SPECIAL MATHEMATICAL METHODS WITH
APPLICATIONS TO MOLECULAR AND ATOMIC PHYSICS

BY

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ABSTRACT

The less common theoretical methods, Green's functions, the theory of continuous groups, and canonical transformations, are applied to study properties of the following: a single particle spin-orbit coupled system in a magnetic field, a linear chain of point charges, the Coulomb potential and Hamiltonians quadratic in coordinates and (or) momentum operators.

RESUME

Les fonctions de Green, la théorie des groupes continus et les transformations canoniques parmi des méthodes théoriques moins générales sont appliquées à l'étude des propriétés d'un système spin-orbité couplé dans un champ magnétique, d'une chaîne linéaire des charges ponctuées, d'un potentiel coulombien et des Hamiltoniens quadratiques en coordonnées et (ou) en moments.
The next village

My grandfather used to say: "Life is astoundingly short. To me, looking back over it, life seems so foreshortened that I scarcely understand, for instance, how a young man can decide to ride over to the next village without being afraid that—not to mention accidents—even the span of a normal happy life may fall far short of the time needed for such a journey"

Franz Kafka
(A short story; Eng. translation W. and E. Muir).
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SUMMARY

In part one, the possibility of calculating the dynamic paramagnetic susceptibility tensor of a spin-orbit coupled system in an external magnetic field, by means of a Green's function formulation of linear response theory, has been considered, with the intention of obtaining results independent of the basis set. The attempt to solve this problem exactly leads to considerable mathematical complexity. Nevertheless, in the limit of zero external field, the calculation simplifies to the point when the relevant Heisenberg equation of motion for the magnetic moment operator can be solved directly to produce an exact Green's function for the system. The Fourier transform with respect to time of this Green's function finally gives a frequency-dependent susceptibility tensor whose resonance frequencies are compared, in a few cases, with the splitting of energy levels calculated by different theories and experimentally observed. This calculation is accomplished in Chapter I.

In Chapter II, a general method for factorizing an exponential function of operators is proposed. The method is applied to factorizing the evolution operator of the spin-orbit coupled system in an external magnetic field, one of the necessary steps in the calculation of the susceptibility tensor of this system. Unfortunately, the expressions cannot be given in closed
form. The method is illustrated with the case \( L = l/2, \ S = l/2 \).

In part two, Chapter III, a Green's function method (a multiple scattering method) is used to calculate the electronic structure of a model for polymers, considered as a linear chain of singly ionized hydrogen atoms. It is found that in the direction perpendicular to the chain there are two regions of different potential. The Green's function method is used to formulate the condition of continuity of a wave function on the boundary between these two regions. This condition leads to a secular equation from which the structure of energy levels can be determined. By the same method a solution is formulated along the chain, which can be regarded as a one-dimensional solid.

In part three, certain calculations are described which are relevant for applied aspects of the theory of the representations of continuous groups associated with the Coulomb potential.

In particular, in Chapter IV a general non-square representation of the symmetry group of the Coulomb Hamiltonian, \( \text{SO}(4) \), has been obtained in terms of 6-Euler angles specifying rotations in 4-dimensional space. The basis states are derived as columns of \( \text{SO}(4) \) rotation matrices. A connection between two possible parametrization of the \( \text{SO}(4) \) group is shown explicitly and some interrelations between involved special functions are derived. These general non-square representations describe the states of 'more than one electron' atoms as well as the degeneracy with respect to \( j \) of an atom in a magnetic field.

In Chapter V, a representation of the \( \text{SO}(4,1) \) group in the space of \( \text{SO}(4) \) spinors and in 4-dimensional Euclidian...
space has been found. The two spaces are linked by linearly transforming variables. It has been shown that, the 4-dimensional hyperspherical harmonics in both 4-dimensional polar co-ordinate systems transform in accordance with the $W = 0$, $Q = 2$ representation of the $SO(4,1)$ group. A set of new recursion relations is derived for the $SO(3)$ group reduced rotation matrices, together with a set of standard recursion relations for the Legendre and Gegenbauer polynomials, all of which are obtained by transforming both forms of the $SO(4)$ group basis states in spinor space into 4-dimensional space. The matrix elements of the non-compact $SO(4,1)$ group generators are given in the $(j,m)$ basis.

In Chapter VI, the discrete classes of the unitary irreducible representations of the group $SO(2,2)$ which leave the magnetic quantum number of the hydrogenic wave functions invariant have been reduced with respect to the representations of the $SO(2,1)$ subgroup. It has been shown that the discrete class of the representations of the $SO(2,2)$ group contain the continuous non-exceptional class and two discrete classes of the $SO(2,1)$ representations once.

In part four, Chapter VII, a Hamiltonian quadratic in coordinate and momentum operators has been diagonalized by a canonical transformation. This method for diagonalizing the Hamiltonian has been applied to the Hamiltonian of angular momentum in a magnetic field, which transforms into one of uncoupled harmonic oscillators.
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**CLAIMS TO ORIGINAL RESEARCH**

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PART ONE

CONTRIBUTIONS TOWARD THE CALCULATION OF THE DYNAMIC PARAMAGNETIC SUSCEPTIBILITY TENSOR OF A SPIN-ORBIT COUPLED SYSTEM IN A MAGNETIC FIELD.
Introduction to part one

Spin-orbit coupling has been extensively studied both experimentally and theoretically in the case of free atoms and ions, ions in a ligand field and diatomic molecules. In recent years theoretical studies have been extended to the solid state, where it is found that spin-orbit coupling takes part in a number of processes, for example: electric dipole transitions in rare earth metals \(^1\), indirect exchange in intermetalics \(^2\), residual attenuation of shear waves in superconductors \(^3\) and the Hall effect in ferromagnets \(^4\), etc.

In more complex systems, the role of spin-orbit coupling has been experimentally verified \(^6, 6, 7\), but the usual theoretical treatment, by means of perturbation of the spin-Hamiltonian, seems not to be adequate, because the relevant wave functions are too complex or unknown.

In this work an attempt is made to study the properties of the spin-orbit coupling term without early reference to a particular basis set.

Consequently, the Heisenberg picture of quantum mechanics is employed. The intention is to calculate the paramagnetic dynamic susceptibility (hereafter referred to as susceptibility) of this system in an external magnetic field.
It is assumed that a molecular system can be divided into two parts, described by two sets of operators. The operators of the first set depend on coordinates only, while the operators of the second set depend on spin and angular momentum. The system is in an oscillating external field. The Hamiltonian takes the form:

\[ H = H_0 + H_1 + H_2(t), \]  

where

- \( H_0 \) includes the kinetic and potential energy operators, and
- \( H_1 = \xi \vec{L} \cdot \vec{S} \),
- \( H_2(t) = \mu_B (\vec{L} + 2\vec{S}) \cdot \vec{H}_{\text{ex}}(t) \),

where \( \xi \) is the isotropic coupling constant and \( \vec{L} \) and \( \vec{S} \) are the angular momentum and spin operators; and
- \( \vec{H}_{\text{ex}}(t) \) is the external field.

The magnetic moment operator is

\[ \vec{\mathcal{M}} = - \frac{\partial H}{\partial \vec{H}} = - \mu_B (\vec{L} + 2\vec{S}). \]  

Although \( H_0 \) depends on the coordinates and \( H_1 \) and \( H_2(t) \) on the coordinates and spin, it is still a good approximation to assume that the eigenstates of the Hamiltonian (1) are a product of eigenstates of \( H_0 \) and eigenstates of the spin, as established by Slater. The change of linear momentum in the magnetic field, \( \vec{p} = \vec{p} - \frac{e}{c} \vec{A} \), (A-vector potential) is not explicitly considered. It may be included by choosing appropriate basis sets.
for calculation of the matrix elements; (Landau wave functions for example). Also, it is assumed that the disturbances induced by magnetic fields on the orbits of the particles do not interfere with the precession of the magnetic moments. In such a case two sets of operators, referring to the orbital and magnetic part of the system, can be considered as independent, in the sense described by Fano. Then, the magnetic properties are described by the density matrix:

$$\rho_1 = Tr_0 \rho,$$  \hspace{1cm} (1.5)

where $\rho_1$ is the reduced density matrix and the trace is taken over the unperturbed eigenstates of particles $2, 3, \ldots, N$, $N$ being the number of particles in the system.

If $\Delta \rho$ is the change in $\rho$ induced by the external perturbation $H_2$, then it can be calculated by linear response theory following the standard procedure of Kubo and others, and the susceptibility is then given in terms of a Fourier transform of a retarded Green's function:\textsuperscript{10}

$$\chi_{j,k}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt e^{i\omega t} \rho_{j,k}(t,0),$$ \hspace{1cm} (1.6)

where $\chi_{j,k}$ is a component of the susceptibility tensor and

$$\rho_{j,k}(t,0) = \delta(t) \langle m_j, m_k(0) \rangle,$$ \hspace{1cm} (1.7)

where $\delta(t)$ is the step function. The appearance of this step function is a manifestation of causality. The angular bracket signifies that the average is taken over the canonical ensemble. The canonical ensemble is characterized by the so-called "natural motion", which is not affected by the external perturbation; that is, the Hamiltonian is given by $H_0 + H_1$ in this model. The perturbation has been developed as a Fourier integral:

$$H_2(t) = \frac{1}{\hbar} \int d\omega e^{i\omega t} H_{ex}(\omega).$$

In linear response theory the time evolution of the components of the magnetic moment operator is given by the
ordinarily, in the full heisenberg picture the equation of motion for the components of the magnetic moment operator is:

\[ m_j(t) = \exp\left(\frac{iH_1 t}{\hbar}\right)m_j(0)\exp\left(-\frac{iH_1 t}{\hbar}\right). \quad (I.8) \]

if only the dynamical evolution of a single magnetic moment is considered. it must be emphasized that (I.9) does not appear in linear response theory.

by considering the structure of the equation of motion (I.9), it can be seen that any attempt to separate the time dependence from the operator dependence will encounter various difficulties.

although linear response theory does not require (I.9) to be solved, such an equation of motion does appear in quantum mechanical problems and it is of interest to consider a method for solving it. a mathematical problem related to solution of (I.9) will be considered in chapter II, since (I.8) is really a special case of (I.9) that is the zero field case.

because the operators \( \hat{L} \) and \( \hat{L} + \hat{2S} \) do not commute it is necessary to factorize the evolution operator in (I.9):

\[ \exp\left(\frac{i\zeta(\hat{L} \cdot \hat{S}) t}{\hbar} + \frac{i\mu_B(\hat{L} \cdot \hat{2S})_\text{ext} t}{\hbar}\right) = \exp\left(\frac{i\zeta(\hat{L} \cdot \hat{S}) t}{\hbar}\right) \exp\left(\frac{i\mu_B(\hat{L} \cdot \hat{2S})_\text{ext} t}{\hbar}\right) C(t), \quad (I.10) \]

where \( C(t) \) is an unknown function of the operators and time.

next, the following expression has to be calculated:

\[ D_j(t) = \exp\left(\frac{i\mu_B(\hat{L} \cdot \hat{2S})_\text{ext} t}{\hbar}\right) C(t) \omega_B(\hat{L} + \hat{2S}_j) \exp\left(-\frac{i\mu_B(\hat{L} \cdot \hat{2S})_\text{ext} t}{\hbar}\right) \]

\[ (I.11) \]
The final answer will be obtained by solving:

$$ m_j(t) = \exp\left[i\zeta(\Delta S)t/\hbar\right] D_j(t) \exp\left[-i\zeta(\Delta S)t/\hbar\right]. $$

(1.12)

It is apparent that this problem is fairly complex.

The problem simplifies considerably if the external field is assumed to be zero; then the equation of motion (1.9) reduces to equation (1.8) and this equation can be solved exactly in the limit of zero field as can the commutator in (1.7). The Fourier transform of the Green's function thus generated gives the exact frequency dependent susceptibility tensor (1.6) for the system. The predicted values of the resonance frequencies are found to be in agreement, in a few cases, with the splitting of the energy levels calculated by different theories, and experimentally observed. This calculation is described in Chapter I.

In Chapter II, a method for factorizing an exponential function of two non-commuting operators is proposed. The method is applied to the evolution operator in (1.9), which is factorized according to (1.10). Unfortunately, the form of the function $C(t)$ depends on the values of $L$ and $S$, and generally cannot be found in closed form, but the method is still applicable, provided an electronic calculator is available for diagonalizing certain higher order matrices. The method is illustrated for a case $L=1/2$ and $S=1/2$, when the calculations can be done analytically.

Even though the results of this part are limited to the case of non-interacting magnetic moments, (1.5), the results of Chapter I provide an insight into structure of the relevant Green's functions, and allow some conclusions of general validity to be drawn. Also the method
for the factorization, presented in Chapter II, may prove useful in other calculations where an evolution operator, having the sum of non-commuting operators in the argument, appears.
CHAPTER I

A GREEN'S FUNCTION FORM FOR THE SUSCEPTIBILITY TENSOR OF A SPIN-ORBIT COUPLED SYSTEM IN THE LIMIT OF ZERO EXTERNAL MAGNETIC FIELD.
1. Introduction

In this chapter an exact form of the susceptibility tensor, (1.6), is calculated. The equation of motion of the components of the magnetic moment operator is:

\[ m_j(t) = \exp\{i(\mathbf{L} \cdot \mathbf{S})t/\hbar\} m_j(0) \exp\{-i(\mathbf{L} \cdot \mathbf{S})t/\hbar\}, \quad (1.1) \]

In the equation of motion (1.1) the time dependence can be separated out of the operator dependence by developing the exponents in a Taylor series. The resulting chain of commutators is expressed as a certain function of a few basic commutators which allows the solution of Equation (1.1) to be found in closed form. From this closed form solution, the time dependent Green's function (1.7) is determined by calculating the appropriate commutator. The susceptibility tensor, (1.6), is obtained by a Fourier transform of this Green's function found in Section 2. Discussion of the results is given in Section 3 and the conclusion in Section 4. Section 2, 3 and 4 together with some parts of the Introduction to this part have been previously published separately.

2. Calculation

The total angular momentum \( \mathbf{J} \) at time \( t \) is given by:

\[ \mathbf{J}(t) = \mathbf{L}(t) + \mathbf{S}(t) \]

where the components of \( \mathbf{L} \) and \( \mathbf{S} \) vary in time according with (1.1). In the case of small external field the operator \( \mathbf{J} \) commutes with the Hamiltonian \( H \), and it is approximately a constant of motion; then the commutators entering (1.7) can be given to the lowest order in the external field as:
Expanding the exponents in (1.1) with $L_j$ in place of $m_j$, gives the equation of motion

$$L_j(t) = L_j(0) + \sum_{k=1}^{\infty} \frac{(it/\hbar)^k}{k!} \left[(L+S), \ldots (L+S), L_j \right].$$

A new notation is now introduced: let

(a) $\eta = \xi t/\hbar$
(b) $\mathcal{Y} = L+S$ (n brackets)
(c) $[(L-S), \ldots (L-S), L_j] = F_n^{j_{n>0}}$
(d) $[(L-S), L_j] = i(LxS)_j = U_j$
(e) $|A| = A$
(f) $A(0) = A$

where $A$ stands for any vector operator

(g) $\sqrt{1+4Y^2} = z$

and

(h) $(L^2+S^2)L_j - (L^2+S^2)L_j = \{ (L+S)_x (L+S) \}_j = V_j$.

In the last equality, the order of factors must be kept as in the curly brackets.

The operators $Y^2, L^2, S^2$ commute between themselves and with $H_1$.

All the brackets in (2.2) can be expressed in terms of $U_j$ and $V_j$ with polynomial coefficients in $\mathcal{Y}$.
\[ F_1 = \frac{1}{2} u_j - o v_j \]
\[ F_2 = -u_j + 1 v_j \]
\[ F_3 = (y^2 + 1) u_j - 1 v_j \]
\[ F_4 = -(2y^2 + 1) u_j + (y^2 + 1) v_j \]
\[ F_5 = (y^2 + 3y^2 + 1) u_j - (2y^2 + 1) v_j \]
\[ F_6 = etc. \]

Thus the brackets can be written generally as

\[ F_n^j = (-1)^{n+1} p_n(y) u_j + (-1)^n v_{n-1}(y) v_j \] (2.4)

where

\[ p_n(y) = \sum_{n=0}^{\frac{n-1}{2}} (-1)^n \frac{(n-m)!}{(n-2m-1)!} \frac{2m}{n} \] (2.5)

with the additional definition that

\[ p_0 = 0 \] (2.6)

Equation (2.5) can be connected with the Chebyshev polynomials of the second kind \textsuperscript{13}, \( u_n(\lambda) \). After formal replacement of

\[ x = \frac{\lambda}{2y} \]

the identity

\[ p_n(y) = \left(\frac{\lambda}{2}\right)^{n-1} u_{n-1} \left(\frac{\lambda}{2}\right) \] (2.7)

follows. Use of inverse operators is purely formal in this presentation,
and expressions containing them stand for a series expansion in which only even positive powers of the operators appear. With the preceding identity, the equation of motion (2.2) becomes:

\[ L_j(n) = L_j(0) - \sum_{k=1}^{\infty} \frac{(-1)^k}{k} P_{k-1}(Y) v_j, \]

(2.8)

where \( U \) is expressed by

\[ U_n(\cos \theta) = \frac{\sin(n+1)\theta}{\sin \theta}, \]

(2.9)

and in this case

\[ \theta = \arccos \frac{1}{2Y}. \]

(2.10)

Substitution of (2.9) in (2.8) gives

\[ L_j(n) = L_j(0) - \sum_{k=1}^{\infty} \frac{(-1)^k}{k} \left( \frac{Y}{1} \right)^{k-2} \frac{\sin(k-1)\theta}{\sin \theta} v_j. \]

(2.11)

The series (2.11) can be brought to the closed form using formula (5) Part III, Section 3C of Ref. 14. This gives

\[ L_j(n) = L_j + A(n) v_j + B(n) v_j, \]

(2.12)

where

\[ A(n) = \frac{2n}{z} \exp(-nz) \sin \frac{nz}{2} z, \]

and

\[ B(n) = \frac{1}{z^2} \left( \exp(-nz) \frac{\sin \frac{nz}{2} z}{\cos \frac{nz}{2} z} + \frac{\sin \frac{nz}{2} z}{z} \right). \]

(2.13)
This is the equation of motion for the components of angular momentum.

However, for the classical Hamiltonian \((L \cdot S)\), no motion is possible. The magnetic moments will orient themselves in a fixed position parallel or anti-parallel to the magnetic field, depending on the sign of \(\zeta\).

In the quantum case they precess around the constant vector \(L+S\), having components along \(L\), \((L \times S)\) and \((L+S) \times (L \times S)\). The commutator of Equation (2.1) decomposes into

\[
[L_j(t), L_q(0)] = [L_j, L_q(0)] = [L_j, L_q] + A(t) [U_j, L_q] + [A(t), L_q] U_j
\]

\[+ B(t) [V_j, L_q] + [B(t), L_q] V_j. \tag{2.15}
\]

Comparing Equation (2.11) and (2.12), it is seen that \(A(n)\) and \(B(n)\) are expressible in terms of Chebishev polynomials in \(\gamma\); so, in order to find the time dependent commutator in (2.15), it is enough to calculate the commutator \([\gamma^{2n}, L_q]\).

\(\gamma^{2n}\) is decomposed by the binomial theorem, as follows

\[
\gamma^{2n} = (L^2 + S^2 + 2L \cdot S)^n = \sum_{s=0}^{n} \binom{n}{s} (L^2 + S^2)^{n-s} L^s S^{n-s} \tag{2.16}
\]

and the only commutator needed is:

\[
[(L \cdot S)^n, L_q] = \sum_{p=1}^{s} (L \cdot S)^{s-p} [(L \cdot S), L_q] (L \cdot S)^{p-1} \tag{2.17}
\]

Also, a term on the right hand side of (2.17) can be represented as a finite series of the commutators (2.3), or from (2.4) and (2.7) in terms of
the Chebyshev polynomials,

\[
(L \cdot S)^{s-p} [L \cdot S, L_q] (L \cdot S)^{p-1} = \sum_{k=0}^{p-1} (-1)^k (p-1) (L \cdot S)^{s-l-p} p^{p+1}
\]

\[
= \sum_{k=0}^{p-1} (p-1) (L \cdot S)^{s-l-p} \left\{ \left( \frac{1}{2} \right)^k u_k (Y) U_{q-k} - \left( \frac{1}{2} \right)^k u_{k-1} (Y) V_q \right\}
\]

Then using expression (3.9) for the Chebyshev polynomials, and the identity:

\[
\exp(i \theta) = \frac{1}{2Y} (1 \pm i z)
\]

the right hand side of Equation (2.18) becomes a binomial equation, giving

\[
(L \cdot S)^{s-p} [(L \cdot S), L_q] (L \cdot S)^{p-1} = \frac{1}{2^p} \left\{ (2L \cdot S + 1 + z)^{p-1} - (2L \cdot S + 1 - z)^{p-1} \right\} V_q
\]

With the operator identity

\[
(1 - A_{1+\ldots+A}^n) = 1 - A^n
\]

the geometrical sum on the right hand side of Equation (2.17) gives,

\[
[(L \cdot S)^{s}, L_q] = \frac{1}{2z} \left\{ (2L \cdot S + z + 1)^s - (2L \cdot S - z + 1)^s \right\} U_q
\]

\[
+ \frac{1}{2^{s-1} z} \left\{ \frac{(2L \cdot S)^s - (2L \cdot S + z + 1)^s}{(1+z)} - \frac{(2L \cdot S)^s - (2L \cdot S - z + 1)^s}{(z-1)} \right\} V_q
\]

With this expression the commutator \([Y^{2n}, L_q]\) becomes,
\[ [Y^{2n}, \ell_q] = \left(-\frac{1}{z} \sum_{s=0}^{n} \left(\begin{array}{c} n \\ s \end{array}\right) (L^2+S^2)^s \right) \frac{1}{z} \sum_{s=0}^{n} \left(\begin{array}{c} n \\ s \end{array}\right) (L^2+S^2)^{n-s} (2L+r \cdot s-z+1)^s (2L+r \cdot s)^s \]

\[ x(2L+r \cdot s-z+1)^s - \frac{1}{z} \sum_{s=0}^{n} \left(\begin{array}{c} n \\ s \end{array}\right) (2L+r \cdot s-z+1)^s (L^2+r \cdot s)^s \]

\[ + \frac{1}{z(1+z)} \sum_{s=0}^{n} \left(\begin{array}{c} n \\ s \end{array}\right) (L^2+S^2)^{n-s} (2L+r \cdot s)^s - \frac{1}{z(z+1)} \sum_{s=0}^{n} \left(\begin{array}{c} n \\ s \end{array}\right) (L^2+S^2)^{n-s} (2L+r \cdot s)^s \]

\[ x(2L+r \cdot s)^s (2L+r \cdot s+1)^s + \frac{1}{z(z-1)} \sum_{s=0}^{n} \left(\begin{array}{c} n \\ s \end{array}\right) (L^2+r \cdot s)^s (2L+r \cdot s)^s \]

\[ - \frac{1}{z(z+1)} \sum_{s=0}^{n} \left(\begin{array}{c} n \\ s \end{array}\right) (L^2+r \cdot s)^s (2L+r \cdot s-z+1)^s \]

\[ = \frac{(Y+z+1)^n}{z} - \frac{(Y^2-z+1)^n}{z} \]

\[ + \left(\frac{2y^2n}{z(z+1)} + \frac{2y^2n}{z(z-1)} \right) \]

\[ \left(\frac{2(Y^2-z+1)}{z(z+1)} + \frac{2(Y^2-z+1)}{z(z-1)} \right) \]

\[ \text{(2.21)} \]

This is again a binomial sum, hence,

\[ [Y^{2n}, \ell_q] = \frac{1}{z} \left( (Y^2+z+1)^n - (Y^2-z+1)^n \right) \]

\[ + \frac{2}{z} \left( \frac{1}{z+1} + \frac{1}{z-1} \right) Y^{2n} \]

\[ P_n \left( \sqrt{Y^2+z+1} \right) - P_n \left( \sqrt{Y^2-z+1} \right) \]

\[ \text{(2.22)} \]

From the definition of \( P_n(Y) \), (2.5) and (2.22),

\[ \left[ \frac{n-1}{2} \right] \]

\[ [P_n(Y), \ell_q] = \sum_{m=0}^{\infty} \frac{(-1)^m (m-1)!}{m!(n-2m-1)!} [Y^{2m}, \ell_q] \]

\[ = \frac{1}{z} \left( P_n \left( \sqrt{Y^2+z+1} \right) - P_n \left( \sqrt{Y^2-z+1} \right) \right) \]

\[ + \frac{2}{z} \left( \frac{1}{z+1} + \frac{1}{z-1} \right) P_n(Y) \]

\[ \text{(2.23)} \]
Using again the closed form expression for the Chebyshev polynomials of the second kind, (2.9) and the summation formula of Reference 14, the same as has been used before for obtaining (2.13), the right hand side of (2.23) can be summed up. With this, and from definition of \( A(t) \) and \( B(t) \) in (2.13), and (2.5), the commutators of (2.15) can be found.

