac{1}{2}\left[\frac{1}{r^q}\left[r, 2m\underset{\sim}{H} \right], 2m\underset{\sim}{H} \right] + \frac{q}{4}\left[\frac{1}{r^{q+1}}, 2m\underset{\sim}{H} \right]$$

$$= \frac{q}{r^{q+1}}\left(2m\underset{\sim}{H}\right) + \frac{(2q+1)}{r^{q+2}}\alpha Z m + (q+1)\left\{\frac{q(q+2)}{4} + (K_1 - K_1^2)\right\}\frac{1}{r^{q+3}} \tag{45}$$

Taking the expectation value of both sides with respect to $|N\kappa\mu\rangle$ we see

$$2q_m E_n \left\langle \frac{1}{r^{q+1}} \right\rangle + (2q+1)\alpha Z m \left\langle \frac{1}{r^{q+2}} \right\rangle + (q+1)\left\{\frac{q(q+2)}{4} + l(l+1)\right\}\left\langle \frac{1}{r^{q+3}} \right\rangle = 0 \tag{46}$$

i.e

$$\left(l+1+\frac{q}{2}\right)\left(l-\frac{q}{2}\right)\langle r^{-q-3}\rangle$$

$$= \frac{2q+1}{q+1}\,\frac{Z}{a_0}\langle r^{-q-2}\rangle - \frac{q}{q+1}\,\frac{Z^2}{n a_0^2}\langle r^{-q-1}\rangle \tag{47}$$

where q is either positive or negative integer or zero. So we see that without any appeal to the properties of the contiguous relations of the hydrogenic wave functions we can get the recursion relation by purely operator algebra.

The invariant operator $\underset{\sim}{K}_1$ anticommutes with $\vec{\sigma}\cdot\hat{r}$ and $\vec{\sigma}\cdot\vec{a}$. Using this property the following operator relations are easily established

$$[\vec{\sigma}\cdot\hat{r}, \underset{\sim}{\beta}] = 2K_1\,\vec{\sigma}\cdot\hat{r}\,\frac{1}{r^2} \qquad \text{where } \beta = 2m\underset{\sim}{H} \tag{48}$$

$$\frac{\vec{\sigma}\cdot\hat{r}}{2(q-1)}\left[\underset{\sim}{\beta}, \frac{\vec{\sigma}\cdot\hat{r}}{r^{q-1}}\right] = \frac{1}{r^q} i p_r + \left(\frac{K_1}{q-1} - \frac{q}{2}\right)\frac{1}{r^{q+1}} \qquad (q \neq 0,\ q \neq 1) \tag{49}$$

And

$$\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^{q-1}} i p_r, \underset{\sim}{\beta}\right] + \left[\frac{q(q-1)+2K_1}{2q}\right]\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^q}, \underset{\sim}{\beta}\right]$$

$$= \vec{\sigma}\cdot\hat{r}\left\{2(q-1)\frac{1}{r^q}\underset{\sim}{\beta} + 2\alpha Z m(2q-1)\frac{1}{r^{q+1}} + \frac{1}{2q}\,\frac{(q^2-1)(q^2-4K_1^2)}{r^{q+2}}\right\} \tag{50}$$

Taking the matrix element

$$\left(\Psi_{N-\kappa\mu} \; (\text{eqn } 50) \; \Psi_{N\kappa\mu} \right)$$

we obtain the following recursion relation for the bound state radial matrix elements which is of frequent use in the rest of the thesis.

$$q(q-2)\left(l+\frac{1}{2}-\frac{q}{2}\right)\left(l+\frac{3}{2}-\frac{q}{2}\right)\left\langle l+1\left|\frac{1}{r^{q+1}}\right| l\right\rangle$$
$$-\alpha Z m\,(q-1)(2q-3)\left\langle l+1\left|\frac{1}{r^{q}}\right| l\right\rangle$$
$$+K_\beta^2\,(q-2)(q-1)\left\langle l+1\left|\frac{1}{r^{q-1}}\right| l\right\rangle = 0 \quad (51)$$

where q is positive integer or zero. The angular operator $\Omega_0 \equiv \hat{z}\cdot(\vec{\sigma}\times\vec{L})$ changes κ to $-\kappa -1$ without affecting the radial part of the function $\Psi_{N\kappa\mu}$ and it commutes with $\underset{\sim}{\beta}$, while it anticommutes with $(2\underset{\sim}{K}_1-1)$. The operators $\vec{\sigma}\cdot\vec{a}\;\Omega_0$ and $\Omega_0\;\vec{\sigma}\cdot\vec{a}$ raise or lower the ℓ values or more precisely κ values of the operand and $\Psi_{N\kappa\mu}$ respectively. The angular operators $\vec{\sigma}\cdot\hat{r}\;\Omega_0$ and $\Omega_0\;\vec{\sigma}\cdot\hat{r}$ preserve the ℓ value of the radial function while changing K_1 to $K_1 + 1$ and $K_1 - 1$ respectively. For completeness we give below what these operators do to the bound state wave functions $\Psi_{N\kappa\mu}$ and $\Psi_{N-\kappa\mu}$ respectively, confining our attention to say $j = 1 - \frac{1}{2}$.

$$\vec{\sigma}\cdot\vec{a}\,\Psi_{N\kappa\mu} = -i\,\frac{a_\kappa}{K_\beta}\,\Psi_{N-\kappa\mu} \quad \text{where } a_\kappa = \left|\sqrt{N^2-\kappa^2}\right| \quad (52)$$

$$\vec{\sigma}\cdot\vec{a}\,\Omega_0\,\Psi_{N\kappa\mu} = i\,\frac{a_{l+1}}{k_\beta}\sqrt{l(l+1)}\;C^{l-\frac{1}{2}\;\;1\;\;l+\frac{1}{2}}_{\mu\;\;0\;\;\mu}\;\Psi_{N\kappa+1,\mu} \quad (53)$$

$$\Omega_0\,\vec{\sigma}\cdot\vec{a}\,\Psi_{N\kappa\mu}$$
$$= i\,\frac{a_l}{K_\beta}\sqrt{l(2l-1)}\;C^{l-\frac{1}{2}\;\;1\;\;l-\frac{3}{2}}_{\mu\;\;0\;\;\mu}\;\Psi_{N+(\kappa-1)\mu} \quad (54)$$

$$\Omega_0 \Psi_{N\kappa\mu} = \sqrt{l(2l+1)}\; C^{l-\frac{1}{2}\;1\;l+\frac{1}{2}}_{\mu\;0\;\mu}\; \Psi_{N-(\kappa+1)\mu} \tag{55}$$

$$\vec{\sigma}\cdot\hat{r}\,\Omega_0 \Psi_{N\kappa\mu} = -i\sqrt{l(2l+1)}\; C^{l-\frac{1}{2}\;1\;l+\frac{1}{2}}_{\mu\;0\;\mu}\; F_{Nl\,(\kappa)}^{(r)}\, \chi^{\mu}_{\kappa+1} \tag{56}$$

$$\Omega_0\, \vec{\sigma}\cdot\hat{r}\, \Psi_{N\kappa\mu} = \sqrt{l(2l-1)}\; C^{l-\frac{1}{2}\;1\;l-\frac{3}{2}}_{\mu\;0\;\mu}\; F_{Nl(\kappa)}\, \chi^{\mu}_{\kappa-1} \tag{57}$$

And the relation for $\Psi_{N-\kappa\mu}$ are

$$\vec{\sigma}\cdot\vec{a}\, \Psi_{N-\kappa\mu} = -i\, \frac{a_{-\kappa}}{k_B}\, \Psi_{N\kappa\mu} \tag{58a}$$

$$\Omega_0 \Psi_{N-\kappa\mu} = -\sqrt{l(2l-1)}\; C^{l-\frac{1}{2}\;1\;l-\frac{3}{2}}_{\mu\;0\;\mu}\; \Psi_{N\kappa-1\mu} \tag{58b}$$

$$\vec{\sigma}\cdot\vec{a}\,\Omega_0 \Psi_{N-\kappa\mu} = \frac{i a_{l-1}}{k_B}\sqrt{l(2l-1)}\; C^{l-\frac{1}{2}\;1\;l-\frac{3}{2}}_{\mu\;0\;\mu}\; \Psi_{N-(\kappa-1)\mu} \tag{59}$$

$$\Omega_0\, \vec{\sigma}\cdot\vec{a}\, \Psi_{N-\kappa\mu} = \frac{i a_l}{k_B}\sqrt{l(2l+1)}\; C^{l-\frac{1}{2}\;1\;l+\frac{1}{2}}_{\mu\;0\;\mu}\; \Psi_{N-(\kappa+1)\mu} \tag{60}$$

$$\Omega_0\, \vec{\sigma}\cdot\hat{r}\, \Psi_{N-\kappa\mu} = \sqrt{l(2l+1)}\; C^{l-\frac{1}{2}\;1\;l+\frac{1}{2}}_{\mu\;0\;\mu}\; F_{Nl-1}\, \chi^{\mu}_{-\kappa-1} \tag{61}$$

$$\vec{\sigma}\cdot\hat{r}\,\Omega_0 \Psi_{N-\kappa\mu} = -\sqrt{l(2l-1)}\; C^{l-\frac{1}{2}\;1\;l-\frac{3}{2}}_{\mu\;0\;\mu}\; F_{Nl-1}\, i\chi^{\mu}_{-\kappa+1} \tag{62}$$

$\Psi_{N-\kappa\mu}$ are defined by $\Psi_{N-\kappa\mu} = F_{N\ell(-\kappa)}\, i\chi_{-\kappa}^{\mu}$ with the help of these results we now proceed to a formal proof of the Pasternack Sternheimer result.

Proof for the Vanishing of $\langle \ell+1 | \frac{1}{r^2} | \ell \rangle$

Consider the matrix element

$$\left(\Psi_{N-\kappa-2,\mu}, \left\{\vec{\sigma}\cdot\vec{a}\,\Omega_0\right\}^0 \left\{\Omega_0\,\vec{\sigma}\cdot\hat{r}\right\}^1 \frac{1}{r^2}\,\vec{\sigma}\cdot\vec{a}\,\Psi_{N\kappa+1\mu}\right) \tag{63}$$

If we take κ positive it is then easy to see that the above equation leads to

$$\sqrt{(l+2)(2l+3)}\; C^{l+\frac{3}{2}\; 1\; l+\frac{1}{2}}_{\mu\; 0\; \mu}\; \frac{a_{l+1}}{K_\beta^2} \left\langle l+1 \left| \frac{1}{r^2} \right| l \right\rangle \tag{64}$$

On the other hand

$$\Omega_0 \frac{1}{r^2}\,\vec{\sigma}\cdot\hat{r}\;\vec{\sigma}\cdot\vec{a} = \frac{1}{K_\beta^2}\,\Omega_0 \frac{1}{r^2}\left\{\alpha Z m + i p_r K_1 - \frac{1}{r} K_1^2\right\} \tag{65}$$

$$= \frac{1}{r^2}\,\vec{\sigma}\cdot\hat{r}\;\vec{\sigma}\cdot\vec{a}\;\Omega_0 + \frac{1}{K_\beta^2}\left(\frac{1}{r^2}\, i p_r - \frac{1}{r^3}\right)\left(1-2K_1\right)\Omega_0 \tag{66}$$

where we made use of the commutation relation between Ω_0 and K_1, $1/r^q$ and ip_r by means of the Equations 10 and 16 (Section I). We see that

$$\left(\frac{1}{r^2}\, i p_r - \frac{1}{r^3}\right) = \frac{1}{2}\left[\mathcal{L}, \frac{1}{r}\right] \text{ and} \tag{67}$$

$$\vec{\sigma}\cdot\hat{r}\,\frac{1}{r^2} = \frac{1}{2\alpha Z m}\left[\frac{1}{2}\left[\vec{\sigma}\cdot\hat{r}, \mathcal{L}\right], \mathcal{L}\right] \tag{68}$$

The operator under consideration is then

$$\left\{ \vec{\sigma}\cdot\vec{a}\,\Omega_0 \right\}^0 \left\{ \Omega_0\, \vec{\sigma}\cdot\hat{r} \right\}^1 \frac{1}{r^2}\, \vec{\sigma}\cdot\vec{a}$$

$$= \frac{1}{2}\left[\underset{\sim}{\beta}, \frac{1}{r} \right](1-2\kappa_1) + \frac{1}{2\alpha Z m}\left[\frac{1}{2}\left[\vec{\sigma}\cdot\hat{r}\,\underset{\sim}{\beta} \right], \underset{\sim}{\beta} \right]_{\vec{\sigma}\cdot\vec{a}} \tag{69}$$

Hence the matrix element

$$\left(\Psi_{N-\kappa-2,\mu}\ \Omega_0\ \vec{\sigma}\cdot\hat{r}\ \frac{1}{r^2}\ \vec{\sigma}\cdot\vec{a}\ \Psi_{N\kappa+1\,\mu} \right) \tag{70}$$

The right hand side vanishes because it is the matrix element of commutators with the Hamiltonian and the expectation value of the commutator of any operator with the Hamiltonian taken with respect to the eigenstates of the latter, vanishes. Hence the left hand side vanishes and we get

$$\left\langle l+1 \right| \frac{1}{r^2} \left| l \right\rangle = 0$$

For the next step we consider the operator

$$\left(\vec{\sigma}\cdot\vec{a}\,\Omega_0 \right)^1 \left(\Omega_0\, \vec{\sigma}\cdot\hat{r} \right)^2 \frac{1}{r^q}\, \vec{\sigma}\cdot\vec{a} \tag{71}$$

The matrix element of this operator between $\Psi_{N-(\kappa+2)\mu}$ and $\Psi_{N\kappa+1\mu}$ is

$$\left(\Psi_{N-\kappa-2,\mu}, \vec{\sigma}\cdot\vec{a}\,\Omega_0\,\Omega_0\,\vec{\sigma}\cdot\hat{r}\,\Omega_0\,\vec{\sigma}\cdot\vec{r}\ \frac{1}{r^q}\ \vec{\sigma}\cdot\vec{a}\ \Psi_{N\kappa+1\,\mu} \right) \tag{72}$$

$$= i\,\frac{a_{l+2}}{K_\beta^2}\sqrt{(2l+3)(l+3)(2l+5)}\; C^{l+\frac{1}{2}\ 1\ l+\frac{3}{2}}_{\mu\ 0\ \mu}\; C^{l+\frac{3}{2}\ 1\ l+\frac{1}{2}}_{\mu\ 0\ \mu}$$

$$(l+2)a_{l+1}\, C^{l+\frac{5}{2}\ 1\ l+\frac{3}{2}}_{\mu\ 0\ \mu} \int_0^\infty F_{Nl+2} \frac{1}{r^q} F_{Nl}\, r^2 dr \tag{73}$$

Since Ω_0 commutes with the Hamiltonian we can factor out $\Omega_0^{\ 2}$ by using the commutation relation

$$\left[\vec{\sigma}\cdot\vec{a}, \Omega_0^2\right] = 2K_1\, \vec{\sigma}\cdot\vec{a} \tag{74}$$

and also

$$\vec{\sigma}\cdot\hat{r}\ \Omega_0 \Omega_0\, \vec{\sigma}\cdot\hat{r} = \underset{\sim}{\varnothing} = \Omega_0^{\ 2} + 2K_1 \tag{75}$$

$$\left[\vec{\sigma}\cdot\vec{a}\ \vec{\sigma}\cdot\hat{r},\ \vec{\sigma}\cdot\hat{r}\ \Omega_0 \Omega_0\, \vec{\sigma}\cdot\hat{r}\right] = 0 \tag{76}$$

The operator can now be written as

$$\vec{\sigma}\cdot\vec{a}\ \Omega_0 \Omega_0\ \vec{\sigma}\cdot\hat{r}\ \Omega_0\, \vec{\sigma}\cdot\hat{r}\ \frac{1}{r^q}\vec{\sigma}\cdot\vec{a} = \underset{\sim}{\varnothing}\ \vec{\sigma}\cdot\vec{a}\ \frac{\vec{\sigma}\cdot\hat{r}\ \Omega_0\ \vec{\sigma}\cdot\hat{r}}{r^q}\ \vec{\sigma}\cdot\vec{a} \tag{77}$$

The procedure hereafter consists of the following general steps. We expand $\vec{\sigma}\cdot\vec{a}\ \vec{\sigma}\cdot\hat{r}$, take Ω_0 to the extreme right and replace $\frac{1}{r^q}\, ip_r$ or $\vec{\sigma}\cdot\hat{r}\ \frac{1}{r^q}\, ip_r$ by appropriate commutators with the Hamiltonian and reduce the operator, after picking out commutators with H, to a sum of terms like $\left(\frac{\text{a factor}}{r^q}\right)$. So the operator becomes

$$\text{Operator} \equiv \vec{\sigma}\cdot\vec{a}\ \vec{\sigma}\cdot\hat{r}\left\{\frac{1}{r^q}\vec{\sigma}\cdot\hat{r}\ \vec{\sigma}\cdot\vec{a} + \frac{1}{K_B^{\ 2}}\left(\frac{1}{r^q}\, ip_r - \frac{1}{r^{q+1}}\right)(1-2K_1)\right\}\Omega_0$$

Expanding

$$\frac{1}{r^q}\vec{\sigma}\cdot\hat{r}\ \vec{\sigma}\cdot\vec{a} = \frac{1}{K_B^{\ 2}}\left(\frac{\alpha Z m}{r^q} + \frac{1}{r^q}\, ip_r \underset{\sim}{K_1} - \frac{K_1^{\ 2}}{r^{q+1}}\right) \tag{78}$$

and rearranging the terms we get

$$\text{Operator} \equiv \underset{\sim}{\mathcal{D}} \frac{\vec{\sigma}\cdot\vec{a}\,\vec{\sigma}\cdot\hat{r}}{K_B^2}\left\{\frac{\alpha Z m}{r^q} + \frac{1}{r^q} i p_r (1-K_1) - (1-K_1^2)\frac{1}{r^{q+1}}\right\}\Omega_0 \tag{79}$$

Now

$$\vec{\sigma}\cdot\hat{r}\,\frac{1}{r^q} i p_r (1-K_1)$$
$$= \frac{1}{2(q-1)}\left[\beta, \frac{\vec{\sigma}\cdot\hat{r}}{r^q}\right](1-K_1) + \vec{\sigma}\cdot\hat{r}\left(\frac{q}{2} - \frac{K_1}{q-1}\right)\frac{1-K_1}{r^{q+1}} \tag{80}$$

When q = 2 we know that

$$\alpha Z m\, \vec{\sigma}\cdot\hat{r}\,\frac{1}{r^2} = \frac{1}{2}\left[\frac{1}{2}\left[\vec{\sigma}\cdot\hat{r}, \underset{\sim}{\beta}\right]\underset{\sim}{\beta}\right]$$

we get when q = 2, the operator

$$\underset{\sim}{O} \equiv \underset{\sim}{\mathcal{D}}\,\vec{\sigma}\cdot\vec{a}\,\frac{1}{2(q-1)K_B^2}\left[2m\underset{\sim}{H}, \frac{\vec{\sigma}\cdot\hat{r}}{r^{q-1}}\right](1-K_1)\Omega_0$$
$$+ \frac{\vec{\sigma}\cdot\vec{a}}{K_B^2}\,\vec{\sigma}\cdot\hat{r}\left\{\frac{\alpha Z m}{r^q} + \frac{q-2}{2}\left(\frac{(q-1)-(q-3)K_1}{q-1} - \frac{2K_1^2}{q-1}\right)\frac{1}{r^{q+1}}\right\}\Omega_0$$

gives

$$\vec{\sigma}\cdot\vec{a}\,\Omega_0\,\Omega_0\,\vec{\sigma}\cdot\hat{r}\,\Omega_0\,\vec{\sigma}\cdot\hat{r}\,\frac{1}{r^2}\,\vec{\sigma}\cdot\vec{a}$$
$$= \underset{\sim}{\mathcal{D}}\,\vec{\sigma}\cdot\vec{a}\,\frac{1}{2K_B^2}\left[2m\underset{\sim}{H}, \frac{\vec{\sigma}\cdot\hat{r}}{r}\right](1-K_1)\Omega_0$$
$$+ \mathcal{D}\,\frac{\vec{\sigma}\cdot\vec{a}}{K_B^2}\,\frac{1}{2}\left[\frac{1}{2}\left[\vec{\sigma}\cdot\hat{r}, \underset{\sim}{\beta}\right], \underset{\sim}{\beta}\right]\Omega_0 \tag{81}$$

Hence taking the matrix element between $\Psi_{N-\kappa-2\mu}$ and $\Psi_{N\kappa+1\mu}$ we get the left hand side as zero so we have

$$\left\langle l+2 \left| \frac{1}{r^2} \right| l \right\rangle = 0$$

When q = 3

Numerically this leads to

$$\alpha Z m \left\langle l+2 \left| \frac{1}{r^3} \right| l+1 \right\rangle - \frac{(l+1)(l+3)}{2}\left\langle l+2 \left| \frac{1}{r^4} \right| l+1 \right\rangle \tag{82}$$

which is seen to be zero from relation 16. Therefore operatorwise we get

$$\vec{\sigma}\cdot\hat{r}\left\{\frac{\alpha Z m}{r^3}-\frac{k_1^2-1}{2}\frac{1}{r^4}\right\}$$

$$=\frac{1}{3}\left\{\left[\vec{\sigma}\cdot\vec{r}\,\frac{1}{r}\,ip_r\,,\underset{\sim}{\beta}\right]+\left(\frac{k_1+1}{2}\right)\left[\frac{\vec{\sigma}\cdot\vec{r}}{r^2},\underset{\sim}{\beta}\right]\right.$$

$$-\frac{1}{\alpha Z m}\left[\vec{\sigma}\cdot\vec{r}\,ip_r\,,\underset{\sim}{\beta}\right]2m\underset{\sim}{H}$$

$$\left.-2k_1\left[\frac{\vec{\sigma}\cdot\vec{r}}{r},\underset{\sim}{\beta}\right]\right\} \tag{83}$$

Collecting all terms we get

$$\text{Operator}=\underset{\sim}{\mathcal{D}}\,\frac{\vec{\sigma}\cdot\vec{a}}{k_B^2}\left\{\frac{1}{4}\left[\underset{\sim}{\beta},\frac{\vec{\sigma}\cdot\vec{r}}{r^2}\right](1-\underset{\sim}{k_1})\right.$$

$$+\frac{1}{3}\left[\vec{\sigma}\cdot\hat{r}\,\frac{1}{r}\,ip_r\,,\underset{\sim}{\beta}\right]+\frac{k_1+1}{6}\left[\frac{\vec{\sigma}\cdot\vec{r}}{r^2},\underset{\sim}{\beta}\right]$$

$$\left.-\left(\frac{1}{3\alpha Z m}\left[\vec{\sigma}\cdot\vec{r}\,ip_r,\underset{\sim}{\beta}\right]+\frac{2}{3}\underset{\sim}{k_1}\left[\frac{\vec{\sigma}\cdot\vec{r}}{r},\underset{\sim}{\beta}\right]\right)\beta\right\}\Omega_0 \tag{84}$$

Since all are commutators with the Hamiltonian the matrix element vanish. So we get

$$\left\langle l+2\right|\frac{1}{r^3}\left|l\right\rangle=0$$

We thus see that the operator

$$\vec{\sigma}\cdot\vec{a}\,\Omega_0\,\Omega_0\,\vec{\sigma}\cdot\vec{r}\,\Omega_0\,\vec{\sigma}\cdot\hat{r}\,\frac{1}{r^q}\,\vec{\sigma}\cdot\vec{a}$$

leads to

$$\left\langle l+2\right|\frac{1}{r^q}\left|l\right\rangle=0,$$ when q = 2,3.

Proof for $\langle \ell+3|\frac{1}{r^q}|\ell\rangle$ for q = 2,3,4

Now consider the operator

$$(\sigma . a\, \Omega_0)^2 (\Omega_0\, \vec{\sigma} . \vec{r})^3 \frac{1}{r^q}\, \vec{\sigma} . \vec{a} \tag{85}$$

The matrix element of this operator

$$\left(\Psi_{N-K-2\,\mu} (\vec{\sigma}.\vec{a}\,\Omega_0)(\Omega_0 \vec{\sigma}.\hat{r})^3 \frac{1}{r^q} \vec{\sigma}.\vec{a}\, \Psi_{NK+1\mu}\right)$$
$$= -iK_B^{-3} a_{\ell+1} a_{\ell+2} a_{\ell+3} (\ell+2)(\ell+3)(2\ell+5)(2\ell+7)\sqrt{\frac{(\ell+4)}{(2\ell+3)}}$$
$$\cdot C^{\ell+\frac{3}{2}\ 1\ \ell+\frac{5}{2}}_{\mu\ 0\ \mu} \cdot C^{\ell+\frac{5}{2}\ 1\ \ell+\frac{7}{2}}_{\mu\ 0\ \mu} \cdot C^{\ell+\frac{7}{2}\ 1\ \ell+\frac{5}{2}}_{\mu\ 0\ \mu}$$
$$\cdot C^{\ell+\frac{5}{2}\ 1\ \ell+\frac{3}{2}}_{\mu\ 0\ \mu}\ C^{\ell+\frac{3}{2}\ 1\ \ell+\frac{1}{2}}_{\mu\ 0\ \mu} \langle \ell+3|\frac{1}{r^q}|\ell\rangle$$
$$= (\text{numerical factor}) \langle \ell+3|\frac{1}{r^q}|\ell\rangle \tag{86}$$

Now we consider

$$\vec{\sigma}.\vec{a}\,\Omega_0\, \vec{\sigma}.\vec{a}\,(\Omega_0\,\Omega_0 \vec{\sigma}.\hat{r})\,\Omega_0\, \vec{\sigma}.\hat{r}$$
$$\Omega_0\, \vec{\sigma}\,\hat{r}\, \frac{1}{r^q}\, \vec{\sigma}.\vec{a}$$
$$= \vec{\sigma}.\vec{a}\,\Omega_0\, \underset{\sim}{\mathcal{D}}\, (\vec{\sigma}.\vec{a}\,\vec{\sigma}.\hat{r}\,\Omega_0)\,\vec{\sigma}.\hat{r}\,(\Omega_0\,\vec{\sigma}.\hat{r}\,\frac{1}{r^q}\,\vec{\sigma}.\vec{a}) \tag{87}$$

We bring Ω_0 in the first bracket to the left while in the second bracket to the right using the relations 14 and 15 (Section II) that is,

$$\vec{\sigma}\cdot\vec{a}\;\vec{\sigma}\cdot\hat{r}\,\Omega_0 = \Omega_0\,\vec{\sigma}\cdot\vec{a}\;\vec{\sigma}\cdot\hat{r} + \left(ip_r + \frac{1}{r}\right)\Omega_0(2K_1 - 1)$$

and

$$\Omega_0 \frac{1}{r^q}\,\vec{\sigma}\cdot\hat{r}\,\vec{\sigma}\cdot\vec{a} = \frac{1}{r^q}\vec{\sigma}\cdot\hat{r}\,\vec{\sigma}\cdot\vec{a}\,\Omega_0 + \frac{1}{K_B^2}(1 - 2\underset{\sim}{K_1})\left(\frac{1}{r^q}ip_r - \frac{1}{r^{q+1}}\right)\Omega_0 \tag{88}$$

With these substitutions the operator becomes

$$\vec{\sigma}\cdot\vec{a}\,\Omega_0\,\underset{\sim}{\mathcal{O}}\,\Omega_0\left\{\vec{\sigma}\cdot\vec{a}\;\vec{\sigma}\cdot\hat{r} + \frac{1}{k_B^2}\left(ip_r + \frac{1}{r}\right)(2K_1 - 1)\right\}\vec{\sigma}\cdot\hat{r}$$
$$\cdot\left\{\frac{1}{r^q}\vec{\sigma}\cdot\hat{r}\,\vec{\sigma}\cdot\vec{a} + \frac{1}{k_B^2}(1 - 2K_1)\left(\frac{1}{r^q}ip_r - \frac{1}{r^{q+1}}\right)\right\}\Omega_0 \tag{89}$$

$$= \vec{\sigma}\cdot\vec{a}\,\underset{\sim}{\mathcal{O}}'\left\{\vec{\sigma}\cdot\vec{a}\,\frac{1}{r^q}\,\vec{\sigma}\cdot\hat{r}\,\vec{\sigma}\cdot\vec{a} + \frac{1}{k_B^2}\vec{\sigma}\cdot\vec{a}\left(\frac{1}{r^q}ip_r - \frac{1}{r^{q+1}}\right)(1 - 2K_1)\right.$$
$$+ \frac{1}{k_B^2}\left(ip_r + \frac{1}{r}\right)\frac{1}{r^q}(2K_1 - 1)\,\vec{\sigma}\cdot\vec{a}$$
$$\left. + \frac{1}{k_B^4}\,\vec{\sigma}\cdot\hat{r}\left(ip_r + \frac{1}{r}\right)\left(\frac{1}{r^q}ip_r - \frac{1}{r^{q+1}}\right)(4K_1^2 - 1)\right\}\Omega_0 \tag{90}$$

Now

$$\frac{1}{r^q}\vec{\sigma}\cdot\hat{r}\,\vec{\sigma}\cdot\vec{a} = \frac{1}{k_B^2}\left\{\frac{\alpha Z m}{r^q} + \left(\frac{q}{2}K_1 - K_1^2\right)\frac{1}{r^{q+1}}\right\} - \frac{1}{2k_B^2(q-1)}\left[\frac{1}{r^{q-1}}, \underset{\sim}{\beta}\right]\underset{\sim}{K_1}$$

and

$$\left(\frac{1}{r^q}ip_r - \frac{1}{r^{q+1}}\right) = \left(\frac{q-2}{2}\right)\frac{1}{r^{q+1}} + \frac{1}{2(q-1)}\left[\underset{\sim}{\beta}, \frac{1}{r^{q-1}}\right]$$