Collecting the factors with the same time dependence, the commutator entering (2.1) becomes,

\[
[L_j(t), L_{q}] = C_{j,q} + 2i \sin \frac{n \pi}{2} \exp(-i \frac{n \pi}{2}) D_{j,q} + 2i \sin \frac{n \pi}{2}(z+2) \exp(-i \frac{n \pi}{2}) E_{j,q} + 2i \sin \frac{n \pi}{2}(z-2) \exp(-i \frac{n \pi}{2}) R_{j,q} + 2 \cos \frac{n \pi}{2} \exp(-i \frac{n \pi}{2}) S_{j,q} + 2 \cos \frac{n \pi}{2}(z+2) \exp(-i \frac{n \pi}{2}) T_{j,q} + 2 \cos \frac{n \pi}{2}(z-2) \exp(-i \frac{n \pi}{2}) W_{j,q} ,
\]

(2.24)

where the components of the tensors are:

\[
\begin{align*}
\rho^1_{C_{j,q}} &= \frac{4}{z^2-1} [L_j, L_q] + \frac{64}{(z-9)(z-1)^2} \frac{V}{q} V J + \frac{32}{(z-1)(z^2-9)} U U J \\
\rho^1_{D_{j,q}} &= \frac{1}{z} [U_j, L_q] + \frac{4}{z(z-1)} V U J + \frac{4}{2z(z-1)} [V_j, L_q] + \frac{8}{z(z-1)^2} V V J \\
\rho^1_{E_{j,q}} &= \frac{1}{z(z+2)} U Q J - \frac{2}{z(z+1)(z+2)} V Q J - \frac{4}{z(z+1)^2(z+3)(z+2)} V V J \\
\rho^1_{R_{j,q}} &= \frac{1}{z(z-2)} U Q J - \frac{2}{z(z-1)(z-2)} V Q J - \frac{4}{z(z-1)^2(z-3)(z-2)} V V J \\
\rho^1_{S_{j,q}} &= \frac{2}{(z^2-1)} [V_j, L_q] + \frac{8}{(z^2-1)^2} V Q V J
\end{align*}
\]
\[ \rho_{j,q}^{-1} = \frac{4}{z(z+1)(z+3)} \quad \rho_{j,q} = \frac{2}{z(z+1)(z+3)} \quad U \quad V \]

The average value of (2.24) over an appropriate basis set, should give the exact time dependent Green's Function for a spin-orbit coupled system \([L_j(t), L_q]\). It consists of the products of time dependent and time independent operators.

Since an independent particle Hamiltonian is assumed, there is no possibility of relaxation processes. The system is in a specified quantum state. Consequently, the poles of the Green's function are purely real and simply the energy differences of these states. In other words, an absorption line is reduced to a delta function shape; the residues of these poles give the transition probabilities.

The orthonormal basis set is taken to be \( |\alpha\rangle \) corresponding to an \( \alpha \) collection of quantum numbers. The time dependent and time independent operators in (2.24) and (2.25) can then be separated by inserting a decomposed unity between them.

After this, the Fourier transform of (2.24) with frequency \( \omega \) gives for the susceptibility, (in the final results the small positive parameter \( \varepsilon \) has been set to zero)

\[ \chi_{j,q}(\omega) = \sum_{\alpha} \frac{1}{2\pi} \int_{-\infty}^{\infty} \left( \frac{1}{z(\omega \alpha^2 + \omega)} + \frac{1}{z(\omega \alpha^2 - \omega)} \right) \langle \chi^\dagger_{j,q} | \alpha \rangle \langle \alpha | |\rangle \]

\[ (2.26) \]
where

\[
 z_a = \sqrt{1+4\langle \alpha \rangle (L+S)^2} |\alpha^\dagger>.
\]  

(2.27)

3. Discussion

The usual interpretation of the Fourier transform of Green's function is that the value of \( \omega \) at the pole gives the energy difference between quantum states, while the residues correspond to transition amplitudes. In an exact calculation, the poles on the real axis should be distributed symmetrically about the imaginary axis, because both back and forth transitions are possible. In this case, in expression (2.26) only half of the poles appear. This is due to the fact that the Green's function has been calculated only in the upper half plane (\( \omega = \omega - i\epsilon \)) and only
symmetrical set of poles in Equation (2.26) will be generated. This can be clarified; the absorption of power is related to:

\[ x_{jq}(\omega) - x_{jq}(\omega) \]

and the solution to (1.6) given by Equation (2.26) gives some operators of higher rank, (2.25) and (2.3, h and d), which can induce transitions between the energy levels. Thus the same pole appears under different residues.

In the present calculation no coupling between different particles has been assumed. It is applicable to one particle spin-orbit coupled system.

In the simplest case of spherical symmetry, \( I + S = J \), and the \( \alpha \) correspond to the \( n, l, m \), set of quantum numbers.

The pole

\[ \omega = \frac{\xi}{2\hbar}[1 + 4J(J+1) - 1] = \pm(\xi/\hbar)J \]

Secondly, a cubic (octahedral) field splits ten degenerate states of the \( d^1 \) configuration into four-fold degenerate \( e^g \) states, and six-fold degenerate \( t^2_g \) states; when the spin-orbit coupling is much stronger then the cubic field, these two groups are separated by \((5/2)\) \( \hbar \), where \( \alpha \) corresponds to the set of quantum numbers \( L=2, m_l=2, S=1/2 \) and \( m_S=1/2 \), which label the component in the wave function; the pole gives the separation:

\[ \omega = \frac{\xi}{2\hbar}[1 + 4(6\pi - 3/4 + 4k^2/3 - 1)] \]

which correspond to the strong spin-orbit coupling, weak field case of Reference 16,
then gives the separation in agreement with experiment.\textsuperscript{16}

The spin-orbit coupling mixes these two groups and splits the \( e_g \) and \( t_{2g} \) states; the \( t_{2g} \) state split into a two-fold and a four-fold degenerate state. According to Kamimura\textsuperscript{17} these two sets are separated by \( 3/2 \). The same components of the wave function as above, gives for the pole

\[
\omega = \xi/2b\left[\sqrt{1+4(6+3/4+2^2+1/2)} - 3\right] = (\xi/6)(3/2).
\]

The singlet case, \( L=0, S=0 \) shows no resonant absorption since \( \omega=0 \) and the present theory reproduces an established fact. The susceptibility tensor has more poles than there are actual resonances in a system. In this respect, it resembles the spectra of an anion in a crystal field where only some of all possible \( SLJ \) states appear, for example in the spectra of \( Gd^{++} \textsuperscript{18} \).

If a non-spherical state vector is developed in angular and spin eigenvectors, then

\[
|\phi\rangle = \sum_{L S} A^L_S |L S\rangle \sum_{M_L M_S} N^L_M |N_L M_S\rangle \quad \text{(3.1)}
\]

and from (2.26) the maximum number of possible resonances is

\[
2^4 \times 3 = 12,
\]

per \( |L S\rangle |N_L M_S\rangle \) component in (3.1).

The factor 3 comes from the fact that the operator \((L+S)^2\) can mix only states with the same magnetic quantum numbers, or states in which
they differ by one, \( (M_L, N_L, M_S, N_S; N_L = M_L + 1, M_S = M_S + 1) \).

4. Conclusion

The exact Green's function for the dynamic paramagnetic susceptibility of a single particle spin-orbit coupled system is shown to generate the Lande interval rule, the experimental separation between \( e_g \) and \( t_{2g} \) states, and the spectra of an ion in a ligand field. Thus while the generalized spectra it predicts have yet to be experimentally detected, the validity of the formulation can be established by these specific examples.
CHAPTER II

A METHOD FOR FACTORIZING AN EXPONENTIAL FUNCTION
OF OPERATORS
1. Introduction:

In this chapter an operator function of the type \( \exp(a+b) \) will be considered.

The aim is to factorize this function \( \exp(a+b) \) and to determine the operator \( C \) in the operator identity:

\[
\exp(b+a) = \exp(b)\exp(a)C
\]  

(1.1)

In general, if the operators \( a \) and \( b \) do not commute, this factorization is possible only in a few special cases. Two independent methods for the factorization have been developed by Feynman\(^1\) and Kumar\(^2\); from a practical point of view neither of these is applicable because the former involves repeated time integrations, and the latter does not provide closed expressions for the coefficients in a Taylor expansion of the operator on the left hand side of (1.1).

In Section 2 of this chapter a method will be described by means of which the operator \( C \) in (1.1) can be found. This method requires the use of an electronic calculator, for diagonalization of relevant matrices.

In Section 3 this method will be applied to the case of the evolution operator of interest namely for \( a=i\gamma /\hbar \) \((\gamma \neq \gamma')\) and \( b=\frac{iAt}{\hbar}(\gamma + \gamma') \cdot \hbar \exp \) and the analytical solution is worked out for \( \gamma = 1/2 \) and \( S=1/2 \) case.
2. Method:

First, recall the definition of an exponential operator. An exponential operator stands for development:

\[ \exp(iA) = \sum_{n=0}^{\infty} \frac{(iA)^n}{n!} = 1 + iA - \frac{A^2}{2!} + \frac{A^3}{3!} - \ldots \]

(2.1)

It will be assumed that the operator \( A \) can be represented in the form of a finite Hermitian matrix, then there is a unitary matrix \( U_A \) which diagonalizes \( A \):

\[ U_A^+ A U_A = D_A = D(A_1, \ldots, A_n), \]

(2.2)

here \( D \) is the diagonal matrix and \( A_1, \ldots, A_n \) are the eigenvalues of the matrix \( A \).

From (2.1) and (2.2) it follows that

\[ U_A^+ \exp(iA) U_A = \exp(iU_A^+ AU) = D(\exp(iA_1), \ldots, \exp(iA_n)) \]

(2.3)

and

\[ \exp(iA) = UD(\exp(iA_1), \ldots, \exp(iA_n))U^+. \]

(2.4)

Also, because the operators \( e^{iA} \) and \( e^{-iA} \) commute

\[ U_A = U_{-A}. \]

(2.5)

The same matrix diagonalizes both \( \exp(iA) \) and \( \exp(-iA) \). Now, it is a simple matter to specify the operator \( C \) in (1.1). This function is given by

\[ C = \exp(-a) \exp(-b) \exp(a+b). \]

(2.6)
Then the exponentials in (2.6) can be expressed according to (2.4) and (2.5).

So, for the operator $C$, (1.1):

$$
C = U_a D \exp(-s_j) \cdots \exp(-s_n) U_x^+ \\
U_b D \exp(-s_1) \cdots \exp(-s_n) U_x^+ \\
U_{a+b} D \exp(-s_{a+b}) \cdots \exp(-s_{n-a-b}) U_x^+ \\
(2.7)
$$

where $U_a, U_b$ and $U_{a+b}$ are the unitary matrices which diagonalize the matrices associated with the operators $a, b$ and $(a+b)$ respectively. The eigenvalues of these operators are $s_{a_i}, s_{b_i}$ and $s_{a_i+b_i}$.

3. Application to the evolution operator for a spin-orbit coupled system in a magnetic field

The results of Section 2 will be now applied to the case of a spin-orbit coupled system in an external magnetic field. The evolution operator for this system is given by (1.1) with:

$$
a = i \hbar \gamma \hat{L} \cdot \hat{S}; \quad b = i \hbar \gamma / n \left( \hat{L}^2 + \hat{S}^2 \right) \hat{H}_{ex}. \quad (3.1)
$$

A matrix representation for the components of the operators $\hat{L}$ and $\hat{S}$ can be obtained from the theory of $O(4)$ group representations. The $O(4)$ group is homomorphic to the $O(3) \times O(3)$ group. The Lie algebra of the $O(3) \times O(3)$ group consists of two mutually commuting vectors $\hat{j}^+$ and $\hat{j}^-$; they commute in the same way as $\hat{L}$ and $\hat{S}$. Therefore one can associate:

$$
\hat{L} \leftrightarrow \hat{j}^+; \quad \hat{S} \leftrightarrow \hat{j}^- \quad (3.2)
$$
Therefore the basis for unitary irreducible representation of the $O(4)$ group, in this case, is a product of the two bases for representations of the $O(3)$ group. Accordingly, the basis states for a representation of the $O(4)$ group are labelled with a pair of $O(3)$ labels such as $(j^+, m^+)$ and $(j^-, m^-)$.

In this basis the matrix elements of the operators (3.2) are:

\[
\begin{align*}
\langle j^+ j^- | j^+ j^- \rangle_{m \pm 1} &= (j^+ \pm m^+ \pm 1)(j^+ \pm m^+) \frac{1}{2} , \\
\langle j^+ j^- | j_0 \rangle_{m \pm 1} &= m^+ , \\
\langle j^+ j^- | j_0 \rangle_{m \pm 1} &= m^- .
\end{align*}
\]

The ladder components of the operators $L$ and $S$ are:

\[
L_\pm = (L_\pm \pm iL_y); \quad L_0 = L_z ,
\]

\[
S_\pm = (S_\pm \pm iS_y); \quad S_0 = S_z .
\]

(3.4)
As usual, it will be assumed that the external field is along z-axis; then the operators $a$ and $b$ of (3.1) are:

$$a = \frac{ie}{2\hbar} \left( L_z S_z + 2L_+ S_+ \right) \tau^z = \frac{ie}{2\hbar} \left( j_+^+- j_-^- + 2j_0^+ j_0^- \right) \tau^z,$$

$$b = \frac{\mu B \text{ex}}{2\hbar} \left( L_0 + 2S_0 \right) = \frac{\mu B \text{ex}}{\xi} \left( j_0^+ j_0^- \right) \tau^z. \quad (3.5)$$

The matrix representation for $a$ and $b$ is easily obtained from (3.3) and (3.5).

A. An illustration: the case where $L = 1/2$ and $S = 1/2$

Reducing the matrix elements of (3.3) to the case $j_0^+ = j_0^- = 1/2$, from (3.5), the operators $a, b$ and $a+b$ become:

$$a = \frac{i\epsilon t}{4\hbar} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad b = \frac{\mu B \text{ex}}{2\hbar} \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix}$$

and

$$a+b = \frac{i\epsilon t}{4\hbar} \begin{pmatrix} 1 + 3v & 0 & 0 \\ 0 & 1-v & 2 & 0 \\ 0 & 2 & -1-v & 0 \\ 0 & 0 & 1 & -3v \end{pmatrix}, \quad (3.6)$$

where

$$v = 2 \frac{\mu B \text{ex}}{\xi}. \quad (3.7)$$

Now, the set of three unitary matrices which diagonalize $a, b$ and $a+b$ has to be found. They can be found by solving the corresponding
eigenvalue problems, to be:

\[ V_a = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}; V_a V_a^+ = 1. \] (3.8)

The matrix \( b \) is already diagonal, so the unitary matrix which "diagonalizes" it is simply the unit matrix:

\[ V_b = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \] (3.9)

The unitary matrix, which diagonalizes the \( a+b \) matrix is:

\[ V_{a+b} = \begin{pmatrix} 1 & 0 & 1/2 & 0 \\ 0 & \frac{2}{\delta + v} & 0 & 1/2 \\ 0 & \frac{\delta - v}{2v} & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \]

where \( \delta = (4+v^2)^{1/2} \) and \( V_{a+b} V_{a+b}^+ = 1 \) (3.10).

The eigenvalues of the matrices \( a, b \) and \( a+b \) given in (3.6) are:

\[ a_i = \frac{-i\tau t}{2\hbar}, \frac{i\tau t}{2\hbar}, \frac{3i\tau t}{4\hbar}, \text{ and } -\frac{i\tau t}{4\hbar}, \]

\[ b_i = \frac{3\mu B_{ext}}{2\hbar}, \frac{\mu B_{ext}}{2\hbar}, \frac{3\mu B_{ext}}{2\hbar}, \text{ and } \frac{3\mu B_{ext}}{2\hbar}, \]

and

\[ a+b; \frac{1}{2}(1+3v)\tau, \frac{1}{2}[-1+(4+v^2)^{1/2}]\tau, \frac{1}{2}[-1-(4+v^2)^{1/2}]\tau \text{ and } \frac{1}{2}(1-3v)\tau. \] (3.11)

where \( v \) is given by (3.7)
These eigenvalues are now substituted into the general expression for \( C \), (2.7), together with the unitary matrices (3.8), (3.9) and (3.10); after some manipulation the following form for the matrix \( C(t) \) in (1.1) is obtained:

\[
C(t) = 2(L_z S_z + L_z^2) - 2(L_z S_z - L_z^2)f_1(t) - 2(L_x L_y - S_x S_y)f_2(t) + 2i(L_x S_y - L_y S_x)f_3(t) + 2i(L_x S_x + L_y S_y)f_4(t),
\]

(3.12)

in which the time dependent functions, \( f_j(t) \), \( j = 1, 2, \ldots, 4 \) are:

\[
f_1 = \cos nt \cos xt \cos vt,
\]

\[
f_2 = -\sin nt \cos xt \cos vt \frac{\mu B}{h v} \cos xt \sin vt + \frac{E}{h v},
\]

\[
f_3 = \frac{E}{h v} \sin nt \cos xt \sin vt - i \frac{\mu B}{h v} \cos nt \sin xt \cos vt + \sin nt \sin xt \cos vt
\]

and

\[
f_4 = -i \frac{\mu B}{h v} \sin nt \sin xt \sin vt,
\]

(3.13)

where

\[
n = \frac{\mu B e}{2h}, \quad \chi = \frac{E}{2h} \quad \text{and} \quad v = \left(n + \chi\right)^{1/2}
\]

(3.14)

The matrices for \( L_z, S_z, L_x, S_x, L_y, S_y \) are easily calculated from (3.3) and (3.4).
The general method presented in Section 1 is when the operators \( a \) and \( b \) can be represented as finite Hermitian matrices. The method is easily generalized to the case of an arbitrary sum of operators.

In the application of this method to the factorization of the evolution operator of a spin-orbit coupled system in an external field, Section 2, the eigenvalues of \( L^2 \) and \( S^2 \) have to be known beforehand, because the form of the matrices for \( L \) and \( S \) depends on these eigenvalues and consequently the form of the function \( C(t) \).

Nevertheless, this method may be useful in practical calculations because it gives the form of the matrix \( C \) in (1.1), in a rather straightforward fashion and, in the case of an evolution operator, leads to a factorization of the time dependence out of the operator dependence in the final expression for the operator \( C \), as has been illustrated in 3A.
REFERENCES AND FOOTNOTES

7. Usually, spin-orbit coupling is not a subject of a separate research or a review article. Various facts referring to it are scattered all over the literature. It is not possible to cover here any significant part of the work done on the subject References quoted so far have only exemplary meaning.

12. The notation \( J = \hat{L} + \hat{S} \) is avoided, because if used it would imply a coupling between \( \hat{L} \) and \( \hat{S} \).
14. V. Mangulis, Handbook of Series for Scientific and Engineers, (Academic Press, New York, 1965) Part III, Sec. 3C, Eq. (5), which is:

\[ \sum_{n=0}^{\infty} \frac{r^n \cos(n\theta + \phi)}{n!} = \exp(r \cos \phi) \cos(\theta + \sin \phi) \]

15. See A.J. Akhiezer et al, Second item of Ref. 10.


17. H. Kamimura; J. Phys. Soc. J. 11, 1171 (1956). The above result is obtained by separating the component of the trigonal field out of the cubic field, after setting \( A = 0 \) in the relevant equation of this paper.


21. The observation that \( L \) and \( \hat{S} \) can be regarded as generators of \( O(4) \) group is due to Professor R.T. Sharp, McGill University, private communication.

PART TWO

ELECTRONIC STRUCTURE OF A LINEAR CHAIN OF POINT CHARGES.
CHAPTER III

A GREEN'S FUNCTION FORM FOR THE SOLUTIONS FOR
THE ONE-ELECTRON PROPERTIES OF A LINEAR CHAIN
Introduction

Long linear molecules are important in polymer chemistry, bio-physics and the physics of organic crystals.

The simplest model of such molecules, if the parts of the molecule do not mutually interact, is a chain of identical atoms with a single electron outside the filled core. There are a number of ways in which this model can be approached theoretically and they fall roughly into two categories:

(i) The one-electron potential is approximated to a form for which the Schrödinger equation can be solved exactly; the wave function describes the properties of the chain as a whole. The classic example of this approach is the Kronig and Penney model of a one-dimensional solid and of a gas of free electrons enclosed within impenetrable boundaries.

(ii) The atomic character of the constituents of the chain is emphasized. It is assumed that the chain is composed of free atoms with overlapping wave functions. The application of some type of molecular orbital theory then leads to solutions for the problem. The one electron potential, being implicitly a sum of the Coulomb potentials is more realistic than the potential in (i), but the wave function is found only approximately.

Representing the potential of the chain in terms of ionized atoms has certain features which are not fully accounted for by (i) and (ii) but before proceeding to a discussion, this model has to be fully described.
For simplicity it will be assumed that there are no core electrons; the chain consists of the point charges separated by a distance "a"; the amount of charge is taken to be $e_0$ where $e_0$ is the charge of an electron (reference to the "hydrogen atom" is deliberately avoided in order not to cause confusion with the two-dimensional hydrogen atom, whose wave functions are used in this calculations).

The appropriate coordinate system for this model is a cylindrical one with the coordinates:

\[ x = r \cos \phi, \]
\[ y = r \sin \phi, \]
\[ z = z \]

and

\[ dv = r \, dr \, d\phi \, dz, \]

where $dv$ is the volume element.

The $z$ axis points along the chain and $r$ is the perpendicular distance to it. The geometry is illustrated at the Figure 1.

The form of the potential function along the chain ($z$ dependence) is different from that in the direction perpendicular to the chain ($r$ dependence) and the potential is clearly independent of $\phi$, due to cylindrical symmetry of the chain. Along the chain the potential is periodic with the period $a$. Within this period, as it will be shown in Section 2 of this Chapter, the potential is a sum of two terms, $V(r) = a/z + bz^2$; the first, $a/z$, term is a one-dimensional Coulomb potential and the second, $bz^2$, is a harmonic oscillator potential.
The distribution of a one-electron potential around a linear chain of point charges; $F_r(r)$ and $F_z(z)$ are the forces on an electron perpendicular to and along the chain, respectively. The boundary which separates the two regions of different potential is taken at the distance $r = \frac{3a}{2}$.
The Coulomb potential is dominant in the vicinity of a charge (small \( z \)); halfway between two charges both terms are of comparable value.

In the perpendicular direction, in the vicinity of the chain, the potential is proportional to the Coulomb potential in two dimensions at large distances from the chain; the distinction between the individual charges is blurred out and the potential becomes proportional to the potential of a continuously charged wire \( \text{lnr} \).

In this Chapter, a solution is formulated which incorporates the foregoing properties of the potential. In Section 2, the form of the potential is analyzed in more detail and the true potential is approximated by a form for which the one-electron Schrödinger equation can be separated with respect to \( r \) and \( z \). The resulting two Schrödinger equations, one for each direction, are formally solved with appropriate boundary conditions.

In Section 3, the perpendicular direction is considered, where there are two regions with the different potentials, for which the radial two-dimensional Schrödinger equation has to be solved separately. The energy levels of the system are obtained from the usual conditions on the wave function at the boundary between these two regions. The Green's function method originally developed for solids \(^4\) and extended to molecules \(^5,6\) has been applied to this case.

In Section 4, the direction along the chain is considered. In this direction an electron "sees" a one-dimensional solid. The boundary conditions are the usual periodic ones \(^1\). The Schrödinger equation is converted into an
integral equation using the appropriate Green's function.

The solution for the chain formulated in this way holds for fairly realistic one-electron potentials. On the other hand, the solution does not depend on the states of individual atoms, in that sense the chain is considered as a whole.

2. The potential of the chain and the Schrödinger equation

The general form of the one-electron potential of the chain \( V(r, z) \) is approximated by the sum of two terms \( V_r(r) \) and \( V_z(z) \), where \( V_r(r) \) and \( V_z(z) \) are potentials in a direction perpendicular to the chain and parallel to the chain respectively. This is equivalent to saying that variation of the parallel potential does not influence the perpendicular component of wave function appreciably. This is certainly true for large distances from the chain. In such a case the Schrödinger equation in cylindrical coordinates can be separated with respect to \( r \) and \( z \). Explicitly,

\[
V(r, z) = -\frac{e^2}{\varepsilon} \frac{1}{\sqrt{r^2+(z-na)^2}} = -\frac{e^2}{\varepsilon} \left( \frac{1}{\sqrt{r^2+a^2}} + \frac{1}{\sqrt{(z-na)^2}} \right) = V_r(r) + V_z(z). \tag{2.1}
\]

As all the terms in equation (2.1) decrease towards infinity as \( 1/r \), the potentials are divergent; therefore instead of considering the potentials one has to consider the force on an electron (Figure 1) in order to find the
potential function.

A. The potential perpendicular to the chain

The force on an electron at distance \( r \) from a point on the chain is:

\[
F_x(r) = -e_0 \left( \frac{r}{(r^2 + \alpha a^2)^{3/2}} \right)
\]  

(2.2)

With the use of a summation formula, the preceding expression becomes

\[
F_x(r) = -e_0 \left( \frac{1}{r^2} + \frac{\mathbf{e}^2}{a^2} \right) \left( \sum_{n=1}^{\infty} \frac{1}{e^{n \alpha}} \frac{2 \pi}{a} \right) = \frac{e_0^2}{2} - I,
\]

(2.3)

where \( J_1(\cdot) \) is a Bessel function of the first order.