In the third term

$$\frac{1}{r^q}ip_r + \frac{1-q}{r^{q+1}} = \frac{2-q}{2}\,\frac{1}{r^{q+1}} + \frac{1}{2(q-1)}\left[\underset{\sim}{\beta}, \frac{1}{r^{q-1}}\right]$$

and also

$$\vec{\sigma}\cdot\hat{r}\left(ip_r+\frac{1}{r}\right)\left(\frac{1}{r^{\gamma}}ip_r-\frac{1}{r^{\gamma+1}}\right)=\vec{\sigma}\cdot\hat{r}\left(-\frac{1}{r^{\gamma}}p_r^2-\frac{\gamma}{r^{\gamma+1}}ip_r+\frac{\gamma}{r^{\gamma+2}}\right)$$

Now using the relations 8 and 10 we get

$$=\left\{\frac{1}{2(\gamma-1)}\left[\underset{\sim}{\beta},\vec{\sigma}\cdot\hat{r}\frac{1}{r^{\gamma}}ip_r\right]+\frac{1}{4}\left[\vec{\sigma}\cdot\hat{r}\frac{1}{r^{\gamma}},\underset{\sim}{\beta}\right]+\frac{K_1}{2\gamma(\gamma-1)}\left[\underset{\sim}{\beta},\frac{\vec{\sigma}\cdot\hat{r}}{r^{\gamma}}\right]\right\}$$

$$+\vec{\sigma}\cdot\hat{r}\left\{\frac{\alpha Zm}{\gamma-1}\frac{1}{r^{\gamma+1}}+\frac{\gamma(3-\gamma)}{4\,r^{\gamma+2}}-\frac{K_1^2}{\gamma}\frac{1}{r^{\gamma+1}}\right\}$$

Hence the operator

$$=\vec{\sigma}\cdot\vec{a}\;\varpi'\left\{\vec{\sigma}\cdot\vec{a}\frac{1}{2k_B^2(1-\gamma)}\left[\frac{1}{r^{\gamma}},\underset{\sim}{\beta}\right]\underset{\sim}{K_1}+\frac{1}{k_B^2}\vec{\sigma}\cdot\vec{a}\frac{1}{\alpha(\gamma-1)}\cdot\right.$$

$$\cdot\left[\underset{\sim}{\beta},\frac{1}{r^{\gamma-1}}\right](1-2K_1)+\frac{1}{k_B^2}\frac{1}{2(\gamma-1)}\left[\underset{\sim}{\beta},\frac{1}{r^{\gamma-1}}\right](2K_1-1)\vec{\sigma}\cdot\vec{a}$$

$$+\frac{1}{k_B^2}\left(\frac{1}{2(\gamma-1)}\left[\underset{\sim}{\beta},\vec{\sigma}\cdot\hat{r}\frac{1}{r^{\gamma}}ip_r\right]+\frac{1}{4}\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^{\gamma}},\underset{\sim}{\beta}\right]\right.$$

$$\left.\left.+\frac{K_1}{2\gamma(\gamma-1)}\left[\underset{\sim}{\beta},\vec{\sigma}\cdot\hat{r}\frac{1}{r^{\gamma}}\right]\right)(4K_1^2-1)\right\}\Omega_0$$

$$+\vec{\sigma}\cdot\vec{a}\;\underset{\sim}{\varpi}'\left\{\frac{1}{k_B^2}\vec{\sigma}\cdot\vec{a}\left(\frac{\alpha Zm}{r^{\gamma}}+\left(\frac{\gamma K_1}{2}-K_1^2\right)\frac{1}{r^{\gamma+1}}\right)\right.$$

$$+\frac{\vec{\sigma}\cdot\vec{a}}{k_B^2}\frac{(\gamma-2)}{2}\frac{(1-2K_1)}{r^{\gamma+1}}+\frac{1}{k_B^2}\vec{\sigma}\cdot\vec{a}\left(\frac{\gamma-2}{2}\right)\frac{1-2K_1}{r^{\gamma+1}}\vec{\sigma}\cdot\vec{a}$$

$$+\frac{1}{k_B^2}\vec{\sigma}\cdot\vec{a}\left(\frac{\gamma-2}{2}\right)\frac{1}{r^{\gamma+1}}(1-2K_1)\vec{\sigma}\cdot\vec{a}$$

$$\left.+\vec{\sigma}\cdot\hat{r}\left(\frac{\alpha Zm}{\gamma-1}\frac{1}{r^{\gamma+1}}+\left(\frac{\gamma(3-\gamma)}{4}-\frac{K_1^2}{\gamma}\right)\frac{1}{r^{\gamma+2}}\right)(4K_1^2-1)\right\}\Omega_0 \tag{91}$$

We see that the first six terms are commutators with the Hamiltonian and do not pose any difficulty. The term to be worried about is

$$\frac{1}{k_B^2}\vec{\sigma}\cdot\vec{a}\left\{\frac{\alpha Zm}{r^{\gamma}}+\left(\frac{\gamma}{2}k_1-k_1^2\right)\frac{1}{r^{\gamma+1}}+\frac{\gamma-2}{\alpha}(1-2k_1)\frac{1}{r^{\gamma+1}}\right\}$$

$$+\frac{1}{k_B^2}\left(\frac{2-\gamma}{\alpha}\right)\frac{1}{r^{\gamma+1}}(2k_1-1)\,\vec{\sigma}\cdot\vec{a}$$

$$+\frac{\vec{\sigma}\cdot\hat{r}}{k_B^4}\left\{\frac{\alpha Zm}{\gamma-1}\frac{1}{r^{\gamma+1}}+\left(\frac{\gamma(3-\gamma)}{4}-\frac{k_1^2}{\gamma}\right)\frac{1}{r^{\gamma+2}}\right\}(4k_1^2-1)$$

Making use of commutation relation between $\vec{\sigma}\cdot\vec{a}$ and $\frac{1}{r^q}$ this can be written as

$$\frac{1}{k_B^2}\vec{\sigma}\cdot\vec{a}\left\{\frac{\alpha Zm}{r^{\gamma}}+\left[(\gamma-2)+\frac{\gamma k_1}{2}-k_1^2\right]\frac{1}{r^{\gamma+1}}\right\}$$

$$+\frac{\vec{\sigma}\cdot\hat{r}}{k_B^4}\left\{\left(\frac{\gamma(\gamma-3)}{4}+\frac{(\gamma+1)(\gamma-2)}{2}k_1+\left[2(\gamma-1)+\frac{1}{\gamma}\right]k_1^2-\frac{4k_1^2}{\gamma}\right)\right\}\frac{1}{r^{\gamma+2}}$$

$$+\frac{\alpha Zm(4k_1^2-1)}{\gamma-1}\frac{1}{r^{\gamma+1}}$$

Now

$$\vec{\sigma}\cdot\vec{a}\,\frac{1}{r^{\gamma}}=\frac{\vec{\sigma}\cdot\hat{r}}{k_B^2}\left\{\frac{\alpha Zm}{r^{\gamma}}-\left[\frac{\gamma}{2}k_1+\left(\frac{\gamma}{\gamma-1}\right)k_1^2\right]\frac{1}{r^{\gamma+1}}\right\}$$

$$+\frac{1}{2(\gamma-1)}\frac{1}{k_B^2}\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^{\gamma-2}},\,\underset{\sim}{\beta}\right]$$

We therefore pick out few more commutators with Hamiltonian namely,

$$\frac{1}{k_B^4}\frac{\alpha Z m}{\alpha(q-1)}\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^{q-2}},\ \underset{\sim}{\beta}\right]+\frac{1}{k_B^4\,2q}\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^{q-1}},\underset{\sim}{\beta}\right]\left((q-2)+\frac{q}{2}k_1-k_1^2\right)$$

and absorb all the factors multiplying $\vec{\sigma}\cdot\hat{r}$ as

$$\frac{1}{k_B^4}\vec{\sigma}\cdot\hat{r}\left\{\frac{(\alpha Z m)^2}{r^q}+\alpha Z m\left(\frac{q^2-3q+1}{q-1}+\frac{5-2q}{q-1}k_1^2\right)\frac{1}{r^{q+1}}\right.$$

$$\left.+(q-3)\left(\frac{q}{4}-\frac{q^2+4}{4q}k_1^2+\frac{k_1^2}{q}\right)\frac{1}{r^{q+2}}\right\} \tag{92}$$

Collecting different terms we get

$$\text{Operator} = \vec{\sigma}\cdot\vec{a}\ \underset{\sim}{\varpi}'\left\{\left(\sum_i \text{Commutators}\right)\right.$$

$$+\frac{\vec{\sigma}\cdot\hat{r}}{k_B^4}\left\{\frac{(\alpha Z m)^2}{r^q}+\alpha Z m\left(\frac{q^2-3q+1}{q-1}+\frac{5-2q}{q-1}k_1^2\right)\frac{1}{r^{q+1}}\right.$$

$$\left.\left.+(q-3)\left[\frac{q}{4}-\frac{q^2+4}{4\cdot q}k_1^2+\frac{k_1}{q}\right]\frac{1}{r^{q+2}}\right\}\right\}\Omega_0 \tag{93}$$

for q = 2,3,4, Equation (92) can also be written as commutation with the Hamiltonian. Thus the operator

$$(\sigma\cdot a\,\Omega_0)^2\left\{(\Omega_0\,\vec{\sigma}\cdot\hat{r})^3\frac{1}{r^q}\vec{\sigma}\cdot\vec{a}\right\}$$

happens to be

$$\varpi''\vec{\sigma}\cdot\vec{a}\left(\sum_i O_{q_i}\right)\Omega_0 \tag{94}$$

where $$\underset{\sim}{\mathcal{D}}'' = \vec{\sigma}\cdot\hat{r}\,\Omega_0\,\underset{\sim}{\mathcal{D}}\,\Omega_0\,\vec{\sigma}\cdot\hat{r} \tag{95}$$

$$\mathcal{O}_{q1} = -\frac{1}{2K_\beta^2(q-1)}\vec{\sigma}\cdot\vec{a}\left[\frac{1}{r^{q-1}},\underset{\sim}{\beta}\right]\underset{\sim}{K_1}$$

$$\mathcal{O}_{q2} = \frac{1}{K_\beta^2\,2(q-1)}\vec{\sigma}\cdot\vec{a}\left[\frac{1}{r^{q-1}},\underset{\sim}{\beta}\right](2K_1-1)$$

$$\mathcal{O}_{q3} = -\frac{1}{K_\beta^2\,2(q-1)}\left[\frac{1}{r^{q-1}},\underset{\sim}{\beta}\right](2\underset{\sim}{K_1}-1)\vec{\sigma}\cdot\vec{a}$$

$$\mathcal{O}_{q4} = -\frac{1}{K_\beta^4\,2(q-1)}\left[\vec{\sigma}\cdot\hat{r}\,\frac{1}{r^{q-1}}\,ip_r,\underset{\sim}{\beta}\right](4K_1^2-1)$$

$$\mathcal{O}_{q5} = \frac{1}{4K_\beta^4}\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^q},\underset{\sim}{\beta}\right](4K_1^2-1)$$

$$\mathcal{O}_{q6} = -\frac{1}{K_\beta^4\,2q(q-1)}\underset{\sim}{K_1}\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^q},\underset{\sim}{\beta}\right](4K_1^2-1)$$

$$\mathcal{O}_{q7} = \frac{\alpha Z m}{K_\beta^4\,2(q-1)}\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^{q-2}},\underset{\sim}{\beta}\right]\underset{\sim}{K_1}$$

$$\mathcal{O}_{q8} = \frac{1}{K_\beta^4\,2q}\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^{q-1}},\underset{\sim}{\beta}\right]\underset{\sim}{K_1}\left\{(q-2) + \frac{qK_1}{2} - K_1^2\right\} \tag{96}$$

For q = 2

$$\mathcal{O}_{2,9} = \frac{(\kappa_1^2-1)}{6K_\beta^4}\left[\vec{\sigma}\cdot\hat{r}\,\frac{1}{r}\,ip_r\,,\underset{\sim}{\beta}\right]$$

$$\mathcal{O}_{2,10} = \frac{(1+\kappa_1)}{12}\,\frac{(\kappa_1^2-1)}{K_\beta^4}\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^2}\,,\underset{\sim}{\beta}\right]$$

$$\mathcal{O}_{2,11} = \frac{(\alpha Zm)^2}{K_\beta^4}\left[\frac{\vec{\sigma}\cdot\hat{r}}{2\alpha Zm}\left(ip_r-\frac{\kappa_1}{r}\right),\underset{\sim}{\beta}\right]$$

$$\mathcal{O}_{2,12} = \frac{(1-\kappa_1^2)}{3K_\beta^4}\left[\frac{\vec{\sigma}\cdot\hat{r}}{2\alpha Zm}\left(ip_r-\frac{1}{r}\right),\underset{\sim}{\beta}\right]\underset{\sim}{\beta} \tag{97}$$

For q = 3

$$\mathcal{O}_{3,9} = \frac{\alpha Zm}{6K_\beta^4}\left[\vec{\sigma}\cdot\hat{r}\,\frac{1}{r}\,ip_r\,,\underset{\sim}{\beta}\right]$$

$$\mathcal{O}_{3,10} = \frac{\alpha Zm}{12K_\beta^4}\left(1+\underset{\sim}{\kappa_1}\right)\left[\frac{\vec{\sigma}\cdot\vec{r}}{r^2}\,,\underset{\sim}{\beta}\right]$$

$$\mathcal{O}_{3,11} = -\frac{1}{3K_\beta^4}\left[\frac{\vec{\sigma}\cdot\hat{r}}{2}\left(ip_r-\frac{\kappa_1}{r}\right),\underset{\sim}{\beta}\right]\underset{\sim}{\beta}$$

For q = 4

$$\mathcal{O}_{4,9} = \frac{1-\kappa_1^2}{30}\left[\vec{\sigma}\cdot\hat{r}\,\frac{1}{r^3}\,ip_r\,,\underset{\sim}{\beta}\right]$$

$$\mathcal{O}_{4,10} = \frac{(1-\kappa_1^2)(6+\kappa_1)}{120}\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^4}\,,\underset{\sim}{\beta}\right]$$

$$\mathcal{O}_{4,12} = \frac{\alpha Z m (3+K_1)}{30}\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^3}, \underset{\sim}{\beta}\right]$$

$$\mathcal{O}_{4,13} = -\frac{1}{15}\left[\vec{\sigma}\cdot\hat{r}\,\frac{1}{r}\,i p_r, \underset{\sim}{\beta}\right]\underset{\sim}{\beta}$$

$$\mathcal{O}_{4,14} = -\frac{1}{30}(1+K_1)\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^2}, \underset{\sim}{\beta}\right]\underset{\sim}{\beta}$$

$$\mathcal{O}_{4,15} = \frac{1}{15\alpha Z m}\left[\vec{\sigma}\cdot\hat{r}\; i p_r, \underset{\sim}{\beta}\right]\underset{\sim}{\beta}^2$$

$$\mathcal{O}_{4,16} = \frac{1}{15\alpha Z m} K_1\left[\frac{\vec{\sigma}\cdot\hat{r}}{r}, \underset{\sim}{\beta}\right]\underset{\sim}{\beta}^2$$

(98)

Thus we see that

$$\left\langle l+1 \left| \frac{1}{r^2} \right| l \right\rangle = 0$$

$$\left\langle l+2 \left| \frac{1}{r^2} \right| l \right\rangle = 0$$

$$\left\langle l+2 \left| \frac{1}{r^3} \right| l \right\rangle = 0$$

$$\left\langle l+3 \left| \frac{1}{r^q} \right| l \right\rangle = 0 \quad \text{for } q = 2,3,4. \tag{99}$$

And by induction, for bound states, we get

$$\left\langle l+L \left| \frac{1}{r^q} \right| l \right\rangle = 0 \qquad 2 \leq q \leq L+1 \tag{100}$$

Section III

Continuum States

The radial part of continuum solutions of the Hamiltonian is derived from bound state functions by analytic continuation which essentially consists in the discrete quantum number N going over to complex number $-i\eta$ where η is any positive number, not necessarily an integer and by replacing the Laguerre polynomials by Laguerre functions defined through Cauchy integrals. The continuous functions are normalized such that

$$\int_0^\infty f_{\eta l}(r)\, f_{\eta' l}(r)\, r^3\, dr \tag{101}$$

Introducing the wave number $k_c = \frac{\alpha Z m}{\eta}$ and appropriately modifying the operator equations and confining our attention to say $j = (l - \frac{1}{2})$

$$\vec{\sigma}\cdot\vec{a}\ \Psi_{\eta\kappa\mu} = -\frac{i}{k_c}\,|k+i\eta|\ \Psi_{\eta-\kappa\mu} \equiv -\frac{i}{k_c}\,a_\kappa \Psi_{\eta-\kappa\mu} \tag{102}$$

$$\Omega_0 \Psi_{\eta\varkappa\mu} = \sqrt{\ell(2\ell+1)}\; C^{\ell-\frac{1}{2},\,1,\,\ell+\frac{1}{2}}_{\mu\;\;0\;\;\mu}\; \Psi_{\eta\,-(\varkappa+1)\,\mu} \tag{103}$$

$$\vec{\sigma}\cdot\vec{a}\;\Omega_0\,\Psi_{\eta\varkappa\mu} = \frac{i a_{\ell+1}}{k_c}\sqrt{\ell(2\ell+1)}\; C^{\ell-\frac{1}{2},\,1,\,\ell+\frac{1}{2}}_{\mu,\,0,\,\mu}\; \Psi_{\eta\,\varkappa+1,\,\mu} \tag{104}$$

$$\Omega_0\,\vec{\sigma}\cdot\vec{a}\;\Psi_{\eta\varkappa\mu} = \sqrt{\ell(2\ell-1)}\;\frac{i a_\ell}{k_c}\; C^{\ell-\frac{1}{2},\,1,\,\ell-3/2}_{\mu,\,0,\,\mu}\; \Psi_{\eta\,\varkappa-1,\,\mu} \tag{105}$$

It is important to note that, while the operator relationships derived in Sections I and II are valid here also, caution has to be exercised in taking matrix elements as some of the radial integrals are likely to be singular.

To begin with let us consider the matrix element

$$\left(\Psi_{\eta\,-\varkappa-2\,\mu},\;(\vec{\sigma}\cdot\vec{a}\;\Omega_0)^0\left\{\Omega_0\vec{\sigma}\cdot\hat{r}\,\frac{1}{r^2}\vec{\sigma}\cdot\vec{a} - \vec{\sigma}\cdot\vec{a}\,\frac{1}{r^2}\vec{\sigma}\cdot\hat{r}\,\Omega_0\right\}\Psi_{\eta\,\varkappa+1\,\mu}\right) \tag{106}$$

which can be written as

$$\left(\Psi_{\eta\,-\varkappa-2\,\mu},\;(\vec{\sigma}\cdot\vec{a}\;\Omega_0)^0\left\{\Omega_0\,\vec{\sigma}\cdot\hat{r}\,\frac{1}{r^2}\vec{\sigma}\cdot\vec{a} - \text{its Adjoint}\right\}\Psi_{\eta\,\varkappa+1\,\mu}\right) \tag{107}$$

This matrix element is evaluated to be

$$i\sqrt{(\ell+2)(2\ell+3)}\; C^{\ell+3/2,\,1,\,\ell+1/2}_{\mu,\,0,\,\mu} \cdot\left\{\frac{a_{\ell+1}}{k_c}\langle \ell+1|\frac{1}{r^2}|\ell\rangle - \frac{a_{\ell+2}}{k_c}\langle \ell+2|\frac{1}{r^2}|\ell+1\rangle\right\} \tag{108}$$

$$= (\text{a numerical factor})\left\{\frac{a_{\ell+1}}{k_c}\langle \ell+1|\frac{1}{r^2}|\ell\rangle - \frac{a_{\ell+2}}{k_c}\langle \ell+2|\frac{1}{r^2}|\ell+1\rangle\right\}.$$

Now consider the difference operator

$$\Omega_0 \vec{\sigma}\cdot\hat{r} \frac{1}{r^2} \vec{\sigma}\cdot\vec{a} - \vec{\sigma}\cdot\vec{a} \frac{1}{r^2} \vec{\sigma}\cdot\hat{r} \Omega_0 \tag{109}$$

Taking Ω_o in the first term to the extreme right we get

$$= \left(\frac{1}{r^2} \vec{\sigma}\cdot\hat{r} \vec{\sigma}\cdot\vec{a} - \vec{\sigma}\cdot\vec{a} \frac{1}{r^2} \vec{\sigma}\cdot\hat{r} \right) \Omega_0 - \frac{1}{k_c^2} \left(\frac{1}{r^2} i p_r - \frac{1}{r^3} \right) (2k_1 - 1) \Omega_0 \tag{110}$$

Applying Equations 16 and 4 of Section I we get

$$= - \frac{1}{k_c^2} \left[\frac{1}{r}, \underset{\sim}{\beta} \right] \Omega_0 - \frac{1}{2k_c^2} \left[\underset{\sim}{\beta}, \frac{1}{r} \right] (2k_1 - 1) \Omega_0 \tag{111}$$

Hence the operator

$$(\vec{\sigma}\cdot\vec{a}\,\Omega_0)^{\circ} \left\{ \Omega_0 \vec{\sigma}\cdot\hat{r} \frac{1}{r^2} \vec{\sigma}\cdot\vec{a} - \text{its Adj} \right\}$$

$$= \frac{1}{2k_c^2} \left[\frac{1}{r}, \underset{\sim}{\beta} \right] \left(\frac{1-2k_1}{2} \right) \Omega_0 \tag{112}$$

The matrix element therefore vanishes and we get the difference equation

$$\frac{a_{\ell+1}}{k_c} \langle \ell+1 | \frac{1}{r^2} | \ell \rangle - \frac{a_{\ell+2}}{k_c} \langle \ell+2 | \frac{1}{r^2} | \ell \rangle = 0 \tag{113}$$

which has a solution

$$\langle \ell+1 | \frac{1}{r^2} | \ell \rangle = \frac{(\text{const})\, k_c}{a_{\ell+1}} \tag{114}$$

$$= \frac{\text{const}\; k_c}{|\ell+1+i\eta|} \tag{115}$$

To evaluate $\langle \ell+2 | \frac{1}{r^3} | \ell \rangle$ we consider the operator

$$(\vec{\sigma}\cdot\vec{a}\,\Omega_0) \left\{ \Omega_0 \vec{\sigma}\cdot\hat{r}\, \Omega_0 \vec{\sigma}\cdot\hat{r} \frac{1}{r^3} \vec{\sigma}\cdot\vec{a} - \vec{\sigma}\cdot\vec{a} \frac{1}{r^3} \vec{\sigma}\cdot\hat{r}\, \Omega_0 \vec{\sigma}\cdot\hat{r}\, \Omega_0 \right\} \equiv \underset{\sim}{Q}_2 \tag{116}$$

Its matrix element

$$\left(\Psi_{\eta-\kappa-2\mu},\ \vec{\sigma}\cdot\vec{a}\ \Omega_0 \left\{ (\Omega_0 \vec{\sigma}\cdot\hat{r})^2 \frac{1}{r^3} \vec{\sigma}\cdot\vec{a} - \text{its Adj} \right\} \Psi_{\eta\kappa+1\mu}\right)$$

gives

$$\frac{1}{k^2} \left(l+2 \right) (2l+5) \sqrt{(l+3)(2l+3)}\ C^{\,l+3/2,\ 1,\ l+\frac{1}{2}}_{\ \mu,\ 0,\ \mu}$$

$$C^{\,l+5/2,\ 1,\ l+3/2}_{\ \mu,\ 0,\ \mu}\ C^{\,l+3/2,\ 1,\ l+5/2}_{\ \mu,\ 0,\ \mu} \Big\{ a_{l+1}\, a_{l+2} \langle l+2 | \frac{1}{r^3} | l \rangle$$

$$- a_{l+2}\, a_{l+3} \langle l+3 | \frac{1}{r^3} | l+1 \rangle \Big\}$$

The following steps will show how the operator reduces to a commutator with Hamiltonian

Let $\underset{\sim}{O}_2$ = L.H.S operator − R.H.S. operator.

As we have already taken care of the left side of the operator we deal only with the right side of the operator.

$$\text{Right operator} = \vec{\sigma}\cdot\vec{a}\ \Omega_0 \underline{\vec{\sigma}\cdot\vec{a} \frac{1}{r^3} \vec{\sigma}\cdot\hat{r}}\ \Omega_0 \vec{\sigma}\cdot\hat{r}\ \Omega_0 \tag{117}$$

$$= \vec{\sigma}\cdot\vec{a}\ \Omega_0 \Big\{ \Omega_0 \vec{\sigma}\cdot\vec{a}\ \vec{\sigma}\cdot\hat{r} \frac{1}{r^3}$$

$$+ \frac{\Omega_0}{k_c^2} \left(\frac{2}{r^4} - \frac{1}{r^3} i p_r \right) (1 - 2K_1) \Big\} \vec{\sigma}\cdot\hat{r}\ \Omega_0 \tag{118}$$

Here the underlined part is handled by the rule (12) of Section I.

$$\therefore\ R.O = \underset{\sim}{\Theta} \left\{ (\vec{\sigma}\cdot\vec{a})^2 \frac{1}{r^3} + \frac{1}{k_c^2} \vec{\sigma}\cdot\vec{a}\ \vec{\sigma}\cdot\hat{r} \left(\frac{2}{r^4} - \frac{1}{r^3} i p_r \right) (1 + 2K_1) \right\} \Omega_0$$

So the complete operator becomes

$$\underset{\sim}{O}_2 = \underset{\sim}{\varpi}\Big\{\vec{\sigma}\cdot\vec{a}\,\frac{1}{r^3}\,\vec{\sigma}\cdot\vec{a} + \frac{\vec{\sigma}\cdot\vec{a}\,\vec{\sigma}\cdot\hat{r}}{k_c^2}\Big(\frac{1}{r^3}\,ip_r - \frac{1}{r^4}\Big)(1-2k_1)$$

$$- \vec{\sigma}\cdot\vec{a}\,\vec{\sigma}\cdot\vec{a}\,\frac{1}{r^3} + \frac{1}{k_c^2}\,\vec{\sigma}\cdot\vec{a}\,\vec{\sigma}\cdot\hat{r}\Big(\frac{2}{r^4} - \frac{1}{r^3}\,ip_r\Big)\cdot$$

$$\cdot\,(1+2k_1)\Big\}\,\Omega_0 \tag{119}$$

Using relation 12 of Section I this reduces to

$$\underset{\sim}{O}_2 \equiv \underset{\sim}{\varpi}\,\frac{\vec{\sigma}\cdot\vec{a}\,\vec{\sigma}\cdot\hat{r}}{2\,k_c^2}\Big\{\frac{1}{r^3}\,ip_r + \Big(\frac{K_1}{2} - 3/2\Big)\frac{1}{r^4}\Big\}\,\Omega_0 \tag{120}$$

and using relation 8, operator becomes

$$\underset{\sim}{O}_2 = \underset{\sim}{\varpi}\,\frac{\vec{\sigma}\cdot\vec{a}}{2\,k_c^2}\Big[2m\,\underset{\sim}{H},\ \frac{\vec{\sigma}\cdot\hat{r}}{r^2}\Big]\,\Omega_0 \tag{121}$$

$$\therefore\ \Big(\Psi_{\eta\,-\kappa-2\,\mu},\ \underset{\sim}{O}_2\ \Psi_{\eta\,\kappa+1\,\mu}\Big) = 0 \tag{122}$$

We then get a difference equation

$$\frac{a_{\ell+1}\,a_{\ell+2}}{k_c^2}\,\langle \ell+2|\,\frac{1}{r^3}\,|\ell\rangle - \frac{a_{\ell+3}\,a_{\ell+2}}{k_c^2}\,\langle \ell+3|\,\frac{1}{r^3}\,|\ell+1\rangle = 0 \tag{123}$$

Which has a solution

$$\langle \ell+2|\,\frac{1}{r^3}\,|\ell\rangle = \frac{\text{const}\ k_c^2}{a_{\ell+1}\ a_{\ell+2}}$$

$$= \frac{\text{const}\ k_c^2}{|\ell+1+i\eta|\ |\ell+2+i\eta|} \tag{124}$$

The Derivation for $\langle \ell+3|\frac{1}{r^4}|\ell\rangle$

The operator which leads to this matrix element is

$$\underset{\sim}{O}_3 \equiv (\vec{\sigma}\cdot\vec{a}\ \Omega_0)^2\Big\{(\Omega_0\,\vec{\sigma}\cdot\hat{r})^3\,\frac{1}{r^4}\,\vec{\sigma}\cdot\vec{a} - \text{its Adj}\Big\} \tag{125}$$

And the matrix element

$$\left(\Psi_{\eta\,-\chi-2\,\mu},\ \underset{\sim}{O}_3\ \Psi_{\eta\,\chi+1\,\mu} \right) \tag{126}$$

yields (# numerical factor)

$$= \# \left\{ \frac{a_{\ell+1}a_{\ell+2}a_{\ell+3}}{k_c^3} \langle \ell+3 | \frac{1}{r^4} | \ell \rangle - \frac{a_{\ell+4}a_{\ell+3}a_{\ell+2}}{k_c^3} \langle \ell+4 | \frac{1}{r^4} | \ell+1 \rangle \right\} \tag{127}$$

And now we shall prove that the matrix element vanishes. Consider (125)

$$\vec{\sigma}\cdot\vec{a}\,\Omega_0\,\vec{\sigma}\cdot\vec{a}\,\Omega_0\,\Omega_0\,\vec{\sigma}\cdot\hat{r}\,\Omega_0\,\vec{\sigma}\cdot\hat{r}\,\Omega_0\,\vec{\sigma}\cdot\hat{r}\,\frac{1}{r^4}\,\vec{\sigma}\cdot\vec{a}$$

$$-\ \vec{\sigma}\cdot\vec{a}\,\Omega_0\,\vec{\sigma}\cdot\vec{a}\,\Omega_0\,\vec{\sigma}\cdot\vec{a}\,\frac{1}{r^4}\,\vec{\sigma}\cdot\hat{r}\,\Omega_0\,\vec{\sigma}\cdot\hat{r}\,\Omega_0\,\vec{\sigma}\cdot\hat{r}\,\Omega_0$$

$$= L.Op - R.Op$$

$$\equiv \text{Left operator} - \text{Right operator}$$

$$= \vec{\sigma}\cdot\vec{a}\,\Omega_0\,\underset{\sim}{\varpi}\,\vec{\sigma}\cdot\vec{a}\,\vec{\sigma}\cdot\hat{r}\,\Omega_0\,\vec{\sigma}\cdot\hat{r}\,\Omega_0\,\vec{\sigma}\cdot\hat{r}\,\frac{1}{r^4}\,\vec{\sigma}\cdot\vec{a}$$

$$-\ \vec{\sigma}\cdot\vec{a}\,\Omega_0\,\vec{\sigma}\cdot\vec{a}\left\{ \vec{\sigma}\cdot\vec{a}\,\vec{\sigma}\cdot\hat{r}\,\frac{1}{r^4}\,\Omega_0 \right.$$

$$\left. +\ \frac{1}{k_c^2}\left(\frac{1}{r^4}\,ip_r - \frac{3}{r^5}\right)\Omega_0(1-2k_1) \right\}.$$

$$\cdot\ \Omega_0\,\vec{\sigma}\cdot\hat{r}\,\Omega_0\,\vec{\sigma}\cdot\hat{r}\,\Omega_0 \tag{128}$$

Where the relation 14 of Section II is used in the right hand side.

$$= \vec{\sigma}\cdot\vec{a}\,\Omega_0\, \underset{\sim}{\varpi} \left\{ \Omega_0\, \vec{\sigma}\cdot\vec{a}\, \vec{\sigma}\cdot\hat{r} + \frac{1}{k_c^2}\left(ip_r + \frac{1}{r}\right)\Omega_0 (2K_1 - 1) \right\} \cdot$$

$$\vec{\sigma}\cdot\hat{r} \left\{ \frac{1}{r^4}\, \vec{\sigma}\cdot\hat{r}\, \vec{\sigma}\cdot\vec{a}\, \Omega_0 + \frac{1}{k_c^2}\left(\frac{1}{r^4} ip_r - \frac{1}{r^5}\right)(1-2K_1)\Omega_0 \right\}$$

$$- \left\{ \vec{\sigma}\cdot\vec{a}\, \Omega_0\, \vec{\sigma}\cdot\vec{a}\, \vec{\sigma}\cdot\vec{a}\, \underset{\sim}{\varpi}\, \frac{1}{r^4}\, \Omega_0\, \vec{\sigma}\cdot\hat{r}\, \Omega_0 \right.$$

$$+ \vec{\sigma}\cdot\vec{a}\, \Omega_0\, \vec{\sigma}\cdot\vec{a}\, \vec{\sigma}\cdot\hat{r}\, \underset{\sim}{\varpi}\, \frac{1}{k_c^2}\left(\frac{3}{r^5} - \frac{1}{r^4} ip_r \right)$$

$$\left. \cdot\, (1+2K_1)\, \Omega_0\, \vec{\sigma}\cdot\hat{r}\, \Omega_0 \right\} \tag{129}$$

Define $\underset{\sim}{\varpi}'' = \vec{\sigma}\cdot\hat{r}\ \Omega_0\, \underset{\sim}{\varpi}\ \Omega_0\ \vec{\sigma}\cdot\hat{r}$ which commutes with $\underset{\sim}{K}_1$, $2m\underset{\sim}{H}$, and therefore with $(\vec{\sigma}\cdot\vec{a})^2$. So the right operator becomes

$$R.O \equiv \vec{\sigma}\cdot\vec{a}\, \underset{\sim}{\varpi}'' \left\{ (\sigma\cdot a)^2 \frac{1}{r^4}\, \vec{\sigma}\cdot\hat{r}\, \Omega_0 + \frac{1}{k_c^2 r^4}(1-2K_1)\, \vec{\sigma}\cdot\hat{r}\, \Omega_0 \right\}$$

$$+ \vec{\sigma}\cdot\vec{a}\, \Omega_0\, \varpi\, \vec{\sigma}\cdot\vec{a}\, \vec{\sigma}\cdot\hat{r}\, \Omega_0 \left\{ \frac{3}{r^5} - \frac{1}{r^4} ip_r \right\} \cdot$$

$$\cdot\, (3-2K_1)\, \vec{\sigma}\cdot\hat{r}\, \Omega_0 \tag{130}$$

The latter term can be modified by switching Ω_0 and $\vec{\sigma}\cdot\vec{a}$ $\vec{\sigma}\cdot\hat{r}$, then we get the right operator as

$$= \vec{\sigma}\cdot\vec{a}\, \underset{\sim}{\varpi}'' \left\{ \vec{\sigma}\cdot\vec{a}\, \vec{\sigma}\cdot\vec{a}\, \frac{1}{r^4}\, \vec{\sigma}\cdot\hat{r} + \frac{1}{k_c^2}(1-2K_1)\, \frac{1}{r^4}\, \vec{\sigma}\cdot\hat{r} \right.$$

$$+ \vec{\sigma}\cdot\vec{a} \left(\frac{3}{r^5} - \frac{1}{r^4} ip_r \right)(3+2K_1)$$

$$\left. + \left(ip_r + \frac{1}{r}\right)\left(\frac{3}{r^5} - \frac{1}{r^4} ip_r \right)(3-2K_1)(2K_1-1)\, \vec{\sigma}\cdot\hat{r} \right\} \Omega_0 \tag{131}$$

As already illustrated in Section II

$$\text{Left op} = \vec{\sigma}\cdot\vec{a}\ \underset{\sim}{\varpi}''\left\{ \text{eqns (96)} + \text{eqn (99)} \right\}\Omega_0 \tag{132}$$

Therefore the complete operator

$$\equiv \text{eqn (132)} - \text{eqn (131)}$$

Using the technique similar to that for bound states and leaving the relevant commutators with Hamiltonian, the part that matters becomes

$$\begin{aligned}
&\vec{\sigma}\cdot\vec{a}\ \underset{\sim}{\varpi}''\Big\{ \frac{1}{k_c^2}\vec{\sigma}\cdot\vec{a}\left(\frac{\alpha Zm}{r^4} + (2k_1 - k_1^2)\frac{1}{r^5}\right) + \frac{2}{k_c^2}\vec{\sigma}\cdot\vec{a}\frac{1}{r^5}(1-2k_1) \\
&\quad - \frac{1}{k_c^2}\frac{1}{r^5}(2k_1-1)\vec{\sigma}\cdot\vec{a} + \vec{\sigma}\cdot\hat{r}\left(\frac{\alpha Zm}{3}\frac{1}{r^5} - \frac{4+k_1^2}{4}\frac{1}{r^6}\right) \\
&\qquad (4k_1^2-1)\Big\}\Omega_0 \\
&- \vec{\sigma}\cdot\vec{a}\ \underset{\sim}{\varpi}''\Big\{ \frac{1}{k_c^2}\vec{\sigma}\cdot\vec{a}\left(\frac{\alpha Zm}{r^4} + (3+4k_1-2k_1^2)\frac{1}{r^5}\right) \\
&\quad + \vec{\sigma}\cdot\hat{r}\cdot\frac{1}{k_c^2}(1+2k_1)\frac{1}{r^4} \\
&\quad + \vec{\sigma}\cdot\hat{r}\left(\frac{\alpha Zm}{3}\frac{1}{r^5} - \frac{1}{4}(k_1^4+2k_1-8)\frac{1}{r^6}\right)\cdot \\
&\qquad \cdot(3+2k_1)(2k_1+1)\Big\}\Omega_0
\end{aligned} \tag{133}$$

This further reduces to

$$\varpi''\frac{\vec{\sigma}\cdot\vec{a}\ \vec{\sigma}\cdot\hat{r}}{k_c^4}\left\{ -\frac{1}{r^4}2m\underset{\sim}{H} - \frac{7}{3}\alpha Zm\frac{1}{r^5} + \left(\frac{5}{4}k_1^2 - 1\right)\frac{1}{r^6}\right\}\cdot(2k_1+1)\Omega_0 \tag{134}$$

$$= \underset{\sim}{\varpi}'' \vec{\sigma}\cdot\vec{a} \frac{1}{k_c^4} \left\{ \frac{1}{6} \left[\vec{\sigma}\cdot\hat{r} \frac{1}{r^3} i p_r , \underset{\sim}{\beta} \right] - \left(\frac{k_1+6}{6} \right) \left[\underset{\sim}{\beta} , \frac{\vec{\sigma}\cdot\hat{r}}{r^4} \right] \right\} . \qquad (135)$$

$$, (2k_1+1)\, \Omega_0$$

Thus the complete operator in the form of commutators with Hamiltonian can be written as

$$(\vec{\sigma}\cdot\vec{a}\,\Omega_0)^2 \left\{ (\Omega_0 \vec{\sigma}\cdot\hat{r})^3 \frac{1}{r^4} \vec{\sigma}\cdot\vec{a} - I_{tr}\ Adj \right\}$$

$$= \underset{\sim}{\varpi}'' \vec{\sigma}\cdot\vec{a} \left(\sum_i \mathcal{O}^c_{4,i} \right) \Omega_0 \qquad (136)$$

where

$$\mathcal{O}^c_{4,1} = - \frac{\vec{\sigma}\cdot\vec{a}}{6 k_c^2} \left[\frac{1}{r^3} , \beta \right] \underset{\sim}{k_1}$$

$$\mathcal{O}^c_{4,2} = \frac{\vec{\sigma}\cdot\vec{a}}{6 k_c^2} \left[\frac{1}{r^3} , \underset{\sim}{\beta} \right] (2k_1 - 1)$$

$$\mathcal{O}^c_{4,3} = \frac{1}{6 k_c^2} \left[\frac{1}{r^3} , \underset{\sim}{\beta} \right] \vec{\sigma}\cdot\vec{a}\ (2k_1 + 1)$$

$$\mathcal{O}^c_{4,4} = \frac{1}{6 k_c^4} \left[\vec{\sigma}\cdot\hat{r} \frac{1}{r^3} i p_r , \underset{\sim}{\beta} \right] (1 - 4 \underset{\sim}{k_1}^2)$$

$$\mathcal{O}^c_{4,5} = \frac{1}{4 k_c^4} \left[\frac{\vec{\sigma}\cdot\hat{r}}{r^4} , \underset{\sim}{\beta} \right] (1 - 4k_1^2)$$

$$\mathcal{O}^c_{4,6} = \frac{7}{24 k_c^4} \left[\frac{\vec{\sigma}\cdot\hat{r}}{r^4} , \underset{\sim}{\beta} \right] (1 - 4k_1^2)$$

$$\mathcal{O}^c_{4,7} = \frac{k_1 - 1}{3 k_c^2} \vec{\sigma}\cdot\vec{a} \left[\frac{1}{r^3} , \underset{\sim}{\beta} \right]$$

$$\mathcal{O}^{c}_{4,8} = \frac{1}{6k_c^4}\left[\vec{\sigma}\cdot\hat{r}\,\frac{1}{r^4}\,i p_r\,,\,\underset{\sim}{\beta}\right](3+2k_1)(2k_1+1)$$

$$\mathcal{O}^{c}_{4,9} = \frac{1}{24k_c^4}(6+k_1)\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^4},\underset{\sim}{\beta}\right](3+2k_1)(2k_1+1)$$

$$\mathcal{O}^{c}_{4,10} = -\frac{3}{4k_c^4}\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^4},\underset{\sim}{\beta}\right](2k_1+3)(2k_1+1)$$

$$\mathcal{O}^{c}_{4,11} = \frac{1}{6k_c^4}\left[\vec{\sigma}\cdot\hat{r}\,\frac{1}{r^3}\,i p_r\,,\,\underset{\sim}{\beta}\right](2k_1+1)$$

$$\mathcal{O}^{c}_{4,12} = \frac{1}{6k_c^4}\left(\frac{k_1+6}{4}\right)\left[\frac{\vec{\sigma}\cdot\hat{r}}{r^4},\underset{\sim}{\beta}\right](2k_1+1)$$

(137)

Thus we get the difference equation

$$\langle l+3|\frac{1}{r^4}|l\rangle\,\frac{a_{l+1}a_{l+2}a_{l+3}}{k_c^3} - \frac{a_{l+2}a_{l+3}a_{l+4}}{k_c^3}\langle l+4|\frac{1}{r^4}|l+1\rangle = 0$$

Which has the solution

$$\langle l+3|\frac{1}{r^4}|l\rangle = \frac{\text{const}\ k_c^3}{|l+1+i\eta|\,|l+2+i\eta|\,|l+3+i\eta|} \tag{138}$$

Thus we have proved that in the continuum case

$$\langle l+1|\frac{1}{r^2}|l\rangle = \frac{\text{const}\ k_c}{|l+1+i\eta|}$$

$$\langle l+2|\frac{1}{r^3}|l\rangle = \frac{\text{const}\ k_c^2}{|l+1+i\eta|\,|l+2+i\eta|}$$

$$<\ell+3|\frac{1}{r^4}|\ell> = \frac{\text{const } R_c^3}{|\ell+1+i\eta|\,|\ell+2+i\eta|\,|\ell+3+i\eta|} \tag{139}$$

And by induction as it would be indicated in Section IV we get the general result

$$<\ell+L|\frac{1}{r^{L+1}}|\ell> = \frac{\text{const } R_c^L}{|\ell+1+i\eta| \cdots |\ell+L+i\eta|} \tag{140}$$

Section IV

Systematics of Operator Algebra

The general result for bound states arises from the matrix element

$$\left(\Psi_{N-\varkappa-2\mu},\ (\vec{\sigma}\cdot\vec{a}-\Omega_0)^{L-1}\left(\Omega_0\vec{\sigma}\cdot\hat{r}\right)\frac{1}{r^q}\,\vec{r}\cdot\vec{a}\ \Psi_{N\,\kappa+1\,\mu}\right) \tag{141}$$

Which will give us

$$\# \ R_B^{-L} <\ell+L|\frac{1}{r^q}|\ell> \tag{142}$$

and the numerical factors will inclube (2L-1) C.G. coefficients and many other ℓ dependent terms.

The parallel result for the continuum basis states arises from the matrix element

$$\left(\Psi_{\eta-\varkappa-2\mu},\ (\vec{\sigma}\cdot\vec{a}-\Omega_0)^{L-1}\left\{(\Omega_0\vec{\sigma}\cdot\hat{r})^L\frac{1}{r^{L+1}}\,\vec{r}\cdot\vec{a} - i\hbar\,\mathrm{Adj}\right\}\Psi_{\eta\,\kappa+1\,\mu}\right) \tag{143}$$

The extreme complexity of the resolution of the appropriate operators into a sum of commutators with the Hamiltonian notices in $<\ell+3|\frac{1}{r^q}|\ell>$, for bound states as well as continuum states, show that the general result would be too complicated to write down.

We notice, for instance, that the invariant operator that multiplies the whole sum of commutators with the Hamiltonian in the cases studied is seen to follow a systematic pattern,

When the operator in the second parenthesis multiplying the invariant Ω_0 is	The operator multiplying the entire sum is
$\vec{\sigma}\cdot\hat{r}\ \mathbb{1}$	$\mathbb{1} = \vec{\sigma}\cdot\hat{r}\ \mathbb{1}\,\mathbb{1}\,\vec{\sigma}\cdot\hat{r}$
$\vec{\sigma}\cdot\hat{r}\,\Omega_0\,\vec{\sigma}\cdot\hat{r}$	$\varpi = \vec{\sigma}\cdot\hat{r}\,\Omega_0\,\Omega_0\,\vec{\sigma}\cdot\hat{r}$ $= \vec{\sigma}\cdot\hat{r}\,\Omega_0\,\vec{\sigma}\cdot\hat{r}\,\vec{\sigma}\cdot\hat{r}\,\Omega_0\,\vec{\sigma}\cdot\hat{r}$
$\vec{\sigma}\cdot\hat{r}\,\Omega_0\,\vec{\sigma}\cdot\hat{r}\,\Omega_0\,\vec{\sigma}\cdot\hat{r}$	$\varpi' = \vec{\sigma}\cdot\hat{r}\,\Omega_0\,\varpi\,\Omega_0\,\vec{\sigma}\cdot\hat{r}$ $=\{\vec{\sigma}\cdot\hat{r}\,\Omega_0\,\vec{\sigma}\cdot\hat{r}\,\Omega_0\,\vec{\sigma}\cdot\hat{r}\}\cdot\{\text{Its Adj}\}$
- - - -	- - - -
$\vec{\sigma}\cdot\hat{r}\,(\Omega_0\,\vec{\sigma}\cdot\hat{r})^{L-1}$	$\tilde{\varpi} = \{\vec{\sigma}\cdot\hat{r}\,(\Omega_0\,\vec{\sigma}\cdot\hat{r})^{L-1}\}\{\text{its Adj}\}$

(144)

Secondly Ω_0 happens to multiply the whole sum on the right. Thirdly one of the important intermediate steps is to manipulate

$$\Omega_0\,\vec{\sigma}\cdot\vec{a}\,\vec{\sigma}\cdot\hat{r}\,\frac{1}{r^q} \qquad \text{and} \qquad \vec{\sigma}\cdot\vec{a}\,\vec{\sigma}\cdot\hat{r}\,\frac{1}{r^q}\,\Omega_0 \tag{145}$$

Such that Ω_0 can be moved to the right or left as required and at the ultimate stage one gets a linear combination of recursion relations.

The essential point to be noted in our demonstration here is that the symmetry of the Coulomb field permits the construction of a variety of angular operators, the matrix elements of which lead to interesting relationships among radial integrals and peculiar selection rules. We collect below, for completeness, the different relations that were proved by the operator technique in the preceding chapters.

1. Pasternack's three term recursion relation between the bound state expectation values.
2. A three recursion relation between $\langle \ell+1|\frac{1}{r^q}|\ell\rangle$'s.
3. Pasternack and Sternheimer result that is $\langle \ell+L|\frac{1}{r^q}|\ell\rangle = 0$

   a. $\langle \ell+1|\frac{1}{r^2}|\ell\rangle = 0$, $\langle \ell+2|\frac{1}{r^2}|\ell\rangle = 0$

   b. $\langle \ell+2|\frac{1}{r^3}|\ell\rangle = 0$

   c. $\langle \ell+3|\frac{1}{r^3}|\ell\rangle = 0$, $\langle \ell+3|\frac{1}{r^2}|\ell\rangle = 0$

   d. $\langle \ell+3|\frac{1}{r^4}|\ell\rangle = 0$

4. For continuum case

$$\langle \ell+1|\frac{1}{r^2}|\ell\rangle = \frac{\text{const}\ k_c}{|\ell+1+i\eta|}$$

$$\langle \ell+2|\frac{1}{r^3}|\ell\rangle = \frac{\text{const}\ k_c^2}{|\ell+1+i\eta|\,|\ell+2+i\eta|}$$

and

$$\langle \ell+3|\frac{1}{r^4}|\ell\rangle = \frac{\text{const}\ k_c^3}{|\ell+1+i\eta|\,|\ell+2+i\eta|\,|\ell+3+i\eta|}$$

It has been proved elsewhere that the zero energy loss limit simplifies the radial integrals considerably. Symmetry helps in the most convenient, though not the most general, evaluation of such integrals.

It is to be emphasized that the radial integrals can be evaluated more simply by actual calculations using the generating functions of the generalized Laguerre polynomials and this derivation, which develops an operator calculus, is not meant to be a substitute but seeks to interpret the result. The key invariants that go to make up the basic units are $\vec{L}$ and $\vec{a}$ which underlie the O(4) invariant group structure of the non-relativistic Coulomb field. Out of these basic units, systems of complicated operators can be built whose matrix elements, evaluated in the basis of the eigenstates of the Coulomb Hamiltonian (discrete or continuum), vanish giving rise to useful selection rules and transition probabilities.

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CHAPTER V

STUDY OF STARK EFFECT

The hydrogen atom in an electric field is perhaps the simplest quantum mechanical problem for which there is no known exact solution. The solution of this problem has application in several areas in solid state physics, such as field controlled photo generation of carriers in solids, trap controlled mobilities, field ionization in plasma physics where the problem can be reduced to a bound charge under the influence of an electric field.[1] Historically the effect of a uniform electric field first observed experimentally by Stark[2] in 1913 on the Balmer series of hydrogen. Even though Voigt[3], as early as 1899, had tried to see the effect on sodium D lines without much success. For the frequency shift Stark gave the following formula

$$\Delta\nu(n_1 n_2 m) \quad = \quad .068n(n_1 - n_2)\varepsilon$$

where ε is in Kilo volt per centimeter.

Later experiments by Sjogram and Kasiner[4] gave a value of 0.0642 for the numerical factor. The range of the electric field used by them was .6 to 1.0 million volt/cm. The year that Bohr proposed his theory of the hydrogen spectrum Epsetein and Schwarzchild[5] explained the Stark effect in terms of quantized orbits. Later in 1926 after the introduction of wave mechanics Schrodinger[6] and Epstein solved the non-relativistic Schrodinger equation for the hydrogen atom in a constant electric field in parabolic coordinates and offerred a satisfactory theory of the non-relativistic Stark effect.

A comprehensive review up to 1935 is available in Condon and Shortly[7] and on up to 1957 in Bethe and Salpeter.[8]

In recent years there has been a renewed interest in the experimental study of the Stark effect, connected with the direct effect of the electric fields on the electron density distributions in atoms. This interest has been stimulated by the development of methods for detecting small splittings of atomic levels, which are of the order of 10^{-4} cm^{-1} in the optical range and 10^{-7} in the radiofrequency range, and a very widespread use of the Stark effect in the spectroscopic method of studying plasma.[9]

The direct classical method of studying the Stark effect is to observe the shift of the centers of gravity of absorption and emission lines of atoms in an electric field.[10] The recent methods of atomic beams propagated perpendicular to the direction of observation of emission and absorption, instead of the observation of vapors, have increased the sensitivity by the factor of 1,000, and the Stark shifts can be observed for as small a field as 10^3 to 10^5 volt/cm. All purely optical methods permit the observation of the frequency shifts of transitions associated with two optical terms, the shift being equal to the sum of energy shifts in upper and lower terms. The novel radiospectroscopic techniques which has a resolution of 10^{-7} cm^{-1} are used to measure the shifts between the sublevels of a given term.

The double radio-optical resonance has made it possible to use the high resolving power of the radiospectroscopic methods to study the Stark effect in excited states of the atoms[11,12]. In this method the radio frequency transitions between the sublevels of the excited state are observed by means of polarization of the scattered resonant light. Some technical difficulties of the double radio-optical resonance method are eliminated in the method of level crossing[14], a change in the angular distribution of the intensity of resonance florescence when the levels are split by an amount larger than the natural width, is observed. In the beat method[15] one observes an anomalous increase in the depth of modulation of the exciting term which are split in the electric field. Only the natural widths of terms put the limit to the sensitivity of these methods.[16-18]

Recently quite a few theoretical and experimental papers[19-22] have appeared on the Stark effect due to high frequency alternating fields. But in this work we study only the Stark effect of a uniform electric field. As the above reference to various literature shows the field of study is very current and experimental advances have necessitated the effort to improve the accuracy of the existing theoretical calculations.

Section I

Group Theory of Hydrogen Atom in a Constant Electric Field

In this section we derive classical invariants of hydrogen atom Hamiltonian in constant electric field for a non-relativistic case. It has been elaborated in Chapter II that non-relativistic Kepler problem admits two vector invariants $\bar{L}$ and $\bar{A}$. It was discussed in Chapter II that the degeneracy of the bound state spectrum is due to the O(4) group structure of the non-relativistic Coulomb Hamiltonian and the Schrodinger equation for hydrogen atom is separable in parabolic and polar coordinates. It is interesting to note that even when a uniform electric field is applied, the Hamiltonian is still separable in parabolic coordinates. It is therefore tempting to probe from the symmetry and group theory point of view why it should be so. The classical discussion of the derivation of the invariants was given by Edmond[23] on suggestion of Lippmann. Edmond shows that $\vec{L}\cdot\vec{E}$ and $\vec{C}\cdot\vec{E}$, where $\vec{C}$ is a generalization of Runge-Lentz-Pauli vector, are the constants of motion. $\vec{C}$ is explicitly given by

$$\vec{C} = \vec{A} - \frac{1}{2ze}[(\vec{r}x\vec{E})x\vec{r}] \tag{1}$$

where $\vec{r}$ is the radius vector.

He also derived some interesting classical relations. They are:

$$\frac{d}{dt}\vec{C} = \frac{3}{2zem}\vec{L}\ x\ \vec{E} \tag{2}$$

$$\vec{L}\cdot\vec{C} = \frac{r^2}{2ze}\vec{E}\cdot\vec{L} \tag{3}$$

and

$$\vec{C}\cdot\vec{r} = r - \left(\frac{L^2}{Ze^2m}\right) \tag{4}$$

The last equation is a generalization of the Keplerian equation of motion in the Coulomb field.

To translate this simple classical picture of invariants into quantum mechanics we have to use proper operators for $\vec{A}$ and $\vec{L}$, because of the basic non-commutativity of x_i and p_{xi}. The appropriate quantum mechanical $\vec{C}$ happens to be

$$\vec{C} = [\hat{r} + \frac{1}{Ze^2m}(\vec{L}x\vec{p} - \vec{p}x\vec{L}) - \frac{1}{2ze}(\vec{r}x\vec{E})\ x\ \vec{r}] \tag{5}$$

If without loss of generality, we take $\vec{E} = \hat{z}F + 0\cdot\hat{x} + 0\cdot\hat{y}$ where F is constant, measuring the strength of the external uniform electric field, then

$$C_x = [\frac{x}{r} + \frac{1}{Ze^2m}[(L_y p_z - L_z p_y) - ihp_x] - \frac{1}{2Ze}(r^2 \cdot 0 - xz)F] \qquad (6)$$

$$C_y = [\frac{y}{r} + \frac{1}{Ze^2m}[(L_z p_x - L_x p_z) - ihp_y] - \frac{1}{2Ze}(r^2 \cdot 0 - y_z)F] \qquad (7)$$

$$C_z = [\frac{z}{r} + \frac{1}{Ze^2m}[(L_x p_y - L_y p_x) - ihp_z] - \frac{1}{2Ze}(r^2 - z^2)F] \qquad (8)$$

and

$$\underset{\sim}{H} = \frac{P^2}{2m} - \frac{Ze^2}{r} - Fez$$

in the non-relativistic Hamiltonian. It can be seen that,

$$[C_z, \underset{\sim}{H}] = 0 \qquad (9)$$

$$[L_z, \underset{\sim}{H}] = 0 \qquad (10)$$

and

$$[C_z, L_z] = 0 \qquad (11)$$

We therefore note that L_Z and C_Z can be used as the constants of the motion. The other commutators are complicated functions of $\vec{C}$, $\vec{L}$, $\vec{r}$, and $\vec{E}$ and it is not easy to see the Lie algebra from these operators. For completeness we give below the commutation relations.

$$[C_x, L_x] = ih \frac{1}{2Ze} xy\ F = ih\ x(\vec{r} x \vec{E})_x$$

$$[C_x, L_y] = ih\ [C_z + \frac{F}{2Ze}(y^2 + z^2)]$$

$$[C_x, L_2] = -ih\ C_y$$

$$[C_y, L_x] = -ih\ [C_z - \frac{F}{2Ze}(x^2 + z^2)]$$

$$[C_y, L_y] = -ih \frac{xy}{2Ze} F = ih\ y\ (\vec{r}x\vec{E})_y$$

$$[C_y, L_z] = ih\ C_x$$

$$[C_z, L_x] = ih\ C_y$$

$$[C_z, L_y] = -ih\ C_x$$

$$[C_z, L_z] = 0 = ih\ Z(\vec{r}x\vec{E})_z \tag{12}$$

Equations (12) definitely show that the invariant group is much larger than O(4). In fact the commutation relations become complicated functions of the five vectors $\vec{C}$, $\vec{L}$, $(p x\vec{E})$ $(\vec{r}x\vec{E})$, and $\vec{E}$. In polar coordinates we can not see clearly what might be the actual group but Barut and Kleinhart[24], using operator representations in parabolic coordinates and also making use of their dialation operator have shown, under the perturbation scheme, that the hydrogen atom under the influence of dipole type of perturbation belongs to O(4,2) group.

Section II

The First Order Stark Effect

The Stark effect was one of the problems to which quantum mechanical perturbation theory was applied successfully as early as 1926 by Schrodinger in his fourth communication,[25] when he developed quantum mechanical perturbation theory. The relativistic Stark effect was discussed by Kramers[26] in the classical sense in 1920. Schlapp[27] calculated some Stark shifts using Darvin wave functions and Rojansky[28] treated the relativistic Stark effect in 1929. But his calculations were not accurate because wave functions he used for the calculation did not include all the degenerate wave functions for the given energy level. In 1955 Luder[29] calculated accurately the first order Stark shifts and the Stark intensities for hydrogen in Pauli approximation. In these earlier papers the complicated Dirac wave functions were always approximated in the calculations. Moreover the experimental error was too large to demand very accurate calculations. As it is mentioned in the introduction, recently the experimental accuracy has been increased by four orders of magnitude, and also the availability of fast computers with vast memory makes it feasible for a very accurate calculations of the first order Stark shifts and the other related quantities of experimental interest. We use here the Dirac wave functions, symmetric Hamiltonian wave functions and compare the result with Luder's calculations and with the experimental results.