The integral \( I \), in (2.3) is estimated, with the use of inequalities, which hold for any \( t \):

\[
\pi t \leq e^{\pi t} - 1 \leq \pi te^{\pi t}
\]

(2.4)

When these inequalities are substituted for the denominator of the integrand, in (2.3), the upper and lower bound of the integral \( I \) become

\[
\frac{e_0^2}{2} \int_0^{\infty} e^{-\pi t} J_1(\frac{\pi t}{a}) dt < I < \frac{e_0^2}{2} \int_0^{\infty} J_1(\frac{\pi t}{a}) dt.
\]

(2.5)

The integration can be performed explicitly to give:

\[
\frac{e_0^2}{ar} \left( \frac{\sqrt{a^2 + r^2} - a}{\sqrt{a^2 + r^2}} \right) < I < \frac{e_0^2}{ra}
\]

(2.6)

For \( r \to 0 \), \( I \to \infty \); the Coulomb term \( \frac{e_0^2}{r^2} \) in (2.3) is dominant.
For $r \to \infty$, $I \to \frac{e^2}{ar}$, the "logarithmic" term $\frac{e^2}{ar}$ in (2.2) is dominant.

The approximate boundary between these two regions can be discerned from the Table 1 where the absolute value of the Coulomb term must lie between the upper and lower bounds of the non-Coulomb term $I$.

**COMPARISON OF THE MAGNITUDE OF THE TWO TERMS IN THE EXPRESSION FOR FORCE (2.3)**

<table>
<thead>
<tr>
<th>Distance $r$</th>
<th>Coulomb Term $\left(\frac{e^2}{r^2}\right)$</th>
<th>Lower Bound of $I$</th>
<th>Upper Bound of $I$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{1}{2}a$</td>
<td>$-\frac{4e^2}{a^2}$</td>
<td>$0.73 \frac{e^2}{a^2}$</td>
<td>$2 \frac{e^2}{a^2}$</td>
</tr>
<tr>
<td>$a$</td>
<td>$-\frac{e^2}{a^2}$</td>
<td>$0.37 \frac{e^2}{a^2}$</td>
<td>$1 \frac{e^2}{a^2}$</td>
</tr>
<tr>
<td>$\frac{3}{2}a$</td>
<td>$-0.44 \frac{e^2}{a^2}$</td>
<td>$0.3 \frac{e^2}{a^2}$</td>
<td>$0.67 \frac{e^2}{a^2}$</td>
</tr>
<tr>
<td>$2a$</td>
<td>$-0.25 \frac{e^2}{a^2}$</td>
<td>$0.27 \frac{e^2}{a^2}$</td>
<td>$0.5 \frac{e^2}{a^2}$</td>
</tr>
</tbody>
</table>

Table 1

The boundary is therefore around $r = \frac{3a}{2}$, and is taken to be at $r = \frac{3a}{2}$.

Below $r = \frac{3a}{2}$ only the Coulomb force term is retained.

$$I^1(r) = -\frac{e^2}{r^2} \quad \text{for } 0 < r \leq \frac{3a}{2}.$$
In (2.3); and above \( r = \frac{3}{2}a \) only the "logarithmic" force term \( F \) is retained:

\[
F_{r}^{II}(r) = \frac{2}{ar} \quad \text{For} \quad \frac{3}{2}a < r < \infty 
\]

Integrating the preceding force terms, gives the potential in the perpendicular direction:

\[
V_{r}^{I}(r) = -\frac{e^{2}}{r} + C_{1} \quad \text{For} \quad 0 < r \leq \frac{3}{2}a \tag{2.7a}
\]

\[
V_{r}^{II}(r) = -\frac{e^{2}}{a} \ln C_{2}r \quad \text{For} \quad \frac{3}{2}a < r < \infty \tag{2.7b}
\]

For later convenience the gauge \( C_{1} \) is determined from the condition:

\[
V_{r}^{I}(r) \bigg|_{r=\frac{3}{2}a} = \frac{e^{2}}{3a} \tag{2.8}
\]

This is the "origin" of the energy scale.

The gauge \( C_{2} \) is determined from the condition that the two potentials are equal at \( r = \frac{3}{2}a \). This gives:

\[
C_{2} = \frac{2e}{3a} \tag{2.10}
\]

E. The potential along the chain

Due to the periodicity of the potential along the \( z \) axis, and its symmetry with respect to reflection through the perpendicular planes, only the interval \( 0 < z < a/2 \), need be considered. The force on an electron is (Figure 1).
The series in (2.11) are in fact the definition of the generalized Riemann zeta functions \( \zeta \); by means of these functions the force can be expressed as:

\[
F_z(z) = -\varepsilon_0^2 \left\{ \frac{1}{z^2} + \frac{1}{a^2} \left[ \zeta(2,1+\frac{z}{a}) - \zeta(2,1-\frac{z}{a}) \right] \right\}. \tag{2.12}
\]

The expression (2.11) can be rearranged into a comparatively fast converging series:

\[
F_z(z) = -\varepsilon_0^2 \left\{ \frac{1}{z^2} - \frac{4z^2}{a^2} \sum_{n=1}^{\infty} \frac{1}{n^3 \left(1 - \frac{2z^2}{n^2a^2}\right)} \right\}. \tag{2.13}
\]

In the interval \(0<z<a/2\) the sum at the right-hand side of (2.13) is a slowly varying function of \(z\). It can be replaced by a constant. The value of the constant is determined from the condition that the force is zero half way between two neighboring charges:

\[
F_z(z) = 0 \quad \left| z = \frac{a}{2} \right. \tag{2.14}
\]

The force \(F_z(z)\) becomes then:

\[
F_z(z) = -\varepsilon_0^2 \left\{ \frac{1}{z^2} - \frac{8z}{a^3} \right\}. \tag{2.15}
\]

and the corresponding potential:

\[
V_z(z) = \varepsilon_0^2 \left\{ \frac{1}{z} + \frac{4z^2}{a^3} \right\}. \tag{2.16}
\]
C. Separation of the Schrödinger equation

The time independent Schrödinger equation is

\[ \left\{ -\frac{\hbar^2}{2m_0} \nabla^2 + V \right\} \psi = E\psi. \quad (2.17) \]

For a potential \( V \) in the form (2.1):

\[ V = V(r,z) = V_r(r) + V_z(z), \]

and for the wave function \( \psi \):

\[ \psi = Y(r,\phi)Z(z), \quad (2.18) \]

in cylindrical coordinates (1.1), (2.17) separates as follows:

\[ \left\{ -\frac{\hbar^2}{2m_0} \left( \frac{1}{r} \frac{\partial}{\partial r} \left[ r \frac{\partial Y(r,\phi)}{\partial r} \right] + \frac{1}{r^2} \frac{\partial^2 Y(r,\phi)}{\partial \phi^2} \right) + \left[ V_r(r) - \Delta \right] Y(r,\phi) = 0 \]

\[ (2.20a) \]

and

\[ -\frac{\hbar^2}{2m_0} \frac{\partial^2 Z(z)}{\partial z^2} + \left[ V_z(z) - \lambda \right] Z(z) = 0; \quad \Delta = E - \lambda, \]

where \( m_0 \) is the electron rest mass, and \( -\lambda \) is the separation constant; the negative sign is chosen in order that \( \lambda \) correspond to the "energy" of a one dimensional Schrödinger equation (2.2a). The total energy of the system, \( E \), is sum of the two eigenvalues of the Schrödinger equations (2.20a) and (2.20b);

\[ E = \lambda + \Delta. \]

3. The solution for the perpendicular direction

Perpendicular to the chain there are two regions with different potential, (2.7a), Region I and (2.7b) Region II. The wave function and its
A method for molecules has been developed in which there are two distinct types of potential within a molecule. Each atom is surrounded by a sphere. An electron "sees" one potential when it is inside the sphere and another when it is in the space between the spheres. The potential inside a sphere depends on the nature of the atom, but outside the sphere the potential is a constant function throughout the molecule. The method requires knowledge of the wave function inside a sphere and of a Green's Function outside the sphere. The energy of the system is then obtained from the condition of continuity for a wave function on the surface of each sphere.

Let the wave function inside a sphere \( \alpha \), of energy \( E \), be \( \psi^A_{\alpha}(r) \); the wave function and Green's Function outside the sphere are \( \psi^B_{E}(r) \) and \( G_{E}(r,r') \). The condition of continuity is\(^5\) that

\[
\psi^B_{E}(r) = \sum_{\alpha} \int_{S_{\alpha}} (G_{E}(r,r'^{\alpha}) \nu \psi^A_{\alpha}(r'^{\alpha}) - \psi^A_{\alpha}(r'^{\alpha}) \nu G_{E}(r,r'^{\alpha})) \cdot dS_{\alpha} \tag{3.1}
\]

The sum includes all spheres. An integral is taken over surface of the sphere \( \alpha \), \( S_{\alpha} \). The secular equation for energy is obtained from (3.1) when \( r = b_{\alpha} \), where \( b_{\alpha} \) is the radius vector of the sphere \( \alpha \).

Moreover, only one "sphere", the circle of radius \( r = \frac{3}{2}a \), is considered and consequently there is ambiguity about which region should be considered "inside" and which "outside". If \( \psi^I, G^I \) and \( \psi^{II}, G^{II} \) are the wave functions and Green's functions in regions I and II respectively, the boundary condition (3.1) at \( r = \frac{3}{2}a \) can be formulated in two equally valid ways:
\[ \psi^I(\vec{r}) = \int \frac{G^I(\vec{r}, \vec{r}^o) \psi^I(\vec{r}^o) - \psi^I(\vec{r}^o) G^I(\vec{r}, \vec{r}^o)}{|\vec{r}| - \frac{3a}{2}} + \psi^I(\vec{r}^o) \psi^I(\vec{r}^o) r^o d\phi, \] 
for \(|\vec{r}| < \frac{3a}{2} \) \hspace{1cm} (3.2a)

or,
\[ \psi^I(\vec{r}) = \int \frac{G^I(\vec{r}, \vec{r}^o) \psi^I(\vec{r}^o) - \psi^I(\vec{r}^o) G^I(\vec{r}, \vec{r}^o)}{|\vec{r}^o| - \frac{3a}{2}} \] 
for \(|\vec{r}| > \frac{3a}{2} \). \hspace{1cm} (3.2b)

The integral is taken along the circumference of a circle \( r^o = \frac{3a}{2} \).

The equations (3.2) have to be solved consistently for \( \psi^I, \psi^I \) and the energy \( \Delta \). The solution requires a knowledge of the Green's function in both regions I and II.

The potential (2.7) is independent on \( \phi \); therefore the complete set \( \{e^{im\phi}\} \) can be used to develop all the quantities appearing in (3.2):

\[ \psi^I_\Delta(r, \phi) = \frac{1}{\sqrt{2\pi}} \sum_{m} e^{im\phi} \gamma^I_{\Delta,m}(r), \] \hspace{1cm} (3.3a)

\[ G^I_\Delta(r, \phi; r^o, \phi^o) = \frac{1}{\sqrt{2\pi}} \sum_{m} e^{im(\phi - \phi^o)} G^I_{\Delta,m}(r, r^o), \] \hspace{1cm} (3.3b)

\[ \psi^II_\Delta(r, \phi) = \frac{1}{\sqrt{2\pi}} \sum_{m} e^{im\phi} \gamma^II_{\Delta,m}(r), \] \hspace{1cm} (3.3c)

and

\[ G^II_\Delta(r, \phi; r^o, \phi^o) = \frac{1}{\sqrt{2\pi}} \sum_{m} e^{im(\phi - \phi^o)} G^II_{\Delta,m}(r, r^o). \] \hspace{1cm} (3.3d)

where \( \vec{r} \) and \( \vec{r}^o \) are two two-dimensional vectors perpendicular to the chain.

The coefficients \( C_{\Delta,m} \) and \( A_{\Delta,m} \) will be determined by the boundary condition.
at \( r = \frac{3}{2} a \), \( \Delta \) is the energy of the system, (2.20a).

The Green's functions satisfy the same equation as the wave functions except for the presence of the "inhomogeneous" delta function at the right hand side of (2.20a). The delta function in cylindrical coordinates has the form:

\[
\delta(r-r_0)\delta(\theta-\theta_0) = \frac{\delta(r-r_0)\delta(\phi-\phi_0)}{r}
\]  

(3.4)

Substituting the developments (3.3) into (2.20a) and with (3.4) after a little manipulation:

\[
\left\{ \begin{array}{l}
\frac{1}{r} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) - \frac{2m}{\hbar^2} [Y_1^{II}(r) - \Delta] - \frac{m}{2} \frac{\delta(r-r')}{r} \delta(\theta-\theta') \delta(\phi-\phi') \\
\end{array} \right.
\]

\[= 0 \]

(3.5a)

\[
\frac{2m}{\hbar^2} \frac{\delta(r-r_0)}{r} \]

(3.5b)

Once, the solutions of (3.5a) are known, the Green's function can be found by a standard technique\(^{10,11}\). If \( Y_1 \) and \( Y_2 \) are two independent solutions of (3.5a) satisfying the boundary conditions at end points of an interval, the Green's function is:

\[
G(r,r') = \frac{2m}{\hbar^2 r_0 W(Y_1,Y_2)} \left\{ \begin{array}{ll}
Y_1(r)Y_2(r'); & r < r_0 \\
Y_2(r)Y_1(r'); & r > r_0
\end{array} \right.
\]

(3.6)

Here the interval is the whole space, \( 0 < r < \infty \). The boundary conditions are: \( Y \) finite for \( r \to 0 \); and \( Y_2 \to 0 \) as \( r \to \infty \). \( W \) is the Wronskian evaluated
at \( r = r_0 \); \( W = Y_1 Y_2 - Y_2 Y_1 \). The indices \( I, II, \lambda \) and \( m \) have been omitted in (3.6). The last equation holds for each of the regions. Now, to determine the solutions of (3.5):

A. Region I. \( 0 < r < \frac{3a}{2} \)

The potential in this region is given by (2.7a)

\[
V^I_2(r) = - \frac{e^2}{r} + \frac{5e^2}{3a}.
\]

With this potential, the Eq. (3.5a) becomes:

\[
\frac{\partial^2 V^I_{\lambda,m}(r)}{\partial r^2} + \frac{1}{r} \frac{\partial V^I_{\lambda,m}(r)}{\partial r} + \frac{2m^2}{\hbar^2 r} + \frac{2m^2}{\hbar^2 r^2} - \frac{2m^2}{\hbar^2} \; Y^I_{\lambda,m}(r) = 0 \tag{3.7a}
\]

\[
\Delta' = \Delta + \frac{5e^2}{3a}.
\tag{3.7b}
\]

This is the Schrödinger equation for a two-dimensional hydrogen atom for which the solutions are found immediately by substitution:

\[
Y^I_{\lambda,m}(r) = r^{-1/2} g(r), \quad r = \frac{1}{2k} x;
\tag{3.8a}
\]

\[
\alpha = \frac{m^2 e^2}{\hbar^2} \sqrt{\frac{1}{-2m^2} \quad \text{and} \quad k^2 = - \frac{\hbar^2}{2m^2} \tag{3.8b} \]

then (3.7) is reduced to Whittaker's equation. The two independent solutions are expressed in terms of Whittaker's functions \(^{12}\)

\[
Y^I_{\lambda,m}(r) = r^{-1/2} \psi_{\lambda,m}(2kr); \tag{3.9a}
\]

\[
Y^I_{\lambda,m}(r) = r^{-1/2} \psi_{\lambda,n}(2kr) \tag{3.9b}
\]
In order to make these functions convergent in the whole interval 0 < r < oo, m has to be restricted to positive integers only. In this case the behaviour of the solutions of the end points of the interval follow from Reference 13.

For m = 0, 1, 2, ...\n\[
\begin{align*}
\text{y}^I_{\text{a},m}(r) & \rightarrow \text{FINITE} & \text{and} & \text{y}^I_{\text{a},m}(r) & \rightarrow 0 \\
\text{y}^I_{\text{d},m}(r) & \rightarrow \infty & \text{and} & \text{y}^I_{\text{d},m}(r) & \rightarrow 0 \\
\text{y}^I_{\text{a},2m}(r) & \rightarrow 0 & \text{and} & \text{y}^I_{\text{a},2m}(r) & \rightarrow \infty
\end{align*}
\]
(3.10)

Since Region I includes zero, the proper solution in this region is (3.9a). The Wronskian evaluated at r^0 is:
\[
\mathcal{W} = -\frac{\Gamma(2m+1)}{\Gamma(m+1/2)} \frac{2\hbar}{r^{2m+1}}
\]
(3.11)

With (3.9), (3.10) and (3.11) the Green's function (3.6) for the Region I is evaluated:
\[
G_{\text{a},2m}(r, r^0) = \begin{cases} 
\frac{m_0 \Gamma(m+1/2)}{2\pi r^{2m+1}} & \text{for } 0 < r < r^0 \\
\frac{M_{\text{a},m}(2\hbar r)\mathcal{W}_{\text{a},m}(2\hbar r^0)}{\pi^2 r^{2m+1}k(2m+1)(rr^0)^{1/2}} & \text{for } r > r^0
\end{cases}
\]
(3.12)

B. Region II, \( \frac{3}{2} < r < \infty \)

The potential in this region is given by (2.7b) and (2.9)
\[
\nabla^2 u = \frac{e^2}{4\pi} \ln C_1 r.
\]
With this potential, the (3.5a) becomes:

\[
\left[ \frac{2}{\Delta_{m}^{II}(r)} \right] + \frac{1}{r} \frac{\Delta_{m}^{II}(r)}{\Delta r} + \frac{2m_{o}}{\hbar^{2}} \left( \frac{2}{a} \ln C_{1} r - \alpha \right) + \frac{m^{2}}{r^{2}} \right] Y_{\Delta_{m}^{II}}^{II}(r) = 0.
\]

(3.13)

Due to the presence of two essential singularities at 0 and \( \infty \), the last equation cannot be solved exactly. Nevertheless, certain features of behaviour of an electron in this potential can be discerned from general considerations. In what follows it will be assumed that a logarithmic potential holds for all space.

An electron cannot "fall" onto the chain because the total energy

\[
E = \frac{\hbar^{2}}{2m_{o} r^{2}} + \frac{e}{a} \ln C_{1} r,
\]

(3.14)

for \( r \to 0 \), becomes large and positive. Approaching to the chain, the kinetic energy, (the first term on the right hand side of (3.14)) becomes at one point, \( (r_{\text{min}}) \), larger than the negative potential energy and the electron will be unable to "fall" on the chain. On the other hand, as the distance increases, the potential energy is positive and increases also, diverging at infinity and an electron cannot penetrate this potential wall.
for an infinite distance. At a certain point \( r_{\text{max}} \) the kinetic energy will become negative and an electron will "swing" back toward the chain. Therefore the motion of an electron for a finite total energy is confined within the interval \( (r_{\text{min}}, r_{\text{max}}) \), consequently, this situation corresponds quantum mechanically to discrete bound states. Since the logarithmic potential is a slowly varying function of distance, it will be assumed that the potential is constant. Since the energy \( \Delta \), in (3.13) is negative, the potential is positive in this region due to the choice of gauge, (2.10) and (2.11), and the expression in square brackets (3.13) is always negative. To introduce a short notation the square brackets in (3.13) will be designated as \( \omega_{\Delta}^2 \),

\[
\omega_{\Delta}^2 = \left[ \frac{2m \omega}{\hbar} \left( \frac{e^2}{\alpha n} \left( \frac{2m \omega}{3 \hbar} - \Delta \right) \right) \right].
\] (3.15)

Solutions of (3.13) are then modified Bessel functions \( I_m \) and \( K_m \):

\[
y_{\Delta,m}^{(1)}(r) = K_m(\omega_{\Delta} r), \quad \text{and} \quad m = 0, 1, 2, \ldots
\] (3.16a)

\[
y_{\Delta,m}^{(2)}(r) = I_m(\omega_{\Delta} r),
\] (3.16b)

\( K_m \) tends to zero as \( r \) tends to infinity; therefore it is a proper
solution of the Schrödinger equation (3.5a) for this region.

Now, the reasons for choice of the gauge (2.10) and (2.11) become apparent. By such choice of gauge one insures that the argument in (3.15) is always different from zero in the interval \( \frac{3a}{2} \pi < r < \infty \). If this is not the case the function \( K_m \) will diverge at the point where
\[
\frac{e^{2}}{a} \ln C_{r} = \Lambda.
\]

From the solution (3.16b), \( I_m \) is finite at \( r = 0 \) for \( m = 0, 1, 2, \ldots \).

The Wronskian of the solutions (3.15) is (the derivative of the logarithm has been ignored):
\[
W = I_m K'_m - K_m I'_m = \frac{1}{r}
\]

With the results (3.15a,b) and (3.17) the Green's function (3.6) for region II is:
\[
G_{\Delta, m}^{II}(r, r') = \frac{m}{\hbar} \left\{ \begin{array}{ll}
I_m(\omega_D r) K_m(\omega_D r') & \text{if } r < r' \\
K_m(\omega_D r) I_m(\omega_D r') & \text{if } r < r'
\end{array} \right. \quad (3.18)
\]

C. The secular equation

The functions appearing in (3.2) are now known. The wave function in Region I is given by (3.3a) and (3.9b) while the Green's function for the same region is (3.12). For region II the wave function is (3.3c) and (3.16a) and the corresponding Green's function is (3.18). Substituting the relevant quantities into (3.2a) we find a relation between the coefficients \( C \) and \( A \), when the sums in (3.3) are restricted to positive integers.
Eq. (3.2b) leads to another relation:

\[ C_{\Delta',m} = \frac{m_o}{\pi^2} \Gamma(2m+\alpha-1/2) \frac{W_{\alpha,m}(2k^0 r^\circ)}{\Gamma(2m+1) k^0} r^\circ \partial_r \partial_r \kappa_m (\omega_d r^\circ) \]

(3.19a)

and

\[ -\kappa_m (\omega_d r^\circ) r^\circ \partial_r \partial_r \kappa_m (\omega_d r^\circ) \]

for \( r^\circ = \frac{3}{2} a \)

For fixed \( m \) the last two equations have to be solved self-consistently because \( \Delta, \kappa \) and \( \alpha \) depend on \( \Delta' \) through (3.7b) and (3.8b).

4. The solution along the chain

The linear chain along the z-axis can be regarded as a one-dimensional solid. The unit cell of this solid is the interval \((-a/2, a/2)\). The wave function \( Z \) has to satisfy boundary conditions at the end points of this unit cell:

\[ Z(a/2) = e^{ika} Z(-a/2) \]

(4.1)

and

\[ Z'(a/2) = -e^{ika} Z'(-a/2) \]
The solution of equation (3.1b) with the boundary condition (3.2) can be expressed in terms of the free particle Green's function, which is a solution of:

$$\frac{\partial^2 G(z,z^0)}{\partial z^2} = \delta(z-z^0)$$ \hspace{1cm} (4.2)

and satisfies the following requirements:

(a) symmetry

$$G(z,z^0) = G(z^0,z)$$ \hspace{1cm} (4.3)

and (b) boundary conditions:

$$G(±a,z) = G(z,±a) = 0.$$ \hspace{1cm} (4.4)

The Green's function which satisfies requirements (4.2) to (4.4) has been given in Ref. 16.

In a slightly modified form, it is:

$$G(z,z^0) = \frac{1}{a} \begin{cases} 
(\frac{a}{2} + z)(\frac{a}{2} - z^0) & ; \ z < z^0 \\
(\frac{a}{2} - z)(\frac{a}{2} + z^0) & ; \ z > z^0 
\end{cases}$$ \hspace{1cm} (4.5)

The differential equation (2.17b) can be converted to the integral form which includes the boundary conditions (4.1):

$$z(z) = \frac{2n}{\pi^2 a} \int_{-a/2}^{a/2} G(z,z^0) \left\{ \psi(z,z^0) \right\} dz^0$$ \hspace{1cm} (4.6)

$$-z(-a/2) \frac{dG(-z^0,-z)}{dz^0} \bigg|_{z^0=-a/2} + z(a/2) \frac{dG(z^0,-z)}{dz^0} \bigg|_{z^0=a/2}$$
or explicitly the potential (2.14):

\[
Z(z) = \frac{1}{a} \int_{-a/2}^{+a/2} \left( \frac{a}{2} + z \right) \left( \frac{a}{2} - Z^0 \right) \frac{2m}{\hbar^2} \left[ \frac{e^2}{z} + \frac{4e^2 z^2}{a^3} + \lambda \right] Z(Z^0) dz
\]

\[
+ \left( \frac{a}{2} - z \right) \left( a^2 + z^2 \right) \frac{2m}{\hbar^2} \left[ \frac{e^2}{z} + \frac{4e^2 z^2}{a^3} + \lambda \right] Z(Z^0) dz^0
\]

\[+ Z(-a/2). \left[ Z\left( \frac{a}{2} - z \right) + e^{ika} Z\left( \frac{a}{2} + z \right) \right].
\]

Eq. (4.7) is the formal complete solution for the component \( Z(z) \) along the chain, the \( z \)-axis, of the total wave function \( \Psi(2,16) \).

The boundary condition on the function in (4.1) is automatically satisfied. The condition on the derivatives is also satisfied as can be seen from the following considerations:

The solution of the equation:

\[
\frac{\partial^2 G'(z,z^0)}{\partial z \partial z^0} = \delta(z-z^0),
\]

with the boundary conditions (4.4), is the same as the solution of (4.2); i.e., the solution of (4.8) is given by (4.5); therefore it follows that

\[
G'(z,z^0) = G(z,z^0).
\]

Now, from (4.8) it is easily seen that the boundary condition on the derivatives in (4.1) is also satisfied by the solution (4.7). The value of the function at the boundary, \( Z(a/2) \) is
determined by the normalization condition.

The integral equation for \( z \), (4.7) is of the Fredholm second kind with an asymmetric kernel. Its solution should give \( \lambda \) as a function of \( k \).

A method similar to this one, using a free particle Green's function, has been proposed for more a general lattice by J. Schulman. Since his Green's function contains the summation over all lattice points, the Green's function (4.5), due to its simple form seems more convenient for use in actual calculations.

5. Conclusion

The solution for the linear chain of point charges by the Green's function method is given by Eq. 's (3.4a), (3.19b) and (4.7). It is of twofold interest. Since the solution incorporates a "realistic" logarithmic potential perpendicular to the chain and the Coulomb plus harmonic oscillator potential along the chain, it will be of interest to see the influence on the band structure resulting from such potentials, as compared to the bands calculated by standard methods. On the other hand, the solution will give insight into the scope of the Green's function method for molecules to which it has not been yet widely applied. The method itself is an important tool for calculating the electronic structure of large molecules, because it intrinsically involves splitting a molecule into smaller parts (by boundaries separating regions of different potentials).
Classical considerations.

The Lagrangian of a particle moving in a logarithmic potential (2.7) is:

$$ L = E - V = \frac{p^2}{2m_0} - \frac{e^2}{a} \ln C_1 r. $$

(A.1)

The equations of motion:

$$ \frac{d}{dt} \frac{\partial L}{\partial \dot{p}} = \frac{\partial L}{\partial p}, $$

(A.2)

become in cylindrical coordinates (1.1):

$$ m \ddot{r} + \frac{e^2}{a} \frac{1}{r} = Q $$

(A.3a)

and

$$ m \dot{\theta} = 0. $$

(A.3b)

The solution of (A.3a) is:

$$ r = \frac{1}{aB_1} \text{erf}^2 \left( - \frac{2B_1 e}{2m_0 a} (t + B_2) \right), $$

where $\text{erf}$ means inverse of error function; the latter defined explicitly in Ref. 16; $B_1$ and $B_2$ are constants of integration and $C_1$ has been set to 1.

The $\dot{\theta}$ dependence is obtained by substitution of (A.4) into (A.3b) and integrating over time. Since the error function is not a periodic function of the argument, the orbit defined by (A.3b) will be open.
REFERENCES


9. ibid, eq. 9.521 (1) p. 1087.


13. ibid, Eq. 13.1.3 p. 504; Eq's. 13.5.1, 13.5.2, p. 508.
15. see Ref. 11, p. 374.
17. See Ref. 11, p. 297.
PART THREE

CONTINUOUS GROUPS AND THE COULOMB PROBLEM
Introduction to part three

A. Survey

Group theory is related to the Coulomb problem in various ways:

First, any group of transformations under which the non-relativistic Coulomb Hamiltonian remains invariant is called the symmetry group or the internal symmetry group, and in this case it is the orthogonal group in 4-dimensions, \( O(4)^1 \).

Second, groups called "mathematical groups" are used in a formal way in atomic spectroscopy in order to provide additional quantum numbers to distinguish states within a given configuration\(^2\).

Third, there are groups borrowed from the theory of elementary particles and nuclear physics commonly called "non-invariance", "dynamical" or "spectrum generating" groups. The largest group of this kind is the dynamical group of the Coulomb potential, the non-compact \( O(4,2) \) group\(^3\), or its covering group \( SU(2,2) \). There are several implications generated by these groups in the Coulomb problem; a few, for illustration will be mentioned.

The bound state solutions of the Coulomb Hamiltonian, hydrogenic wave function are bases for a unitary irreducible representation of \( O(4,2) \) group\(^3\). This is true even when the \( O(4,2) \) group is restricted to its subgroup, the de Sitter \( O(4,1) \) group\(^4\). Consequently, the simpler \( O(4,1) \) group...
can be used as the dynamical group for the Coulomb potential.

The other important subgroup of the $O(4,2)$ group is the $O(2,1) \times O(3)$ group which embodies four models for an atom: the Schrödinger, the Klein-Gordon, the Dirac and Biedenharn and the Dirac model. Additionally, Cunningham has shown that any integer power of a radial coordinate is that part of a tensor with respect to the $O(2,1)$ group, which allows calculations of radial integrals between states with the same energy and consequently leads to an explanation of the Pasternak-Sternheimer selection rule.

The same rule has been derived independently by Armstrong, also on the basis of group theoretical arguments but somewhat outside the framework of the $O(4,2)$ group. Armstrong relates only the radial part of the hydrogenic wave function to the basis of a unitary irreducible representation of the $O(2,1)$ group; the results concerning tensorial properties of a power of the radial coordinate and evaluation of the matrix elements are identical to those in Ref. 6.

The method of Armstrong has been extended by Herrick and Sinanoglu to relate the radial part of the hydrogenic wave function to a representation of the larger $O(3,2)$ group. The difficulty in calculating the radial matrix elements of powers of the radial coordinate, encountered in Refs. 5 and 6 has been circumvented. This result is a significant step forward in the group theoretical calculation of radial integrals in atomic spectroscopy. The same authors have shown that the continuum radial wave functions are the basis for a representation of the $O(2,1)$ group and these functions are incorporated.
Barut and Kleinert have found in realizing the $O(4,2)$ group in the 3-dimensional space, that the dipole operator is expressed in terms of the generators of the $O(4,2)$ group; consequently, electromagnetic dipole transitions can be described group theoretically.

The advances mentioned above are not relevant to the studies in this part, but serve to illustrate the richness of the possibilities offered by the application of the theory of continuous groups to problems connected with the Coulomb potential. General discussion of the meaning of, and future use of groups in molecular and atomic physics, together with an extensive bibliography, can be found in Ref. 10.

B. Notation

In this part, the expression "unitary irreducible representation" is shortened to "representation".

The symmetry group of the non-relativistic Coulomb Hamiltonian, $O(4)$, is isomorphic with the group of rotations in 4-dimensional space, $R^4$. The matrices with determinant $+1$ constitute the subgroup of the $O(4)$ group, the $SO(4)$ group, which is isomorphic with the group of proper rotations in 4-dimensional space. Because, in this part, the parity will not be considered the inversion operator is excluded and the $SO(4)$ group is considered to be the symmetry group of the Coulomb Hamiltonian.

The representations of the $SO(4)$ group are labelled with the eigenvalues
of two Casimir invariants $C_1$ and $C_2$. Within a representation there are two ways of labelling the basis states. One way uses the indices of the SO(3) subgroup $(j,m)$. In this case the 6 generators of the SO(4) group form two vectors, the angular momentum vector $\mathbf{L}$ and the Runge-Lenz vector $\mathbf{K}$, which defines the plane of the orbit. The components of the vector $\mathbf{L}$ constitute the generators of the SO(3) group with respect to which $\mathbf{K}$ is a vector. This arrangement corresponds to separating out the Schrödinger equation in the spherical coordinates. It will be referred throughout this part as the $(j,m)$ scheme.

On the other hand, the SO(4) group is isomorphic to SO(3) x SO(3) group. The “magnetic quantum numbers” of the two SO(3) group $m^+$ and $m^-$ are used to label states within a representation of the SO(4) group. The corresponding set of generators is given by two mutually commuting vectors $\mathbf{j}^+$ and $\mathbf{j}^-$. This is the $(m^+,m^-)$ scheme and it corresponds to separating the Schrödinger equation in the parabolic coordinates.

A representation can be labelled with the eigenvalues of these two "angular momentum" operators $\mathbf{j}^+$ and $\mathbf{j}^-$ instead of with the two customary Casimir invariants $C_1$ and $C_2$; these two pairs are linked through:

$$\frac{1}{2}C_1 = \frac{1}{2}(\mathbf{L}^2 + \mathbf{K}^2) = (\mathbf{j}^+)^2 + (\mathbf{j}^-)^2$$

$$\frac{1}{2}C_2 = \mathbf{L} \cdot \mathbf{K} = (\mathbf{j}^+)^2 - (\mathbf{j}^-)^2$$

also

$$\mathbf{L}^2 = \mathbf{J}^2 = j(j+1) + \mathbf{K}^2 = j(j+1)$$
This notation for the SO(4) group is that of Sharp 11.

C. Purpose of the work

As is well known the bound state hydrogenic wave functions belong to the special class of the SO(4) group representations called "square", which are characterized by:

\[ j^+ = j^- = \frac{1}{2} n; \quad c_2 = \hat{L} \cdot \hat{K} = 0 \]

\[ n = 0, 1, 2, \ldots, \]

or in standard notation by \([0, n+1]\); here \(n+1\) is the energy quantum number of the hydrogenic wave function. For a square representation \(\hat{L} \cdot \hat{K} = 0\), i.e. the angular momentum is perpendicular to the plane of the orbit. Indeed, a square representation is the only one possible in a 3-dimensional space; but in the case of atoms with more than one electron, the angular momentum vector, \(\hat{L}\), and Runge-Lenz vector, \(\hat{K}\), of the individual electrons add up independently to form resultants which are not necessarily equal; to characterize such states a general non-square representation of the SO(4) group is needed. 12

Describing an atom in a constant magnetic field also requires a non-square representation, as can be seen from the following considerations: let \(n+1, \ell, m\) be the usual quantum numbers specifying the hydrogenic eigenstates; in free space \(\ell\) is always in the interval \(0 \leq \ell \leq n\), this corresponds to the square representation \(j^+ = j^- = \frac{1}{2} n\) (1.2), if a constant magnetic field is present than \(m < \ell < n\), which means from Eq. (1.2) that

\[ j^+ = \frac{1}{2} (n+m) \quad \text{and} \quad j^- = \frac{1}{2} (n-m) \quad \text{i.e. a non-square representation of the} \]
SO(4) group is involved.

The same conclusion can be reached by considering the change of momentum in a magnetic field. The presence of a magnetic field removes the isotropy of space. The momentum operator, \( \hat{p} \), is replaced by \( \hat{p} \rightarrow \frac{\hbar}{c} \hat{A} \)
where \( \hat{A} \) is a vector potential, consequently \( \hat{L} \cdot \hat{R} \) is no longer necessarily zero, i.e. the angular momentum is not perpendicular to the orbit.

For these two reasons, in Chapter IV, the problem of deriving the general, non-square representations of the \( SO(4) \) group is considered. It turns out that it is possible to construct such non-square representations in the \( SO(4) \) parameter space of 6-Euler angles by specifying the rotations in 4-dimensional space. It is expected that in a later stage of this research these non-square representations will be linked with the physical space and may prove useful in studying the properties of more than one electron atoms and atoms in magnetic fields. In Chapter V, the de Sitter Group, \( SO(4,1) \), is considered. This group can also be used as the dynamical group of the Coulomb problem because when a basis is chosen in which the \( SO(4) \) subgroup is diagonal, two classes of its unitary irreducible representations contain the bound states of the Coulomb potential.

In 3-dimensional coordinate space, these bound states are the solutions of the non-relativistic Coulomb Hamiltonian, namely the hydrogenic wave functions. The solutions of the same Hamiltonian in 3-dimensional momentum space are related to the hyperspherical harmonics in 4-dimensional space through Fock's transformations. These hyperspherical harmonics are basis states for the square representations of the \( SO(4) \) group.
The main concern of Chapter V is to study the relation of the hyperspherical harmonics to the representation of the SO(4,1) group in 4-dimensional space, since the non-compact generators of this group act as ladder operators for \( n \), the energy quantum number, and consequently this representation of the SO(4,1) group has two important applications.

(i) It can be used to study the transformation properties of the radial parts of the hydrogenic wave functions, which are still not fully understood; the radial parts alone cannot be a basis function for a representation of a group because the radial functions are not fully orthogonal; the radial functions have to be multiplied by other mathematical functions, so that total product functions are orthogonal and can be the basis for an irreducible representation of the SO(2,1) group \(^7\) or SO(3,2) group \(^8\).

(ii) The representation is relevant to a group theoretical description of an atom in an external magnetic field, when the SO(4) symmetry is broken. The group which leaves the magnetic quantum number, \( m \), unchanged is the SO(2,1) \( \times \) SO(2) group in the SO(4,1) group framework; if the full dynamical group SO(4,2) is considered, then the required subgroup is SO(2,2) \( \times \) SO(2).

Thus instead of the usual reduction for the field free case, SO(4,1) \( \supset \) SO(4), the reduction SO(4,1) \( \supset \) SO(2,1) \( \times \) SO(2) is more appropriate when a field is applied. The representation of the SO(4,1) group, established in this paper will facilitate this reduction. Interest in (i) and (ii) motivated this research.

As mentioned above, the subgroup of the SO(4,2) group, which leaves the magnetic quantum number, \( m \), unchanged, is the SO(2,2) group. The
generators of the \( \text{SO}(2,2) \) group act as ladder operators on the \( n \) and \( \ell \) quantum numbers and thus the radial part of the hydrogenic wave function is related to a basis for a representation of this group. Because the \( \text{SO}(2,2) \) group can be decomposed into the \( \text{SO}(2,1) \times \text{SO}(2,1) \) group; the representations and other properties of the \( \text{SO}(2,2) \) group are easily derived from those of the \( \text{SO}(2,1) \) group which are known in great detail. Analogously with the \( \text{SO}(4) \) group, the representations of the \( \text{SO}(2,2) \) group considered are those in which the subgroup \( \text{SO}(2,1) \) is diagonal. This type of representation and its relation to the \( \text{SO}(2,1) \times \text{SO}(2,1) \) representations is studied in Chapter VI.
CHAPTER IV

THE NON-SQUARE REPRESENTATIONS OF THE SO(4) GROUP
1. Introduction

The SO(4) group is a group of all real, orthogonal $4 \times 4$ matrices with determinant +1. It is isomorphic with the group of proper rotations in 4-dimensional space. This group is an internal symmetry group of the non-relativistic Coulomb Hamiltonian.

As mentioned above, the hydrogenic wave function transforms according to the square representations of the SO(4) group. (13).

Because of the relevance of the general non-square representations of this group to the description of 'more than one electron' atoms and atoms in magnetic fields, the problem of constructing such general representations will be the main concern of this chapter.

The minimum number of dimensions of space which can carry all irreducible representations of the SO(4) group is 416. This requirement is obviously not satisfied in 3-dimensional "physical" space, nor in 4-dimensional space, where the generators of the SO(4) group induce rotations of the coordinates, since the coordinates are linked through an invariant Hermitian form. This is why only square representations appear in 4-dimensional space.

The parameter space of the SO(4) group consists of the 6 Euler angles specifying a rotation in 4-dimensional space. The number of independent
variables is 5, because the "cosine law" imposes an extra condition on the parameters. Therefore this parameter space is large enough to carry all irreducible representations of the SO(4) group.

Two different parameterizations of the SO(4) group elements are possible. One emphasizes rotations in 3-dimensional "physical" space, as referred to as the \((j,m)\) scheme. The second parameterization uses the fact that the SO(4) group is homomorphic to the SO(3) x SO(3) group. In this case the parameters are two independent sets of SO(3) Euler angles; this parameterization is referred to as the \((m^+, m^-)\) scheme (see IR and Ref. 11).

In Section 2 of this Chapter the connection between the two parameterizations is established and the form of the generators in the \((j,m)\) parameter space is found. In the \((m^+, m^-)\) parameter space the generators are just two commuting sets of SO(3) generators. In part 3 a general rotation matrix is calculated in the \((j,m)\) scheme, any column of which is then a basis state of a general representation of the SO(4) group.

The columns of the rotation matrices are operand states for the generators found in Section 2. In Section 4 several applications of the preceding results are presented; they are (A) an expansion for Gegenbauer polynomials in terms of 3-j symbols (B) the connection between Gegenbauer polynomials and SO(3) reduced rotation matrices (C) an addition theorem for Gegenbauer polynomials and (D) an addition theorem for hyperspherical harmonics.

2. The Generators of the SO(4) Group in the \((j,m)\) Scheme

In the \((j,m)\) scheme, the three components of the vector \(L\) induce rotations in 3-dimensional "physical" space; these three generators form the SO(3) subgroup of the SO(4) group, with respect to which the remaining three generators, \(K\), constitute a vector.
In the \((m^+,m^-)\) scheme, the generators are divided into two mutually commuting vectors \(j^+\) and \(j^-\) which correspond to the \(SO(3) \times SO(3)\) factorization of the \(SO(4)\) group. The two sets of generators are connected by:

\[
\frac{1}{2}(L^+K^-) = j^+ = j^- = \frac{1}{2}(L^+K^-) \quad (2.1)
\]

In this space the 4-coordinate axes are labelled with indices \((1,2,3,\text{ and } 4)\); the metric tensor for the space is

\[
g_{11} = g_{22} = g_{33} = g_{44} = 1, \text{ and zero otherwise.}
\]

The generators \(L_1, L_2\) and \(L_3\) induce rotations in the \((2,3)\), \((3,1)\) and \((1,2)\) planes and the generators \(K_1, K_2\) and \(K_3\) induce rotations in the \((1,4)\), \((2,4)\), and \((3,4)\) planes respectively.

**Connection between the two parametrizations**

There are two different parametrizations of the group elements according to the two schemes. In the \((m^+,m^-)\) scheme, a group element is expressed as a product of two independent rotations, each characterized by a set of \(SO(3)\) Euler angles \((a_1^+, a_2^+, a_3^+)\) and \((a_4^+, a_5^+, a_6^+)\):

\[
g_{j^+}^j((a_1^+, a_2^+, a_3^+)) g_{j^-}^j((a_4^+, a_5^+, a_6^+)) = e^{ia_1^+ J_3^+ e^{i a_2^+ J_2^+ e^{i a_3^+ J_3^+}} e^{i a_4^+ J_3^+ e^{i a_5^+ J_2^+ e^{i a_6^+ J_3^+}}}, \text{ where } i = \sqrt{-1}.
\]

In the \((1,m)\) scheme it is known that a group element can be represented as a product of two \(SO(3)\) rotations in an element of the type \(e^{ia K}\), therefore:

\[
g_{LK}((a_1, \ldots, a_6)) = e^{ia_1 L_3^+ a_2 L_2^+ a_3 L_3^+ a_4 K_3^+ a_5 L_2^+ a_6 L_3}. \quad (2.3)
\]
Using (2.1) to re-express generators $L$ and $K$ in (2.3) in terms of $j^+$ and $j^-$ together with the fact that $j^+$ and $j^-$ commute, the two parametrizations for the same group element are related through the identity:

$$g_{L+K}(a_1, \ldots, a_6) =$$

$$= g_{j^+}((a_1, a_2, a_3)) g_{j^+}((a_4, a_5, a_6)) g_{j^-}((a_1, a_2, a_3)) g_{j^-}((-a_4, a_5, a_6))$$

$$= g_{j^+(a_1^', \ldots, a_6^')}. \tag{2.4}$$

The last line follows from the fact that the products of the elements $g$ belonging to the same subgroup can be expressed as a single subgroup element with new parameters $a'$ which are functions of the original $a$'s. The simplest matrix representation of the rotations in 4-dimensional space (Appendix A, Eq. Al) are used to discern the actual connection, which is:

$$\cos^2 \frac{\alpha_{\frac{1}{2}}}{2} = (\cos \frac{\alpha_{2}}{2} \cos \frac{\alpha_{5}}{2})^2 + (\sin \frac{\alpha_{2}}{2} \sin \frac{\alpha_{5}}{2})^2 - \frac{1}{2} \sin \alpha_2 \sin \alpha_5 \cos (a_3 a_4),$$

or

$$\cos \alpha_{\frac{1}{2}} = \cos \alpha_2 \cos \alpha_5 - \sin \alpha_2 \sin \alpha_5 \cos (a_3 a_4); \tag{2.5}$$

$$\tan \frac{1}{2}(a_{1} + a_{3}') =$$

$$\frac{\cos \frac{\alpha_{2}}{2} \cos \frac{\alpha_{5}}{2} \sin^2 (a_{1} + a_{3} + a_{4} + a_{5}) - \sin \frac{\alpha_{2}}{2} \sin \frac{\alpha_{5}}{2} \sin^2 (a_{1} - a_{3} - a_{4} + a_{6})}{\cos \frac{\alpha_{2}}{2} \sin \frac{\alpha_{5}}{2} \cos^2 (a_{1} + a_{3} + a_{4} + a_{6}) + \sin \frac{\alpha_{2}}{2} \cos \frac{\alpha_{5}}{2} \cos^2 (a_{1} - a_{3} - a_{4} + a_{6})}.$$
\[ \tan \frac{1}{2}(\alpha'_1 - \alpha'_3) = \frac{a'_2 \sin^2 \frac{\alpha'_5}{2} \sin^2 \frac{1}{2}(\alpha_1 + \alpha_3 + \alpha_4 + \alpha_6)}{\cos^2 \frac{\alpha'_2}{2} \sin^2 \frac{1}{2}(\alpha_1 + \alpha_3 + \alpha_4 + \alpha_6) + \sin^2 \frac{\alpha'_2}{2} \cos^2 \frac{1}{2}(\alpha_1 + \alpha_3 + \alpha_4 + \alpha_6)} \]

\[ \cos \frac{\alpha'_5}{2} = \frac{a'_2 \cos^2 \frac{\alpha'_5}{2} + (\sin^2 \frac{\alpha'_2}{2} \sin^2 \frac{\alpha'_5}{2}) - \frac{1}{2} s_{\alpha_2} s_{\alpha_5} \cos(\alpha_3 - \alpha_4)}{2} \]

or

\[ \cos \alpha'_5 = \cos \alpha'_2 \cos \alpha'_5 - \sin \alpha_2 \sin \alpha_5 \cos(\alpha_3 - \alpha_4); \]

Equations (2.5) and (2.6) are the same except for the sign of \( \alpha_4 \), in consequence of the fact that an SO(4) rotation in the \((m^+, m^-)\) scheme can be decomposed into two SO(3) rotations, equal in magnitude, in the two mutually perpendicular planes.

The Equations (7.5) and (2.6) also represent a general connection between the parameters of the product of the two SO(3) group elements. The parameters of the resulting element are on the left.
hand side of (2.6) or (2.7), the parameters of the factors are \((a_1, a_2, a_3)\) and \((a_4, a_5, a_6)\), in, for example, (2.5).

**6. Realization of the Generators in the Parameter Space**

In the \((m^+, m^-)\) scheme, the generators assume the form of two sets of \(SO(3)\) generators with corresponding variables \((a_1, a_2, a_3)\) and \((a_4, a_5, a_6)\) as given for example in Ref. 17. The generators in the \((j, m)\) scheme can be obtained by the well-known method of mapping a group into itself by multiplication of group elements with an infinitesimal group element. This method is illustrated for \(SO(3)\) in Ref. 18 and applied to non-compact groups in Refs. 16 and 19. The method requires the explicit form of the general matrix of rotation in 4-dimensional space. This matrix is formed according to (2.3) from the matrices of rotations around 4-coordinate axes (Appendix A.1). By employing "left" multiplication the following result, expressed in terms of 'ladder' operators \(L_+ = L_1 + L_2\) and \(K_+ = K_1 + K_2\), is obtained:

\[
L_+ = e^{+i\alpha_6} \left\{ -i \alpha_3 + \sin \alpha_5 \alpha_5 + i \cos \alpha_5 \alpha_6 \right\};
\]

\[
L_3 = -i \alpha_6;
\]
\[
k_2 = \frac{\cota_2}{\sin a_4} \left( \cota_2 (\cos^2 a_5 e^{i a_3} + \sin^2 a_5 e^{i a_3}) a_1 + \right.
\]
\[
+ i (\cos^2 a_5 e^{i a_3} - \sin^2 a_5 e^{-i a_3}) a_2,
\]
\[
\left. + (\cos^2 a_5 e^{i a_3} + \sin^2 a_5 e^{-i a_3}) \cota_2 \cos a_4 \cota_5 a_3 \right)
\]
\[
- \sin a_4 \sin a_5 a_4 - \cos a_4 \cos a_5 a_5 + \frac{\cos a_4 a_5}{\sin a_5 a_6} \right)\]

\[
k_3 = -\frac{1}{\sin a_4} \left( \sin a_3 \sin a_5 a_1 + \cos a_3 \sin a_5 a_2 + \right.
\]
\[
- \cota_2 \sin a_3 \sin a_5 a_3 + \cos a_5 \sin a_4 a_4 - \cos a_4 \sin a_5 a_6 \right)
\]

The second Casimir invariant \(C_2\) with these generators, is different from zero, therefore they correspond to non-square representations of the \(SO(4)\) group. Direct commutation verifies the commutation law.

3. The rotation matrices of the \(SO(4)\) group

A basis state for an irreducible representation of the \(SO(4)\) group in the \((j,m)\) scheme can be any column of a rotation matrix. The generators which act on such a basis state are given by (2.7). To find the rotation matrices, the matrices of group elements depending on one parameter will be calculated initially in the \((j,m)\) scheme. These matrices would be required in decompositions of a general group element which are not the decompositions.
of (2.2) or (2.3); for example in Ref. 20, the decomposition of a group element involves $K_2$, and the form of the generators is simpler than using (2.3) which involves $K_3$, but the rotation matrices are more complicated than in the decomposition involving $K_3$.

The matrix elements of the group elements in the $(m^+, m^-)$ scheme are just the product of two SO(3) rotation matrices. In the $(j, m)$ scheme the matrix elements of the group elements depending on the components of the L vector are, by definition, the SO(3) rotation matrices, $\exp[i\alpha_1]$ and $\exp[i\alpha_2]$ can be decomposed as follows:

$$\begin{align*}
\{\alpha_1\} &= e^{i\pi L_3} - i\alpha_3 e^{i\pi L_2} \quad \text{and} \\
\{\alpha_2\} &= e^{i\pi L_3} - i\alpha_3 e^{i\pi L_2}
\end{align*}$$

(3.1)

the only matrix element to be calculated is of the type:

$$\langle j^+ | i\alpha_3 | j^- \rangle,$$

(3.2)

where $j^+$ and $j^-$ are related to the two Casimir invariants of the SO(4) group (1.1) and the $a, m$ are the familiar SO(3) group indices.
It is advantageous to find the element in the \((m^+, m^-)\) scheme first and to transform the result back into the basis of the \((j, m)\) scheme.