The theory of the first order Stark effect is well known (Bethe[8]). The Dirac Hamiltonian with Coulomb field and the uniform electric field is given by

$$H\psi = (\rho_1 \vec{\sigma}\cdot\vec{p} + \rho_3 m_o C^2 - \frac{Ze^2}{r} - e\phi)\,\psi = E\psi \qquad (13)$$

The second order equation, to sufficient approximation and with $\phi = -ZF$ will be

$$H = \underbrace{\frac{p^2}{2m_o} - \frac{Ze^2}{r}}_{H_o} - \underbrace{\frac{p^4}{8m_o^3C^2} - \frac{Ze^2}{4m_o^3C^2r^3}\vec{\sigma}.\vec{L}}_{H_1} \pm \underbrace{ezF}_{H_2} + \underbrace{\frac{e}{4m_o^2C^2}\left(\sigma[p,z]F\right)}_{H_3} \qquad (14)$$

Let us designate the first two terms as H_0, third and fourth terms as H_1, ezF as H_2 and remaining terms as H_3.

H_0 is the non-relativistic Schrodinger Hamiltonian for the Coulomb field. H_1 is the spin orbit coupling term and H_2 is perturbation due to the external electric field. In his paper Schrodinger, using the parabolic coordinates and neglecting H_1 and H_3 showed through perturbation calculations that

$$E_{o+2} = -\frac{e^2}{2a_o}\left(\frac{Z}{n}\right)^2 + \frac{3}{2} e a_o F \frac{n}{Z} n_F - \frac{1}{32}\frac{(e a_o F)^2}{e^2/2a_o}\left(\frac{n}{Z}\right)^4 \{17n^2 - 3n_F^2 - 9m_\ell^2 + 19\} + \text{---} \tag{15}$$

Here a_o is the first Bohr orbit for hydrogen and $n_F = (n_1 - n_2)$ is the so called electric quantum number. The above equations works well when the electric field is large so that the splitting in the energy level is large compared to the spin orbit splitting.

If H_2 and H_3 are neglected then using Pauli's two component wave equation we see that

$$E_{o+1} = -\frac{e^2}{2a_o}\left(\frac{Z}{n}\right)^2 - \frac{\alpha^2 e^2}{2a_o}\left(\frac{Z}{n}\right)^4 \left(\frac{n}{j+\frac{1}{2}} - 3/4\right) \tag{16}$$

We notice that the spin orbit splitting (to the first approximation) goes as Z^4 whereas the first order Stark splitting varies as Z^{-1}. For hydrogen, for n = 2, the field for which the spin orbit splitting and the Stark splitting are of the same order of magnitude is 3×10^3 volt/cm and it drastically increases to 10^5 volt/cm for Z = 2, and 0.8 10^6 volt/cm for Z = 3. Experimentally we can not produce electric field more than 10^7 or 10^8 volt/cm, and hence for high Z values (Z > 5) we need a very accurate treatment of the problem. As $\Delta E_{s\cdot o}$ becomes equal to $\Delta E_{e\cdot f}$ the problem is really complicated and neither ℓ nor j or κ is a good quantum number. Only n and μ are good quantum numbers and one has to use degenerate perturbation theory. Depending upon values of these n and μ we will have $2(n-\mu)$ dimentional matrices which have to be diagonalize to get the energy eigenvalues and the eigenvectors. The eigenvectors would be a mixture of all values according to the Kramer's degenerate perturbation theory. The details of the theory are worked out in the Luder's paper.[29]

The Dirac wave functions are given by

$$\psi^{\mathcal{B}}_{N\kappa\mu}(r,\theta,\phi) = \begin{pmatrix} g_{n\kappa}(r)\,\chi^{\mu}_{\kappa}(\theta,\phi) \\ -i f_{n\kappa}(r)\,\chi^{\mu}_{-\kappa}(\theta,\phi) \end{pmatrix} \tag{17}$$

Where

$$g_{n\kappa}(r) = -\frac{1}{\sqrt{\Gamma(2\gamma_k+1)}}\sqrt{\frac{\Gamma(2\gamma_k+n+|k|+1)\,(1+\epsilon(n,k))}{\Gamma(2\gamma_k+1)\,(n-k)!\,4N(N-\kappa)}}$$

$$\cdot\, e^{-\frac{Zr}{Na_0}}\left(\frac{2Zr}{Na_0}\right)^{\gamma_k-1}\cdot\left\{-(n-k)\,{}_1F_1\begin{pmatrix}-n+k+1 \\ 2\gamma_k+1,\ \frac{2Zr}{Na_0}\end{pmatrix}\right.$$

$$\left.+(N-\kappa)\,{}_1F_1\begin{pmatrix}-n+k \\ 2\gamma_k+1,\ \frac{2Zr}{Na_0}\end{pmatrix}\right\}$$

and

$$f_{n\varkappa}(r) = -\frac{1}{\sqrt{\Gamma(2\gamma_k+1)}}\sqrt{\frac{\Gamma(2\gamma_k+n-k+1)\,(1-\epsilon(n,k))}{\Gamma(2\gamma_k+1)\,(n-k)!\,4N(N-\varkappa)}}$$

$$\cdot\, e^{-\frac{Z\xi}{Na_0}}\left(\frac{2Z\xi}{Na_0}\right)^{\gamma_k-1}\cdot\Big\{(n-k)\,\cdot$$

$${}_1F_1\begin{pmatrix}-n+k+1 \\ 2\gamma_k+1, & \frac{2Z\xi}{Na_0}\end{pmatrix} + (N-\varkappa)\,{}_1F_1\begin{pmatrix}-n+k \\ 2\gamma_k+1, & \frac{2Z\xi}{Na_0}\end{pmatrix}\Big\}$$

where

$$\gamma_k = \pm\sqrt{|\varkappa|^2-(\alpha Z)^2} \qquad |\varkappa| \equiv k$$

$$N(n,k) = N = \sqrt{n^2-2(n-k)\left(k-\sqrt{k^2-(\alpha Z)^2}\right)} \tag{18}$$

$$\epsilon(n,k) = \frac{1}{\sqrt{1+\left(\frac{\alpha Z}{n-k+\gamma_k}\right)^2}}$$

$${}_1F_1\begin{pmatrix}a \\ b\,;\, x\end{pmatrix} = 1+\frac{a}{b}x+\frac{a(a+1)}{b(b+1)\,2!}x^2+\cdots$$

$g_{n\kappa}$ and $f_{n\kappa}$ are tabulated by Payne[30] for various values of n and κ. The Hamiltonian including perturbation is

$$H = H_o' + V$$

where

$$H_o' = H_o + H_1 \quad \text{of Eqn. 14}$$

and

$$V = - Fez$$

where F is a constant. e is the charge on the electron and z is the distance in the z direction, Ze is the charge on the nucleus.

Then the matrix elements of the Hamiltonian are

$$H_{kk'}^{\mu\mu'} = \langle\psi_{n\kappa\mu}^{D}(r,\theta,\phi)|H|\psi_{n\kappa'\mu'}^{D}\rangle \qquad (19)$$

The H_o' part gives the diagonal matrix elements whereas

$$\langle\psi_{n\kappa\mu}^{D}(r,\theta,\phi)|r|\psi_{n\kappa'\mu'}^{D}(r,\theta,\phi)\rangle \qquad (20)$$

part gives off diagonal elements.

The Evaluation of the Off Diagonal Elements

Since $\chi_{\kappa}^{\mu}(\theta,\phi) = \sum_{\tau} C_{\mu-\tau}^{\ell(\kappa)}\,{}_{\tau}^{\frac{1}{2}}\,{}_{\mu}^{j(\kappa)}\; Y_{\ell(\kappa)}^{\mu-\tau}(\theta,\phi)\; \chi_{\frac{1}{2}}^{\tau}$

And we can write Fez as Fer cos θ. Substituting in Equation (20) we get

$$Fe \langle \psi_{n\kappa\mu}^{D}(r,\theta,\phi) | V | \psi_{n\kappa'\mu'}^{D}(r,\theta,\phi)\rangle$$

$$= \left[g_{n\kappa}(r) \langle\chi_{\kappa}^{\mu}| + i f_{n\kappa} \langle\chi_{-\kappa}^{\mu}| \right] r\cos\theta \begin{bmatrix} g_{n\kappa'}\, \chi_{\kappa'}^{\mu'} \\ -i f_{n\kappa'}\, \chi_{-\kappa'}^{\mu'} \end{bmatrix}$$

$$= \left[\int_0^\infty g_{n\kappa}(r)\, g_{n\kappa'}(r)\, r^3 dr + \int_0^\infty f_{n\kappa}(r)\, f_{n\kappa'}(r)\, r^3 dr \right] \cdot \langle \chi_\kappa^\mu \,|\, \cos\theta \,|\, \chi_{\kappa'}^{\mu'} \rangle \tag{21}$$

because

$$\langle \chi_{-\kappa}^\mu(\theta,\phi) \,|\, \cos\theta \,|\, \chi_{\kappa'}^{\mu'}(\theta,\phi) \rangle = \langle \chi_\kappa^\mu(\theta,\phi) \,|\, \cos\theta \,|\, \chi_{-\kappa'}^{\mu'}(\theta,\phi) \rangle$$

The angular part is evaluated using the Racah algebra and Wigner Eckert theorem.

$$\langle \chi_\kappa^\mu | Y_1^0 | \chi_{\kappa'}^{\mu'} \rangle = \delta_{\mu\mu'}\, C_{\mu' \; 0 \; \mu}^{j(\kappa') \; 1 \; j(\kappa)} \langle j'(\kappa) \| Y_1 \| j(\kappa) \rangle \cdot \sum_{\tau\tau'} C_{\mu-\tau \; 0 \; \mu'-\tau'}^{l(\kappa) \; 1 \; l(\kappa')} \tag{22}$$

The results are listed below.

$$\begin{aligned} \langle \chi_{\kappa_f}^\mu | \cos\theta | \chi_{\kappa_i}^\mu \rangle &= \frac{\sqrt{j_i^2 - \mu^2}}{2j} \quad \text{if } j_f - j_i = -1 \\ &= \frac{\sqrt{(j_i+1)^2 - \mu^2}}{2(j_i+1)} \quad \text{if } j_f - j_i = +1 \\ &= \frac{-\mu}{2j_i(j_i+1)} \quad \text{if } j_f - j_i = 0 \\ &= 0 \quad \text{if } \kappa_i = \kappa_f \end{aligned} \tag{23}$$

Evaluation of Dirac Radial Integrals

The radial integrals involved are

$$\int_0^\infty g_{n\kappa}(r)\, g_{n\kappa'}(r)\, r^3 dr + \int_0^\infty f_{n\kappa}(r)\, f_{n\kappa'}(r)\, r^3 dr$$
$$= C(n, \gamma_\kappa, k, N_\kappa)\, C(n \gamma_{\kappa'}, k', N(n,\kappa')) \Big\{ \int_0^\infty [-(n-\kappa)\,\phi_1(\kappa) + (N(n,\kappa)-\kappa)\,\phi_2(\kappa)][-(n-\kappa')\,\phi_1(\kappa') + (N(n,\kappa')-\kappa')\,\phi_2(\kappa')]\, r^3 dr$$
$$+ \sqrt{\frac{(1-\epsilon(n,\kappa))(1-\epsilon(n,\kappa'))}{(1+\epsilon(n,\kappa))(1+\epsilon(n,\kappa'))}} \int_0^\infty [(n-k)\,\phi_1(\kappa) + (N-\kappa)\,\phi_2(\kappa)]\,[(n-k')\,\phi_1(\kappa') + (N_{\kappa'}-\kappa')\,\phi_2(\kappa')]\, r^3 dr \Big\} \tag{24}$$

where

$$C(n, \gamma_\kappa, N(n,\kappa)) = \frac{1}{\sqrt{\Gamma(2\gamma_\kappa+1)}} \sqrt{\frac{\Gamma(2\gamma_\kappa+n-k+1)(1+\epsilon(n,\kappa))}{\Gamma(2\gamma_\kappa+1)\,\Gamma(n-k+1)\cdot 4\cdot N(N-\kappa)}} \tag{25}$$

$$\phi_1(\kappa) = e^{-\frac{Zr}{Na_0}} \left(\frac{2Zr}{Na_0}\right)^{\gamma_\kappa-1} {}_1F_1\left(\begin{matrix}-n+k+1 \\ 2\gamma_\kappa+1;\ \frac{2Zr}{Na_0}\end{matrix}\right) \tag{26}$$

$$\phi_2(\kappa) = e^{-\frac{Zr}{Na_0}} \left(\frac{2Zr}{Na_0}\right)^{\gamma_\kappa-1} {}_1F_1\left(\begin{matrix}-n+k \\ 2\gamma_\kappa+1,\ \frac{2Zr}{Na_0}\end{matrix}\right) \tag{27}$$

By replacing κ by κ', $N(n,\kappa)$ by $N(n,\kappa')$, and γ_κ by $\gamma_{\kappa'}$, one can easily write $\phi_1(\kappa')$, $\phi_2(\kappa')$ and $C(n, r_{\kappa'}, \kappa', n(n,\kappa'))$ so the general integrals involved are of the type (apart from constant multiplying them)

$$\int_0^\infty \phi_1(\kappa)\,\phi_1(\kappa')\,r^3\,dr,\quad \int_0^\infty \phi_1(\kappa)\,\phi_2(\kappa')\,r^3\,dr,$$

$$\int_0^\infty \phi_2(\kappa)\,\phi_1(\kappa')\,r^3\,dr$$

and
$$\int_0^\infty \phi_2(\kappa)\,\phi_2(\kappa')\,r^3\,dr \tag{27a}$$

Let us denote them by I_{11}, I_{12}, I_{21}, and I_{22}. We have then

$$I_{11} = \int_0^\infty e^{-\frac{Zr}{Na_0}} \left(\frac{2Zr}{Na_0}\right)^{\gamma_\kappa - 1} {}_1F_1\left({-n+\kappa+1 \atop 2\gamma_\kappa+1}\,;\, \frac{2Zr}{Na_0}\right) e^{-\frac{Zr}{Na_0}} \left(\frac{2Zr}{N(n,\kappa')a_0}\right)^{\gamma_\kappa' - 1} {}_1F_1\left({-n+\kappa'+1 \atop 2\gamma_\kappa'+1}\,;\, \frac{2Zr}{Na_0}\right) r^3\,dr \tag{28}$$

When we expand both ${}_1F_1\left({\alpha \atop \beta};x\right)$ functions as the power series as

$${}_1F_1\left({\alpha \atop \beta};x\right) = 1 + \frac{\alpha}{\beta}x + \frac{\alpha(\alpha+1)}{\beta(\beta+1)2!}x^2 + \cdots$$

$$= \sum_{s=0} \frac{(\alpha)_s}{(\beta)_s\, s!}\, x^s$$

$${}_1F_1\left({\alpha' \atop \beta'};x'\right) = \sum_{q=0} \frac{(\alpha')_q}{(\beta')_q\, q!}\,(x')^q$$

After substitution and integration and changing the dummy summation variables we get

$$I_{11} = \left(\frac{2}{N(n,\kappa)a_0}\right)^{\gamma_\kappa - 1} \left(\frac{2}{N(n,\kappa')a_0}\right)^{\gamma_{\kappa'} - 1} \sum_{s=0}^{\infty} \left\{ C(s) \left(\frac{1}{\lambda}\right)^{\gamma_\kappa + \gamma_\kappa' + 2 + s} \cdot \Gamma\left(\gamma_\kappa + \gamma_\kappa' + s + 2\right) \right\} \tag{29}$$

where

$$C(s) = \sum_{q=0}^{s} A(s-q)\,B(q) \;;\; A(s-q) = \frac{(\alpha)_{s-q}}{(2\gamma_k+1)_{s-q}(s-q)!}\left(\frac{2}{N_k a_0}\right)^{s-q}$$

and

$$B(q) = \frac{(\alpha')_q}{(2\gamma_k'+1)_q\, q!}\left(\frac{2}{N_k' a_0}\right)^q \;;\; A(0) = 1$$

$$\lambda = \left(\frac{1}{N(n,k)} + \frac{1}{N(n,k')}\right)\frac{1}{a_0} \;;\; B(0) = 1 = C(0) \tag{30}$$

In a similar way we can evaluate I_{22}, I_{12}, and I_{21}. Substituting these into the Equation (24) we arrive at

$$\begin{aligned}
&\int_0^\infty g_{nk}(r)\,g_{nk'}(r)\,r^3 dr + \int_0^\infty f_{nk}(r)\,f_{nk'}(r)\,r^3 dr \\
&= C\left(n, \gamma_k, k, N(n,k)\right) C\left(n, \gamma_k', k', N(n,k')\right) \\
&\Big[\Big\{ (n-k)(n-k') I_{11} + \left(N(n,k)-k\right) \cdot \\
&\left(N(n,k')-k'\right) I_{22} - (n-k)\left(N(n,k')-k'\right) I_{12} \\
&- (n-k')\left(N(n,k)-k\right) I_{21} \Big\} \\
&+ \sqrt{\frac{\left(1-\epsilon(n,k)\right)\left(1-\epsilon(n,k')\right)}{\left(1+\epsilon(n,k)\right)\left(1+\epsilon(n,k')\right)}} \Big\{ (n-k)(n-k') I_{11} \\
&+ (N_k - k)(N_{k'} - k') I_{22} + (n-k)(N_{k'} - k') I_{12} \\
&+ (n-k')(N_k - k) I_{21} \Big\} \Big]
\end{aligned} \tag{31}$$

Hence

$$V_{\kappa\kappa'}^{\mu\mu'} = \langle \psi^{D}_{N\kappa\mu}(r,\theta,\varphi) \,|V|\, \psi^{D}_{N\kappa'\mu'}(r,\theta,\varphi) \rangle$$

$$= \sum_{\tau} Fe\ \delta_{\mu\mu'}\, C^{j(\kappa)\ 1\ j(\kappa')}_{\mu\ \ 0\ \ \mu}\, C^{l(\kappa)\ 1\ l(\kappa')}_{\mu-\tau\ 0\ \mu-\tau}$$

$$\langle j'(\kappa') \| Y_1 \| j(\kappa) \rangle \cdot C(n, \gamma_\kappa, \kappa, N_\kappa)$$

$$C(n, \gamma_{\kappa}', \kappa', N_{\kappa'}) \Big[\Big(1 + \sqrt{\frac{(1-\epsilon)(1-\epsilon')}{(1+\epsilon)(1+\epsilon')}}\Big)(n-k)$$

$$(n-k')I_{11} + (N_\kappa - k)(N_{\kappa'}' - k')\, I_{22})$$

$$- \Big(1 - \sqrt{\frac{(1-\epsilon)(1-\epsilon')}{(1+\epsilon)(1+\epsilon')}}\Big)\big((n-k)(N' - k')I_{12}$$

$$+ (n - k')(N - k)\, I_{21}\big) \Big] \qquad (32)$$

where

$$\varepsilon' = \varepsilon(n,k') \qquad \varepsilon = (n,k) \qquad N' = N(n,k'), \text{ etc.}$$

Equation (32) gives the off diagonal elements of the energy matrix.

The Diagonalization of the Energy Matrix

Let

$$\phi_i(r,\theta,\phi) = \sum_k a_{ik}\, \psi^{D}_{n\kappa\mu}(r,\theta,\phi)$$

where the summation is over k $a_{i\kappa}$'s are chosen such that

$$\langle\phi_i(r,\theta,\phi)|H|\phi_j(r,\theta,\phi)\rangle = E_i\, \delta_{ij} = E_n^{(o)} + \Delta E_n^{(1)} + \Delta E_n^{(fs)}$$

and

$$\langle\psi_i|\phi_j\rangle = \delta_{ij}$$

Since the Hamiltonian is Hermitian we can use Jocobi method to diagonalize it. Diagonalization has been carried by using a standard available subroutine from the computer library, through which roots and vectors are available.

Application of Relativistic Symmetric Hamiltonian to Stark Effect

As it is discussed in Chapter II, the approximate relativistic Symmetric Hamiltonian is given by

$$H_{sym} = H_D + H_{ff}$$

where H_D is the Dirac Coulomb Hamiltonian and

$$H_{ff} = \rho_2 \frac{\vec{\sigma}\cdot\vec{r}}{r} \kappa \left(\sqrt{1 + \left(\frac{\alpha Z}{k}\right)^2} - 1\right)$$

The Hamiltonian for the electron in the Coulomb field with the unperturbed symmetric Hamiltonian is

$$H = H_{sym} - FeZ \tag{33}$$

$$= H_{sym} + V \tag{34}$$

The wave functions of the symmetric Hamiltonian are

$$\psi^{S}_{N\kappa\mu} = \begin{pmatrix} g^{S}_{n\kappa}(r) & \chi^{\mu}_{\kappa}(\theta,\varphi) \\ -i f^{S}_{n\kappa}(r) & \chi^{\mu}_{-\kappa}(\theta,\varphi) \end{pmatrix} \tag{35}$$

where s refers to the Symmetric Hamiltonian wave function.

And

$$g^{s}_{n\kappa}(r) = \frac{1}{\sqrt{2\varsigma^2-1}}\left\{\sqrt{(\varsigma+1)(\varsigma+\epsilon_N)}\,F_{Nl(\kappa)}(r) - S_\kappa\sqrt{(\varsigma-\epsilon_N)(\varsigma-1)}\,F_{N\tau(\kappa)}(r)\right\}$$

$$f^{s}_{n\kappa}(r) = \frac{1}{\sqrt{2\varsigma^2-1}}\left\{\sqrt{(\varsigma+1)(\varsigma-\epsilon_N)}\,F_{Nl(\kappa)}(r) - S_\kappa\sqrt{(\varsigma+1)(\varsigma+\epsilon_N)}\,F_{N\tau(\kappa)}(r)\right\}$$

Here

$$\zeta = \varepsilon_N \sqrt{1 + (\frac{\alpha Z}{\kappa})^2} \qquad \varepsilon_N = \frac{E_N}{m} = \frac{1}{\sqrt{1 + (\frac{\alpha Z}{n})^2}}; \ \bar{\ell}(\kappa) = \ell(-\kappa)$$

We have

$$H_{sym}|\psi^{s}_{n\kappa\mu}(r,\theta,\phi)> = E_N|\psi^{s}_{n\kappa\mu}(r,\theta,\phi)> \tag{36}$$

We treat V as the perturbation and we have to evaluate

$$V^{\mu\mu'}_{\kappa\kappa'} = <\psi^{s}_{n\kappa\mu}(r,\theta,\phi)|V|\psi^{s}_{n\kappa'\mu'}(r,\theta,\phi)> \tag{37}$$

The evaluation is similar to exact Dirac case, but for the fact that radial integrals are easier to evaluate. In fact integrals are same as the one encountered in non-relativistic calculations. The diagonalization is also similar.

Section III

The Second Order Stark Effect

When we are considering the transition between nondegenerate states, the contribution from the first order effect is zero and we go for the second or higher order corrections to the energy shifts. In actuality even for the hydrogen atom, as in the hydrogen maser[37], the energy levels are split due to the hyperfine structure. In the case of the alkali atoms such splitting can be observed in the optical range. The second order correction is given by

$$\Delta E_n^{(2)} = \sum_m{}' |V_{nm'}|^2/(E_n^{(0)} - E_m^{(0)}) \ ; \ V_{nm'} = <\psi_n|V|\psi_{m'}> \tag{38}$$

The prime on the sum means $n \neq m$. If many matrix elements are surviving, then the correct second order correction is obtained by diagonalization of

$$\left| \sum_{m}{}' \frac{V_{nm} V_{mn'}}{E_n^{(0)} - E_m^{(0)}} - \Delta E_n^{(2)} \delta_{nn'} \right| = 0 \tag{39}$$

If the second order perturbation matrix does not connect the degenerate states by way of one or more intermediate states m, i.e., if

$$\sum_{m} \frac{V_{nm} V_{mn'}}{E_n^{(0)} - E_m^{(0)}} = 0$$

when $n \neq n'$ then Equation (39) leads to (38) which is the simple formula for the quadratic Stark effect. In the first section we evaluated $V_{nn}^{\kappa\kappa'}$, which in the general case becomes

$$Fe \langle \psi_{Nk\mu}, z\,\psi_{Nk'\mu'} \rangle = \sum_{\tau} Fe\, \delta_{\mu\mu'}\, C^{j(k)\ 1\ j(k')}_{\mu\ \ 0\ \ \mu} \cdot C^{\ell(k)\ 1\ \ell(k')}_{\mu-\tau\ 0\ \mu-\tau} \langle j(k') \| Y_1 \| j(k) \rangle R_{nn'}^{\varkappa\varkappa'}(r) \tag{40}$$

Where $R_{nn'}^{\kappa\kappa'}(r)$ is the part involving the radial integral

$$\begin{aligned} R_{nn'}^{\varkappa\varkappa'}(r) = {} & C(n, \gamma_k, k, N(n,k))\, C(n', \gamma_{k'}, k', N(n,k')) \cdot \\ & \cdot \Bigg\{ \left(1 + \sqrt{\frac{(1-\epsilon(n,k))(1-\epsilon(n',k'))}{(1+\epsilon(n,k))(1+\epsilon(n',k'))}} \right) \Big((n-k)(n'-k')\, I_{11}' \\ & + \big((N(n,k)-\varkappa)(N(n',k')-\varkappa') \big) I_{22}' \Big) \\ & - \left(1 - \sqrt{\frac{(1-\epsilon(n,k))(1-\epsilon(n',k'))}{(1+\epsilon(n,k))(1+\epsilon(n,k))}} \right) \Big[(n-k)(N(n',k')-\varkappa') I_{12}' \\ & + (n'-k')(N(n,k)-\varkappa)\, I_{21}' \Big] \Bigg\} \end{aligned} \tag{41}$$

I'_{11}, I'_{22}, I'_{21} and I'_{12} are defined in (27.a) wherein we have to replace $n\kappa'\mu$ by $n'\kappa'\mu'$. In the Pauli approximation these reduce to

$$\begin{aligned} \langle n j \mu_j | z | n', j-1, \mu_j \rangle &= R^{jj'}_{nn'}(r)\sqrt{j^2-\mu^2} \\ \langle n j \mu_j | z | n' j \mu_j \rangle &= R^{jj}_{nn'}(r)\,\mu_j \\ \langle n j \mu_j | z | n' j+1\, \mu_j \rangle &= R^{jj+1}_{nn'}(r)\sqrt{(j_i+)^2-\mu_j^2} \end{aligned} \tag{42}$$

Here $R^{jj'}_{nn'}(r)$ include the reduced matrix element $\langle j(n')||y_1||j(\kappa)\rangle$ and the radial part. They are independent of μ_j. Using these results we get

$$\Delta E_n^{(2)} = (A + B\mu_j^2)\, e^2 F^2 \tag{43}$$

with

$$\begin{aligned} A &= \sum_{n'}{}' \left\{ R^{j,j+1}_{nn'}(r)\frac{(j+1)^2}{E^{(0)}_{nj} - E^{(0)}_{n'j+1}} + \frac{R^{jj-1}_{nn'}(r)\; j^2}{E^{(0)}_{nj} - E^{(0)}_{n'j-1}} \right\} \\ B &= \sum_{n'}{}' \left\{ \frac{R^{jj}_{nn'}(r)}{E^{(0)}_{nj} - E^{(0)}_{n'j}} - \frac{R^{j,j+1}_{nn'}(r)}{E^{(0)}_{nj} - E^{(0)}_{n'j+1}} - \frac{R^{jj-1}_{nn'}}{E^{(0)}_{nj} - E^{(0)}_{n'j-1}} \right\} \end{aligned} \tag{44}$$

In the present work we have not attempted to calculate A and B using exact Dirac Function for two reasons. Firstly for atoms of low atomic numbers, as will be shown in Section IV, the difference between the values of the matrix elements calculated by exact Dirac and Pauli approximation is very small even in the first order ($\simeq 10^{-6}$ cm^{-1} for $Z = 1$, $n = 2$, $\kappa = +1$ term). So in the second order, required accuracy can be attained by using Pauli approximation. On the other hand for high Z values where relativistic effects might be pronounced we need to include the other sensitive effects like screening, electron correlation, hyperfine splitting, etc. For the same reason calculations of the oscillator strength f_{mn} or the transition probability are deferred.

If the energy $E_{n'}^{(o)}$, for one or more levels is close to $E_n^{(o)}$, the second order correction to the energy of the level n is large, as $E_n^{(o)} - E_{n'}^{(o)}$ is in the denominator, we cannot use Equation (38) and the shift of the energy level must be found by exact diagonalization of the matrix of the operator $(H_o' + \underset{\sim}{V})$. For two closely spaced nondegenerate levels $E_1^{(o)}$ and $E_2^{(o)}$ (with $E_1^{(o)} > E_2^{(o)}$), this leads to the stationary values

$$E_1 = + \frac{1}{2}\sqrt{(E_1^{(0)} - E_2^{(0)})^2 + 4|V_{12}|^2}$$

$$E_2 = - \frac{1}{2}\sqrt{(E_1^{(0)} - E_2^{(0)})^2 + 4|V_{12}|^2}$$

The origin from which the energy is measured is at $\frac{1}{2}(E_1^{(o)} - E_2^{(o)})$. If $2|V_{12}| << E_1^{(o)} - E_2^{(o)}$ then the energy values

$$E_{\substack{1\\2}} = \frac{1}{2}(E_1^{(0)} - E_2^{(0)}) \pm \frac{|V_{12}|^2}{(E_1^{(0)} - E_2^{(0)})}$$

are the same as given by the second order perturbation theory for the non degenerate levels, whereas for $2|V_{12}| >> E_1^{(o)} - E_2^{(o)}$ the values $V_{12} = E_1 = -E_2$ are the same as given by first order perturbation theory and hence a linear effect is predicted. For the intermediate cases we find the mixture of both the first order and the second order effects.