Consequently from (2.1):

\[
\begin{align*}
\langle j^+ | j^- | e \rangle & = \langle j^+ | j^- | e \rangle_{a} \\
\langle m^+_a m^-_a | m^+_b m^-_b \rangle & = \delta_{m^+_a m^+_b} \delta_{m^-_a m^-_b} - e^{i \alpha(m^+_a - m^-_a)} \\
& = \delta_{m^+_a m^+_b} \delta_{m^-_a m^-_b} - e^{i \alpha}\ . \\
\end{align*}
\]

with \(-j^+ \leq m^- \leq j^+\).

The states of the \((m^+, m^-)\) scheme can be expressed in terms of those of the \((j, m)\) scheme using the Clebsch-Gordan coefficients:

\[
\begin{align*}
| j^+ j^- m \rangle & = \Sigma_{m^+} \langle j^+ j^- m^+ | j^+ j^- m^- \rangle | j^+ j^- m^+ \rangle \\
& = \langle j^+ j^- m^+ | e \rangle | j^+ j^- m^- \rangle \\
& = \delta_{m^+_a m^+_b} \delta_{m^-_a m^-_b} - e^{i \alpha}\ . \\
\end{align*}
\]

The matrix element is obtained by substituting expansion (3.4) into (3.2) and using the result of (3.3):

\[
\begin{align*}
\langle j^+ j^- | e \rangle & = \langle j^+ j^- | e \rangle_{a} \\
\langle j^+_a m^+_a | j^-_b m^-_b \rangle & = \delta_{m^+_a m^+_b} \delta_{m^-_a m^-_b} - e^{i \alpha}\ . \\
\end{align*}
\]

Because:

\[
m = m^+ + m^- \text{ or } m^+ - m^- = m^+ - m^- = m^+ - 2m^+ .
\]
the matrix element (3.5) assumes the following form, in terms of Wigner 3-j symbols:

\[
\begin{align*}
\langle j^+ j^- | e^{i\theta} | j_a j_b m \rangle &= [(2j_a + 1)(2j_b + 1)]^{1/2} x \\
&\times e^{-i\lambda m + i\lambda m} \left( j^+ j^- j_a \right) \left( j^+ j^- j_b \right)
\end{align*}
\]

The Kronecker delta in (3.5) ensures that only a single \( m \) enters (3.6) and the subscripts are therefore dropped.

The same matrix elements have been calculated by Biedenharn and Talman\(^{20}\) and in Ref. 1, Appendix, but this derivation is somewhat clearer and includes more general matrix elements.

The general rotation matrix in the \((j,m)\) scheme is obtained by taking matrix elements of the expression (2.3):

\[
\begin{align*}
\langle j^+ j^- | g_{LK}(\alpha_1, \ldots, \alpha_6) | j^+ j^- \rangle &= D_{j_b j_a \alpha_1 \alpha_2 \alpha_3 \alpha_4 \alpha_5 \alpha_6} (j_a j_b m_a m_b) \\
&= [(2j_b + 1)(2j_a + 1)]^{1/2} x \\
&\times \Sigma_m e^{-2i\theta m} \left( j^+ j^- j_b \right) \left( j^+ j^- j_a \right)
\end{align*}
\]

where \( D \) is introduced as a convenient shorthand for the matrix element, and \( d \) is an \( SO(3) \) reduced rotation matrix.

For fixed \( j_b \) and \( \bar{m}_b \), the matrix element (3.7) is a basis
state for a general irreducible representation of the SO(4) group, with the generators in the form of (2.7). The 'left' subscripts have to be fixed due to the derivation of the generators by left multiplication. For \( j_b = m_b = 0 \) the only representation possible is a square one with \( j^+ = j^- \).

To be consistent with the positive exponent in the definition of the group elements (2.3), the reduced rotation matrices in (3.7) are those defined in Ref. 21.

The norm of the rotation matrices (3.7) is most easily found by considering the invariant integral \( I \) in the group space:

\[
I = \int f(g) dg. \tag{3.8}
\]

From (2.4) and (2.5) it is evident that the integral (3.8) in the \((j,m)\) parameter space remains the same as in the \((m^+,m^-)\) space because the parameters in the \((m^+,m^-)\) scheme can be expressed as those in the \((j,m)\) scheme which are a product of two SO(3) rotations, (2.6) and the associated following comment. Moreover, an adjustment for the range of parameters has to be made: in the \((m^+,m^-)\) parameter space the range is \(0 < a_4 < \pi\). The weight functions in the two space are:

\[
d\nu_{j^+j^-} = \sin a_1 \sin a_5 da_1 \cdots da_6 \quad \text{and} \quad d\nu_{L_4} = \sin^2 a_4 \sin a_5 da_1 \cdots da_6. \tag{3.9}
\]

The value of the integral (3.8) is then for \(1/4\) less in \((j,m)\) parameter space than in \((m^+,m^-)\) parameter space.

In the \((m^+,m^-)\) scheme, the rotation matrices are just the product of two SO(3) matrices. The orthogonality is then given by:
the rotation matrices and the Gegenbauer polynomials

The relation of the rotation matrices given by (3.7) to the basis functions for a square representation of the $SO(4)$ group, which are hyperspherical harmonics, will be considered first.

The rotation matrices transform a basis function from point $(\bar{x}_1, \ldots, \bar{x}_4)$ to the point $(x_1, \ldots, x_4)$, which is specified by six Euler angles of rotation $(\alpha_1, \ldots, \alpha_6)$ in the polar spherical coordinate system, appropriate for the $(j, m)$ scheme:

\begin{equation}
\begin{split}
J^+ (\alpha_1, \alpha_2, \alpha_3) D (\alpha_4, \alpha_5, \alpha_6) \times \\
J^- \frac{2(2n)^4}{(2j_+^a + 1)(2j^-_a + 1)}
\end{split}
\end{equation}

Consequently, in the $(j, m)$ scheme the orthogonality relation is:

\begin{equation}
\begin{split}
\langle j_1^a \mid j_2^b \rangle \left( \sum_{a=1}^{b} \sum_{m} \sum_{l} \sum_{k} \delta_{j_1^a} \delta_{j_2^b} \delta_{j_1} \delta_{j_2} \delta_{m} \delta_{m} \pi(2n)^3 \right) \frac{2^2}{(2j_+^a + 1)(2j^-_a + 1)}
\end{split}
\end{equation}

4. Some applications
The basis functions are the hyperspherical harmonics \( Y \) as defined by Sharp\(^{11} \) with the additional phase factor \((-1)\), which is the factor of proportionality between the functions and the rotation matrices.

For \( j^+ = j^- = (\frac{1}{2})n_j \)

the connection between the hyperspherical harmonics and the SO(4) rotation matrices (3.7) is \(^{22} \)

\[
\mathbf{\mathbf{y}}^n_{l_m}(x_1, \theta, \phi) = \sum_{l', m'} D_{l, m, l', m'}(\sigma_1, \ldots, \sigma_6) \mathbf{\mathbf{y}}^n_{l', m'}(\overline{x}, \overline{\theta}, \overline{\phi}),
\]

where since \( j \) is always an integer in a square representation it is replaced by \( l \).

At the point on the 4th axis where

\( x = \theta = \phi = 0; \) then \( x_1 = x_2 = x_3 = 0 \) and \( x_4 = \rho \),

and the hyperspherical harmonics have the value,

\[
\mathbf{\mathbf{y}}^n_{l_m}(0, 0, 0) = \delta_{l, 0} \delta_{m, 0} \frac{1}{\sqrt{2}} \pi^{(n+1)}.
\]

The point specified in (4.3) is transformed by \( R^{-1} \), where \( R \) is a general rotation (2.3) formed from the matrices of rotation around the 4-coordinate axis (Appendix A) into the
point with coordinates given by (4.1). The Euler and the polar angles are related by,

\[ \alpha_4 = -x; \quad \alpha_5 = 0; \quad \alpha_6 = \phi, \]

and \( \alpha_1, \alpha_2, \alpha_3 \) being arbitrary (4.5).

Therefore the basis functions, the hyperspherical harmonics, do not depend on \( \alpha_1, \alpha_2, \) and \( \alpha_3 \). By omitting derivatives with respect to these variables, and using the relations, (4.5), the generators given by (2.8) reduce to their standard form in the \((j, m)\) scheme in 4-dimensional spherical coordinates, (4.1). Then, with (4.3) and (4.4), equation (4.2) provides a link between the rotation matrix elements and the hyperspherical harmonics:

\[
\sum_{\ell=0}^{n} \sum_{m=-\ell}^{\ell} \psi_{\ell m}(x, \theta, \phi) = \left[ \frac{2^{2\ell+1}(n-\ell)!}{n!(n+\ell+1)!} \right]^{1/2} \left[ \frac{\ell!(\ell+1)!}{(2\ell+1)!} \right] (-i sin \theta)^{\ell+1} \cos \theta \]

\[
\times \sum_{\ell=0}^{n} \sum_{m=-\ell}^{\ell} 
\left[ \frac{2^{2\ell+1}(n-\ell)!}{n!(n+\ell+1)!} \right]^{1/2} \left[ \frac{\ell!(\ell+1)!}{(2\ell+1)!} \right] (-1)^{m} \frac{m}{\ell} (\cos \theta) \]

\[
\times \sum_{p=0}^{\ell} (-1)^{m-p} 2^{n-m-2i\chi m} \left( \begin{array}{c} \ell+1 \\ m-p \end{array} \right) \left( \begin{array}{c} \ell+1 \\ m \end{array} \right) \left( \begin{array}{c} \ell+1 \\ 0 \end{array} \right)
\]

where the \( \psi_{\ell m} \) are Gegenbauer polynomials and the \( \chi \) are associated Legendre polynomials, and \( m \) and \( \ell \) are integers.
By comparing the two sides of (4.6) a new relation for the Gegenbauer polynomials is obtained,

\[ 2^\ell \ell! \left[ \frac{(n-\ell)!}{(n+\ell)!} \right] \frac{1}{2} (\ell+1)! C_{n-\ell}^{\ell+1}(\cos \chi) = \]

\[ = \ell + (-1)^{\ell-n-m} e^{2i\chi m+} \begin{pmatrix} \ell \frac{1}{2} \frac{1}{2} n \frac{1}{2} \ell \\
 m+ m- 0 \end{pmatrix} \]

(4.7)

For some special values of \( \ell \) the last equality reduces to an expansion of the trigonometric functions in terms of Wigner 3-j symbols: for \( \ell = n \)

\[ \sin^n \chi = \frac{\sqrt{(2n+1)!}}{(-1)^n 2^n n!} \sum_{m=1}^{n+1} (-1)^m e^{-2i\chi m+} \begin{pmatrix} \ell \frac{1}{2} \frac{1}{2} n \frac{1}{2} \ell \\
 m+ m- 0 \end{pmatrix} = \]

(4.8)

B. Gegenbauer polynomials and SO(3) reduced rotation matrices

Considering only the square representation of (3.7) another relation for the Gegenbauer polynomials, involving reduced SO(3) matrices, can be derived. The rotation matrix of \( \exp(i\chi \hat{K}_2) \) is calculated in two ways: the first uses the factorization (3.1) and calculates the matrix elements by (3.7), in the second, the matrix element is calculated by following the procedure for calculating the matrix elements of \( \exp(i\chi \hat{K}_3) \), namely (3.3) through (3.6). Comparing the two results gives,
The closure relation for reduced $SO(3)$ matrices\textsuperscript{21} is used to sum up the right hand side of (4.9). The left hand side is calculated from (4.7). Thus (4.9) becomes:

\begin{equation}
(4.10)
\end{equation}

The last equality holds only for $\ell + m = 2$ even, otherwise it reduces to zero.

C. An addition theorem for Gegenbauer polynomials

An addition theorem for Gegenbauer polynomials is obtained from the general formula for multiplication of two $SO(4)$ rotation matrices, namely

\begin{equation}
(4.11)
\end{equation}
for the case for which:

\[ j^+ = j^- = \frac{1}{2} \text{,} \quad j_\text{b} = m_\text{b} = 0; \]
\[ a_1 = a_2 = a_3 = a_5 = a_6 = 0; \quad a_1'' = a_2'' = a_3'' = a_5'' = a_6'' = 0; \]
\[ a_4' = x_1 \quad \text{and} \quad a_4'' = x_2' \]

then

\[ a_1 = a_2 = a_3 = a_5 = a_6 = 0; \]
\[ a_4 = x_1 + x_2' \]

and (4.11) becomes after setting \( j = L \), the addition theorem for Gegenbauer polynomials, (4.12):

\[
(1)^{\ell_1 \ell_2 \ell_3} \left[ \frac{(n-\ell)!}{(n+\ell+1)!} \right] \frac{1}{2} \left[ \sin(x_1 + x_2) \right]^{\ell_1 + 1} \left[ \cos(x_1 + x_2) \right]^{\ell_2 + 1} \]
\[ = \sum_{k_1} (i)^{\ell_1} (2)_{\ell_2} (2)_{\ell_3} \left[ \frac{(2^{\ell_1}+1)(\text{parity})}{(n^2 + 1)(\text{parity})} \right]^{\frac{1}{2}} \left[ \sin x_1 \right]^{\ell_1} \left[ \cos x_1 \right]^{\ell_2 + 1} \left[ \cos x_1 \right] \times \]
\[ \sum_{m'} \left( \frac{2n}{2n} \frac{1}{2n} \right)^{\ell_1} \left( \frac{1}{2n} \frac{1}{2n} \right)^{\ell_2} \left( \frac{1}{2n} \frac{1}{2n} \right)^{\ell_3} \]

The standard addition theorem cannot be derived from the SO(4) group framework since its derivation requires a change in the number of dimensions of the space.

D. An addition theorem for the hyperspherical harmonics

By applying the rotation \( \exp(i \chi K_3) \) to the hyperspherical harmonics (4.5) a more general addition theorem is obtained.
\[ \psi_{nlm}^n(x, \theta, \phi) = \sum_{l} \mathcal{Y}_{lm}^{(2l+1)(2l'+1)} e^{i x^m} \times \]
\[ \left\{ \Gamma_{m+} e^{2i x^m} \left( \frac{1}{2} n + \frac{1}{2} l \right) \left( \frac{1}{2} n - m \right) \right\} \mathcal{Y}_{lm}^{n}(x', \theta', \phi') \] (4.13)

where the coordinates are related by,
\[
\cos x = \sin x \sin x' \cos \theta + \cos x \sin x' \\
\cos \theta = \frac{\sin x' \cos \theta - \cos x' \sin x}{\sin x}
\] and \( \phi = \phi' \).

The special case of (4.14) for \( \theta = 0 \) is (4.12), with \( x' = x_1 \)
and \( x' = -x_2 \).

5. Conclusion

Even though the results of this work are mostly applied mathematical ones, the original motivation of the author for it was an interest in extending the theory of the \( SO(4) \) group representations to allow calculation of 'non-square' wave functions for atoms with more than one electron, in a later stage of the research. These functions, in a sense, incorporate the effect of electron-electron interactions and would also be a suitable choice for describing an atom in a magnetic field, Section 1C.
CHAPTER V

THE REPRESENTATION OF THE SO(\(4,1\)) GROUP IN 4 - DIMENSIONAL EUCLIDIAN AND SPINOR SPACE
1: Introduction

A. Preliminaries

The unitary irreducible representations of the SO(4,1) group were derived by Thomas. The representations are labelled by two invariants (p,q) which are related to the Casimir Invariants (Q,W). Thomas also calculated the matrix elements of the generators. The list of representations was later corrected by Newton who labelled the representations with (Q,W). Additional representations have been added by Dixmier.

The square representations of the SO(4) group are contained in two unitary irreducible representations of the SO(4,1) group, Table 1. The minimum number of dimensions of space to carry all irreducible representations of the SO(4,1) group and SO(4) groups are six and four respectively. Therefore a representation of SO(4,1) in 4-dimensional space is admissible only if both Casimir invariants are specified; 4-dimensional space has only three independent dimensions with respect to the SO(4) group, since the 4-coordinates are linked through an invariant Hermitian form, and consequently one Casimir invariant has to be specified; this is usually the second invariant, q or W, and is set to zero. Therefore only square representations occur.

There are two ways to label basis states in an irreducible representation of the SO(4) group; each corresponds to a different linear combination of the generators. One uses the homomorphism of the SO(4) group to the group SO(2) x SO(2): the basis states and relevant set of generators are then in the (j,m) scheme, Both schemes are used.
## COMPARISON OF THE NOTATIONS FOR TWO CLASSES OF THE SO(4,1) GROUP REPRESENTATIONS

<table>
<thead>
<tr>
<th>Representation</th>
<th>THOMAS</th>
<th>NEWTON</th>
<th>SO(4) CONTENT</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>q=0</td>
<td>class I</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>-\frac{1}{2} &lt; p &lt; 1</td>
<td>W=0</td>
<td>n &gt; 0</td>
</tr>
<tr>
<td></td>
<td>p+\frac{1}{2} = i\sigma</td>
<td>0 &lt; Q &lt; \frac{9}{4}</td>
<td></td>
</tr>
<tr>
<td></td>
<td>\sigma \text{ real}</td>
<td>\frac{9}{4} \leq Q &lt; \infty</td>
<td></td>
</tr>
<tr>
<td></td>
<td>q=0</td>
<td>class II</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>W=0</td>
<td>n &gt; s</td>
<td></td>
</tr>
<tr>
<td></td>
<td>p=s</td>
<td>Q=-(s-1)(s+2)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>s=1,2,3,...</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Table 1.

The eigenvalue spectra of the two Casimir invariants for two classes of the SO(4,1) group representations relevant to the Coulomb problem, are shown in the notations of Thomas and Newton. Representation "1" contains all bound states; representation "2" contains only states for n > s.
B. Methods and results

The basis for the square representations of the SO(4) group in 3-dimensional space are hydrogenic wavefunctions; in addition there are two other bases for both SO(4) schemes: one in spinor space and one in 4-dimensional Euclidean space. The notation is established in Section 2. The matrix elements of the generators of Thomas, which are in the \( (m^+, m^-) \) scheme, are reformulated in terms of their tensor properties and then are reformulated in the \( (j, m) \) scheme, (Section 3).

In 3-dimensional space the representation of the SO(4) group generators has been found in spherical coordinates, the \( (j, m) \) scheme, and in parabolic coordinates, the \( (m^+, m^-) \) scheme.

The spinor space and 4-dimensional space are explicitly connected through a linear transformation of the variables. In addition to the already known compact generators of the SO(4,1) group, the relative simplicity of spinor space permits 4-noncompact SO(4,1) group generators to be constructed. These generators together form a representation of the SO(4,1) group in spinor space. The basis states in this spinor space transform according to representation 1 of Table 1, with

\[ q = 0 \text{ and } p = 0, \]

or

\[ W = 0 \text{ and } Q = 2. \quad (1.1) \]

These basis states and generators will be transformed into 4-dimensional
Euclidean space, when the states become hyperspherical harmonics in the
\((j,m)\) scheme, and functions related to the \(SO(3)\) reduced rotational matrices
in the \((m^+,m^-)\) scheme. The transformed states are the bases for the square
representation of the \(SO(4)\) group in 4-dimensional space. The transformation
properties (1.1) remain the same. The non-compact \(SO(4,1)\) group generators
assume comparatively simple forms. A similar but different method of using
spinor space has been employed to study certain representations of the Lorenz
group and the \(U(2,2)\) group.

This representation, with the matrix elements of the \(SO(4,1)\) group
generators from Section 3, permit derivation of the set of standard recursion
relations for the Legendre and Gegenbauer polynomials and a set of new re-
cursion relations for the \(SO(3)\) reduced rotation matrices, and prove the
validity of (1.1) and of the representation of the \(SO(4,1)\) group based on
(1.1), Section 4.

C. Remarks

While preparing the manuscript, our attention was drawn to the paper
of Han, where the representation of the \(SO(4,1)\) group generators in 4-
dimensional space is found which corresponds to the representation 1 in
Table 1 with

\[
q = 0 \quad \text{and} \quad p = -1/2,
\]
or
\[
W = 0 \quad \text{and} \quad Q = 9/4,
\]

(1.2)

which differs from the representation in the present work which uses (1.1).
With Han's generators, the hyperspherical harmonics in both the $(j,m)$ and $(m^+,m^-)$ schemes do not transform correctly, but their linear combination should. This further indicates that the choice of (1.1) for the values of the $SO(4,1)$ group Casimir invariants is natural for the hyperspherical harmonics and consequently for the hydrogenic wavefunctions. The relation between Han's generators and the ones used herein, is given in Appendix B.

The content of this Chapter, without significant changes, has been published.

2. The generators of the $SO(4,1)$ group

As an attempt to promote a unified notation for continuous groups, the notation for the $O(4,2)$ group has been truncated to give the notation for the $SO(4,1)$ group. The compact axes are labelled 1, 2, 3 and 5, and the non-compact axis is labelled 0.

The generators of the $SO(4,1)$ group commute between themselves

$$[L_{jk}, L_{ks}] = i(g_{jl} L_{ks} - g_{js} L_{ks} - g_{kl} L_{js} + g_{ks} L_{jl})$$

where $i = \sqrt{-1}$

$j, k, l, s = 0, 1, 2, \ldots, 5$

$g_{11} = g_{22} = g_{33} = g_{55} = 1$

$g_{00} = -1$ (2.1)

and zero otherwise.

The compact generators can be represented by

$$L_{lj} = -i(x_j x_l + x_l x_j)$$

with $l, j = 1, 2, 3$ or 5. (2.2)
and the non-compact generators by

\[ L_0 = x_0^2 \partial + x_j^3 x_j, \]

where

\[ x_0 = i x_0^1 \text{ and } x_0^1 \text{ is a real variable.} \]  

(2.3)

A. The generators for the \((n^+, n^-)\) scheme

In the \((n^+, n^-)\) scheme the generators are given by

\[
\begin{align*}
    j^+_1 &= \frac{1}{2} \left( (L_{23} + iL_{31}) + (L_{15} + iL_{25}) \right) ; \\
    j^+_2 &= \frac{1}{2} \left( (L_{15} + iL_{25}) \right) ; \\
    j^+_3 &= \frac{1}{2} \left( (L_{12} + L_{35}) \right) ; \\
    j^-_0 &= \frac{1}{2} \left( (L_{03} + iL_{05}) \right) ; \\
    S^+_2 &= \frac{1}{2} \left( (L_{01} + iL_{02}) \right) .
\end{align*}
\]  

(2.4)

The \((j^+_1, j^-_0)\) and \((j^+_2, j^-_3)\) generate two mutually commuting \(SO(3)\) subgroups with respect to which \(P_\pm\) and \(S_\pm\) transform like \(\frac{1}{2}\) tensors; namely:

\[
\begin{align*}
    [j^+_1, S_-] &= P_+ ; & [j^+_1, P_-] &= S_+ ; \\
    [j^-_0, P_+] &= S_- ; & [j^-_0, S_+] &= P_- ; \\
    [j^+_2, S_\pm] &= \mp \frac{1}{2} S_\pm ; & [j^+_2, P_\pm] &= \mp \frac{1}{2} P_\pm ; \\
    [j^+_3, S_-] &= P_+ ; & [j^+_3, P_-] &= S_+ ; \\
    [j^-_3, P_+] &= S_- ; & [j^-_3, S_+] &= P_- ; \\
    [j^-_0, S_\pm] &= \mp \frac{1}{2} S_\pm ; & [j^-_0, P_\pm] &= \mp \frac{1}{2} P_\pm ; \\
    [j^-_2, P_+] &= [j^-_2, S_-] = [j^-_2, S_+] = [j^-_2, P_-] = 0 .
\end{align*}
\]  

(2.5)
For these commutation relations it is seen that the pairs \((P_+, S_-)\) and \((S_+, P_-)\) form the 1/2 and -1/2 components of a 1/2 tensor with respect to the \(j^+\) subgroup, and that the pairs \((P_-, S_-)\) and \((S_+, P_+)\) form the 1/2 and -1/2 components of a 1/2 tensor with respect to the \(j^-\) subgroup.

**B. The generators for \((j, m)\) scheme**

In the \((j, m)\) scheme the generators assume the standard form,

\[
L_+ = L_{23} + i L_{31} \quad L_0 = L_{12}.
\]

\[
K_+ = L_{15} + i L_{25} \quad K_0 = L_{35}.
\]

\[
L_{03} = \frac{1}{\sqrt{2}} (P_+ - P_-);
\]

\[
iL_{05} = \frac{1}{2} (P_+ - P_-);
\]

and

\[
S_+.
\]

The \(L_+, L_, \) and \(L_0\) are generators of the \(SO(3)\) subgroup with respect to which the generators \(K_+, K_-\) and \(K_0\) form a vector, the non-compact generators \(S_+, S_-\) and \(L_{03}\) form a spherical vector and \(L_{05}\) is a scalar.

**3. The matrix elements of the generators**

**A. The matrix elements in the \((j^+, -)\) scheme**

The matrix elements of the generators have been calculated by Thomas in the \((m^+, m^-)\) scheme for the whole range of eigenvalues of two Casimir operators for unitary representations of the \(SO(4,1)\) group.
To make the notation consistent with the tensor properties of $P_\pm$ and $S_\pm$, and for future reference, the matrix elements are reformulated as:

\[
\begin{align*}
\langle j_b^- j_b^- | P_\pm | j_a^+ j_a^- \rangle &= \\
\langle j_a^+ j_b^- \rangle \langle j_b^- j_a^- \rangle \langle j_a^+ j_b^- \rangle \langle j_b^- j_a^- \rangle \langle j_b^+ j_b^- | P_\pm | j_a^+ j_a^- \rangle
\end{align*}
\]

(3.1)

Similarly for $P_\pm$,

\[
\begin{align*}
\langle j_b^+ j_b^- | S_\pm | j_a^+ j_a^- \rangle &= \\
\langle j_a^+ j_b^- \rangle \langle j_b^- j_a^- \rangle \langle j_a^+ j_b^- \rangle \langle j_b^- j_a^- \rangle \langle j_b^+ j_b^- | S_\pm | j_a^+ j_a^- \rangle
\end{align*}
\]

(3.2)
The \( g \) and \( q \) are the eigenvalues of two Casimir invariants which specify an irreducible representation of the \( SL(4,1) \) group and \( \langle \cdot | \cdot \rangle \) are Clebsh-Gordan coefficients and \( \langle \cdot | \cdot \cdot | \cdot \rangle \) are reduced matrix elements. The matrix elements are different from zero only in four cases:

\[
\begin{align*}
\pm \frac{3}{2} & \quad \text{and} \quad \pm \frac{1}{2} \\
& \quad \text{and} \quad \pm \frac{1}{2}
\end{align*}
\] (3.3)

### B. The reduced matrix elements

For these non-zero cases in the Clebsh-Gordan coefficients, the reduced matrix elements are:

\[
\begin{align*}
\langle j^+ j^- | p | \langle j^+ j^- | pq \rangle 
& = \langle j^+ j^- | p | \langle j^+ j^- | pq \rangle \\
& = \frac{(j^+ j^- p + 1) (j^+ j^- q + 2)}{2 (2j^+2)(2j^-2)} \\
\langle j^+ j^- | j^+ j^- | p | \langle j^+ j^- \rangle 
& = \langle j^+ j^- | j^+ j^- | p | \langle j^+ j^- \rangle \\
& = \frac{(j^+ j^- - q - 1) (j^+ j^- q + 1)}{2 (2j^+2)(2j^-2)} \\
\langle j^+ j^- | j^+ j^- | p | \langle j^+ j^- \rangle 
& = \langle j^+ j^- | j^+ j^- | p | \langle j^+ j^- \rangle \\
& = \frac{(j^- j^- - q - 1) (j^- j^- q + 1)}{2 (2j^-2)} \\
\langle j^+ j^- | j^+ j^- | p | \langle j^+ j^- \rangle 
& = \langle j^+ j^- | j^+ j^- | p | \langle j^+ j^- \rangle \\
& = \frac{(j^- j^- - p - 1) (j^- j^- q + 1)}{2 (2j^-2)} \\
\langle j^+ j^- | j^+ j^- | p | \langle j^+ j^- \rangle 
& = \langle j^+ j^- | j^+ j^- | p | \langle j^+ j^- \rangle \\
& = \frac{(j^- j^- - p - 1) (j^- j^- q + 1)}{2 (2j^-2)}
\end{align*}
\]
Because the representations are unitary, the generators \( L_{ij} \) are Hermitian, therefore \( P_+ \) and \( P_- \) are Hermitian conjugates of each other, and \( S_+ \) and \( S_- \) are an anti-Hermitian conjugate pair.

C. The matrix elements in the \((l,m)\) scheme

In the \((j,m)\) scheme, the reduced matrix elements (3.4) are unchanged. Applying then the Wigner-Eckart theorem to the tensors (2.6), the matrix elements are:

\[
\begin{align*}
\langle j_b^+ j_b^- | S_\pm | j_a^+ j_a^- \rangle &= \langle \frac{1}{2} \pm \frac{1}{2} | \frac{1}{2} \pm \frac{1}{2} \rangle \\
\times [3(2j_a+1)(2j_b+1)(2j^-+1)]^{\frac{1}{2}} &\langle j_a \frac{1}{2} | j_b \frac{1}{2} \rangle \begin{pmatrix} j_b & j_a \\
\frac{1}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} j_b & j_a \\
\frac{1}{2} & \frac{1}{2} \end{pmatrix} \times \\
\langle j_b^+ j_b^- | L_{03} | j_a^+ j_a^- \rangle &= E_{m_a^b} \sqrt{2} \langle j_a \frac{1}{2} | j_b \frac{1}{2} \rangle \\
\times [3(2j_a+1)(2j_b+1)(2j^-+1)]^{\frac{1}{2}} &\langle j_b \frac{1}{2} | j_a \frac{1}{2} \rangle \begin{pmatrix} j_b & j_a \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} j_b & j_a \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2} \end{pmatrix} \times \\
\langle j_b^+ j_b^- | L_{05} | j_a^+ j_a^- \rangle &= E_{m_a^b} \sqrt{2} \langle j_a \frac{1}{2} | j_b \frac{1}{2} \rangle \\
\times [3(2j_a+1)(2j_b+1)(2j^-+1)]^{\frac{1}{2}} &\langle j_b \frac{1}{2} | j_a \frac{1}{2} \rangle \begin{pmatrix} j_b & j_a \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} j_b & j_a \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2} \end{pmatrix} \times \\
\end{align*}
\]
where

\[ w(j_b^+ a^- j_a^+ j_a^-) = \langle j_b^+ j_a^- | L_{05} | j_a^+ j_a^- \rangle \]

and \( w(\ldots) \) is a Racah coefficient. The results can be verified directly by inserting the expansion

\[
\begin{vmatrix}
  j^+ & j^- \\
  m^+ & m^-
\end{vmatrix} = L_{j,m} \begin{vmatrix}
  j^+ & j^- \\
  m & m
\end{vmatrix} \begin{vmatrix}
  j^+ & j^- \\
  m & m
\end{vmatrix}
\]

into Equation (3.1).

The generators \( L_{03} \) and \( L_{05} \) leave \( m \) unchanged, and together with \( L_{35} \) they constitute the SO(2,1) subgroup which commutes with \( L_{11} \). This subgroup is of interest in calculations involving an external magnetic field. The generator \( L_{05} \) also leaves \( j \) unchanged.

4. The representation of the SO(4,1) group

In this section the known forms of the square representations of the SO(4) group are extended to include the SO(4,1) group representation.
A. The representation of the SO(4,1) group in the \((m^+, m^-)\) scheme, and a method of constructing non-compact SO(4,1) group generators.

The basis states for the square representation of the SO(4) group in the \((m^+, m^-)\) scheme have been obtained by Sharp by superimposing two orthogonalized SO(3) states in Spinor variables \((\mu, \theta)\) and \((\xi, \zeta)\). For a square representation \(j^+ = j^- = \frac{1}{2}n\), the basis states are:

\[
|j^+ j^- \rangle = \sum_{m^+ m^-} \left( \frac{(3n+m^+)! (3n-m^-)! (3n+m^-)! (3n-m^+)!}{n!} \right)^{1/2} \cdot \hat{r}^m_{m'} (\frac{m^+}{2} \cdots \frac{m^-}{2}) \cdot \hat{r}^{m'}_{m} (\frac{m^+}{2} \cdots \frac{m^-}{2}) \cdot |m^+ m^- \rangle,
\]

where \(-j^- < m^- < j^+\), and \(m'\) is restricted to non-negative factorials.

The square representations of the SO(4) group appear in the representations of the SO(4,1) group only with \(q=0\) (Table 1), and only two matrix elements of the non-compact generators differ from zero, \((3,1)\) and \((3,3)\) for \(n_b = n_a + 1\). For the non-compact
generators to commute with the compact ones according to (2.5) they have to contain at least first derivatives with respect to the spinor variables, (4.1). In addition the non-compact generators change the $n$ of the operand states, (4.1) to $n + 1$. Therefore the following form of the non-compact generators is proposed:

$$G_t = \Sigma_{i,j,k} A_t^{i,j,k} \gamma_i \gamma_j \gamma_k + \Sigma_{l} B_t^{l} \partial \gamma_l',$$

(4.2)

where $i,j,k,$ and $l = 1,2,3$ or 4, $\gamma_i$ is the spinor variable, $\mu, \nu, \xi$ or $\xi$, and $G_t$ is a non-compact generator. The $A_t$ and $B_t$ are coefficients.

From the identity,

$$G_t \left| \begin{array}{c} n \\ m \end{array} \right> = C_t \left| \begin{array}{c} n+1 \\ m-1 \end{array} \right> + D_t \left| \begin{array}{c} n-1 \\ m+1 \end{array} \right>, \quad (4.3)$$

where $m^*_t$ is related to $m^*$ by the operation of a particular generator $G_t^*$, (3.1). With a non-compact generator in the form (4.2), and the states (4.1), the solutions for the $A_t$ and $B_t$, which do not depend on $n$, can be found, as well as the solutions for $C_t$ and $D_t$. The results of this lengthy straightforward calculation for the coefficients is:

$$C_t = n! \left< \begin{array}{c} n+1 \\ m \end{array} \right| G_t \left| \begin{array}{c} n \\ m-1 \end{array} \right>_{q,p=0}, \quad (4.4)$$

$$D_t = n! \left< \begin{array}{c} n-1 \\ m \end{array} \right| G_t \left| \begin{array}{c} n \\ m+1 \end{array} \right>_{q,p=0}.$$
The non-compact generators appropriate for the \((m^+, m^-)\) scheme, (2.3) or (2.4) are:

\[
\begin{align*}
S_+ &= \frac{1}{\sqrt{2}} (1 + \eta \xi_3 + \xi \xi_7 + \xi \xi_8 + \xi \xi_9) + \frac{1}{\sqrt{2}} (0 \xi_4 - 1) \xi_7 ; \\
S_- &= \frac{1}{\sqrt{2}} (1 + \xi \xi_3 + \xi \xi_7 + \xi \xi_8 + \xi \xi_9) + \frac{1}{\sqrt{2}} (0 \xi_4 - 1) \xi_7 ; \\
P_+ &= \frac{1}{\sqrt{2}} (1 + \eta \xi_3 + \eta \xi_7 + \eta \xi_8 + \eta \xi_9) + \frac{1}{\sqrt{2}} (n \xi_4 + 1) \xi_7 ; \\
P_- &= \frac{1}{\sqrt{2}} (1 + \xi \xi_3 + \xi \xi_7 + \xi \xi_8 + \xi \xi_9) + \frac{1}{\sqrt{2}} (n \xi_4 + 1) \xi_7 ;
\end{align*}
\]

For completeness, the set of 6 compact SO(4) generators is:

\[
\begin{align*}
\mathbf{j}_+ &= \eta \xi_3 + \xi \xi_7 + \xi \xi_8 + \xi \xi_9 ; \\
\mathbf{j}_- &= \xi \xi_3 + \eta \xi_7 + \eta \xi_8 + \eta \xi_9 ; \\
\mathbf{j}_0 &= \frac{1}{2} (\eta \xi_3 + \xi \xi_7 + \xi \xi_8 + \xi \xi_9) ;
\end{align*}
\]

Direct calculation verifies their commutation laws (2.1) and (2.5).

The appearance of \(n\) in (4.4) is because the 4-dimensional space is too small to carry all unitary irreducible representations of the SO(4,1) group. This can be seen from the following considerations:

The norm of the basis states with respect to \(n\) can be determined in two ways:

(i) the norm of the next highest state can be generated from the norm of the next lowest state using the matrix elements of the non-compact generator.

or (ii) the norm can be determined by dividing the state with the square root of its length. But the form of a generator has
to depend on \( p, q \) and \( n \) in order to produce the compact matrix elements of the non-compact generator.

The simplest solution is to adopt the norm for the states as determined from (1), when the form of a generator will remain free of the representation indices, and the basis is orthogonal, but the length of the basis states is \((n!)^{1/2}\) instead of 1. Therefore the set of generators, (4.5) and (4.6), together with the basis states

\[
\left| \begin{array}{c}
\frac{n}{m^+ \cdot m^-}
\end{array} \right> = (n!)^{1/2} \left| \begin{array}{c}
\frac{n}{m^+ \cdot m^-}
\end{array} \right>,
\]

constitute the representation of the SO(4,1) group in the \((m^+, m^-)\) scheme in spinor space, with \( p \) and \( q \) equal to zero (Table 1).

This representation is now transformed into 4-dimensional Euclidean space by a change of variables effected by a matrix \( T \):

\[
T_1 \begin{pmatrix}
\chi_1 \\
\chi_2 \\
\chi_3 \\
\chi_4
\end{pmatrix} = \begin{pmatrix}
\eta \\
\zeta \\
\theta \\
\xi
\end{pmatrix}
\]

where

\[
T_1 = \begin{pmatrix}
-1 & -i & 0 & 0 \\
1 & -i & 0 & 0 \\
0 & 0 & 1 & i \\
0 & 0 & 1 & -i
\end{pmatrix}
\]

and \( T^{-1} = \frac{1}{2} T_1 \cdot T_1 \) are brought to the form (4.6).
To arrive at a convenient form of the representation of the $SO(4,1)$ group in 4-dimensional space in the $(m^+,m^-)$ scheme, it is necessary to express the basis states, and the generators in polar variables defined by

\[
x_1 = e^{-\rho} \cos \omega \cos \alpha
\]

\[
x_2 = e^{-\rho} \cos \omega \sin \alpha
\]

\[
x_3 = e^{-\rho} \sin \omega \cos \beta
\]

\[
x_4 = e^{-\rho} \sin \omega \sin \beta
\]

and

The volume element of this system is $g_A$ defined by

\[
g_A = \frac{1}{2} e^{2\rho} \sin 2\omega
\]

The spinor variables are linked with these polar variables through Eq. (4.8). The non-compact generators (4.5) become in these polar variables:

\[
S^\pm = \frac{1}{\sqrt{2}} e^{i\theta} \left( i \cosh \rho \cos \omega \pm \sinh \rho \sin \omega, -i \sinh \rho \sin \omega \pm i \cosh \rho \cos \omega \right)
\]

and

\[
P^\pm = \frac{1}{\sqrt{2}} e^{i\theta} \left( -\cosh \rho \sin \omega \pm \sinh \rho \cos \omega, i \sinh \rho \cos \omega \pm i \cosh \rho \sin \omega \right)
\]

The compact generators assume the familiar form:

\[
j^+_t = \frac{1}{2} e^{i(\alpha + \beta)} \left( i \omega, -i \omega + i \sigma_3 \beta - i \sigma_3 \alpha \right);
\]

\[
j^-_t = \frac{1}{2} e^{i(\alpha - \beta)} \left( i \omega, +i \omega + i \sigma_3 \beta + i \sigma_3 \alpha \right);
\]

\[
\gamma^+_t = -\frac{1}{2} \left( \sigma_3 \alpha + \sigma_3 \beta \right);
\]

\[
\gamma^-_t = -\frac{1}{2} \left( \sigma_3 \alpha - \sigma_3 \beta \right);
\]

and

\[
\gamma^0_t = -\frac{1}{2} \left( \sigma_3 \alpha - \sigma_3 \beta \right).
\]
The basis states \((\pm \pm)\) become after a little manipulation:

\[
\begin{pmatrix}
n \\ \pm \pm
\end{pmatrix} = (-1)^{n+n'} c^{-n'} (c i \alpha)^{n+n'} (c i \beta)^{-n-m} d^{\frac{1}{2}} n_{m}^{-} (2\omega)
\]  

(4.12)

where \(d \cdot (2\omega)\) is an SO(3) reduced rotation matrix as defined in Ref.17. The range of parameters is

\[
0 < p < \omega, \quad 0 < \omega < \pi/2, \quad 0 < \alpha \, \text{and} \, \beta < \pi
\]

The length of these states in system A, (4.9) is

\[
\left(\begin{pmatrix} n \\ \pm \pm \end{pmatrix} \right)^{2} \sum_{\pm \pm} \frac{n}{[2(n+1)(n+2)]^{\frac{1}{2}}}
\]

(4.13)

Since the \(p\) appear explicitly in the non-compact generators (4.9) and in the basis states (4.2), the integrals involving these states will diverge unless the exponential radial dependence, \(\exp(-p)\), is used in system A, (4.9), instead of the usual linear dependence on \(p\).

Applying the non-compact generators (4.10) to the basis states (4.12) gives a set of eight new recursion relations for the SO(3) group reduced rotation matrices. Reducing the general matrix elements of the non-compact generators (3.1) and (3.2) to the case \(j = j = n\), and replacing \(\omega\) by \(\omega\) so that the reduced SO(3) group rotation matrices depend on a single argument,

\[
S_{+} \text{ gives } [^{2} n (1, \cos \omega)^{+}(m^{+} m^{-})]^{2} h^{n}_{m}^{-} (\omega) - \sin \omega d^{\frac{1}{2}} n_{m}^{-} (\omega) = \]

\[
-2[^{2} n (1, \cos \omega)^{+}(m^{+} m^{-})]^{\frac{1}{2}} h^{n}_{m}^{-} (\omega) \]

(4.14)
\[ P_+ \text{ gives } [\frac{1}{2}(n+2) (+\cos \omega) \pm (n^+ n^-)] \pm 2 \frac{1}{n} \frac{1}{m} (\omega) = \sin \frac{1}{2} \cos \frac{1}{2} \pm (\frac{1}{m^+ m^-} (\omega)) \]

\[ S_+ \text{ gives } [\frac{1}{2}(n+2) (+\cos \omega) \pm (m^+ m^-)] \pm 2 \frac{1}{n} \frac{1}{m} (\omega) = \sin \frac{1}{2} \cos \frac{1}{2} \pm (\frac{1}{m^+ m^-} (\omega)) \]

and

\[ P_- \text{ gives } [\frac{1}{2}(n+2) (-\cos \omega) \pm (n^- n^+)] \pm 2 \frac{1}{n} \frac{1}{m} (\omega) = \sin \frac{1}{2} \cos \frac{1}{2} \pm (\frac{1}{m^+ m^-} (\omega)) \]

where \( S_+ \) and \( P_+ \) are the particular generators which lead to the recurrence relations.

B. The representation of the SO(4,1) group in the \((j,m)\) scheme

The basis state and the set of generators for the \((j,m)\) scheme are obtained from those for the \((m^+, m^-)\) scheme by substitution.

\[ \alpha = \frac{1}{\sqrt{2}} (\theta - \xi), \quad (4.15) \]

\[ \beta = \frac{1}{\sqrt{2}} (\theta + \xi). \]

The basis states become,

\[ \left| n, m \right> = \frac{[2k+1]! (n-k)! (n+k+1)!}{\sqrt{n+k+1}} \frac{1}{\sqrt{2}} \frac{(n-k-2s)!}{s! (n-k-2s)! (2k+2s+1)!} \left| m \right> \]

where
where $\mathcal{L}$ replaces $j$, which is always an integer in a square representation. The set of non-compact generators (2.6) in the $(j,m)$ scheme become, after substitution of (4.15) into (4.5),

\[
S = \frac{1}{\sqrt{2}} \left( 1 + \eta \frac{a^n + \beta \beta}{\eta} + \frac{1}{2\sqrt{2}} (a^2 - \beta^2 + 2) \beta \right),
\]

\[
S' = \frac{1}{\sqrt{2}} \left( 1 + \xi \frac{a^n + \beta \beta}{\eta} + \frac{1}{2\sqrt{2}} (a^2 - \beta^2 + 2) \eta \right),
\]

\[
L_{03} = \frac{1}{\sqrt{2}} \left( 1 + \xi \frac{a^n + \beta \beta}{\eta} + \frac{1}{2\sqrt{2}} (a^2 + \beta^2 + 2n\xi + 2) \eta + \alpha \right),
\]

\[
L_{05} = \frac{1}{\sqrt{2}} \left( 1 + \xi \frac{a^n + \beta \beta}{\eta} + \frac{1}{2\sqrt{2}} (a^2 + \beta^2 - 2n\xi - 2) \beta + \alpha \right),
\]

and the compact generators become

\[
L_+ = \sqrt{2} (\beta \eta - \xi \beta), \quad L_- = \sqrt{2} (\beta \eta + \xi \beta), \quad L_0 = \eta \frac{a^n - \xi \beta}{\eta},
\]

\[
K_+ = \sqrt{2} (\alpha \beta - \eta \beta), \quad K_- = \sqrt{2} (\xi \beta - \alpha \beta), \quad K_0 = \alpha \beta + \beta \beta \alpha.
\]
By analogy with $4A$, the representation is transformed into

4-dimensional Euclidean space

\[
\begin{pmatrix}
x_1 \\
x_2 \\
x_3 \\
x_4
\end{pmatrix} =
\begin{pmatrix}
T_2 \\
\zeta \\
\beta \\
\alpha
\end{pmatrix}
\]

where

\[
T_2 = 2/2 \begin{pmatrix}
1/\sqrt{2} & 1/\sqrt{2} & 0 & 0 \\
1/\sqrt{2} & 1/\sqrt{2} & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & i
\end{pmatrix},
\]

\[
T_2^{-1} = \frac{1}{2} T_2^+ = \frac{1}{2} \begin{pmatrix}
1/\sqrt{2} & 1/\sqrt{2} & 0 & 0 \\
1/\sqrt{2} & 1/\sqrt{2} & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & -i
\end{pmatrix}
\]

and the basis states and the generators are expressed in polar variables appropriate to the $(j, m)$ scheme:

\[
x_1 = e^{-\rho} \sin x \sin \phi, \quad x_2 = e^{-\rho} \sin x \sin m \rho, \quad x_3 = e^{-\rho} \sin x \cos \phi, \quad x_4 = e^{-\rho} \cos x.
\]

The volume element of this system is $g_B$

\[
g_B = e^{-4\rho} \sin^2 x \sin \theta.
\]

The range of parameters is

\[
0 \leq \rho < +\infty, \quad 0 \leq x \leq \pi, \quad 0 \leq \theta \leq \pi, \quad 0 \leq \phi \leq 2\pi.
\]
The non-compact generators (4.17) become,

\[
S_x = e^{i\phi} (i (\epsilon^0 + 2e^{-\rho}) \sin \chi \sin \Theta \phi (\epsilon^0 - 2e^{-\rho}) \cos \chi \sin \Theta \phi - (\epsilon^0 - 2e^{-\rho}) \cos \chi \sin \Theta \phi)
\]

\[
S_y = \sin \chi \sin \Theta \phi (\epsilon^0 - 2e^{-\rho}) \cos \chi \sin \Theta \phi - (\epsilon^0 - 2e^{-\rho}) \cos \chi \sin \Theta \phi
\]

\[
L^{03} = \frac{1}{2 \sqrt{2}} \left( (\epsilon^0 + 2e^{-\rho}) \sin \chi \cos \Theta \phi (\epsilon^0 - 2e^{-\rho}) \cos \chi \sin \Theta \phi - (\epsilon^0 - 2e^{-\rho}) \sin \chi \sin \Theta \phi + 2 \epsilon^0 \cos \chi \sin \Theta \phi \right)
\]

(4.21)

The compact generators (4.18) take the usual form \(^{35}\),

\[
L_x = e^{i\phi} (i \phi + \epsilon \Theta \phi) ; L_y = -i \epsilon \phi ; L_z = e^{i\phi} (i \sin \Theta \phi + i \epsilon \Theta \phi \cos \Theta \phi) \cos \Theta \phi
\]

(4.22)

The basis states (4.16) become, after manipulation (Appendix C) the hyperspherical harmonics,

\[
| \ell, m, n \rangle = (i)^{\ell} \frac{\left( \frac{1}{2} \right)^{\left( \ell - n \right)} \ell ! (2 \ell + 1) ! (n + \ell + 1) !}{(2 \ell + 1) ! (\ell + m) !} \left( \frac{2 \ell + 1}{(n+\ell+1) !} \right)^{\frac{1}{2}}
\]

\[
e^{-n \rho} (\sin \chi)^{\frac{\ell + 1}{2}} (\cos \chi)^{\frac{\ell + 1}{2}} P^m_c (\cos \Theta) e^{i \phi}
\]

(4.23)

where \( P^m_c \) is a Gegenbauer polynomial, and \( P^m_c (\cos \Theta) \) is an associated Legendre polynomial as defined in reference \(^{36}\).

The same state, apart from normalization, has been derived on group theoretical grounds by Sharp \(^{11}\).
The length, the norm of the states (4.23) is
\[
\left\langle n \middle| n \right\rangle^{\frac{1}{2}} = (-1)^{n-q} \frac{2n}{(n+1)(n+2)}^{\frac{1}{2}}.
\]

Similarly, as in 4A, the known matrix elements in
the \((j,m)\) scheme (3.4), the set of non-compact operators (4.10) and the states (4.23), allow the recursion relations for the hyperspherical harmonics to be derived. All of them will not be written explicitly, because the functions of two variables are involved, instead, several examples will be considered in which only one function appears. The following recursion relations are all known, nevertheless they will be derived because they establish the representation given in (4.10) for non-compact generators and the basis states (4.23).