The application of electric field sometimes removes the forbiddenness of the transition. To see this let us consider the two states $\psi_1^{(o)}$ and $\psi_2^{(o)}$ with energies $E_1^{(o)}$ and $E_2^{(o)}$ described above. Let their wavefunctions in electric field be ψ_1 and ψ_2, respectively. Let as further suppose that there is a third non-degenerate state $\psi_3^{(o)}$ with energy $E_3^{(o)}$ which is connected only with the state $\psi_1^{(o)}$. In the absence of electric field $\psi_1 = \psi_1^{(o)}$ and $\psi_2 = \psi_2^{(o)}$ and the spectrum consists of a single line. When the field is applied, each of the state ψ_1 and ψ_2 becomes the mixture of the unperturbed states $\psi_1^{(o)}$ and $\psi_2^{(o)}$. Therefore there will be two lines in the spectrum with frequencies $\omega_1 = \frac{E_3^{(o)} - E_1}{h}$ and $\omega_2 = \frac{E_3^{(o)} - E_2}{h}$. The intensity of the ω_1 line is practically independent of the electric field. Whereas that of the line ω_2 is proportional to $\left(\frac{|V_{12}|}{E_1^{(o)} - E_2^{(o)}}\right)^2$, i.e., the square of the electric field. Thus the appearance of the line with frequency ω_2 is regarded as a sign that the forbiddenness of the transition is removed.

Section IV

Calculation and Results

The first order Stark shifts are calculated for n = 2,3,4,5, and 6 for the atoms with atomic numbers z = 1,2,...........9,29,39,49,59,69, 79,89 and 99 (and are stored on that tape). The values for the electric fields used are dependent upon the Z values such that the fine structure splitting and the Stark shifts are of the same order of magnitude. The dimensionality of the matrix, which is to be diagonalized, depended on the values of n and μ. For example n = 3 and $\mu = \frac{1}{2}$, k can take values -1, +1, -2, +2, -3. Hence we had a 5 x 5 matrix to be diagonalized. For n = 6, $\mu = \frac{1}{2}$, 3/2, 5/2, 7/2 and 9/2, the matrices were 11, 9, 7, 5, and 3 dimensional and the energy level splits into 36 components. Even after the application of the electric field the energy levels ($nx\mu$) and ($nk-\mu$) are not separated hence the energy levels for μ and $-\mu$ are still degenerate. This phenomena gives an added important tool to the experimentalist and has been abundantly used in the Stark shift measurements by the level crossing method and the method of beats.

For low values of the atomic number the difference between the calculations of the energy shift using the exact Dirac and Pauli approximations as is to be expected, is of the order of 10^{-3} to 10^{-8} cm^{-1}, and hence we were not able to show the difference on the graph. Table I gives the calculations for various values of the field for n = 2 and Z = 4. The energy level with $\kappa = -n$ and $\mu = (n-\frac{1}{2})$ is not affected by the electric field. So we take its energy as the reference level and calculate the shifts of other sub-levels for a given n value.

Figures 2 through 6 give the splittings of different terms. In Figure 2, we have graphed the splitting of n = 2 and Z = 4 term. The electric fields used for the calculations range from 0.0 to 351.4 Kv/cm in a step of 50 Kv. cm^{-1}. The fine structure splitting is of the order of 93.3542 cm^{-1}. In the electric field the κ degeneracy is broken and $2S_{\frac{1}{2}}^{\frac{1}{2}}$ and $2P_{\frac{1}{2}}^{\frac{1}{2}}$ states separate out. We notice that there is no level crossing here. But if one applies a magnetic field parallel to the electric field then $P_{3/2}$ ($\mu = -3/2$) level will cross $P_{\frac{1}{2}}(\mu = \frac{1}{2})$ term and one can use the level corssing method to study the shifts.

In Figure 3, we have graphed n = 3 terms for Z = 1 as well as Z = 3, for the field strength 0 to 700 and 0 to 70,000 volts cm^{-1} respectively. Sample calculations for these cases are given in Table II (see also at the end of the Appendix). Table III gives the field strengths at which the various levels cross.

In Figure 4, we have graphed n = 4 for Z = 2, for the field strength 0 to 3500 volts cm^{-1}. Table IV gives the field strength at which different levels cross. Figure 5 is drawn for n = 5 and Z = 2. Here we

TABLE I

STARK SHIFT CALCULATIONS FOR n = 2, Z = 4

j	μ	κ	F Million Volt cm^{-1}	Stark Shift Using Dirac Wave Functions cm^{-1}	Stark Shift Luder's Calculations cm^{-1}
3/2	½	-2	0.2	0.294231	0.294461
			0.4	1.171366	1.172346
			0.6	2.615130	2.617216
			0.8	4.599243	4.602874
			1.0	7.089028	7.094558
			1.2	10.043625	10.051319
			1.4	13.418507	13.428542
½	½	-1	0.2	- 89.796186	- 89.745283
			0.4	- 86.546617	- 86.494786
			0.6	- 83.612549	- 83.560100
			0.8	- 80.992480	- 80.939678
			1.0	- 78.676516	- 78.623625
			1.2	- 76.647472	- 76.594715
			1.4	- 74.882425	- 74.829977
½	½	-1	0.2	- 97.206534	- 97.158236
			0.4	-101.333210	-101.286590
			0.6	-105.711072	-105.666219
			0.8	-110.315251	-110.272252
			1.0	-115.12094	-115.079953
			1.2	-120.104668	-120.065689

TABLE II

STARK SHIFT CALCULATIONS FOR n = 3, Z = 1 and Z = 3

n = 3							
Z = 1				Z = 3			
F volt/cm	Exact Dirac cm^{-1}	Lüden's Work cm^{-1}	Symmetric Hamiltonian cm^{-1}	F Kvolt/cm	Exact Dirac cm^{-1}	Lüden's Work cm^{-1}	Symmetric Hamiltonian cm^{-1}
$j = 5/2$ $\mu = 1/2$ $\kappa = (-3)$							
100.4	.0106138	.0106138	.033873	10	.164407	.164430	.16693234
200.8	.0336720	.0336720	.0667746	20	.606753	.606834	.333864
300.2	.0623209	.0623225	0.1001620	30	1.238854	1.239033	.500797
401.6	.0942006	.0942023	0.1335493	40	1.998812	1.999106	.6677293
502.0	.128098	.12810132	0.166936	50	2.851092	2.851529	.834661
$j = 5/2$ $\mu = 3/2$ $(\kappa = -3)$							
100.4	.0717517	.07175615	.017638	10	.0126984	.0126980	.0881902
200.8	.0223443	.0223448	.0352761	20	.0485502	.0485499	.176380
301.2	.0399033	.0399037	.0529142	30	.102377	.102381	.264570
401.6	.0582793	.0582797	.0705523	40	.168795	.168805	.352760
502.0	.0770098	.0770115	.0881904	50	.243659	.243668	.440951

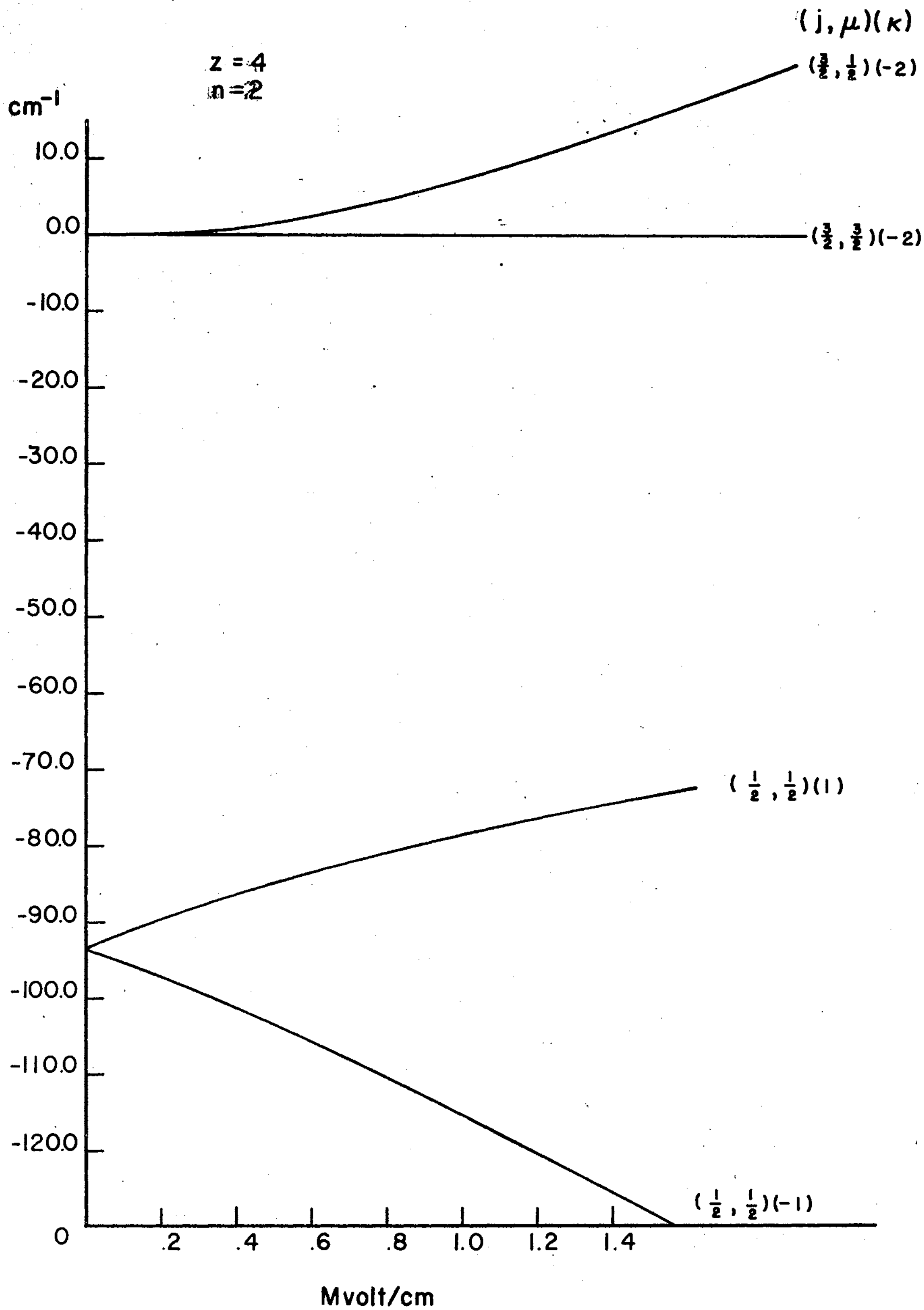

Figure 2. The First Order Stark Shift for $n = 2$, $Z = 4$

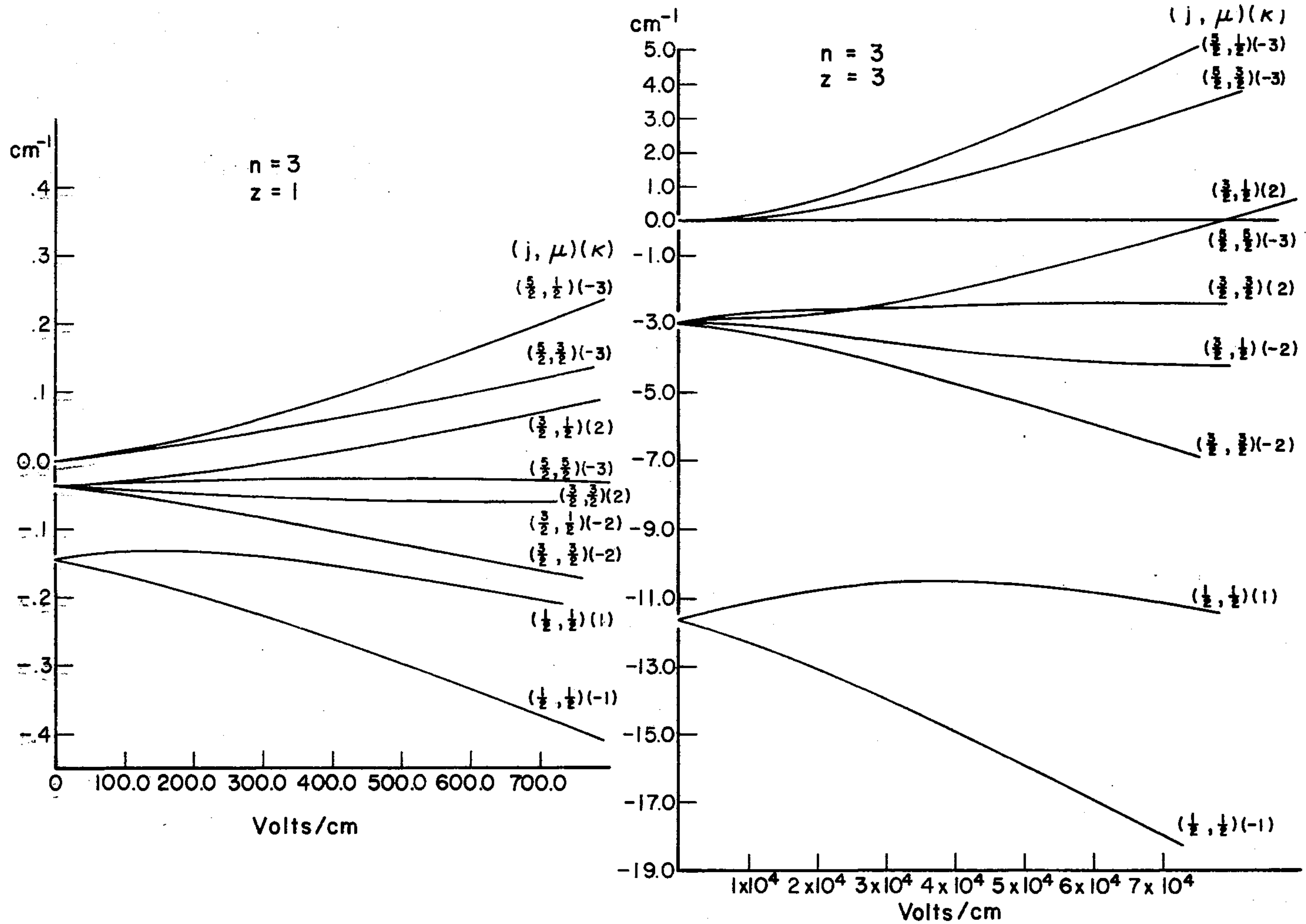

Figure 3. The First Order Stark Shift for n = 3, Z = 1 and Z = 3

TABLE III

LEVEL CROSSING FIELDS FOR n = 3, Z = 1, and Z = 3

j	μ	(κ)	j'	μ'	(κ')	Z = 1	Z = 3
3/2	½	(2)	3/2	3/2	(+2)	100.0 volt cm^{-1}	2.7×10^{4} volts/cm
3/2	½	(2)	5/2	5/2	(-3)	350.0 volts/cm	7.75×10^{4} volts/cm

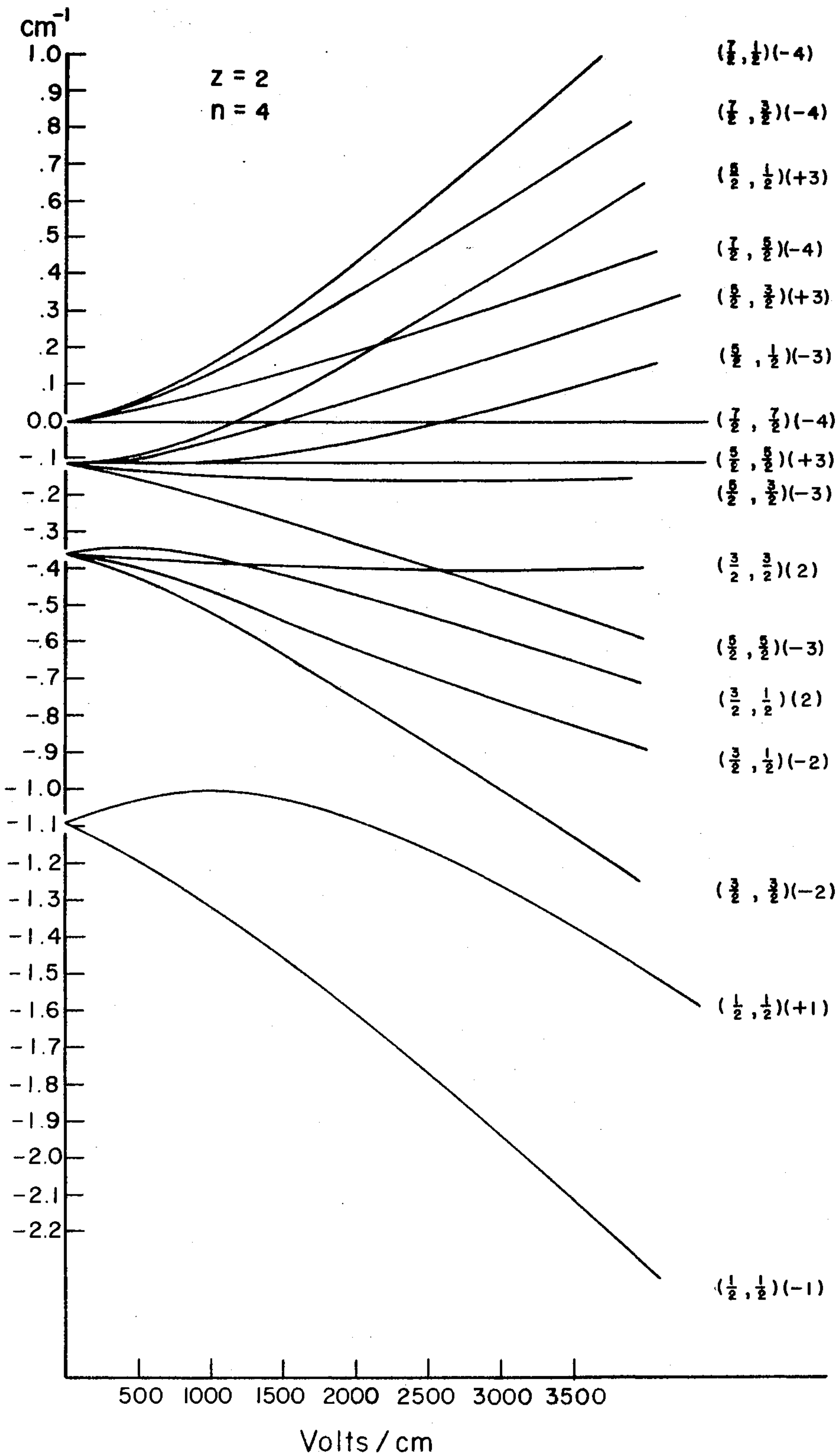

Figure 4. The First Order Stark Shifts for n = 4, Z = 2

TABLE IV

LEVEL CROSSING FIELDS FOR n = 4, Z = 2

j	μ	κ	j'	μ'	κ'	Level Crossing Fields
5/2	½	(−3)	5/2	5/2	(+3)	1120.0 volts/cm
5/2	½	(+3)	7/2	7/2	(−4)	1130.0 volts/cm
5/2	3/2	(+3)	7/2	7/2	(−4)	1500.0 volts/cm
5/2	½	(+3)	7/2	5/2	(−4)	2425.0 volts/cm
5/2	½	(−3)	7/2	7/2	(−4)	2650.0 volts/cm

can notice the complexity of the splitting. In Figure 6, we draw the splitting for n = 6 and Z = 3. However, only $\mu = \frac{1}{2}$ terms are graphed as the inclusion of all the 36 levels will lead to no understandable and clear picture. In Figure 7 we show the effect of electric field on the transition $(2P^{1/2}_{3/2} \rightarrow 2P^{1/2}_{1/2})$ as a function of Z.

From Figures 2 through 6 we see that the term $(j \simeq n - \frac{1}{2}, \mu = n - \frac{1}{2})$ does not have first order Stark effect. Hence to study the effect of an electric field on terms like $2P^{3/2}_{3/2}$, $3D^{5/2}_{5/2}$, $4f^{7/2}_{7/2}$, $5g^{9/2}_{9/2}$ and $6h^{11/2}_{11/2}$ we have to use the second order perturbation calculations.

Figure 8 shows the energy level shifts which are calculated by using the Symmetric Hamiltonian. Because of the O(4) symmetry there is no spin orbit splitting and the shifts are very linear. Junge and Steubing[31,32] have experimentally measured Stark shifts in 10π component of H_β line and 18π component of H_γ line. Table V gives comparison of experimental and theoretical values of proportionality constant a. Between 5000 and 12000 v/cm the shift is linear. In Figure 9a we have plotted the results for 10π component of H_β and in 9b we plotted 18π component of H_γ. For fields below 5000 v/cm the shift is quadratic than linear. The experimental results of Kessner who used fields from 48 kv/cm to 98 kv/cm agree with non relativistic calculations of Schrodinger and Epstein.

Steubing and Gunther have done Stark shift measure on HeII 4686 line.[(33)] The field strength in their experiment varies from 50 to 110 kv/cm. In Figure 10 we give the calculated and experimental results. In this case the difference in the results from Dirac and Symmetric Hamiltonian is very small.

Steubing and Hengevoss[34] have done similar measurements on all

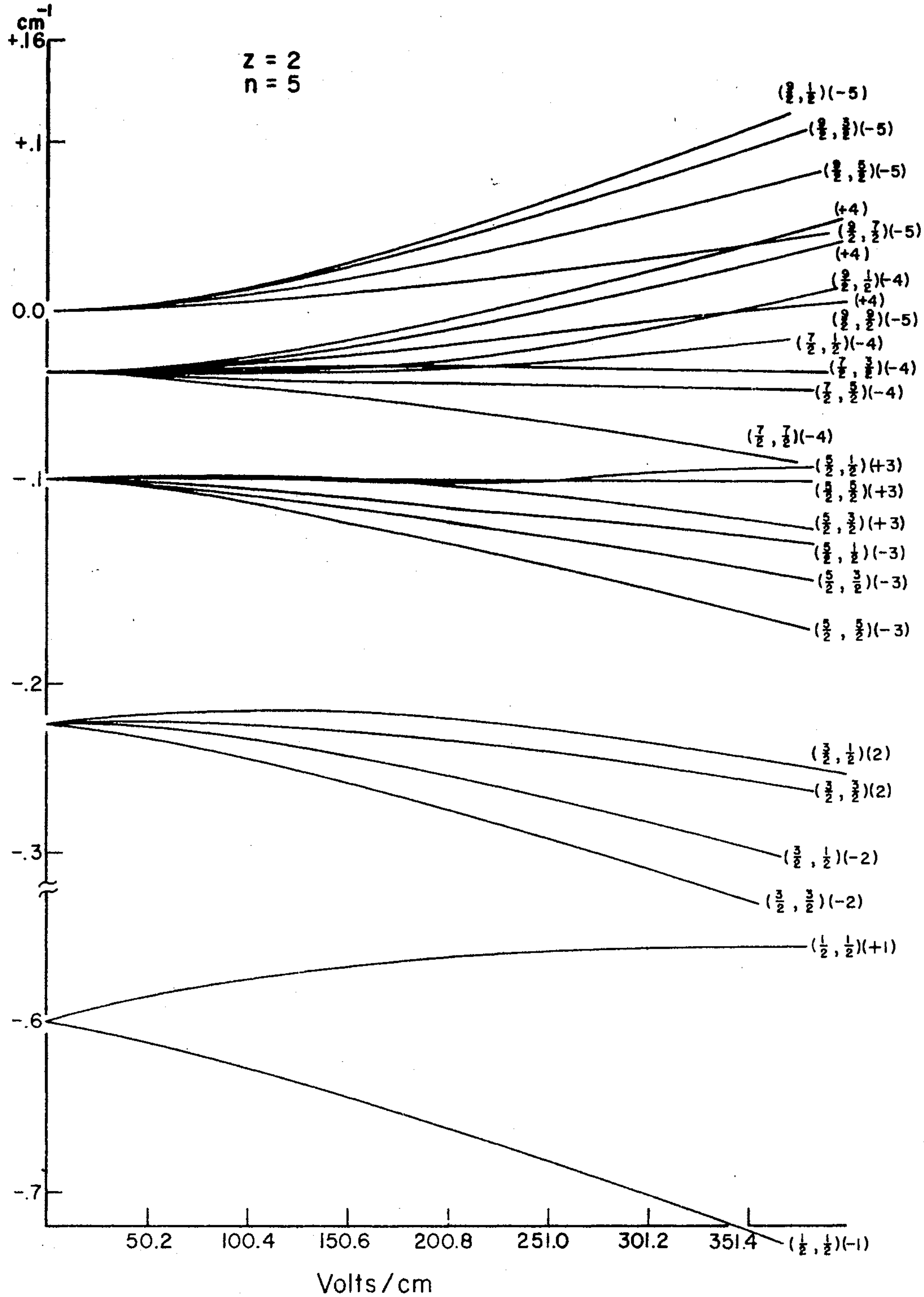

Figure 5. The First Order Stark Shifts for n = 5, Z = 2

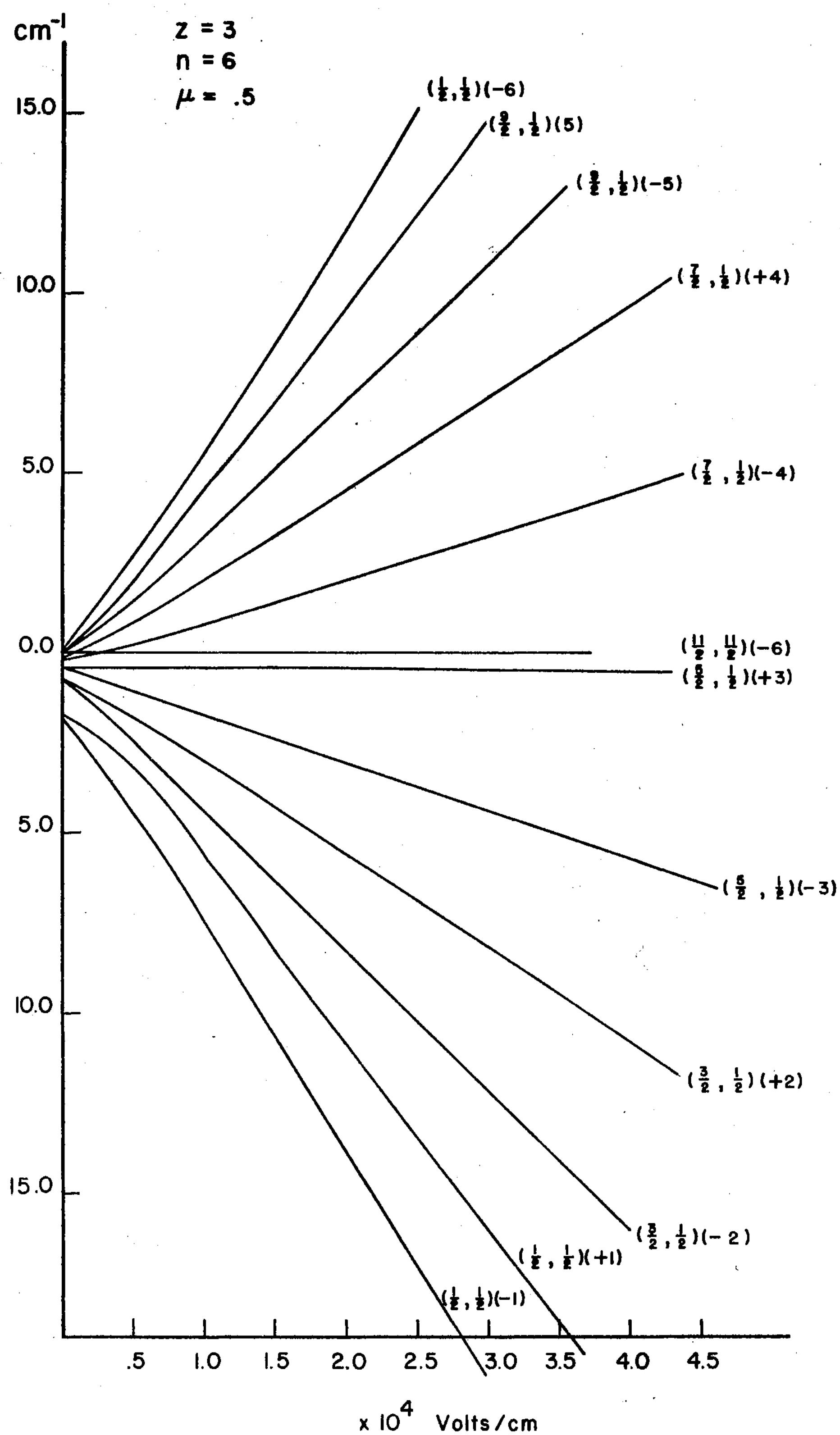

Figure 6. The First Order Stark Shifts for n = 6, Z = 3 and $\mu = \frac{1}{2}$

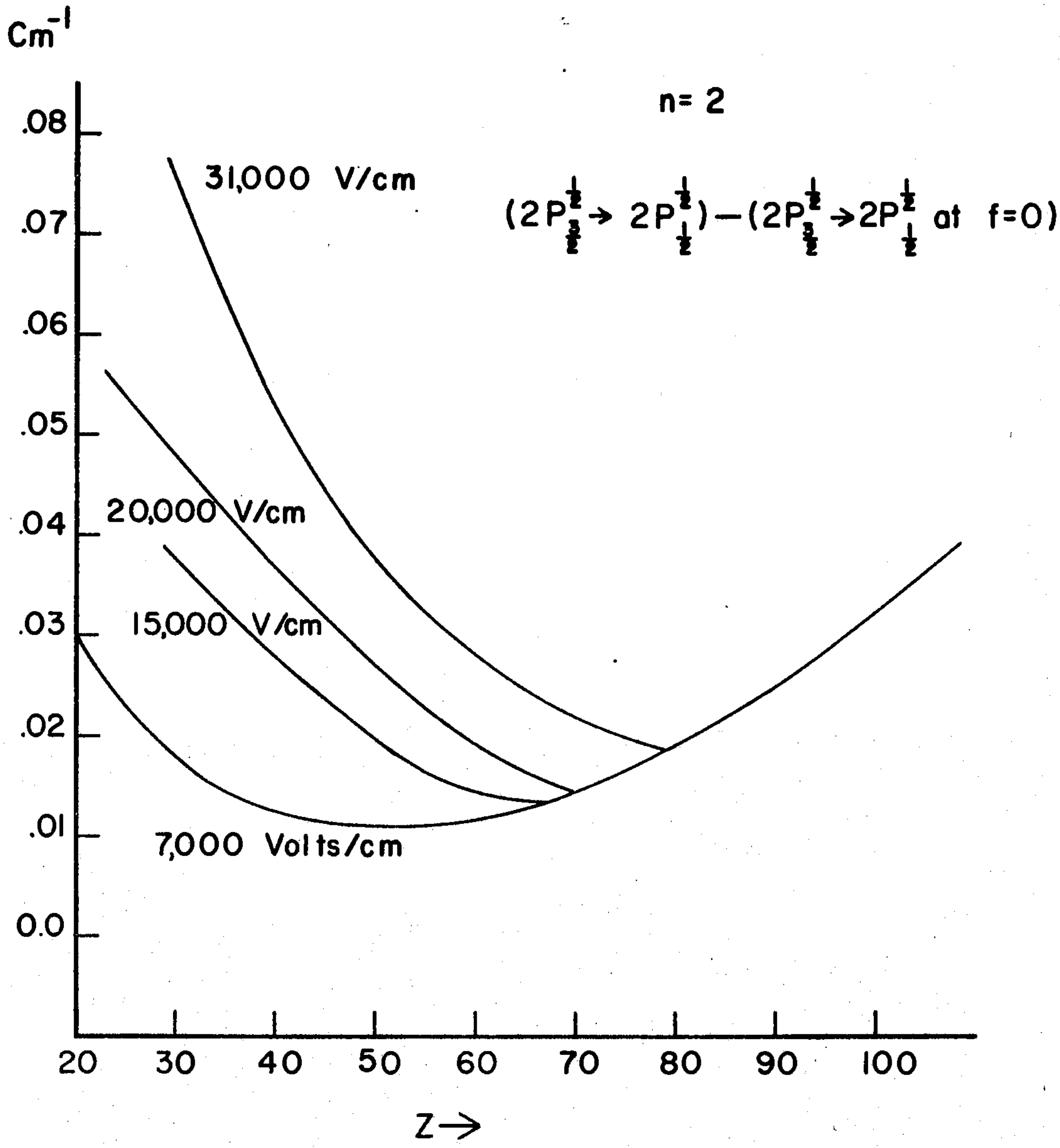

Figure 7. Z Dependence of the Transition $(2P^{1/2}_{3/2} \rightarrow 2P^{1/2}_{1/2})$ on the Electric Field

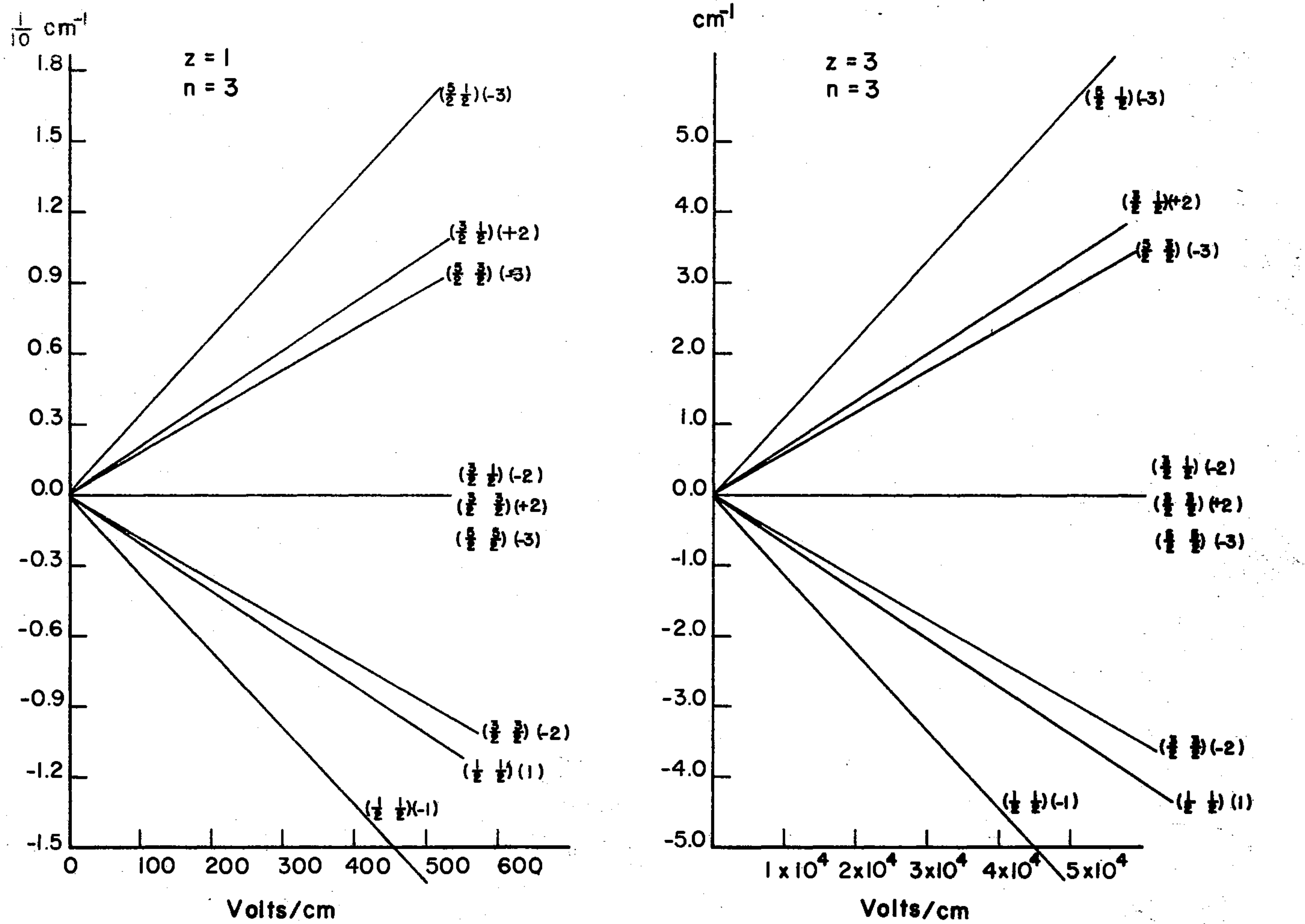

Figure 8. The First Order Stark Shifts for n = 3, Z = 1 and Z = 3 Using Symmetric Hamiltonian

TABLE V

PARAMETER FOR THE FIRST ORDER STARK EFFECT

n	n_f	$n\,n_f$	First Order Stark Constant in $cm^{-1}/Kv\ cm^{-1}$ Dirac	Symmetric	Experimental
2	1	2	.05631	.052788	
3	2	6	.06317	.055645	
			.06497	.055445	
	1	3	.06545	.067181	
			.0624		
			.06450	.05855	
4	3	12	.06421	.05706	
	2	8	.06421	.06659	.06449
			.06411	.05945	
	1	4	.06439	.06682	.06428
			.06423	.06082	
			.06402	.05739	
5	4	20	.06395	.05815	
	3	15	.06395	.06619	.06402
			.06385	.05981	
				.06662	
	2	10	.06453	.06111	
				.05849	
	1	5	.06421	.06605	
				.06629	
				.05988	
				.06186	

strong π and σ components of HeII 3203 line. Range of the field here again was 50 to 110 kv/cm. The proportionality constant is 6.402 $cm^{-1}/Mv.\ cm^{-1}$. Level splitting in deuteron were measured by Steubing et al.[35] Their results for 8π of D_β and 15π of D_γ give the value of a as 6.44 and 6.48 $cm^{-1}/Mv.cm^{-1}$. Steubing and Lebowsky have done the measurements of shifts in crossed electric and magnetic fields[36].

The linear Stark effect is possible only in hydrogen and hydrogen like atoms, and hence the range of its validy is limited. For all non-degenerate energy levels the contribution from first order Stark effect is zero. The phenomena of hyperfine structure lifts the degeneracy even for hydrogen like atoms with nonzero nuclear spin. The Lamb shift also eliminates the degeneracy between $2S_{\frac{1}{2}}$ and $2P_{\frac{1}{2}}$ states. In addition to this intrinsic difficulty the experimenters prefer to use the levels like 2P(3/2, 3/2) or 3D(5/2, 5/2) which give linear shifts in Paschen Back effect. Hence most of the recent experimental work reported in the literature is of the second order Stark effect. Table VI gives such calculations and measurements. Level splitting in Li was observed by Budick, Marcus and Novick[14]. Following is the brief description of their experiment.

The Lithium atoms in the form of a beam are excited by resonance radiation (transition 3P - 2S) and are in a magnetic field. At a field strength 915 G the sub-levels $2P_{3/2}(\mu = -3/2)$ and $2P_{\frac{1}{2}}(\mu = \frac{1}{2})$ cross. This is registered as the resonance behavior of the intensity of fluorescence at angle 90^o with the direction of the exciting radiation. When the constant electric field E, parallel to the magnetic field H, is applied, the sub-levels $2P_{3/2}$ and $2P_{1/2}$ are unequally shifted and cross at a different value of the magnetic field. Actually there are

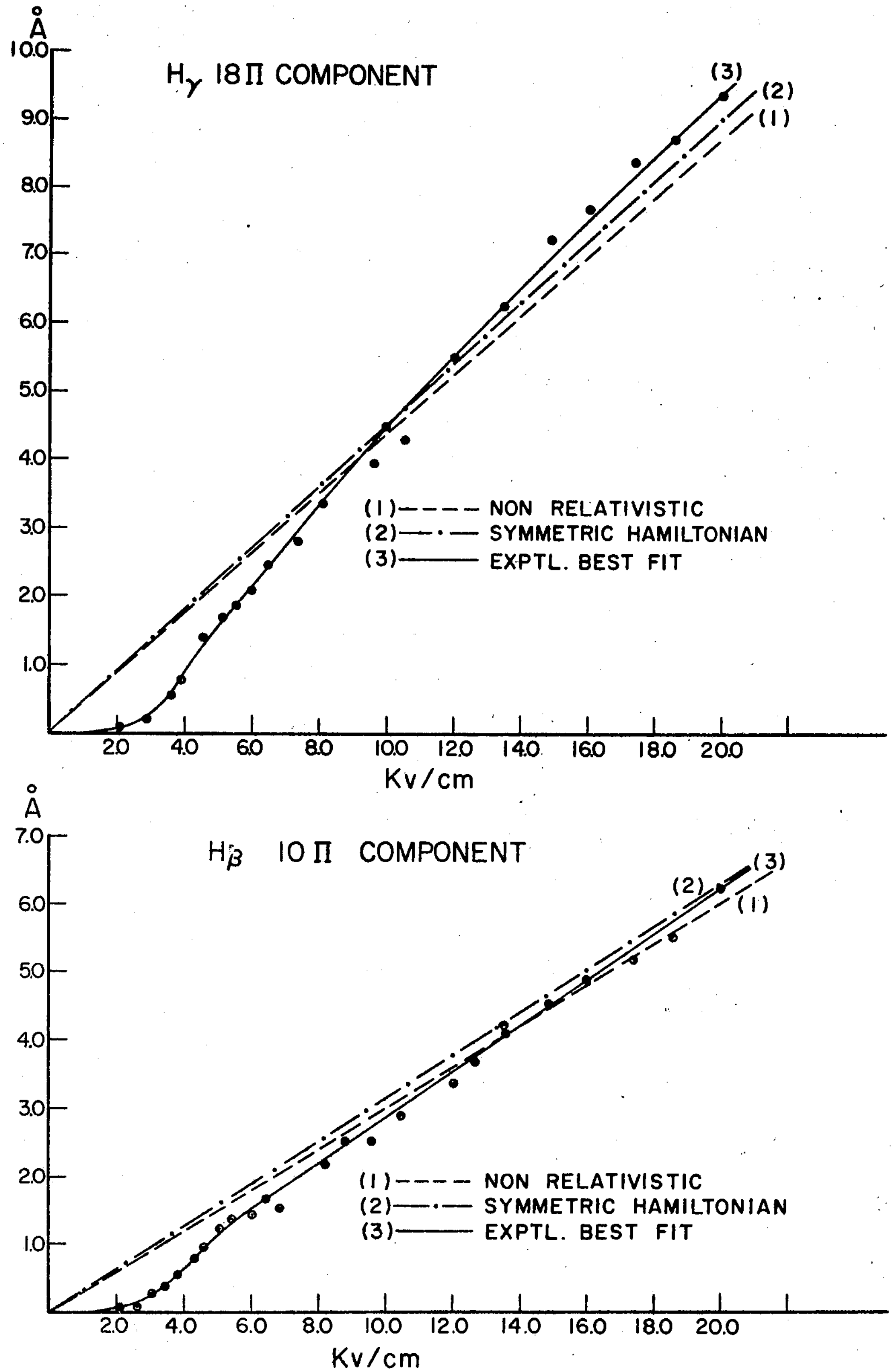

Figure 9. Experimental and Theoretical Stark Shifts of H_{β} and H_{γ} Lines

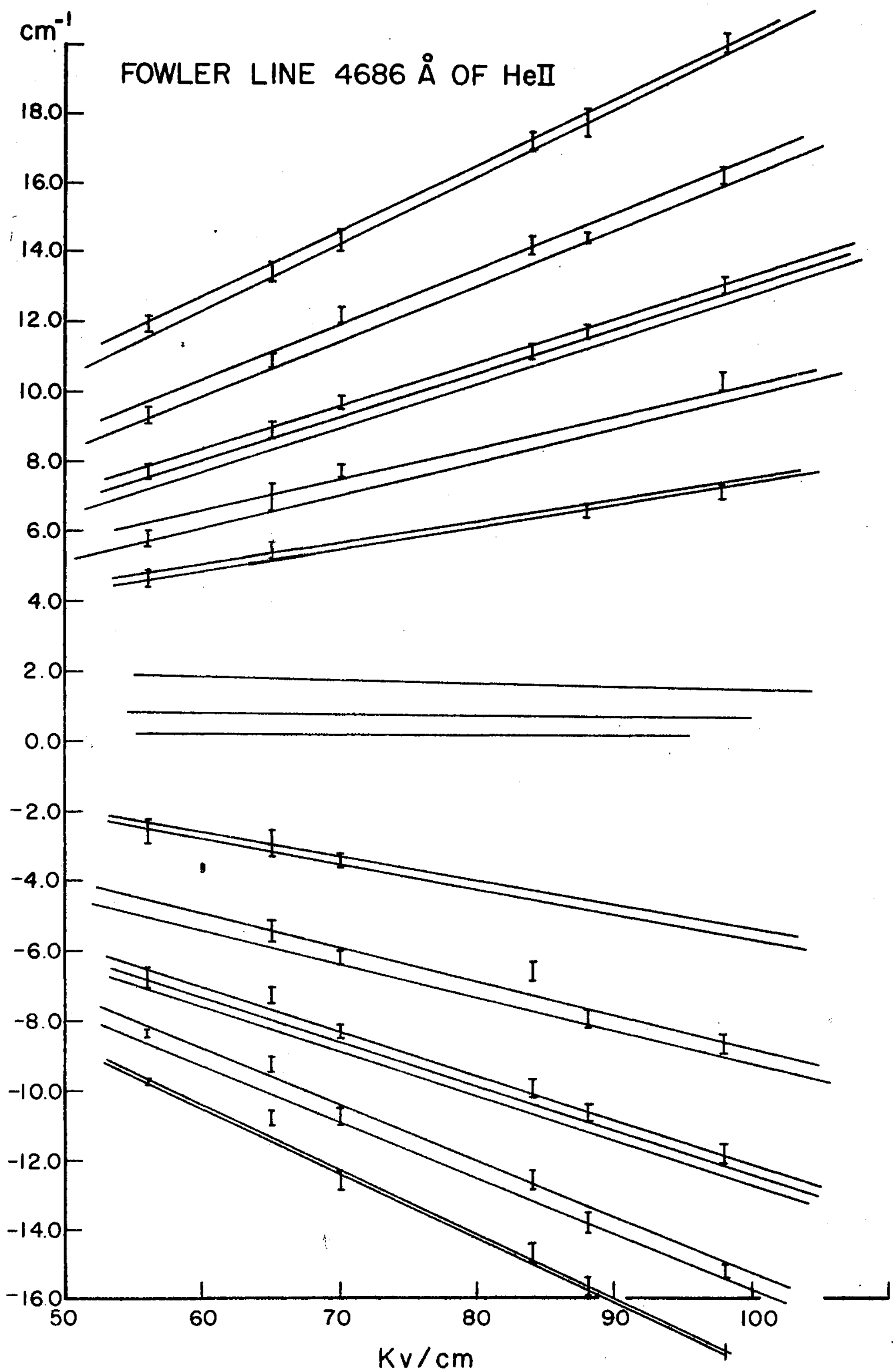

Figure 10. Experimental and Theoretical Stark Shifts of 4686Å Line of He II

TABLE VI

EXPERIMENTAL AND THEORETICAL STARK SHIFTS FOR Rb AND Cs in $Mc/(kv/m)^2$

Nucleus	State	(cal)	(cal)	(expt)		Exptal. crossing fields (kv/cm)	
Rb^{85}	$6^2P_{3/2}$	3.34	- .494	-0.521	0.021	8.77 10.95	0.18
Rb^{87}	$6^2P_{3/2}$	3.34	-0.494	-0.521	.021	14.3	
Cs^{133}	$7^2P_{3/2}$	9.03	-1.05	1.077	.043	11.07 13.5	.02
Cd	5^3P_1	8.5	1.3	1.70	.07		
Hg	6^3P_1	5.5	0.92	1.57	.06		

TABLE VII

PARAMETER FOR QUADRATIC STARK EFFECT IN ALKALI ATOMS

Atom	Transition	Observed Value γ	Method of Observation	Calculated γ
Li^7	2p - 2s	$+(4 \pm 2)\ 10^{-7}$	Shift of the centre of	2.7×10^{-7}
	3p - 2s	$-(1.4 \pm 0.3)10^{-4}$	gravity of absorption	1.1×10^{-4}
	2p - 4s	$-(1.9 \pm 0.4)10^{-4}$	line	1.5×10^{-4}
Na^{23}	$3p_{1/2}$ - 3s	-7.6×10^{-7}	Atomic Beam Method	-7.4×10^{-7}
	$3p^{\pm3/2}_{3/2} \rightarrow 3s$	-4.1×10^{-7}		-4.1×10^{-7}
	$3p^{\pm1/2}_{3/2} \rightarrow 3s$	-11.1×10^{-7}		-10.6×10^{-7}
	$3p^{\pm3/2}_{3/2} \rightarrow 3s$	4.1×10^{-7}	Double Refraction Method	10.6×10^{-7}
	$3p^{\pm1/2}_{3/2} \rightarrow 3s$	11.0×10^{-7}		10.6×10^{-7}
K^{39}	5p - 4s	-3.4×10^{-6}	Shift of center of	-3.3×10^{-5}
	6p - 4s	-1.6×10^{-4}	gravity of absorption	-1.8×10^{-4}
	4s(F=2)	$-(2.53 \pm .25) \times 10^{-12}$	line	-3.1×10^{-12} -3.0×10^{-12}
	4s(F=1)	$-(2.21 \pm 0.17)\ 10^{-12}$	Level crossing method	-3.3×10^{-12}
Rb^{85}	5p - 5s	$-(2.0 \pm .2) \times 10^{-6}$	Radiospectroscopic method	-0.9×10^{-6} -2.0×10^{-6}
	$5p^{\pm3/2}_{3/2}$ - 5s	$-(1.8 \pm .2) \times 10^{-6}$		0.6×10^{-6} 1.8×10^{-6}
	$5p^{\pm1/2}_{3/2}$ - 5s	$-(3.0 \pm .4) \times 10^{-6}$		1.9×10^{-6} 2.9×10^{-6}
Cs^{133}	7p - 6s	-1.18×10^{-4}	Comparison with Hyperfine Structure Splitting	-1.17×10^{-4} -1.63×10^{-4}
	$7p^{\pm1/2}_{3/2}$ - 6s	-1.46×10^{-4}		-2.3×10^{-6} -4.0×10^{-6}
	$6p^{\pm3/2}_{3/2}$ - 6s	$-(4.0 \pm .8) \times 10^{-6}$		-3.8×10^{-6}
	$6p^{\pm1/2}_{3/2}$ - 6s	$-(6.2 \pm 1) \times 10^{-6}$		4.9×10^{-6} 5.9×10^{-6} 6.0×10^{-6}

TABLE VII (Continued)

Atom	Transition	Observed Value γ	Method of Observation	Calculated γ
C_s^{133}	$6p_{1/2} - 6s$	$-(3.8\pm.6)\mathrm{x}10^{-6}$	Level Crossing method	-3.1×10^{-6} -3.8×10^{-6} -3.4×10^{-6}
	6s(F=4) to 6s(F=3)	$-(.76\pm.01)\mathrm{x}10^{-10}$	Radiospectroscopic method	$-0.82\mathrm{x}10^{-10}$ $-0.79\mathrm{x}10^{-10}$ $-0.99\mathrm{x}10^{-10}$

Table VII gives comparison of observed and calculated constants for the quadratic Stark shift $\Delta\nu$ of frequencies of transitions in Alkali metal atoms. The constant γ is defined by the relation $\Delta\nu = \gamma\varepsilon^2$ where $\Delta\nu$ is in cm^{-1}, ε in kv/cm and γ is in $cm^{-1}/kv/cm)^2$.

two possible crossings, i.e., of $P_{1/2}^{1/2}$ and $P_{1/2}^{-1/2}$ with $P_{3/2}^{-3/2}$. Hence one can measure the shifts in the levels in terms of magnetic field. It was found that the size of the shift measured with the change in the magnetic field has the relation $\Delta H = (.056 \pm .011)\varepsilon^2$. H is in gauss and ε in kv/cm. This result is in good agreement with the theoretical results

$$\Delta H = .048\ \varepsilon^2$$

For completeness we reproduce here (in Table VII) the table given by Bounch, Bruevich and Khodov which gives a comparison of observed and calculated constants for the quadratic Stark shifts.

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CHAPTER VI

CONCLUSIONS AND SUGGESTIONS FOR FURTHER WORK

In this work we have taken up the problem of nonrelativistic, relativistic and approximate relativistic p-e system to study the symmetries. In doing so it has been found that the classification of the bases for the irreducible representations of the groups 0(4), 0(4,1) and SU(2,2) x 0(4) to which p-e bound system belongs shows a cohesive connection. The relativistic p-e bound system has wave function which are solutions of the well known Dirac equation. These form the bases for the $\Upsilon_{\frac{1}{2}}\sigma$ irreducible reoresentation of the 0(4,1) group. On the other hand Schrodinger coulomb problem belongs to the invariant group 0(4) and the non-invariant group 0(4,2). Its solutions form the basis functions for the Υ_{0},σ irreducible representation of the group 0(4,1).

The most interesting thing from the symmetry point of view is that the relativistic symmetric Hamiltonian, even though it has the invariant group 0(4) and the dynamical group of SLj(2,c) $\otimes$ SU(2,2) has solutions that also form the basis functions for the irreducible representation $\Upsilon_{\frac{1}{2}},\sigma$. In other words the approximate symmetric Hamiltonian introduced by Biedeharn and Swamy does incorporate the spin without losing the invariant group structure of the nonrelativistic Hamiltonian. This aspect of it might be of use to the particle physicists who have the problem of incorporating relativistic invariance into successful SU(3) group for elementary particles.

We have also been able to arrive at the solutions of the relativistic symmetric Hamiltonian in the momentum space, in closed form, in contrast to the solutions of Dirac Coulomb Hamiltonian in the momentum space, whose wave functions can only be obtained numerically. The complexity of the Schrödinger differential equation in the momentum space or its counter part, the symmetric Hamiltonian, is due to the fact that the Coulomb potential is prescribed in coordinate space, and in the quantum mechanics the operators $\underset{\sim}{X}$'s and p's do not commute. In spite of this the wave functions of the relativistic symmetric Hamiltonian in the momentum space are in closed form. They are related to the momentum space wave functions of the Schrodinger equation in the limiting process. The relativistic symmetric Hamiltonian itself goes over in to free field Dirac Hamiltonian (plane wave equation) in the limiting process $(\alpha Z) \to 0$.

The structure of the nonrelativistic Hamiltonian for Coulomb field or for that matter even the harmonic oscillator, is very simple in the Fock-Bargmann space which is a complex mixture of both coordinate and momentum spaces. Thus we took advantage of the simplicity of the structure of the Hamiltonian and the wavefunctions in this space to study certain properties. The parabolic and the spherical wavefunctions for the nonrelativistic Coulomb problem were obtained in the Fock-Bargmann space and it has been shown that they are connected through the Clebsch-Gordan theorem.

It is also possible to establish the Clebsch-Gordan connection of the free field (external electric field) and Stark wavefunctions of the hydrogen atom in the coordinate space by direct evaluation of the transformation coefficients in accordance with the Dirac Transformation Theory. Using the symmetry properties one can give a group theoretical derivation of this result as it is done in this thesis. The proof on the lines of the Transformation Theory uses the contiguous relations between the hypergeometric functions of variables in the coordinate space which one can not generalize to wave functions in other spaces. On the other hand the symmetry arguments and the proof along group theoretical lines is independent of coordinate and one immediately knows that Clebsch-Gordan connection holds good in momentum and Fock-Bargmann spaces as well.

This result is valuable for the relativistic symmetric Hamiltonian. This Hamiltonian has very complicated structure in parabolic coordinates. It is difficult to solve as an eigen equation. But the existence of the vector invariants J and K, and the O(4) invariance of the Hamiltonian immediately leads us to the conclusion that its wavefunctions in the parabolic coordinates must be connected to the wavefunctions in the spherical coordinates through the Clebsch-Gordan theorem. The deep practical interest in expressing the wavefunctions in parabolic coordinates consists in its applicability to study the Stark affect.

The symmetry property can also be used to evaluate certain radial integrals involving multipole operators, of interest in electric and magnetic transitions, and bound state wavefunctions of the nonrelativistic Coulomb problem. We have been able to derive the Pasternack recursion relation for the expectation values and the Pasternack Sternheimer result for the vanishing of certain radial matrix elements using O(4) x SU(2) group generators. Thus the properties which were thought to be accidental due to the structure of the radial wavefunctions has a deeper group theoretic meaning.

In case of the continuum state wavefunctions we were able to obtain the numerical values of the matrix elements up to a constant using the operator techniques. The operators which lead to these matrix elements follow a systematic trend. These operators can be reduced to a sum of commutation relations between multipole operators and the Hamiltonian whose matrix elements with respect to appropriate basis functions vanish giving the desired result.

As an application of the Symmetric Hamiltonian to a problem of experimental interest the study of Stark effect was taken up. The calculations obtained using relativistic Symmetric Hamiltonian wavefunctions and Dirac wavefunctions were compared with Luder's work and with the experimental results of Steubing and Junge on H and H lines. The theoretical and experimental values of first order Stark Shifts in various components of HeII 4686 line were also compared. The results show that for field strengths 5000 v/cm to 12000 v/cm the Stark shift is linear but for fields below 5000 v/cm the shift is more quadratic than linear, which is as it should be, because at low fields (as is described in Chapter V, Section 3) the linear Stark effect goes over into the quadratic Stark effect for levels which are very close. The calculations using Pauli wavefunctions agree very well with experimental results for hydrogen lines but for HeII and LiIII the discrepancy is noticeable. The first structure splitting which varies as the fourth power of the atomic number becomes quite large as Z increases whereas first order Stark effect varying approximately as Z^{-1} gets smaller. Hence, the fields for which the fine structure is nullified get larger.

The shifts are also dependent on n. As n increases the fine structure splitting becomes small whereas the Stark shifts get larger. For fairly high Z therefore, and for n = 6 or 7 the situation becomes so complicated that without very accurate calculations (accuracy about 10^{-5} cm^{-1}) one cannot tell certainly which level is crossing only on the basis of experimental work.

Figures 9 and 10 show that Symmetric Hamiltonian gives reliable shifts for medium electric field strengths. One difference between the results obtained using the Symmetric Hamiltonian and those of the exact Dirac Hamiltonian, of advantage in experimental work, is that the shifts vary linearly with the applied field. In this respect there is an additional superiority over the non-relativistic, where also the shifts are linear, in as much as they are dependent on the j value of the state. Thus, we conclude that the effect of symmetry is to linearize the shifts without suppressing their j dependence or spin dependence.

The use of Stark shifts to measure the electric fields is a standard technique in experimental plasma physics. One usually uses the shifts in the Balmer lines. Because of the presence of other ions the shape of Stark component is distorted and depends on the density of electrons in the plasma at the point of observation. An accurate Stark profile calculation, therefore, gives valuable information not only on the electric field but also on the electron density and the temperature of the plasma which are of immense importance in controlling thermonuclear reaction. In short accurate first order Stark shifts do give valuable information on energy levels of hydrogen like atoms in electric fields of experimental importance.