The operation of the generators \(S_\pm\) on a basis state for which \(\gamma=\ell\) is
\[
\begin{align*}
S_+ | n \rangle_m^\ell &= | n+1 \rangle_m^{\ell+1} + | n \rangle_m^{\ell+1} | n+1 \rangle_m^{\ell-1} \\
S_- | n \rangle_m^\ell &= | n-1 \rangle_m^{\ell+1} + | n \rangle_m^{\ell+1} | n-1 \rangle_m^{\ell-1} \\
&+ | n \rangle_m^{\ell-1} | n \rangle_m^{\ell+1} | n-1 \rangle_m^{\ell-1}.
\end{align*}
\]

The identity (4.24), with the representation of the non-compact generators (4.21) and the states (4.23) splits into two equations, one for each exponent \(c^{-\frac{(n+1)p}{2}}\), after the matrix elements have been calculated from (3.4) and (3.9) for the case \(p=0\), \(q=0\) and \(j^+ = j^- = n\).
This procedure gives four standard recursion relations for the associated Legendre polynomials of a real variable, (five are actually found, but two are identical)

\((2l+1)\sin\theta P^m_l(\cos\theta) = P^{m+1}_{l-1}(\cos\theta) = P^{m+1}_{l+1}(\cos\theta)\);

\[\sin^2\theta + \cos^2\theta = 1\]

\[\frac{m}{\sin \theta} P^m_l(\cos\theta) - \frac{m}{\sin \theta} P^m_{l-1}(\cos\theta) = P^m_{l-1}(\cos\theta)\]

\[(2l+1)\sin\theta P^m_l(\cos\theta) = (l-m+1)(l-m+2)P^m_{l+1}(\cos\theta) - (l+m)(l+m-1)P^m_{l-1}(\cos\theta)\] \hspace{1cm} (4.25)

Another two recursion relations can be derived from the identity

\[\begin{align*}
\langle L_0 | \ell | m \rangle &= \langle \ell+1 | L_0 | \ell \rangle + \\
&+ \langle \ell-1 | L_0 | \ell \rangle + \\
&+ \langle \ell+1 | L_0 | \ell \rangle + \\
&+ \langle \ell-1 | L_0 | \ell \rangle \\
\end{align*}\] \hspace{1cm} (4.26)

This gives

\[(2l+1)\cos\theta P^m_l(\cos\theta) = (l-m+1)P^m_{l+1}(\cos\theta) + (l+m)P^m_{l-1}(\cos\theta)\] \hspace{1cm} (4.27)

\[\cos\theta P^m_l(\cos\theta) - \sin\theta P^m_{l-1}(\cos\theta) = (l+m)P^m_{l-1}(\cos\theta)\]
Thus six out of eight possible recursion relations appear. The remaining two recursion relations can be derived by applying the compact SO(4,1) group generators (4.22) to the states (4.23). In particular, from the identity

\[ L_+ \left| \ell \right. \ell \m \right. = \left< \ell \ell \ell. \ell \ell m+1 \right. \left| \ell \ell \ell m \right. = \ell \ell \ell m+1 \right. \]  

(4.28)

the two remaining recursion relations follow,

\[ \delta_0 p^m_L(\cos \theta) - \text{cot} \theta p^m_L(\cos \theta) = p^{m+1}_L(\cos \theta), \]  

(4.29)

\[ 3 \delta_0 p^m_L(\cos \theta) + \text{cot} \theta p^m_L(\cos \theta) = -\ell (\ell \ell \ell \ell \ell m+1 + \ell m-1 p^m-L(\cos \theta). \]  

The \( N_+ \) gives the second recursion relation of (4.25); the \( K_0 \) gives the second recursion relation of (4.27); \( L_0 \) gives a trivial result. The recursion relations (4.25), (4.27) and (4.29) are in a form which corresponds to that of the generators. The relations easily reduce to their standard form as in reference 36, by eliminating the derivatives with respect to \( \theta \).

Thus to obtain all the recursion relations group theoretically, the SO(4,1) group representation has to be used. It is of interest to note that, if it is assumed that all the recursion relations for the Legendre polynomials are known, and contained in (4.25), (4.27) and (4.29), then consideration of the full dynamical group of the Coulomb potential SO(4,2) cannot give new recursion relations. A representation of the SO(4,2) group in 4-dimensional space, with the hyperspherical harmonics as basis states, has to coincide with the representation of the SO(4,1)
group. In this sense, it is sufficient to use the SO(4,1) group as the dynamical group for this system, instead of the more complex SO(4,2) group.

The corresponding recursion relations for the Gegenbauer polynomials are most easily derived from the operation of the non-compact generators on the basis state with $m = \ell$. From

$$
S_+ | n \ell \rangle = \langle n+1 \ell+1 | S_+ | n \ell \rangle | n+1 \ell+1 \rangle +
$$

$$
+ \langle n-1 \ell+1 | S_+ | n \ell \rangle
$$

(4.30)

two standard recursion relations are obtained, after changing the indices to:

$$
v = \ell + 1; \quad k = n - 1;
$$

(4.31)

namely:

$$(k+2v)C_k^v(\cos \chi) - \cot \chi \partial C_k^v(\cos \chi) = 2vC_{k+1}^v(\cos \chi);$$

(4.32)

$$kC_k^v(\cos \chi) + \cot \chi \partial C_k^v(\cos \chi) = -2vC_{k-1}^v(\cos \chi).$$

The operation of the generators $S_-$ and $L_{03}$ does not lead to a different recursion relation in this case. As $iL_{05}$ does not change either $\ell$ or $m$, it can be applied to an arbitrary state:

$$
iL_{05} | n \ell m \rangle = \langle n+1 \ell+1 | iL_{05} | n \ell m \rangle | n+1 \ell m \rangle +
$$

$$
+ \langle n-1 \ell+1 | iL_{05} | n \ell m \rangle | n-1 \ell m \rangle
$$

(4.33)
to give two more recursion relations

\[ k \cos x C_k^\nu(\cos x) - \sin x \partial_x C_k^\nu(\cos x) = (k+2\nu-1)C_{k-1}^\nu(\cos x) \]

\[ (k+2\nu) \cos x C_k^\nu(\cos x) + \sin x \partial_x C_k^\nu(\cos x) = (k+1)C_{k+1}^\nu(\cos x) \]

Equations (4.32) and (4.34) give four recursion relations for the Gegenbauer polynomials. The remaining recursion relation can be derived by applying any of the generators \( K_+ \), \( K_- \) and \( K_0 \) to the basis states (4.23) with \( m = \frac{1}{2}, m = -\frac{1}{2} \), respectively. The result is

\[ -\partial_x C_k^\nu(\cos x) = 2\nu\sin x C_{k+1}^{\nu+1}(\cos x) \]

The last recursion relation is the only one which can be derived by use of the compact generators. Similarly, as in the case of the Legendre polynomials, the full set of recursion relations for the Gegenbauer polynomials is contained in a representation of the \( \text{SO}(4,1) \) group.

5. Concluding remarks

Two points of interest emerge.

First, the connection between the space of the \( \text{O}(4) \) spinors and 4-dimensional Euclidean space: apart from the theoretical interest, it is an advantage in practical calculations, since various operations are far more easily performed in spinor space than in Euclidean space; by the coordinate transformations (4.8) and (4.19), one can always arrive at the corresponding set of operations expressed in the appropriate coordinates in 4-dimensional
space from those in spinor space.

Second, the explicit representation of the SO(4,1) generators found, should facilitate reduction of SO(4,1) with respect to its different subgroups.

As mentioned in the introduction, it is known that the radial part of the hydrogenic wave function is linked with the basis for a unitary irreducible representation of the SO(2,1) group. The radial wave functions depend on \( n \) and \( l \). The wave-function dependence on \( m \) can be eliminated by considering the SO(2,1) group generators which leave this quantum number \( m \) unchanged, namely the \( L_{35} \), \( L_{05} \) and \( L_{03} \) which constitute the Lie algebra of the SO(2,1) group.

This suggests that in the reduction of \( \text{SO}(4,1) \rightarrow \text{SO}(2,1) \times \text{SO}(2) \) in which \( L_{12} \) generates the \( \text{SO}(2) \) group, the radial wavefunctions are contained in a basis in which the subgroup \( \text{SO}(2,1) \) is diagonal. The same reduction is of interest in considering the group theoretical description of an atom in a magnetic field where \( \text{SO}(4,1) \rightarrow \text{SO}(2,1) \times \text{SO}(2) \).

The non-compact generators (4.10) and (4.21) can be transformed into 3-dimensional "physical" space by reversing the procedure in Reference 3. It will be of interest to compare such transformed generators with the existing representations of the \( \text{SO}(4,1) \) group in 3-dimensional space \(^{28,29} \), or with the representations of the \( \text{SO}(4,2) \) group in 3-dimensional space \(^{9} \).

The representations of the \( \text{SO}(4,1) \) group found in this paper for \( q = 0 \) and \( p = 0 \), representation 1 of Table 1, fall within the chain of reduction of certain important classes of the \( \text{O}(4,2) \) group representations \( \text{O}(4,2) \rightarrow \text{SO}(4,1) \rightarrow \text{SO}(4) \), the sub-
class (1) of Reference 4.

In this paper the representation of the generators of the SO(4,1) group has been found for which the hyperspherical harmonics are basis state, belonging to the representation 1 of Table 1 with \( p = 0 \) and \( q = 0 \).

The recursion relations of the SO(3) reduced rotation matrices, the Legendre polynomials and the Gegenbauer polynomials have been derived by group theoretical arguments alone, consequently they are of intrinsic interest in the study of the connections between these functions and the group representations.
CHAPTER VI

REDUCTION OF THE DISCRETE CLASS OF REPRESENTATIONS OF THE $\text{SO}(2,2)$ GROUP WITH RESPECT TO THE REPRESENTATIONS OF THE $\text{SO}(2,1)$ GROUP.
1. Introduction and method

The generators of the full dynamical $SO(4,2)$ group which leave the magnetic quantum number, $m$, unchanged, constitute the Lie algebra of the $SO(2,2)$ group. As emphasized in the introduction to this part, the group is important for studying the transformation properties of the radial part of the hydrogenic wave function, and for developing a group theoretical description of an atom in a magnetic field.

To be consistent with the notation of Chapter V, the notation proposed for the $SO(4,2)$ group by Yada has been adopted. The compact axes are labelled with the indices 1, 2, 3 and 5, while the two non-compact axes are 0 and 6. The metric tensor for this space is:

$$g_{11} = g_{22} = g_{33} = g_{55} = 1 \quad \text{and} \quad g_{00} = g_{66} = -1.$$  

The generators can be represented in the usual form of differential operators:

$$L_{a,b} = -i(x_a \delta_{b} - x_b \delta_a)$$

$$a, b = 0, 1, 2, 3, 5, 6,$$  

and $l = \sqrt{-1}$,  

which commute according to:

$$[L_{a,b}, L_{c,d}] = i(g_{ac} L_{bd} - g_{ad} L_{bc} - g_{bc} L_{ad} + g_{bd} L_{ac}).$$  

The generators of the group of interest here, $SO(2,2)$, leave the hermitian quadratic form, $x_3^2 + x_5^2 - x_0^2 - x_6^2$, invariant.
Indices 1 and 2 do not appear in the defining Hermitian form (1.3) because the generators which commute with $L_{12}$ (the magnetic operator) should not contain these indices. These generators are

$$L_{35}, L_{36}, L_{03}, L_{05} \text{ and } L_{06} \quad (1.4)$$

and they form the Lie algebra of the $SO(2,2)$ group.

The generators of the $SO(2,1)$ subgroup are:

$$L_{35}, L_{03}, \text{ and } L_{05} \quad (1.5)$$

The representation of these generators in their parameter space, established by Kihlberg\textsuperscript{16}, has been used to form the eigenvalue equation for the Casimir invariant of the $SO(2,1)$ group. It turns out that this eigenvalue equation is formally the same as one found by Mukunda\textsuperscript{37} when reducing the 'homogeneous Lorentz group,' $SO(3,1),$ with respect to the non-compact $SO(2,1)$ subgroup. By following similar lines to Mukunda, the $SO(2,1)$ content in the discrete series of the $SO(2,2)$ group representations is determined in the next section.

2. Calculations

According to Kihlberg\textsuperscript{16}, the basis states for a representation of the $SO(2,2)$ group in parameter space are of the form:

$$|ab\rangle = e^{i(a+1)\mu} e^{ib\nu} f(\rho, \phi) \quad (2.1)$$
The range of parameters is:

\[ 0 < \rho, \psi < 2\pi \quad \text{and} \quad -\infty < \mu, \nu < \infty \quad (2.2) \]

The eigenvalues of the first and second Casimir invariants of the SO(2,2) group are related to \( a \) and \( b \) by:

\[ I^2 = -a^2 - b^2 - 1 \quad \text{and} \quad I^4 = -ab, \quad (2.3) \]

The expressions for the 3 generators of the SO(2,1) subgroup (1.5) found in Ref. 16 are:

\[ L_{35} = -\partial_\rho, \]
\[ L_{03} = \cos \rho \cos \psi \partial_\rho + \sin \rho \sin \psi \partial_\psi - \sin \psi \cos \rho \partial_\mu + \cos \psi \partial_\nu, \]

and

\[ L_{05} = \sin \rho \cos \psi \partial_\rho + \cos \psi \sin \rho \partial_\psi - \cos \psi \cos \rho \partial_\mu - \sin \psi \partial_\nu. \]

When the derivatives over \( \mu \) and \( \nu \) have been replaced by the eigenvalues, \( i(a+1) \) and \( i b \), the generators (1.5), assume the following form:

\[ L_{35} = -\partial_\rho, \]
\[ L_{03} = \cos \rho \cos \psi \partial_\rho + \sin \rho \sin \psi \partial_\psi - (a+1) \sin \psi \partial_\mu + ib \cos \psi \]

\[ + \cos \psi \partial_\nu, \quad (2.4) \]

and

\[ L_{05} = \sin \rho \cos \psi \partial_\rho + \cos \psi \sin \rho \partial_\psi - (a+1) \cos \psi \partial_\mu - ib \sin \psi \partial_\nu. \]

The Casimir operator of the SO(2,1) group is:
The solution of the eigenvalue problem:

\[ Q \begin{pmatrix} a \\ b \\ q \\ s \end{pmatrix} = \begin{pmatrix} a \\ b \\ q \\ s \end{pmatrix}, \tag{2.6} \]

has to be found; where \( q \) is an eigenvalue of \( Q \) and \( s \) is an eigenvalue of the "commuting" generator, \( L_{35} \).

When the Casimir operator (2.5) is expressed in terms of the generators (2.4), the resulting form of (2.6) can be separated with respect to the variables \( \psi \) and \( p \):

The operand state in Eq. (2.1) is then in the unnormalized form:

\[ \begin{pmatrix} a \\ b \\ q \\ s \end{pmatrix} = e^{ip} g_{qs}^{ab}(\psi), \tag{2.7} \]

where \( s = 0, \pm 1, \pm 2 \ldots \)

The range of values for \( s \) follows from the boundary conditions at the end points of the allowed interval for \( p \), (2.2).

The equation for \( g(\psi) \) is:

\[ -\delta^2 \psi + 2i(a+i) \cot \psi \psi - 2hs \cosh \psi + \frac{8(a+i)}{\sin^2 \psi} - [s^2 - b^2 + (a+i)^2] g(\psi) = q \cdot g(\psi), \tag{2.8} \]

Changing the variables and the function to:

\[ \psi = iu; \quad t = \cosh u \text{ and } g(t) = (t^2 - 1)^{-i(a+i)} W(t), \tag{2.9} \]
yields an equation for $W(t)$

$$
\left\{-\left(t^2-1\right) \frac{\partial}{\partial t} - \frac{2s}{t^2} \right\} W(t) + \frac{s^2 - 21bst}{t^2 - 1} \right\} W(t) = q \cdot W(t)
$$

(2.10)

Equation (2.10) is identical to the Equation of Mukunda.

The allowed range of values of $q$ follows from the theory of the SO(2,1) group representations.

For the sake of convenience, these values are summarized in Table 1:

**THE REPRESENTATION OF THE SO(2,1) GROUP**

<table>
<thead>
<tr>
<th>Eigenvalues of Casimir invariant $q = -j(j+1)$</th>
<th>Spectrum of the &quot;commuting&quot; generator $L_{35}, s$:</th>
<th>Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>$j = \frac{1}{2}$</td>
<td>$N, 1, 2$</td>
<td>Main series</td>
</tr>
<tr>
<td>$0 &lt; p &lt; \infty$</td>
<td>$\frac{1}{2}, \frac{3}{2}$</td>
<td>Continuous non-exceptional class</td>
</tr>
<tr>
<td>$-\frac{1}{2} &lt; j &lt; 0$</td>
<td>$0, 1, 2$</td>
<td>Continuous part of supplementary series</td>
</tr>
<tr>
<td>$j = s - 1$</td>
<td>$s, s+1, \ldots$</td>
<td>Discrete part of supplementary series bounded below</td>
</tr>
<tr>
<td>$s = \frac{1}{2}, 1, \frac{3}{2} \ldots$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$j = s - 1$</td>
<td>$-s, -s - 1, \ldots$</td>
<td>Discrete part of supplementary series bounded above</td>
</tr>
<tr>
<td>$s = \frac{1}{2}, 1, \frac{3}{2} \ldots$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
In order to make the notation consistent, the spectrum of the Casimir invariant as presented in Ref. 16 is taken with the opposite sign.

For the values of \( q \) in Table 1, the solutions of (2.10) are known \(^{16,37,38}\). In the terminology of Vilenkin \(^{23}\), they are Jacoby functions:

\[
d_{j}^{s,ib}(t) \quad \text{and} \quad q = -j(j+1) \tag{2.11}
\]

Khilberg has shown that the double valued representations of the \( \text{SO}(2,1) \) group have to be considered in the decomposition of the \( \text{SO}(2,2) \) group into the \( \text{SO}(2,1) \times \text{SO}(2,1) \) group \(^{16}\). This means that \( s \) can take half integral values as well as integral ones. The Jacobi functions (2.11) are defined if both \( s \) and \( ib \) take simultaneously integral or half integral values, not necessarily the same.

The two Casimir invariants of the \( \text{SO}(2,1) \) group are related to \( a \) and \( b \) \(^{16}\) by

\[
I_{1}^{2} = -\frac{1}{4} [(b-a)^{2}+1] \tag{2.12}
\]

and

\[
I_{2}^{2} = -\frac{1}{4} [(b+a)^{2}+1]
\]

or equivalently by
Because \( \{b \} \) has to be an integer or half integer, this method is applicable only to representations of the \( SO(2,2) \) group which are built from discrete classes of representations of the \( SO(2,1) \) group. When the range of \( l_1 \) and \( l_2 \) belongs to the discrete class of the \( SO(2,1) \) group representations, Table 1, \( \{b \} \) is given by:

\[
\{b \} = \frac{1}{2} (m_1 - m_2)
\]

The absolute value comes from the associative properties of the group product, \( SO^{(1)} (2,1) \times SO^{(2)} (2,1) = SO^{(2)} (2,1) \times SO^{(1)} (2,1) \). The higher value of two \( m \)'s can be regarded as belonging to the group \( SO^{(1)} (2,1) \). In this way \( \{b \} \) will always have positive values or zero.

The eigenstates of the Casimir operator of the \( SO(2,1) \) group are obtained from (2.7), (2.8), and (2.11); they are unnormalized:

\[
\begin{pmatrix} a \\ b \\ q \\ s \end{pmatrix} = \left( t^2 - 1 \right)^{-\frac{1}{2}} i(a+1) \begin{pmatrix} \rho & 0 \\ 0 & i \rho \end{pmatrix} d^3 \{b \} (t)
\]

where

\[
q = \frac{1}{2} (j + \frac{3}{2}) \quad \text{and} \quad \{b \} = 0, 1, \ldots \quad s = 0, 1, \ldots \quad s = \frac{1}{2}, \frac{3}{2}
\]

and \( \{b \} = 0, 1, \ldots \) or \( \{b \} = \frac{1}{2}, \frac{3}{2} \).
and the range of \( j \) is given in Table 1.

As is known, the representations belonging to the continuous exceptional class are not needed in the completeness relation for the set of basis states of the \( \text{SO}(2,1) \) group representations. This completeness relation is satisfied with only the states \((2,1j)\) then from (2.14) and (2.15) and Table 1 it can be concluded that the discrete class of the \( \text{SO}(2,2) \) representations \((ib=0, \frac{1}{2}, 1, \ldots)\) contains the continuous non-exceptional class and two discrete classes of the \( \text{SO}(2,1) \) representation once.

The scalar product for the states \((2,1s)\) can be derived from the one defined in Ref. 37 which is for the states belonging to the continuous non-exceptional class:

\[
\int_{0}^{2\pi} \int_{-\infty}^{\infty} d\rho \int_{-\infty}^{\infty} dze^{i(s-s')\rho} \psi_{s,ib}(z) \overline{\psi_{s',ib'}(z)} = 2\pi \delta_{s,s'} \delta(p-p') \left( \frac{p}{p \tanh p} \right)
\]

where \(-\infty < s < \infty \) and \( 0 < p < \infty \).

For the discrete class the scalar product is:

\[
\int_{0}^{2\pi} \int_{1}^{\infty} d\rho \int_{1}^{\infty} dze^{i(s-s')\rho} \psi_{s,ib}(z) \overline{\psi_{s',ib'}(z)} = \frac{2}{2k+1} \delta_{s,s'} \delta_{k,k'}
\]

where \( k \) stands for either \( s \) or \( s' \) which are the upper or lower bounds of the "commuting" generating \( L_{35} \) in two inequivalent
representations of the discrete classes of the $SO(2,1)$ group
with
\[ k = \begin{cases} s, & s = s, s+1, \\ s', & s = -s, -s-1, \end{cases} \]

(Table 1)

Changing the variable in the last two equations to:

\[ z = \coth u \quad \text{and} \quad dz = -\csch^2 u \, du \]

gives for the scalar product of the states (2.15) with the change $t = \coth u$

\[
\int dp \int_0^\infty \csch^2 u \, e^{i(s-s')p} \, ds,ib \, (u) \, d^{s,ib}_{k-1} \, (u) = 2\pi \delta \frac{\delta (p-p')}{s,s', p \tanh p} \tag{2.18}
\]

and

\[
2\pi \int dp \int_0^\infty \csch^2 u \, e^{i(s-s')p} \, ds,ib \, (u) \, d^{s',ib}_{k-1} \, (u) = \frac{2}{2k-1} \delta_{s-s'} \delta_{k,k} \tag{2.19}
\]

Therefore, the complete orthonormal set of basis states for the representation of the $SO(2,1)$ group in which the $SO(2,1)$ group is diagonal for the continuous non-exceptional class is

\[
\begin{pmatrix} a \\ b \\ s \end{pmatrix} = \frac{e^{i\sigma \theta}}{\Gamma(2)(c^{-1})} \frac{1}{2} \frac{1}{(a+1)} \, ds,ib \, (c) \, \frac{1}{2+ip} \tag{2.20}
\]
where \( -\infty < s < \infty \) integer steps, \( j = -\frac{1}{2} + ip \) and 
\( 0 < p < \infty \), and two discrete classes, one bounded below, and the other bounded above given by:

\[
\begin{pmatrix}
  a & b \\
  j & s
\end{pmatrix} = \left( \frac{2k-1}{4\pi} \right)^{1/2} e^{isp\left(t^2-1\right)} \cos \left( (a+1) \right) d_{k-1} (t),
\]

(2.21)

where \( k = \frac{s}{2}; s = \frac{s+1}{2}, \ldots; j = s-1 \), \( s = -s, -s-1, \ldots; j = s-1 \).

with \( k \neq s \)

\( ib = 0, \frac{1}{2}, 1, \ldots \)

and \( s, s \) are integers or half integers, depending on the value of \( ib \).

3. Concluding remarks:

The basis states found in the preceding section (2.20) and (2.21) can be used to calculate the matrix elements of finite "rotations" between states labelled with different subgroup indices. These matrix elements are important in transforming one set of basis vectors for a representation of the \( SO(2,2) \) group into another which is labelled with a different subgroup, using the method of induced representations.
These states, (2.20) and (2.21) are helpful in calculating the Clebsh-Gordan coefficients for the $SO(2,2)$ group and the $SO(2,1)$ group.

In order to define the scalar product of (2.18) and (2.19) the parameter scale (2.2) has to be extended, Equations (2.18) and (2.19). This points out the limitation of the method of Ref. 16 which uses the space of the parameters of the maximal compact subgroup to construct the representations of the whole group. These parameters do not allow the scalar product to be constructed in the usual way.