Suggestion for Further Work

If it is possible to describe spin orbit interaction in the frame work of Symmetric Hamiltonian, to a first order approximation, it will then be possible to study by numerical methods how close one can predict the actual level shifts using the Symmetric Hamiltonian wavefunctions. Group theoretical study of the hydrogen atom in the electric field itself is an interesting problem, to which not much attention has been paid. A more difficult problem would be the study of hydrogen atom in crossed electric and magnetic fields, especially with respect to its relation to the invariance and non-invariance groups and the energy spectrum.

Second and higher order Stark shifts in levels like 2P(3/2, 3/2), D(5/2, 5/2) or on other lines in alkali atoms can be calculated on the basis of the Symmetric Hamiltonian. This basis is suited for such calculations because of the simple structure of the radial functions as compared to Dirac wavefunctions. The theoretical study of Stark shifts of the impurity levels in solids needs lots more attention than has been given, as also the study of electroabsorption of Wanier excitons in semi-conductors.

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APPENDIX

Here we give the listing of computer programs used in the calculations reported in Chapter V. There are two mainline programs.

RGKU : In this program the metrix elements of the Stark interaction are calculated using the solutions of the Symmetric Hamiltonian. The matrices are diagonalized and the Stark shifts are printed in the units of $(\text{meter})^{-1}$.

RGK1 : In this program the matrix elements are calculated using exact Dirac wavefunctions and the Pauli wavefunctions. The metrices are diagonalized and the Stark shifts are printed in the unit of $(\text{meter})^{-1}$.

The first program involves only one subroutine 'GIVENS'. Whereas the second program involves 3 subroutines, 'DIRACL', 'DGAMMA', AND 'GIVENS'. 'DGAMMA' calculates gamma functions in the radial integrals using the Bernouli numbers. Subroutine DIRACL calculates E(n,k), N(n,k) and the radial integrals I_{11}, I_{12}, I_{21} and I_{22}.

GIVENS

The subroutine diagonalizes a given hermitian matrix and gives the roots and vectors.

All calculations are carried out in double precision.

PROGRAM RGKU

```
FORTRAN IV G LEVEL  18                  MAIN

      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION   A(6),  B(6),  C(7),  D(5),  BETA(6),   CXI(6)
      DIMENSION   CPEN(7), CMEN(7), CPONE  (7), CMONE(7)
      DIMENSION          Y(5),   Z(5),  T(5),   W(5)
      DIMENSION   AY(6),  BY(6), CY(6),    DY(6)
      DIMENSION   ROOT(11),          CRATCH(15,5)
      DIMENSION      RM (12,12),  VECT (15,15)
      DIMENSION   ARRAY(66),    X(10)
      DIMENSION BX (10) , BX2 (10)
      DIMENSION  ROOTD(12)
          DIMENSION  FL ( 6,10 )
      EXTERNAL  GIVENS
C     THIS PROGRAMME CALCULATES MATRIX ELEMENTS OF THE OPERATOR Z
C     IN THE BASIS OF SYMMETRIC HAMILTONIAN
      DO 4  I= 1,15
       DO 4  J= 1,5
    4  CRATCH(I,J) =00.0
      DO 15  I=1,  15
      DO 15  J=1,  15
      AB=  1.0
      VECT(I,J)  =1.0+ AB* .005379813
   15  AB= AB+1.0
      N1  = 3 + 2
      N2  = 2
      FL ( 6,1 )  = 2510.0 * 40.0
      FL ( 5,1 )  = 2510.0 * 40.0
      FL ( 4,1 )  = 2510.0 * 40.0
      FL ( 3,1 )  = 5020.0 * 20.0
      FL ( 2,1 )  = 5020.0 * 20.0
      E  = 1.6021D-19
      ANOT  = 5.2917D-11
      PLC  = 6.626D-34
      VL  = 2.99793D+08
      ALPHA=1.0/137.0388
   14 AN=N1
      N1M1 = N1-1
      N1M2  = 2*N1 -2
      RMU=0.5
      IRMU  = 1
      DO 90 J=1, 12
      DO 90 K=1, 12
   90 RM(K,J)=00.00
   35  RJ=    1.5
C     XN IS ORDER OF THE MATRIX TO BE DIAGONALIZED
      XN =  (AN- RMU)*2.0
      N =XN
      IF ( N.LE.1 )  GO TO  125
C     NSIZE IS THE LENGTH OF THE EIGEN VECTOR.
      NSIZE =N
C     KEY NUMBER OF EIGENVECTORS NEEDED
      KEY  = -N
C     X'S ARE THE RESULT AFTER ANGULAR INTEGRATION
      DO 40 I=1,  N1M1
      IF(RMU.GE.RJ) GO TO 39
      AX=(RJ**2.0-RMU**2.0)**.5
      X (I)  = AX /( 8.0 * RJ )
      GO TO 40
   39 X(I)=0.0
```

FORTRAN IV G LEVEL 18 MAIN

```
      40 RJ=RJ+1.
         RJ=0.5
         DO 50 I=1,N1M1
         IF(RMU.GT.RJ) GO TO 49
         X(I+N1-1)=- RMU
         GO TO 50
      49 X(I+N1-1) = 0.0
      50 RJ=RJ+1.0
         CHAR  = 1.0
      51  K1  = 1
         IZ  = CHAR
         F  =    FL(N1,1 ) *(10.0)**(IZ-1)
         ENCNV  = ( ALPHA *E*CHAR**2)**2/(2.0*ANOT*PLC*VL)
         ALFHA  = ALPHA * CHAR
         DO 10 I=1,N1
         FI=I
      10 CXI(I)=((1.0+(ALFHA/FI)**2 )/(1.0+(ALFHA/AN )**2  ))**.5
         S=1.0
         DO 5 I=1,N1
         A(I)=-1.5*AN*(AN**2-(  S  )**2)**.5
       5 S=S+1.0
         DO 16  I= 1,  N1
         S=I
      16   C(I)        = .5*(3.* AN**2 - S*(S-1.0))
         EN=1.0/(1.0+(ALFHA/AN)**2  )**.5
         EV = .51*(10.0)**6
C        FNEV IS  BINDING ENERGY IN EV.
         ENEV = (EN-1.)*EV
         DO 60 I=1,N1
         CPEN (I) =(CXI(I)+EN)**.5
         CMEN (I) =(CXI(I)-EN)**.5
         CPONE (I)  = (CXI(I)+1.0)**.5
         CMONE (I)  = (CXI(I)-1.0)**.5
      60 BETA(I)=((CXI(I)**2  -1.0)*(CXI(I)**2  -EN**2  ))**.5
         J= 1
          DO 7C  I=  1, N1M1
         K  = J+1
         SUY1  = CPEN(J)*CPEN(K) +CMEN(J)* CMEN(K)
         Y(I)  =CPONE(J)* CPONE(K) *SUY1
         Z(I)  =CMONE(J)* CMONE(K) *SUY1
         SUY2  = CPEN(J)*CMEN(K) +CMEN(J)* CPEN(K)
         W(I)   =CMONE (J)* CPONE(K)* SUY2
         T(I)   =CPONE (J)* CMONE(K)* SUY2
      70  J=  J+1
         DO  24  I= 1, N1M1
         AY(I)  =  A(I) * Y(I) + A(I+1)* Z(I)
         BY(I)  = A(I+1) * Y(I) + A(I) *Z(I)
         CY(I) =C(I+1) * W(I)
         DY(I) =C(I+1) * T(I)
         BX (I) = ((2.0*CXI(I)**2-1.0)*(2.0*CXI(I+1)**2.0-1.0))**.5
         BX2(I)=(2.0*CXI(I)**2-1. )*8.0*RJ*(RJ+1.0)
      24  CONTINUE
      52 CONVF  = -2.0*F*(ANOT/ALPHA)**2/(E*CHAR**5)
         V  = CONVF
         V1  = V
         DC  91  I=  1,  N1M1
         FI  =I
         M=N1+I-1
```

```
FORTRAN IV G LEVEL  18                    MAIN

                RM(2*I-1,2*I)= V1* 2.* X(M )*(2.*A(I )*CXI   (I)-   FI *BETA(I))
               X/BX 2(I)
                RM ( 2* I-1, 2*I+1)=( AY(I)-CY(I))* X(I)*V1 / BX (I)
                RM ( 2* I, 2*I+2) =   X(I)* ( BY(I  )+DY(I  )) *V1 / BX (I)
             91  CONTINUE
                M = 2.0 * RMU
                N3  = 2. * RMU + XN - 1.0
                L=1
                DO 110 K=M      ,N3
                DO 109  J=M,K
                ARRAY(L)=  RM(J,K)
            109  L=L+1
                DO 110 J=K,N3
            110 RM(J,K)=RM(K,J)
            800 FORMAT(1H0,/,7(1X,D16.8) /    )
                DO 120 K=M,N3
            120 WRITE(6,8C0) (RM(K,J),J=M,N3)
                CALL GIVENS ( N,KEY,NSIZE,ARRAY,CRATCH,ROOT,VECT)
                DO 54 I = 1,N
                ROOT (I)  = ROOT (I) * ENCNV
             54 WRITE ( 6,856 ) IZ,N1,K1,IRMU,I,F,ROOT(I)
            856 FORMAT ( 2X, 3I2 , 2I3,2( 5X, D24.16 ))
                DELF =  FL(N1,1 ) *(10.0)**(IZ-1)
                F  = F + 2.0 * DELF
                K1  = K1+ 1
                   IF ( K1.GE.7  ) GO TO 122
                GO TO 52
            122 CHAR = CHAR +1.
                IF ( CHAR.GE.3  . ) GO TO 34
                    GO TO 51
             34 RMU=RMU+1.0
                    IRMU  = IRMU + 1
                IF(RMU.GT.AN) GO TO 125
                GO TO 35
            125  N1 = N1-1
                IF ( N1.LT.N2 )  GO TO 130
                GO TO 14
            130 STOP
                END
```

0.0	-0.24309496D 08	0.72199766D 09	0.0	0.0	0.0	0.0
-0.24309496D 08	0.0	0.0	0.645756610D 09	0.0	0.0	0.0
0.72199766D 09	0.0	0.0	-0.217443650D 08	0.67111694D 09	0.0	0.0
0.0	0.645756610D 09	-0.217443650D 08	0.0	0.0	0.51257024D 09	0.0
0.0	0.0	0.67111694D 09	0.0	0.0	-0.16607714D 08	0.517779250D 09
0.0	0.0	0.0	0.51257024D 09	-0.16607714D 08	0.0	0.0
0.0	0.0	0.0	0.0	0.517779250D 09	0.0	0.0

Z N					F IN VOLTS/METER	(METER)⁻¹
1	4	1	1	1	0.10040000000000000D 06	0.68741538802849230D 02
1	4	1	1	2	0.10040000000000000D 06	0.53496484237785870D 02
1	4	1	1	3	0.10040000000000000D 06	0.23050013302401350D 02
1	4	1	1	4	0.10040000000000000D 06	-0.74171161185668220D-08
1	4	1	1	5	0.10040000000000000D 06	-0.23050013309818470D 02
1	4	1	1	6	0.10040000000000000D 06	-0.53496484245202990D 02
1	4	1	1	7	0.10040000000000000D 06	-0.68741538810266350D 02

0.0	-0.72928489D 08	0.21659930D 10	0.0	0.0	0.0	0.0
-0.72928489D 08	0.0	0.0	0.193726980D 10	0.0	0.0	0.0
0.21659930D 10	0.0	0.0	-0.652330950D 08	0.201335080D 10	0.0	0.0
0.0	0.193726980D 10	-0.652330950D 08	0.0	0.0	0.153771070D 10	0.0
0.0	0.0	0.201335080D 10	0.0	0.0	-0.498231430D 08	0.155333780D 10
0.0	0.0	0.0	0.153771070D 10	-0.498231430D 08	0.0	0.0
0.0	0.0	0.0	0.0	0.155333780D 10	0.0	0.0

1	4	2	1	1	0.30120000000000000D 06	0.20622461640854770D 03
1	4	2	1	2	0.30120000000000000D 06	0.16048945271335760D 03
1	4	2	1	3	0.30120000000000000D 06	0.69150039907204080D 02

```
1 4 2  1  4      0.30120000000000000D 06      -0.22251348355700470-07
1 4 2  1  5      0.3012CCCCCCCCC000D 06       -0.69150039929455420 02
1 4 2  1  6      0.30120000000000000D 06      -C.16048945273560900 03
1 4 2  1  7      0.30120000000000000D 06      -0.2062246164307991D C3

0.C              -0.12154748D 09  0.36099883D 1C  0.0             0.0             0.0             0.0

-0.12154748D 09  0.0              0.0             0.32287830D 1C  C.0             0.0             0.0

0.36099883D 10   0.0              0.0             -0.10872182D 09 0.33555847D 10  0.0             0.0

C.C              0.32287830D 1C   -0.10872182D C9 0.0             0.0             0.25628512D 10  0.0

C.C              0.0              0.33555847D 1C  0.0             0.0             -0.83038571D 08 0.25888963D 10

0.C              C.C              0.0             0.25628512D 10  -0.83038571D 08 0.0             0.0

C.C              C.0              0.0             0.0             0.25888963D 10  0.0             C.C
1 4 3  1  1      0.50200000000000000D 06       0.3437076940142462D 03
1 4 3  1  2      0.50200000000000000D 06       0.2674824211889294D 03
1 4 3  1  3      0.50200000000000000D 06       0.1152500665120068D 03
1 4 3  1  4      0.50200000000000000D 06      -0.37085580592834110-07
1 4 3  1  5      0.5C2CC00CCCCCCC00D 06       -0.1152500665490923D 03
1 4 3  1  6      0.50200000000000000D 06      -0.2674824212260149D 03
1 4 3  1  7      0.50200000000000000D 06      -0.3437076940513317D 03

0.0              -0.17016647D 09  0.50539836D 10  0.0             C.0             0.0             0.0

-0.17016647D 09  0.0              0.0             0.45202962D 10  0.0             0.0             0.0

0.50539836D 10   C.0              0.0             -0.15221055D 09 0.46978186D 10  0.0             0.0

0.C              0.45202962D 10   -0.15221055D C9 0.0             0.0             0.35879917D 10  C.0

C.C              0.0              0.46978186D 10  0.0             0.0             -0.11625400D 09 0.36244548D 10

C.C              C.0              0.0             0.35879917D 10  -0.11625400D 09 0.0             C.C

C.C              0.0              0.0             0.0             0.36244548D 10  0.0             C.C
```

PROGRAM RGKI

```
FORTRAN IV G LEVEL  18                    MAIN

               IMPLICIT REAL*8(A-H,O-Z)
               COMMON CONP  , CONM
               COMMON Q
               DIMENSION  CONP (10) , CONM (10)
               DIMENSION  CONSTA (6) , CONSTB(6)
                DIMENSION  DL M (6,6)     , CONST (6) , CNP(6) , CNM(6)
                DIMENSION      Z1 (6)   ,  Z2 (6) ,  W1 (6) ,  T 1 (6), CONS (10)
               DIMENSION RED(10,2,9,5,11) , REDL (10,2,9,5,11)
               DIMENSION  ROOTD(12), UDERL (12)
                 DIMENSION DNKZ(6)
               DIMENSION  FL ( 6,10 )
               DIMENSION  GKP(6) , DNK(6), ENK(6), GAM1(6), GAM2(6) , GAM3(6)
               DIMENSION   A(6),  B(6),C(7,2),  D(5),  BETA(6),   CXI(6)
               DIMENSION CC(7,2), BB (7)
               DIMENSION            Y(5),   Z(5),  T(5),   W(5)
               DIMENSION   AY(6),  BY(6), CY(6),    DY(6)
               DIMENSION   ROOT(11),        CRATCH(15,5)
               DIMENSION     RM (12,12),  VECT (15,15)
               DIMENSION   ARRAY(66),    X(10)
               DIMENSION ROWLD (11)
               DIMENSION   Q(6)
               DIMENSION   Y1 (5)
               DIMENSION RML (12,12) , UDER(15),  UDRAY(66)
               EXTERNAL  DIRAC 1  , DGAMMA
               EXTERNAL  GIVENS
           200 FORMAT (  6(F10.8 ) )
           300 FORMAT(1H0,4D15.7)
           800 FORMAT(1H0,/,7(1X,D16.8) /     )
           750 FORMAT ( 1H0,////, 25X, 'RMU  =' , D15.7, 15X,  ' N1  = ' , I1
             1 //, 10X, 'F  = ', D 15.7, 'VOLT/METER ', 15X, ' Z  =',D15.7)
           850 FORMAT ( 1H0 , 20X, 'ROOT (', I2, ' )  = ', D28.9,//, 5X, 8(D15.7)//)
             1 //)
               DO 4  I=  1,15
                DO 4  J= 1,5
             4  CRATCH(I,J) =00.0
               DO 15  I=1,  15
               DO 15  J=1,  15
               AB=  1.0
               VECT(I,J)  =1.0+ AB* .005379813
            15  AB= AB+1.0
               DO 90 J=1, 12
               DO 90 K=1, 12
               RML (K,J)  = 00.0
            90 RM(K,J)=00.00
               N1  = 5
               N2  = 3
               FL  (6, 1 )  = 2510.0 *40.0
               FL  (5, 1 )  = 2510.0 *40.0
               FL ( 4, 1 )  = 2510.0 *40.0
               FL (3, 1 )  =  5020.0 * 2.0*10.0
               FL (2, 1 )  = 5018.0*2.0 *10.0
               E  = 1.6021D-19
               ANOT  = 5.2917D-11
               PLC  = 6.626D-34
               VL  = 2.99793D+08
               ALPHA=1.0/137.0388
               SIGMA  = 0.0
               READ ( 5, 200 )  ( Q (I), I= 1,6 )
```

```
      1000 FORMAT ( 1X, I1 ,  D17.8)
        14 AN=N1
           N1M1 = N1-1
           N1M2  = 2*N1 -2
           N1M3  = 2* N1 - 1 + 2
           RMU=0.5
           IRMU  = 1
        35  RJ=    1.5
           XN =  (AN- RMU)*2.0
           N =XN
           IF ( N.LE.1 )  GO TO  125
           NSIZE =N
           KEY = -N
           DO 40 I=1,  N1M1
           IF(RMU.GE.RJ) GO TO 39
           AX=(RJ**2.0-RMU**2.0)**.5
           BX  = .25
           X(I)=AX/(8.0*BX  *RJ)
           GO TO 40
        39 X(I)=0.0
        40 RJ=RJ+1.
           RJ=0.5
           DO 50 I=1,N1M1
           IF(RMU.GT.RJ) GO TO 49
           BX 2 =  2.0 * RJ * ( RJ + 1.0 )
           X(I+N1-1)=- RMU/BX2
           GO TO 50
        49 X(I+N1-1) = 0.0
        50 RJ=RJ+1.0
           CHAR  = 2.0
        51 K1  = 1
           IZ  =  CHAR
           IZH  = IZ
           ALPHA = ALPHA * CHAR * DSQRT (5.1D+05)
           F  =    FL(N1,1 ) *(10.0)**(IZ-1)
           ENCNV  = (ALPHA*CHAR/AN)**2
             CALL     DIRAC1(N1,AY,BY,CY,DY,A,BB,CC,D,DNK,ENK,CHAR)
        52 CONVF  = -2.0*F*(ANOT/ALPHA)**2/(E*CHAR**5)
           V  = CONVF
           V1  = F* ANOT
       757 FORMAT ( 1X, D12.4, 7X, I3, I3, 2(5X, D15.7))
           DO  91  I=  1,  N1M1
           FI  =1
           M=N1+I-1
           CONSTA(I)  = CONP (I)  * CONP ( I+1 )
           CONSTB(I)  = CONM (I)  * CONM ( I+1 ) / CONSTA (I)
           RM ( 2* I, 2*I+2) =   X(I)* ( BY(I  )-DY(I  ))  * CONSTB(I)*V 1
           RM ( 2* I-1, 2*I+1)=( AY(I)-CY(I))* X(I) *V 1
           XCON  = 2.0 * X(M) * CONM (I) / CONP(I) *V1
           CKC  =  CC(I,1) * (AN - FI ) **2 +CC(I,2)*( DNK (I) **2-FI**2)
           CLC  =  2.0 * ENK (I) * ( AN - FI ) * DNK (I)  *BB(I)
           RM(2*I-1,2*I)  =-XCON * ( CKC - CLC ) / ( 1.0 + ENK (I) )
           RM (2*I, 2*I )  =(ENK (I)  -1) * 5.1D+05
            RM ( 2*I-1, 2*I-1 )  = RM ( 2*I , 2*I )
           J  = I+1
           FJ  = J
           RML (2*I-1, 2*I )  =-1.5 * AN/CHAR* X(M) * DSQRT ( AN**2-FI**2)*V1
           RML (2*I,2*I+2)    =-1.5 * AN/CHAR* X(I) * DSQRT ( AN**2-FJ**2)*V1
```

FORTRAN IV G LEVEL 18 MAIN

```
              RML (2*I-1, 2*I+1)= -1.5 * AN/CHAR* X(I) + DSQRT ( AN**2-FI**2)*VI
              RML (2*I,2*I) =-0.5*(ALFHA/AN)**2*(1.0+ENCNV*(AN/FI-.75))
              RML ( 2*I-1 , 2*I-1)  = RML( 2*I  , 2*I   )
         91   CONTINUE
              RM (2*N1-1, 2*N1-1 )  = ( ENK (N1)-1 ) * 5.1D+05
              RML (2*N1-1,2*N1-1 ) = -0.5 *(ALFHA/AN)**2  *( 1.0 +0.25 * ENCNV )
              M = 2.0 * RMU
              N3  = 2. * RMU + XN - 1.0
              L=1
              DO 110 K=M      ,N3
              DO 109  J=M,K
              UDRAY(L)  = RML (J,K)
              ARRAY(L)=  RM(J,K)
        109   L=L+1
              DO 110 J=K,N3
              RML (J,K)  = RML (K,J )
        110 RM(J,K)=RM(K,J)
         53 CALL GIVENS (N,KEY,NSIZE,ARRAY, CRATCH,ROOT,VECT)
            CALL GIVENS ( N,KEY,NSIZE,UDRAY,CRATCH,UDER,VECT )
            UDERL(N) = RML ( 2*N1-1,2*N1-1 ) *E/(PLC*VL)
             ROOTD(N)  =RM ( 2*N1-1,2*N1-1 ) *E/(PLC*VL)
            NM   = N1 -4
            DO 54 I=1,N
            ROOT (I)  = ROOT (I) * E/(PLC*VL ) - ROOTD(N)
            UDER (I)  = UDER (I) * E/ ( PLC* VL ) - UDERL(N)
        851 FORMAT ( 1H0, 5X,   I2, 10X, D 28.20,  20X, D28.20 , 5X, D24.16 )
             RED (IZH,NM,K1,IRMU,I )  = ROOT (I)
            REDL (IZH,NM,K1,IRMU, I )  = UDER (I)
         54 WRITE ( 6,856 ) IZ,N1,K1,IRMU,I,F,ROOT(I), UDER (I)
        855 FORMAT (1X,5I3, D14.7, 2D22.14)
        856 FORMAT ( 2X, 3I2 , 2I3,3( 5X, D24.16 ))
            DELF =  FL(N1,1 ) *(10.0)**(IZ-1)
            F  = F + DELF* 2.0
            K1  = K1+ 1
               IF ( K1.GE.9  ) GO TO 122
            GO TO 52
        122 CHAR = CHAR + 1.0+  SIGMA
            CHAR  = CHAR - SIGMA
            IF ( CHAR.GE.3  . ) GO TO 34
            GO TO 51
         34 RMU=RMU+1.0
            IRMU  = IRMU + 1
            NM1  = 2*N1
            IF(RMU.GT.AN) GO TO 125
            GO TO 35
        125 DO 126  J= 2, NM1
            JM1  = J-1
            DO 126 I = 1,JM1
            IRMU  = J-I
            F  =    FL(N1,1 ) *(10.0)**(IZ-1)
            DELF =  FL(N1,1 ) *(10.0)**(IZ-1)
            IF ( IRMU.GE.N1)  GO TO 126
            DO 126 K1  = 1,9
            F  = F + DELF*2.0
             WRITE (6,856 ) IZH,N1,K1,IRMU,I,F, RED(IZH,NM,K1,IRMU,I)  ,
           X  REDL (IZH,NM,K1, IRMU,I)
        126 CONTINUE
       1125  N1 = N1-1
```

```
FORTRAN IV G LEVEL  18                    MAIN

 0172             IF ( N1.LT.N2 )  GO TO 130
 0173             GO TO 14
 0174         130 STOP
 0175             END
```

FORTRAN IV G LEVEL 18 DIRAC1

```
      SUBROUTINE DIRAC1(N1,AY,BY,CY,DY,A,BB,CC,D,DNK,ENK,CHAR)
      IMPLICIT  REAL* 8  ( A-H , O-Z )
      COMMON CONP  , CONM
      COMMON Q
      DIMENSION Q(6)
        DIMENSION DNKZ(6)
      DIMENSION  CONP (10) , CONM (10)
      DIMENSION CC(7,2), BB (7)
       DIMENSION     CP1(12),    CP2 (12), CSUM (12) ,  SPS (10), SMS (10)
       DIMENSION        Z1 (6)   ,  Z2 (6) ,  W1 (6) ,  T 1 (6), CONS (10)
      DIMENSION  GKP(6) , DNK(6), ENK(6), GAM1(6), GAM2(6) , GAM3(6)
      DIMENSION   A(6),  B(6),C(7,2),  D(5),  BETA(6),   CXI(6)
      DIMENSION  CONSTA (6) , CONSTB(6)
       DIMENSION  DL M (6,6)     , CONST (6) , CNP(6) , CNM(6)
      DIMENSION           Y(5),   Z(5),   T(5),    W(5)
      DIMENSION   AY(6),  BY(6), CY(6),     DY(6)
      DIMENSION    Y1 (5)
       AN = N1
      N1M1  = N1 -1
       N1M3  =   2 * N1 + 1
      ALPHA=1.0/137.0388
      ALPHA = ALPHA * CHAR
      DO 5  I= 1, N1
      FI =I
      GKP(I)  =  DSQRT  (FI **2- ALPHA **2 )
      SFI =  FI - GKP (I)
      SFI  = 2. * (AN - FI)* SFI
      DNK (I) = DSQRT   ( AN**2 - SFI )
      DNKZ(I) = DSQRT   ( AN**2 - SFI )/ CHAR
      AZ  = ( ALFHA / ( AN - FI+ GKP (I))) ** 2
      AZ = DSQRT  ( 1. + AZ )
      ENK (I)  = 1.0 / AZ
      CNP(I) = DSQRT  (( 1. + ENK (I)) /(4. * DNK (I) * ( DNK (I)+FI)))
      CNP(I)  = CNP (I) * DSQRT ((2.0 / DNKZ(I) )** 3 )
      IF ( I. EQ. N1 )  GO TO  4
      CNM (I)   = CNP (I)* DSQRT (( DNK (I) + FI )/ ( DNK(I)-FI ))
      GO TO 6
    4 CNM (I)    = CNP (I)
    6  CALL DGAMMA ( 2. * GKP(I)+1., RES , ERR )
      GAM1 (I) = RES
      CALL  DGAMMA    ( 2.* GKP (I) + AN - FI + 1. , RES , ERR )
      GAM2 (I) = RES
      CALL  DGAMMA (AN-FI+1.,RES, ERR )
      GAM3 (I)  = RES
      CONP(I)  =(CNP(I)/ GAM1(I)  )* DSQRT ( GAM2 (I)         /GAM3(I))
      CONM(I)  =(CNM(I)/ GAM1(I)  )* DSQRT ( GAM2 (I)         /GAM3(I))
    5  CONTINUE
       DO  10  I= 1, N1M1
      FI  = I
      DO  12  K= 1, 2
      J = I+ K -1
      FJ  = J
      DLM (I,J )  =  ( DNK (I) + DNK (J)) / (DNK (I) * DNK (J))*CHAR
      C1  = ( 2.0 / DNKZ(J) ) ** ( GKP (J) - 1.0)
      C2  = ( 2.0 / DNKZ(I) ) ** ( GKP (I) - 1.0)
      C3  = ( 1.0/DLM(I,J)) **( GKP (I) + GKP (J) +1.0)
       C123 = C1 * C2 * C3 * CONP (I) * CONP (J)
      DO 15  IKJ = 1,  2
```

```
            AB =  IKJ -1
            DO  15   IJK = 1  , 3
            CD  = IJK -1
            CP1 (1) = 1.0
            ALP  = 1.0
            BET  =  1.0
             GK=2.* GKP(I)   +1.0
             ALP1  =  - AN +  FI + AB
            N1M4  = N1M3-I-J
            IF ( N1M4.EQ.0 ) GO TO 19
             DO 40  IA  =  2, N1M4
            ALP  = ALP*  ALP1
            ALP1  = ALP1  +1.0
            BET  =  BET * GK
            SQ  = IA
         51 CALL   DGAMMA  ( S Q ,  RES ,  ERR )
             CP1 ( IA  )  =  ( ALP /(BET * RES ))
         40  GK  = GK +1.
         42 ALPP = 1.0
             BETP =  1.0
            ALPP1 =  -AN + FI + AB + CD
             AET2  =  2. * GKP (J)  +  1.0
            CP 2 (1)  = 1.0
            DO  50  IB =  2  , N1M4
            ALPP = ALPP * ALPP1
            BETP  =  BETP* AET2
            ALPP1  = ALPP1 + 1.0
            BQ  = IB
             CALL   DGAMMA  (BQ , RES , ERR )
             CP2  (IB ) = ( ALPP/(BETP * RES ))* ( DNK (I) / DNK (J)) **IB
         50  AET2 = AET2 +1.0
            SUMM = 0.0
            CSUM (1)  = 1.0
             DO 20 IS = 1, N1M4
            S =  IS
            IF ( IS . EQ. 1 ) GO TO 31
            SUM  = 0.0
             DO 30  IQ =  1,  IS
            QS = IQ
            ISQ  = IS  -IQ +1
         30  SUM  =  SUM + CP1( ISQ ) * CP2 ( IQ )
            CSUM (IS ) = SUM * ( 2.0 /DNKZ(I))**(IS -1 )
         31 CALL   DGAMMA ( GKP (I) + GKP (J) + S + 1.0 , RES , ERR )
         20  SUMM = SUMM +  CSUM (IS ) * RES / DLM (I,J )** IS
         19 IF  ( AB-1. )  21 ,22 ,22
         21  IF  (  CD -1.0 )  23 , 25 , 26
         23  C(I,2) =  C123 * SUMM
            GO TO 15
         25  B( I)  =  C123 * SUMM
            GO TO 15
         26   IF ( I. GE . N1-1 )  GO TO 14
        126  D( I)  =  C123 * SUMM
            GO TO 15
         22  IF  (  CD -1.0 )  27 ,28,  15
         27  C(I,1) =  C123 * SUMM
            GO TO 15
         28  A( I)  =  C123 * SUMM
            GO TO 15
```

```
FORTRAN IV G LEVEL  18                DIRAC1

              14  D(I) = 0.0
              15 CONTINUE
                 IF ( K.EQ.2 ) GO TO 10
                 CC (I, 2)  = C ( I, 2)
                 CC (I,1 ) = C (I,1 )
                 BB (I)  = B(I)
              12 CONTINUE
              10  CONTINUE
                 DO  60  I = 1,  N1M1
                 FI  =I
                 J = I+ 1
                 FJ  = J
                 SK1  = DSQRT(( 1. + ENK (I) ) * ( 1.0 + ENK (J)) )
                 SK2  = DSQRT(( 1. - ENK (I) ) * ( 1.0 - ENK (J)) )
                 SPS (I) = ( SK1  + SK2  ) / SK1
                 SMS (I)  =( SK 1  - SK 2) / SK1
                 Y(I)  = ( AN - FI ) *  ( AN - FI - 1. ) *  SPS (I)
                 Y1 (I)  = Y (I)
                 Z (I)  =  ( DNK (I) + FI ) * (DNK (J) + FJ ) * SPS (I)
                 W ( I)  = ( DNK (J) + FJ ) *  ( AN - FI ) *  SMS  (I)
                 W1 (I)   =( DNK (J)  - FJ ) *  SMS (I) * ( AN- FI )
                 Z1 ( I)  =( DNK (I) - FI ) *( DNK (J) - FJ ) * SPS (I)
                 T1 (I) = ((DNK(I)-FI ) ) *(AN - FJ )*  SMS (I)
                 T  (I) = ( DNK(I)+FI )   *(AN - FJ )*  SMS (I)
                 Z 2 (I)  =  2.0 * ENK (I)  *(AN     - FI ) * DNK (I)
              60 CONTINUE
                 DO  24  I= 1, N1M1
                 AY (I) = A (I) * Y (I) + B (I) * Z(I)
                 BY (I)  = A(I) * Y (I) + B(I) * Z1 (I)
                 CY(I) =C(I,1) * W(I)   + T(I) * D(I)
                 DY(I) =C(I,1) *W1(I) + D(I)  * T1 (I)
              24  CONTINUE
                 RETURN
                 END
```

FORTRAN IV G LEVEL 18 DGAMMA

```
      SUBROUTINE  DGAMMA ( XX,GX, ERR )
      IMPLICIT  REAL* 8  ( A-H , O-Z )
      COMMON CONP  , CONM
      COMMON Q
      DIMENSION  CONP (10) , CONM (10)
      DIMENSION   C(6)  , CONS (10)
      IF ( XX-57. ) 6,6, 4
    4  ERR = 2.
      GX =  1. D 75
      RETURN
    6 X=XX
      RR =  1.0 D - 10
      ERR= 0.0
      GX = 1.0
      IF ( X-2. ) 50, 50,  15
   10 IF  ( X-2.0 ) 110 , 110 , 15
   15  X = X-1.0
      GX = GX * X
      GO TO  10
   50 JK = X
      AX = JK
      IF ( X-1. )  60 , 120 , 110
   60  IF ( X- RR ) 62 , 62 , 80
   62  Y = AX - X
      IF ( Y. GE. 0.0 ) GO TO 40
      AB        = -Y
      GO TO 63
   40 AB        = Y
   63 IF ( AB      -RR ) 130 , 130 , 64
   64 IF (1.0- Y - RR ) 130 , 130 , 70
   70 IF ( X-1.0 ) 80 , 80 , 110
   80 GX = GX/X
      X = X+1.
       GO TO 70
  110 Y = X-1.
      GY  = -0.05149930 * Y
      DO  111  K= 1, 6
  111 GY = ( Q (K) + GY ) * Y
      GY = 1.0 + GY
      GX = GX* GY
  120 RETURN
  130 ERR = 1.
      RETURN
      END
```

```
FORTRAN IV G LEVEL  18                  GIVENS

0001                  SUBROUTINE GIVENS(NX,NROOTX,NJX,A,B,ROOT,VECT)
0002                  IMPLICIT REAL*8(A-H,O-Z)
              C        QCPE PROGRAM NUMBER 62.1.   SEPTEMBER, 1966.
              C        EIGENVALUES AND EIGENVECTORS BY GIVENS METHOD.
              C        CALCULATES EIGENVALUES AND EIGENVECTORS OF REAL SYMMETRIC MATRIX
              C        BY THE MODIFIED GIVENS METHOD.  THE PARAMETERS ARE...
              C            NX      ORDER OF MATRIX
              C            NROOTX  NUMBER OF ROOTS WANTED.  MOST NEGATIVE ROOTS ARE
              C                     FOUND FIRST.  IF NO VECTORS ARE WANTED, MAKE THIS
              C                     NUMBER NEGATIVE.
              C            NJX     ROW DIMENSION OF VECT ARRAY.  SEE 'VECT' BELOW.
              C                     NJX MUST BE NOT LESS THAN NX.
              C                    FORM, I.E. OCCUPYING NX*(NX+1)/2 CONSECUTIVE
              C                    LOCATIONS.
              C            B       SCRATCH ARRAY USED BY GIVENS.  MUST BE AT LEAST
              C                     NX*5 CELLS.
              C            ROOT    ARRAY TO HOLD THE EIGENVALUES.  MUST BE AT LEAST
              C                    NROOTX CELLS LONG.  THE NROOTX SMALLEST ROOTS ARE
              C                     ORDERED LARGEST FIRST IN THIS ARRAY.
              C            VECT    EIGENVECTOR ARRAY.  EACH COLUMN WILL HOLD AN
              C                     EIGENVECTOR FOR THE CORRESPONDING ROOT.  MUST BE
              C                     DIMENSIONED WITH 'NJX' ROWS AND AT LEAST 'NROOTX'
              C                     COLUMNS, UNLESS NO VECTORS
              C                     ARE REQUESTED (NEGATIVE NROOTX).  IN THIS LATTER
              C                     CASE, THE ARGUMENT VECT IS JUST A DUMMY, AND THE
              C                     STORAGE IS NOT USED.
              C        THE ARRAYS A AND B ARE DESTROYED BY THE COMPUTATION.  THE RESULTS
              C        APPEAR IN ROOT AND VECT.
              C        THE ORIGINAL REFERENCE TO THE GIVENS TECHNIQUE IS IN OAK RIDGE
              C        REPORT NUMBER ORNL 1574 (PHYSICS), BY WALLACE GIVENS.
              C        THE METHOD AS PRESENTED IN THIS PROGRAM CONSISTS OF FOUR STEPS,
              C        FIRST, THE INPUT MATRIX IS REDUCED TO TRIDIAGONAL FORM BY THE
                       !I COMMENTS  DELETED
0003                   DIMENSION B(NX,5),A(1),ROOT(NROOTX),VECT(NJX,NROOTX)
0004                   EQUIVALENCE (TEMP,ITEMP), (TM,ITM)
              C        ETA IS A CONVERGENCE LIMIT USED TO DETERMINE WHEN THE ROOTS
              C        HAVE BEEN FOUND TO SUFFICIENT ACCURACY.
              C            A       MATRIX STORED BY COLUMNS IN PACKED UPPER TRIANGULAR
              C        ALL MODIFICATIONS OF THE ORIGINAL METHOD...
              C        THIS LIMIT SHOULD BE ADJUSTED TO PROVIDE MAXIMUM ACCURACY ON
              C        A GIVEN COMPUTER.
              C        SUGGESTED TOLERANCES... 2.0E-8 FOR IBM 7090, UNIVAC 1108.
              C        1.0E-10 FOR CDC 3600.
0005                  ETA=1.0D-10
0006                   DELTA = ETA
0007                  SMALL=ETA*1.0D-3
              C        IDEGEN IS A FACTOR USED TO DETERMINE IF TWO ROOTS ARE CLOSE
              C        ENOUGH TO BE CONSIDERED DEGENERATE FOR PURPOSES OF ORTHOGONALI-
              C        ZING THEIR VECTORS.  IF THE DIFFERENCE BETWEEN TWO ADJACENT
              C        ROOTS IS AT LEAST 'IDEGEN' FIGURES LESS THAN THE LARGEST ROOT
              C        (MAGNITUDE), THEN ORTHOGONALIZATION WILL OCCUR.
0008                   IDEGEN = 5
0009                   SQRT2 = 1.4142135624
0010                   N = NX
0011                  NROOT= IABS(NROOTX)
0012                   NJC = NJX
0013                     IF (NROOT.EQ.0) GO TO 1001
0014                     IF (N-1) 1001,1010,105
```

```
FORTRAN IV G LEVEL  18                  GIVENS

 0015        1010   ROOT(1) = A(1)
 0016               IF (NROOTX.GT.0) VECT(1,1) =1.0
 0017               GO TO 1001
 0018        105    CONTINUE
             C      NSIZE   NUMBER OF ELEMENTS IN THE ARRAY
 0019               NSIZE = (N*(N+1))/2
 0020               NM1 = N - 1
 0021               NM2 = N - 2
             C      PRELIMINARY BUSINESS.  SCALE THE MATRIX TO PREVENT OVERFLOWS.
             C      NOTE THAT IF OVERFLOW OCCURS HERE, ALL IS LOST...
             C      HOWEVER, OVERFLOW IS QUITE UNLIKELY.
             C      AN APPROPRIATE TEST IS NOT INCLUDED, SINCE IBM'S FORTRAN IV
             C      CONTAINS NO EASY WAY OF TESTING FOR OVERFLOW.
 0022        85     CONTINUE
 0023               ANORM = 0.
 0024               J = 1
 0025               K = 1
 0026        86     DO 80 I=1,NSIZE
 0027               IF (I.NE.J) GO TO 81
 0028               ANORM = ANORM + A(I)**2/2.
 0029               K = K+1
 0030               J = J+K
 0031               GO TO 80
 0032        81     ANORM = ANORM + A(I)**2
 0033        80     CONTINUE
 0034               ANORM  =DSQRT(ANORM)*SQRT2
 0035               IF (ANORM .EQ.0.) GO TO 1001
             C      SCALE MATRIX TO NORM OF 1.  OVERALL SCALE FACTOR IS ANORM.
 0036               DO 91 I=1,NSIZE
 0037        91     A(I) = A(I)/ANORM
             C      TRIDIA SECTION.
             C      TRIDIAGONALIZATION OF SYMMETRIC MATRIX
 0038               ID = 0
 0039               IA = 1
 0040                 IF (NM2.EQ.0) GO TO 201
 0041               DO 200  J=1,NM2
             C      J         COUNTS ROW  OF A-MATRIX TO BE DIAGONALIZED
             C      IA        START OF NON-CODIAGONAL ELEMENTS IN THE ROW
             C        ID      INDEX OF CODIAGONAL ELEMENT ON ROW BEING CODIAGONALIZED.
 0042               IA = IA+J+2
 0043                 ID = ID + J + 1
 0044                 JP2 = J + 2
             C      SUM SQUARES OF NON-CODIAGONAL ELEMENTS IN ROW J
 0045                 II = IA
 0046               SUM = 0.0
 0047                 DO 100  I=JP2,N
 0048                 SUM = SUM + A(II)**2
 0049        100      II = II + I
 0050                 TEMP = A(ID)
 0051               IF (SUM.GT.SMALL) GO TO 110
             C      NO TRANSFORMATION NECESSARY IF ALL THE NON-CODIAGONAL
             C      ELEMENTS ARE TINY.
 0052         120  B(J,1) = TEMP
 0053                 A(ID) = 0.0
 0054               GO TO 200
             C      NOW COMPLETE THE SUM OF OFF-DIAGONAL SQUARES
 0055        110      SUM =DSQRT(SUM + TEMP**2)
             C      NEW CODIAGONAL ELEMENT
```

```
 0056              B(J,1)  =-DSIGN(SUM,TEMP)
            C       FIRST NON-ZERO ELEMENT OF THIS W-VECTOR
            C       FORM REST OF THE W-VECTOR ELEMENTS
 0057                 B(J+1,2) =DSQRT((1.0 +DABS(TEMP)/SUM)/2.0)
 0058                 TEMP =DSIGN(0.5/(B(J+1,2)*SUM),TEMP)
 0059                 II = IA
 0060                 DO 130 I=JP2,N
 0061                 B(I,2) = A(II)*TEMP
 0062       130       II = II + I
            C       FORM P-VECTOR AND SCALAR.  P-VECTOR = A-MATRIX*W-VECTOR.
            C       SCALAR = W-VECTOR*P-VECTOR.
 0063               AK = 0.0
            C       IC       LOCATION OF NEXT DIAGONAL ELEMENT
 0064                 IC = ID + 1
 0065               J1 = J + 1
 0066               DO 190  I=J1,N
 0067               JJ = IC
 0068               TEMP = 0.
 0069               DO 180  II=J1,N
            C       I        RUNS OVER THE NON-ZERO P-ELEMENTS
            C       II       RUNS OVER ELEMENTS OF W-VECTOR
            C         CHANGE INCREMENTING MODE AT THE DIAGONAL ELEMENTS
 0070               TEMP = TEMP + B(II,2)*A(JJ)
 0071               IF (II.LT.I) GO TO 210
 0072       140     JJ = JJ + II
 0073               GO TO 180
 0074       210     JJ = JJ + 1
 0075       180     CONTINUE
            C       BUILD UP THE K-SCALAR (AK)
 0076               AK = AK + TEMP*B(I,2)
 0077              B(I,1)= TEMP
            C       MOVE IC TO TOP OF NEXT A-MATRIX 'ROW'
 0078       190     IC = IC + I
            C       FORM THE Q-VECTOR
 0079               DO 150  I=J1,N
 0080        150   B(I,1) = B(I,1) - AK*B(I,2)
            C       TRANSFORM THE REST OF THE A-MATRIX
            C       JJ       START-1 OF THE REST OF THE A-MATRIX
 0081                 JJ = ID
            C       MOVE W-VECTOR INTO THE OLD A-MATRIX LOCATIONS TO SAVE SPACE
            C       I        RUNS OVER THE SIGNIFICANT ELEMENTS OF THE W-VECTOR
 0082               DO 160  I=J1,N
 0083               A(JJ) = B(I,2)
 0084               DO 170  II=J1,I
 0085               JJ = JJ + 1
 0086        170   A(JJ)=A(JJ)-2.0*(B(I,1)*B(II,2)+B(I,2)*B(II,1))
 0087       160     JJ = JJ + J
 0088       200     CONTINUE
            C       MOVE LAST CODIAGONAL ELEMENT OUT INTO ITS PROPER PLACE
 0089       201       CONTINUE
 0090              B(N-1,1)= A(NSIZE-1)
 0091               A(NSIZE -1) = 0.0
            C       SHIFT ALL CODIAGONAL ELEMENTS DOWN ONE PLACE TO TAKE ADVANTAGE
            C       OF FORWARD INDEXING (I.E. FIRST CODIAGONAL ELEMENT MUST BE ZERO).
 0092               DO 205 J=1,NM1
 0093                 NMJ = N - J
 0094        205   B(NMJ+1,1) = B(NMJ,1)
 0095              B(1,1) = 0.
```

```
      C      STURM SECTION.
      C      STURM SEQUENCE ITERATION TO OBTAIN ROOTS OF TRIDIAGONAL FORM
      C      MOVE DIAGONAL ELEMENTS INTO SECOND N ELEMENTS OF B-VECTOR.
      C      THIS IS A MORE CONVENIENT INDEXING POSITION.
      C      OF B-VECTOR FOR USE IN STURM SEQUENCE EVALUATION.
              ALIMIT = 1.0
             JUMP=1
             DO 70  J=1,N
             B(J,2)=A(JUMP)
             B(J,3) = B(J,1)**2
         70  JUMP=JUMP+J+1
      C      ROOT(I) HOLDS LOWER LIMIT OF EIGENVALUE I.
      C      B(I,4) HOLDS UPPER LIMIT OF EIGENVALUE I.
        320   DO 310  I=1,NROOT
              ROOT(I) = -ALIMIT
        310   B(I,4) = +ALIMIT
      C      ISOLATE THE ROOTS.  SMALLEST IS SOUGHT FIRST.
              DO 330  I=1,NROOT
      C      IMPROVE THE TRIAL ROOT
        500  TRIAL = (ROOT(I) +B(I,4))*0.5
             IF(DABS(B(I,4)-ROOT(I)).LE.DELTA) GO TO 330
      C      FORM STURM SEQUENCE.
      C      THE TRIAL VALUE.
        350  NOMTCH = 1
              F1 = 1.0
             SIGN1=+1.
              DO 360  J=1,N
              DIAG = B(J,2) - TRIAL
             IF (B(J,1).NE.0.)GO TO 410
        420     F0 = DIAG*SIGN1
              GO TO 400
        410   F0 = DIAG*F1
             IF (B(J-1,1).NE.0.)GO TO 430
        440     F0 = F0 - B(J,3)*SIGN2
              GO TO 400
        430   F0 = F0 - B(J,3)*F2
        400   IF (F0) 450,460,470
        460  SIGN0=SIGN1
              GO TO 510
        480  IF (F0*SIGN1.GT.0.0) GO TO 510
             GO TO 520
        470  SIGN0=+1.
              IF (F1) 520,480,510
        450  SIGN0=-1.
              IF (F1) 510,480,520
        520  NOMTCH = NOMTCH + 1
        510   F2 = F1
              F1 = F0
             SIGN2=SIGN1
             SIGN1=SIGN0
        360   CONTINUE
      C      ESTABLISH NEW BOUNDS FOR REMAINING ROOTS.
              DO 540  J=I,NROOT
             IF (J.GE.NOMTCH) GO TO 610
      C      NEW UPPER BOUND FOR THIS ROOT
        600   B(J,4) = TRIAL
              GO TO 540
      C      NEW LOWER BOUND FOR THIS ROOT
```

```
      610  IF (ROOT(J).LT.TRIAL)  RCCT(J) = TRIAL
      540  CONTINUE
       5C2 GC TC 500
      330  CONTINUE
      C    REVERSE THE ORDER OF THE EIGENVALUES, SINCE CUSTOM DICTATES
      C    'LARGEST FIRST'.
           NRT = NRCOT/2
           DC 10 I=1,NRT
           SAVE = ROOT(I)
           NMIP1 = NROOT - I + 1
           RCCT(I) = RCCT(NMIP1)
      10   ROOT(NMIP1) = SAVE
           TOLER = CMAX1(DABS(ROOT(1)),DABS(ROOT(NROOT)))*10.**(-IDEGEN)
      C    TRIVEC SECTICN.
      C    EIGENVECTORS OF CODIAGCNAL FCRM
      807  CONTINUE
      C    QUIT NOW IF NO VECTCRS WERE REQUESTEC.
           IF (NROOTX.LT.0) GO TO 1C02
      C    SET INITIAL VALUES TO VECTORS TO TRY TO SOLVE THE
      C    DEGENERACY PROBLEM FCR MCST CASES.
           CO 15 I=1,N
           AI = I
           DO 15 J=1,NROOT
      15   VECT(I,J) = 1.0 + AI*.CO5379813
      C    DON'T GET EXCITED.  THE CCNSTANT IS JUST A FACTOR TO TRY TO
      C    DESTROY CYCLES IN THE STARTING VECTCRS.  THIS HELPS CUT THE
      C    ALGCRITHM IN SOME CASES WITH MANY DEGENERACIES.
           DO 7CC  I=1,NROOT
           AROOT = ROOT(I)
      C    CRTHCGONALIZE IF THE CIFFERENCE BETWEEN ADJACENT ROOTS IS
      C    AT LEAST 'IDEGEN' FIGURES LESS THAN THE LARGEST ROOT (MAGNITUDE).
             IF (I.EQ.1) GO TO 710
      715  IF(DABS(RCCT(I-1)-ARCCT).LE.TCLER) GO TO 720
      710  IA = -1
      720  IA = IA + 1
           ELIM1 = A(1) - ARCCT
           ELIM2 = B(2,1)
           JUMP = 1
           DO 750  J=1,NM1
           JUMP = JUMP+J+1
      C    GET THE CORRECT PIVOT EQUATION FOR THIS STEP
          IF(DABS(ELIM1).LT.DABS(B(J+1,1))) GC TC 760
      C    FIRST (ELIM) EQUATION IS THE PIVOT THIS TIME
           IF(DABS(ELIM1).LE.DELTA) ELIM1 =DSIGN(DELTA,ELIM1)
           B(J,2) = ELIM1
           B(J,3) = ELIM2
           B(J,4) = 0.
          TEMP = B(J+1,1)/ELIM1
      C    SAVE FACTOR FOR THE SECONC ITERATION.  MARK IT AS CASE 1
      C      THIS HOCUS-POCUS WITH TEMP-ITEMP AND TM-ITM IS JUST TO PLACE
      C      A FLAG BIT IN THE LOWER BIT POSITION OF B(J,5).  THE CUMBROUS
      C      CODE IS BECAUSE IBM'S FCRTRAN IV DOES NOT HAVE MASKING OPS.
             ITM = (ITEMP/2)*2
             B(J,5) = TM
           ELIM1 = A(JUMP)-ARCCT - TEMP*ELIM2
           ELIM2 = B(J+2,1)
           GC TC 750
      C    SECCND ECUATION IS THE PIVOT THIS TIME.
```

```
FORTRAN IV G LEVEL  18                GIVENS

0179        760     B(J,2) = B(J+1,1)
0180                B(J,3) = A(JUMP) - ARCCT
0181                B(J,4) = B(J+2,1)
0182                TEMP = ELIM1/B(J+1,1)
            C       SAVE FACTOR FOR SECOND ITERATION.  MARK IT AS CASE 2
0183                  ITM = (ITEMP/2)*2 + 1
0184                  B(J,5) = TM
0185                ELIM1 = ELIM2 - TEMP*B(J,3)
0186                ELIM2 = -TEMP*B(J+2,1)
0187        750     CONTINUE
0188                IF(DABS(ELIM1).LE.DELTA) ELIM1 =DSIGN(DELTA,ELIM1)
0189                B(N,2) = ELIM1
0190               B(N,3) = 0.
0191               B(N,4) = 0.
0192                B(N-1,4) = 0.
0193                ITER = 1
0194                  IF (IA.NE.0) GO TO 800
            C       BACK SUBSTITUTE TO GET THIS VECTOR
0195        790     L = N + 1
0196                DO 780  J=1,N
0197                L = L - 1
0198        780     VECT(L,I) =(VECT(L,I) - VECT(L+1,I)*B(L,3) - VECT(L+2,I)*
                  X             B(L,4))/B(L,2)
0199                GO TO (820,800),ITER
            C       SECOND ITERATION.  (BOTH ITERATIONS FOR REPEATED-ROOT VECTORS)
0200        820     ITER = ITER + 1
0201        890     ELIM1 = VECT(1,I)
0202                DO 830  J=1,NM1
0203                  TM = B(J,5)
0204                  ITEMP = MOD(ITM,2)
0205                  IF (ITEMP.NE.0) GO TO 840
            C       CASE ONE.
0206        850     VECT(J,I) = ELIM1
0207                ELIM1 = VECT(J+1,I) - ELIM1*B(J,5)
0208                GO TO 830
            C       CASE TWO.
0209        840     VECT(J,I) = VECT(J+1,I)
0210                ITEMP = (ITM/2)*2
0211                ELIM1 = ELIM1 - VECT(J+1,I)*TEMP
0212        830     CONTINUE
0213                VECT(N,I) = ELIM1
0214                GO TO 790
            C       ORTHOGONALIZE THIS REPEATED-ROOT VECTOR TO OTHERS WITH THIS ROOT
0215        800       IF (IA.EQ.0) GO TO 885
0216                  DO 860 J1=1,IA
0217                K = I - J1
0218                TEMP = 0.
0219                DO 870  J=1,N
0220        870     TEMP = TEMP + VECT(J,I)*VECT(J,K)
0221                DO 880  J=1,N
0222        880     VECT(J,I) = VECT(J,I) - TEMP*VECT(J,K)
0223        860     CONTINUE
0224        885     GO TO (890,900),ITER
            C       NORMALIZE THE VECTOR
0225        900     TEMP = 0.
0226                DO 910  J=1,N
0227        910     TEMP = TEMP + VECT(J,I)**2
0228                  TEMP = 1.0/DSQRT(TEMP)
```

```
                  DO 920  J=1,N
                  VECT(J,I) = VECT(J,I)*TEMP
          920     CONTINUE
          700     CONTINUE
          C       SIMVEC SECTION.
          C       ROTATE CODIAGONAL VECTORS INTO VECTORS OF ORIGINAL ARRAY
          C       LOOP OVER ALL THE TRANSFORMATION VECTORS
                 IF (NM2 .EQ.0) GO TO 1002
                  JUMP = NSIZE - (N+1)
                  IM = NM1
                  DO 950  I=1,NM2
                  J1 = JUMP
          C       MOVE A TRANSFORMATION VECTOR OUT INTO BETTER INDEXING POSITION.
                  DO 955  J=IM,N
                  B(J,2) = A(J1)
          955     J1 = J1 + J
          C       MODIFY ALL REQUESTED VECTORS.
                  DO 960  K=1,NROOT
                  TEMP = 0.
          C       FORM SCALAR PRODUCT OF TRANSFORMATION VECTOR WITH EIGENVECTOR
                  DO 970  J=IM,N
          970     TEMP = TEMP + B(J,2)*VECT(J,K)
                  TEMP = TEMP + TEMP
                  DO 980  J=IM,N
          980     VECT(J,K) = VECT(J,K) - TEMP*B(J,2)
          960     CONTINUE
                  JUMP = JUMP - IM
          950     IM = IM - 1
          1002    CONTINUE
          C       RESTORE ROOTS TO THEIR PROPER SIZE.
                  DO 95 I=1,NROOT
          95      ROOT(I) = ROOT(I)*ANORM
            1001 RETURN
                  END
```

ZN	F in Volts/Meter	Dirac (Meter)$^{-1}$	Luden (Meter)$^{-1}$
2 5 1 1 1	0.1004000000000000D 07	0.6132734153368510D 03	0.6132876534017269D 03
2 5 1 1 2	0.1004000000000000D 07	0.4630189226265065D 03	0.4630255112345330D 03
2 5 1 1 3	0.1004000000000000D 07	0.3020241198721342D 03	0.3020304026242811D 03
2 5 1 1 4	0.1004000000000000D 07	0.1429502785278018D 03	0.1429531955926213D 03
2 5 1 1 5	0.1004000000000000D 07	-0.1705497513432056D 02	-0.1705358785856515D 02
2 5 1 1 6	0.1004000000000000D 07	-0.1785249695214443D 03	-0.1785254180161282D 03
2 5 1 1 7	0.1004000000000000D 07	-0.3408538582501933D 03	-0.3408570604638662D 03
2 5 1 1 8	0.1004000000000000D 07	-0.5015610369641795D 03	-0.5015657689659856D 03
2 5 1 1 9	0.1004000000000000D 07	-0.6748704324089922D 03	-0.6748818959002383D 03
2 5 2 1 1	0.3012000000000000D 07	0.1897829691807507D 04	0.1897870842115022D 04
2 5 2 1 2	0.3012000000000000D 07	0.1426976180837024D 04	0.1426953770814966D 04
2 5 2 1 3	0.3012000000000000D 07	0.9446920595627744D 03	0.9447081200024113D 03
2 5 2 1 4	0.3012000000000000D 07	0.4642940180569421D 03	0.4643005933966488D 03
2 5 2 1 5	0.3012000000000000D 07	-0.1706236248766072D 02	-0.1706068250094540D 02
2 5 2 1 6	0.3012000000000000D 07	-0.4998449302164372D 03	-0.4998484515643213D 03
2 5 2 1 7	0.3012000000000000D 07	-0.9835537087591365D 03	-0.9835667152043898D 03
2 5 2 1 8	0.3012000000000000D 07	-0.1465488703327486D 04	-0.1465504463243531D 04
2 5 2 1 9	0.3012000000000000D 07	-0.1959441489750287D 04	-0.1959479892028496D 04
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2 5 3 1 2	0.5020000000000000D 07	0.2391047888148110D 04	0.2391076772250701D 04
2 5 3 1 3	0.5020000000000000D 07	0.1587413845370756D 04	0.1587439670257736D 04
2 5 3 1 4	0.5020000000000000D 07	0.7856557857610751D 03	0.7856653941520490D 03
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2 5 3 1 6	0.5020000000000000D 07	-0.8212047301346902D 03	-0.8212116436052602D 03
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