A remark should be made concerning the reduction of the $SO(4,2)$ group with respect to its $SO(2,2)xSO2$ subgroup. Yao showed that an extra invariant is necessary to fully characterize the representations of the $SO(4,2)$ group in the reduction $SO(4,2)\supset SO(4)\times SO(2)$. An analogous situation exists in the reduction $SO(4,2)\supset SO(2,2)\times SO(2)$. In addition this invariant operator should be cubic in the $SO(4,2)$ generators, preliminary calculations show that this operator is a combination of the two vectors $A$ and $B$ with components:

$$A \{L_{01}, L_{41}, L_{15}\} \quad \text{and} \quad B \{L_{02}, L_{23}, L_{25}\}.$$ 

In this Chapter it has been shown that the work of Mukunda on the unitary representations of the $SO(2,1)$ in an $O(2,1)$ basis can be applied to reduce the discrete class of the $SO(2,2)$ group representations with respect to the $SO(2,1)$ group with an identical result to that of Reference 37. Equations (2.18), (2.19), (2.20) and (2.21) of this Chapter.
Throughout this work the following parametrization of the group elements in the \((j, m)\) scheme is used:

\[
\begin{align*}
\mathbf{g}_L^1(a_1) &= e^{i a_1 L_1} = \\
&= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos a_1 & \sin a_1 & 0 \\ 0 & -\sin a_1 & \cos a_1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \\
\mathbf{g}_K^1(a_4) &= e^{i a_4 K_1} = \\
&= \begin{pmatrix} \cos a_4 & 0 & 0 & \sin a_4 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -\sin a_4 & 0 & 0 & \cos a_4 \end{pmatrix} \\
\mathbf{g}_L^2(a_2) &= e^{i a_2 L_2} = \\
&= \begin{pmatrix} \cos a_2 & 0 & -\sin a_2 & 0 \\ 0 & 1 & 0 & 0 \\ \sin a_2 & 0 & \cos a_2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \\
\mathbf{g}_K^2(a_5) &= e^{i a_5 K_2} = \\
&= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos a_5 & 0 & \sin a_5 \\ 0 & 0 & 1 & 0 \\ 0 & -\sin a_5 & 0 & \cos a_5 \end{pmatrix}
\end{align*}
\]
$g_{L_3}(a_3) = e^{ia_3L_3} = \begin{pmatrix}
\cos a_3 & \sin a_3 & 0 & 0 \\
-sin a_3 & \cos a_3 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 
\end{pmatrix}$

and

$g_{K_3}(a_6) = e^{ia_6K_3} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & \cos a_6 & \sin a_6 \\
0 & 0 & -\sin a_6 & \cos a_6 
\end{pmatrix}$ (A.1)

These matrices represent rotations around the 4-coordinate axes; the direction is defined in Ref. 22. The corresponding element in the $(m^+, m^-)$ scheme are obtained from:

$g_{\pm k}(a_k) = e^{\pm \frac{ia_k}{2}(L_k \pm K_k)}$ (A.2)

The general rotation $R$ is given by the Eq.s (2.3) and (2.4) in Chapter IV. When a rotation is applied to a function, the coordinates are transformed by $R^{-1}$. 
APPENDIX B

Han has obtained a representation of the SO(4,1) group in 4-dimensional space by constructing an $E_4$ algebra relevant to the problem. His non-compact generators are expressed in terms of a 4-vector $p^i$, called a "Shirokov operator" which transforms irreducibly with respect to the SO(4) group. The relation between Han's non-compact generators $(B, S)$ and those found in Chapter V $(B', L_05)$ $(B'$ has components $L_{01}, L_{02}, L_{03})$ in the notation of Chapter V is:

$$
iB = \sqrt{2}B' + 2(x \cdot x) + \frac{q}{x} - (x \cdot p)^2 - \frac{1}{2}p$$

$$iS = -\sqrt{2}L_05 + (x \cdot p)x_5 - \frac{5}{2}x_5 + p_5$$

The two vectors $x$ and $p$ have components $(x_1, x_2, x_3)$ and $(\alpha_1, \alpha_2, \alpha_3)$, respectively, and $p_5$ by $\alpha x_5$.

The difference arises from the arbitrariness in determining the 4-vector $p^i$, i.e., any vector which transforms irreducibly with respect to the SO(4) sub-group can be identified with 4 non-compact generators of the SO(4,1) group. Han's choice is $p = x$, compared to that in Chapter V which is given by $(B.1)$.

When expressed in spinor coordinates using $(4.8)$ of Chapter V for example, Han's generators do not contain the term which lowers $n$ to $n-1$. Therefore the hyperspherical harmonics in their normal form $(4.23)$, Chapter V, cannot be the basis state for the Han generators (although a linear combination with respect to $i$ and $m$ may possibly transform correctly).
After the spinor variable in the basis states in (4.16) of Chapter V have been replaced by the spherical ones of (4.20) via (4.18), the sums in the expression for the basis states (4.16) takes the following form, (without the normalization factor)

\[ S_s = \sum_{r=0}^{s} \frac{(-1)^r (s+r)! (\cos \Theta)^{n-r-2s} (\sin \Theta)^{2s}}{s! (n-r-2s)! (2l+2s+1)!} \]  \hspace{1cm} (C.1)

and

\[ S_t = \sum_{r=0}^{t} \frac{(-1)^r (s+r)! (\sin^2 \Theta)^{m+2t} (\cos \Theta)^{l-m-2t}}{t! (m+t)! (l-m-2t)! 2^{2t}} \]  \hspace{1cm} (C.2)

by developing

\[(\sin^2 \Theta)^s = (1-\cos^2 \Theta)^s,\]

into the binomial series it is found for \( S_s \)

\[ S_s = \sum_{r=0}^{s} \binom{s}{r} \left( \frac{(l+s)!}{(n-r-2s)! (2l+2s+1)! (s-r)!} \right) (-1)^r (\cos \Theta)^{n-2r} \]  \hspace{1cm} (C.3)

The coefficient in curly brackets may be calculated as follows:

First the index \( s \) is replaced:

\[ \text{s} = t + p, \]

then two identities from Ref. 36 for the Gamma functions are used

\[ (n-l-2p-2t)! = \frac{(n-l-2n)!}{2^{2t} (n+l+1+p)!}, \]

and

\[ (2l+2s+1)! = \Gamma(2l+2s+2) = \frac{(2l+2s+1)!}{\sqrt{\pi} \Gamma(l+s+1) \Gamma(l+s+1/2)}, \]  \hspace{1cm} (C.4)
After the last replacements, the coefficient in (C.3) becomes:

\[
\frac{1}{(2k+1)^2} \frac{1}{(n-1-2p)!}\binom{3}{p-1} \binom{2}{p-1} \binom{2}{p-1} \binom{3}{1}.
\]

From the well-known formula for the value of the hypergeometric function, \( \mathcal{F}_1(...) \), for the argument 1, and using the duplication formula for the Gamma function once more,

\[
\Sigma_s = \frac{(l+s)!}{p(n-l-2s)! (2l+2s+1)! (s-p)!} \frac{(2)^{n-l} (n-p)!}{(2)^{2p-n-2p} (n-l-2p)! (n+l+1)!} \]

and

\[
S_n = \frac{(-1)^s (n-p)!}{(n+l+1)!} \sum_{p=0}^{l} \frac{(2\cos \chi)^{n-2p}}{(n-l-2p)!} \binom{l}{p} \binom{s}{p} C_{n-l}(\cos \chi) \]

where \( C_{n-l}(\cos \chi) \) is a Gegenbauer polynomial, and the sum is restricted to the non-negative factorials.

Similarly, the sum (C.2) leads to

\[
S_l = \frac{(2m)!}{(k+m)!} (-1)^{m} \binom{k}{m} (\cos \theta) \binom{m}{l}.
\]

Substitution of the sums, (C.7) and (C.8) into Eq. (4.16) of the Chapter V together with the normalization factor give finally the basis states (4.23).
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PART FOUR

CANONICAL TRANSFORMATIONS IN QUANTUM CHEMISTRY
Introduction to Art four

In the Hamilton formulation of mechanics, the co-ordinates and the momenta of particles are regarded as equally independent variables. A system of \( n \) particles is represented by a point in \( 6n \) dimensional phase space which moves in time in accordance with Hamilton's equations. Any set of transformations in the phase space which leave these equation invariant is called "canonical".

In a canonical transformation, the new co-ordinates and momenta are expressed in terms of both the old co-ordinates and the old momenta. These transformations are the largest possible class of transformations admissible for a given system.

The "physical" co-ordinates and momenta of a system are "mixed" under a canonical transformation and consequently the Hamiltonian is altered, but the new eigenvalues and their separations are related to those of the initial Hamiltonian. The properties of motion induced by a new Hamiltonian remain the same as those of the old Hamiltonian. In this respect, the group of canonical transformations resembles the role that the dynamical groups have in describing a system when some of the elements of the group do not commute with the Hamiltonian but act on the quantum numbers as ladder operators. Indeed, there are indications that these two groups, the dynamical group of a system and the group of canonical transformations, are connected.

The unpopularity of canonical transformations compared with point transformations is partly due to the fact that the point transformations are simpler to implement than the full set of canonical transformations which in general mix co-ordinates and momenta.
mentioned above: The set of point transformations which leave
the Hamiltonian invariant is often referred to as the "symmetry
of the system, but in the Hamilton formalism there is no dis-
tinction between coordinates and momenta, therefore there is
no reason not to extend the term "symmetry" to include the
full set of canonical transformations, regardless of the non-
invalance of the Hamiltonian under these transformations.

As an example of the use of canonical transformations,
the problem of diagonalizing Hamiltonians expressed as quadratic
forms of both the coordinates and momenta will be considered in
Chapter VII, and the general method is used to study the motion
of angular momentum in a magnetic field under which conditions
the Hamiltonian will be canonically transformed to take the form
of two uncoupled oscillators.

Canonical transformations are being increasingly used
in quantum chemistry and nuclear physics to study various
systems such as the Coulomb potential, the many body problem,
the three body problem, etc.
CHAPTER VII

DIAGONALIZATION OF HAMILTONIANS EXPRESSED
IN "MIXED" QUADRATIC FORMS OF COORDINATES
AND MOMENTA BY A CANONICAL TRANSFORMATION
1. Introduction

A quantum mechanical system is described by a set of 2n canonically conjugate operators consisting of

n coordinates: \(x_1, x_2, \ldots, x_n\)

and

n momenta: \(p_1, p_2, \ldots, p_n\) \hspace{1cm} (1.1)

By definition, the canonical transformation of \(x\) and \(p\) preserves the canonical commutational relations between operators (1.1)

\[
[x_a, p_b] = [x_a, p_b] = \delta_{ab}, \hspace{1cm} (1.2)
\]

where \(a, b = 1, \ldots, n\)

and \(x_a\) and \(x_b\) are the canonically transformed variables.

If a canonical transformation is linear, then it can be represented by:

\[
\bar{x}_a = \sum_{b=1}^{n} M^{(1)}_{ab} x_b + \sum_{c=1}^{n} M^{(2)}_{ac} p_c , \hspace{1cm} (1.3)
\]

and

\[
\bar{p}_a = \sum_{d=1}^{n} M^{(3)}_{ad} x_d + \sum_{e=1}^{n} M^{(4)}_{ae} p_e . \hspace{1cm} (1.4)
\]

or in matrix form by:

\[
\begin{pmatrix}
\bar{x}_1 \\
\vdots \\
\bar{x}_n \\
\bar{p}_1 \\
\vdots \\
\bar{p}_n
\end{pmatrix} = M
\begin{pmatrix}
x_1 \\
\vdots \\
x_n \\
p_1 \\
\vdots \\
p_n
\end{pmatrix} \hspace{1cm} (1.4)
\]
where the \(2n \times 2n\) matrix \(M\) has the form:

\[
M = \begin{pmatrix}
M^{(1)} & M^{(2)} \\
M^{(3)} & M^{(4)}
\end{pmatrix}
\]

(1.5)

and the \(n \times n\) submatrices \(M^{(1)}, M^{(2)}, M^{(3)}\) and \(M^{(4)}\) consist of the elements \(M_{ab}, M_{cd}, M_{ef}\) and \(M_{gh}\) respectively; these elements define the canonical transformation (1.3).

It has been shown that a linear transformation is canonical if the transformation matrix \(M\) (1.5) satisfies the condition:

\[
M \tilde{M} = K
\]

(1.6)

where \(\tilde{M}\) means the transpose of \(M\).

The matrix \(K\) is given by:

\[
K = \begin{pmatrix}
0 & I \\
-I & 0
\end{pmatrix}
\]

(1.7)

in which \(I\) is an \(n \times n\) unit matrix.

2. Diagonalization of quadratic Hamiltonians

A. General method

The most general form of a Hamiltonian which is quadratic in both co-ordinates and momentum operators (1.1) is:

\[
H = \sum_{a,b=1}^{n} H^{(1)}_{ab} x_a x_b + \sum_{c,d=1}^{n} H^{(2)}_{cd} x_c p_d + \sum_{e,f=1}^{n} H^{(3)}_{ef} p_e x_f + \sum_{g,h=1}^{n} H^{(4)}_{gh} p_g p_h
\]

(2.1)

or equivalently, the Hamiltonian (2.1) can be put in the matrix form:
\[ H = \tilde{y} A y \]  
\[ \text{(2.2)} \]
where \( y \) is a 2n dimensional vector:
\[ y = \begin{pmatrix} x_1 \\ \vdots \\ x_n \\ p_1 \\ \vdots \\ p_n \end{pmatrix} \]  
\[ \text{(2.3)} \]
and the matrix \( A \) is:
\[ A = \begin{pmatrix} H(1) & H(2) \\ H(3) & H(4) \end{pmatrix} \]  
\[ \text{(2.4)} \]
The nxn submatrices \( H(1), H(2), H(3) \) and \( H(0) \) have elements \( H_{ab}, H_{cd}, H_{ef} \) and \( H_{gh} \) respectively.

The matrix \( A \) can always be assumed symmetrical; since \( x_a \) and \( x_b \) and \( p_a \) and \( p_b \) commute for all \( a,b = 1, \ldots, n \) the submatrices \( H(1) \) and \( H(4) \) are obviously symmetrical.

The problem in this section is to determine a linear transformation of the co-ordinates and momenta (1.1) specified by an unknown matrix \( P \), which satisfies two conditions:

(i) the transformation must diagonalize the Hamiltonian (2.1) or (2.2):
\[ P A P = D_A \]  
\[ \text{(2.5)} \]
and

(ii) the transformation must be canonical, i.e. condition (1.6) is satisfied by a matrix \( P \),
Similarly, \( x_c \) and \( p_d \) commute for all \( c \) and \( d = 1, \ldots, n \) except when \( c = d \), but because the Bohr quantization rule requires the replacement of \( x_c p_c \) by \( \frac{1}{2}(x_c p_c + p_c x_c) \). When \( c = d \), it follows that

\[
\mathcal{H}^{(3)} = \mathcal{H}^{(2)},
\]

so that the matrix \( \mathbf{A}(2.4) \) is always symmetrical.

To determine the matrix \( \mathbf{P} \), condition \((2.5)\) is replaced by an auxiliary condition \((2.7)\)

\[
\mathbf{P} \mathbf{A} \mathbf{P} = \mathbf{B},
\]

where \( \mathbf{B} \) is an unspecified matrix.

Because the matrix \( \mathbf{K} \) \((1.7)\) is orthogonal:

\[
\mathbf{K}^{-1} = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix},
\]

The inverse of \( \mathbf{P} \), \( \mathbf{P}^{-1} \), can be found from \((2.6)\)

\[
\mathbf{P}^{-1} = \mathbf{K} \mathbf{P} \mathbf{K},
\]

By multiplying condition \((2.7)\) with \( \mathbf{P}^{-1} \) from the left, and by replacing \( \mathbf{P}^{-1} \) from \((2.9)\):

\[
\mathbf{A} \mathbf{P} = \mathbf{K} \mathbf{P} \mathbf{K} \mathbf{B}
\]

The matrix \( \mathbf{B} \) is now specified by the condition that

\[
\mathbf{K} \mathbf{B} = \mathbf{D},
\]

where \( \mathbf{D} \) is a diagonal matrix with elements \( \lambda_1, \lambda_2, \ldots, \lambda_{2n} \).
The set of linear equations contained in (2.10) for elements of the matrix $P$ and for $\lambda_1, \ldots, \lambda_{2n}$, can be solved only for those values of $\lambda$ which are roots of the equation:

$$|A - \lambda K| = 0.$$  \hfill (2.12)

Because matrix $A$ is symmetrical and matrix $K$ has the form (1.7), the polynomial equation for $\lambda$ (2.12) is invariant for the replacement $\lambda$ by $-\lambda$. Explicitly (2.12) with $A$ given by (2.4) and $K$ by (1.7) has the form:

$$\begin{pmatrix}
H(1) & H(2) + \lambda I \\
H(3) - \lambda I & H(4)
\end{pmatrix} = 0. \hfill (2.13)$$

Because $H(3) = H(2)$ the value of the determinant in (2.13) does not change with the replacement $\lambda$ by $-\lambda$. This means that if $\lambda$ is a solution then $-\lambda$ is also a solution. Therefore the elements of the diagonal matrix $D(2.11)$ can be arranged in the following order $\lambda_1, \ldots, \lambda_n, -\lambda_1, \ldots, -\lambda_n$, that is

$$D = \begin{pmatrix}
D_1 & 0 \\
0 & -D_1
\end{pmatrix}, \hfill (2.14)$$

where $D$ has elements $\lambda_1, \ldots, \lambda_n$.

Once the roots $\lambda_1, \ldots, \lambda_n$ of (2.12) have been found, the columns of matrix $P$ are determined from

$$A(P_k) = \lambda_k K(P_k), \hfill (2.15)$$

with $k = 1, \ldots, s \ldots, 2n$. 

where the elements of the column vector \( P_k \) (where \( k \) signifies the \( k \)th column) are \( P_{kj} \), with \( j = 1, \ldots, 2n \), and \( P_s \) is a specific \( P_k \) column vector.

It is possible to establish that the matrix \( P \) determined by means of (2.15) is canonical: multiplying (2.15) by the transpose of \( P_s \) from the left, and then the equation (2.15) for \( (P_s) \) by the transpose of \( P_k \) from the left gives:

\[
(P_s) A(P_k) = \lambda_k (P_s) K(P_k) \quad (2.16)
\]

and

\[
(P_k) A(P_s) = \lambda_s (P_k) K(P_s). \quad (2.17)
\]

Since the matrix \( A \) is symmetric (2.4) and \( K \) skew-symmetric, (1.7)

\[
(P_s) A(P_k) = (P_k) A(P_s) \quad (2.18)
\]

\[
(P_s) K(P_k) = -(P_k) K(P_s)
\]

The identity (2.18) follows from the theorem of congruent matrices:

a matrix congruent to symmetric (skew-symmetric) matrix is itself symmetric (skew-symmetric).

Subtracting (2.17) from (2.16), with the relations of (2.18) gives:

\[
0 \approx (\lambda_k + \lambda_s) (P_s) K(P_k), \quad (2.19)
\]

\[
k, s = 1, \ldots, 2n
\]

Therefore \( (P_s) K(P_k) \) is always zero except in the case when \( \lambda_k + \lambda_s \) is zero, i.e. for \( t = s + n \) where \( s = 1, \ldots, n \); the \( k \) index
of the positive eigenvalues and \( t \) is the index of the negative eigenvalues.

\[
(P_s)_k (P_k) = \begin{cases} 
0 & \text{for } s + k = n, \\
A_k & \text{otherwise}
\end{cases}
\] (2.20)

Collecting all equations (2.16) (over the whole range of \( k \) and \( s \)) for \( 2n \) columns of \( P \) into a single matrix form, gives

\[
\overline{P} \overline{A} \overline{P} = \overline{P} \overline{K} \overline{P} \overline{D}.
\] (2.21)

From (2.20) it is seen that the elements of the columns of \( P \) can be normalized in such a way that

\[
\overline{P} \overline{K} \overline{P} = \overline{K},
\] (2.22)

or

\[
\overline{P} \overline{K} \overline{P} = \overline{K}.
\]

Then (2.21), with \( D \) in the form (2.14), becomes

\[
\overline{P} \overline{A} \overline{P} = \begin{pmatrix} 0 & D_1 \\ D_1 & 0 \end{pmatrix} = \overline{A}.
\] (2.23)

The matrix \( \overline{A} \) (2.23) is now easily diagonalized by the canonical matrix \( T \)

\[
T = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{1} & 1 \\ \sqrt{1} & -1 \end{pmatrix}.
\] (2.24)
that is

$$\tilde{T} A \tilde{T}^{-1} = \begin{pmatrix} D_1 & 0 \\ 0 & D_1 \end{pmatrix} \tilde{A}$$  \hspace{1cm} (2.25)

The Hamiltonian associated with matrix (2.25) has the form of the sum of uncoupled harmonic oscillator Hamiltonians:

$$\tilde{H} = \sum_{a=1}^{n} \lambda_a \left( \frac{-1}{x_a^2} + \frac{-2}{p_a^2} \right).$$  \hspace{1cm} (2.26)

In summary: the procedure for diagonalizing the general Hamiltonian in the form (2.1) consists of three steps:

(i) the Hamiltonian (2.1) has to be made symmetric by using the commutational relations (1.2) and the Bohr quantization rule.

(ii) the matrix A has to be associated with this Hamiltonian and the polynomial equation (2.12) solved. The roots of these equations are symmetrically distributed around zero. Then the columns of the P matrix are determined except for the normalizing factor from (2.15), and the P matrix is then normalized according to (2.22).

The Hamiltonian is then transformed with this matrix to the form (2.23).

Finally (iii) the Hamiltonian (2.23) is transformed by a matrix T (2.24) to a diagonal form (2.25) or explicitly (2.26).

B. Application to the Hamiltonian of angular momentum in a magnetic field.

The general method for diagonalizing quadratic Hamiltonians...
(2.1) (section A) is applied to the Hamiltonian of angular momentum in a magnetic field:

\[ H = \mu_B \hat{L} \cdot \vec{H}_{\text{ex}} \]  

(2.27)

where

\[ \hat{L} = r \times p, \]

and \( \mu_B \) is the Bohr magneton.

\( H_{\text{ex}} \) is a constant magnetic field and is assumed to point along the z axis.

Explicitly, the Hamiltonian (2.27) is:

\[ H = \mu_B (x_1 p_2 - x_2 p_1) H_{\text{ex}} \]  

(2.28)

After symmetrizing (2.28), the form of matrix \( A \) (2.4) is,

in this case:

\[
A = \begin{pmatrix}
0 & 0 & 0 & 1 \\
0 & 0 & -1 & 0 \\
0 & -1 & 0 & 0 \\
1 & 0 & 0 & 0
\end{pmatrix}
\]  

(2.29)

The equation to be solved is (2.12):

\[
|A - \lambda \mathbf{E}| = 
\begin{pmatrix}
0 & 0 & \lambda & 1 \\
0 & 0 & -1 & \lambda \\
-\lambda & -1 & 0 & 0 \\
1 & -\lambda & 0 & 0
\end{pmatrix} = 0
\]  

(2.30)

The solutions of (2.30) are

\[ \lambda_k = i, -i, -1, 1 \]  

(2.31)

with \( k = 1, \ldots, 4 \).
The $P$ matrix determined from (2.15) is, after normalization
\[
P = \sqrt{\frac{1}{2}} \begin{pmatrix}
1 & 1 & 0 & 0 \\
-1 & -1 & 0 & 0 \\
0 & 0 & 1 & 1 \\
0 & 0 & 1 & 1
\end{pmatrix}_{(2.32)}
\]

One can verify that this matrix is canonical (1.6) the matrix (2.32) transforms the Hamiltonian (2.29) into:
\[
\tilde{P} A P = -1 \begin{pmatrix}
0 & 0 & -1 & 0 \\
0 & 0 & 0 & 1 \\
-1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0
\end{pmatrix} = \tilde{A} \quad (2.33)
\]

Then the Hamiltonian (2.33) is diagonalized by the matrix $T$ (2.24):
\[
\tilde{T} \tilde{A} T = \begin{pmatrix}
-1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix} = \tilde{A} \quad (2.34)
\]

The Hamiltonian (2.34) has an explicit form:
\[
\tilde{H} = -\frac{\xi_1^2}{2} + \frac{\xi_2^2}{2} - \frac{p_1^2}{2} + \frac{p_2^2}{2} \quad (2.35)
\]

The result (2.35) has been obtained previously by a different method.\(^6\)

In fact the steps from (2.31) to (2.34) are unnecessary since equation (2.26) shows that the form of the Hamiltonian is specified by the roots of the equation (2.12). Indeed in this case with the roots (2.31) one can use (2.26) directly to obtain (2.35).

3. Conclusion

In this Chapter it has been shown how the method of canonical
transformations can be used to simplify apparently complicated Hamiltonians. Because the explicit form of a canonical transformation is often of no interest in practical calculations while the form of transformed Hamiltonian is of interest, it is only necessary to solve Equation (2.12) for \( \lambda \) when the transformed Hamiltonian is immediately found from (2.6).
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CLAIMS TO ORIGINAL RESEARCH

Chapter I
(i) The method of decoupling the chain of equations for the Green's function of the spin-orbit coupled system, Eqs. (2.2) - (2.25).
(ii) The form of the susceptibility tensor, Eqs. (2.26) and (2.27).
(iii) The statement, after Eq. (3.1), concerning the maximum number of possible resonances for a spin-orbit system.

Chapter II
(i) The method for factorizing an exponential function of operators, Eqs. (2.1) - (2.7).
(ii) The explicit factorization for the case $a = L \cdot S - b = (L + 2S), L = 1/2$ and $S = 1/2$, Eqs. (3.1) - (3.14).

Chapter III
(i) The derivation of the potential functions for the chain, Eqs. (2.2) - (2.6) and Eqs. (2.11) - (2.14); together with the explicit form for these functions, (2.15a and b) and Eq. (2.16).
(ii) The solution for the energy levels of the chain in the perpendicular direction, Eq. (3.19a and b).
(iii) The formal solution for the wave function and the energy levels along the chain, Eq. (4.7)
Chapter IV

(1) The connection between the two sets of parameters for the SO(4) group Eq. (2.5) and (2.6).

(ii) The explicit form of the generators in (j,m) parameter space, Eq. (2.8).

(iii) The relations between the Gegenbauer polynomials and the SO(3) reduced rotational matrices (4.10).

Chapter V

(i) The matrix elements of the generators in the (j,m) scheme, Eqs. (3.5) - (3.7).

(ii) The method of constructing the non-compact generators Eqs. (4.2) - (4.4); together with the form of these generators in spin or space in the (m,m) scheme, Eq. (4.5) and (j,m) scheme, Eq. (4.17).

(iii) The transformation from spin or space to 4-dimensional Euclidian space in the (m,m) scheme, Eq. (4.8) and the form of the generators in Euclidian space, Eq. (4.10).

(iv) The recursion relation for the SO(3) reduced rotational matrices, Eq. (4.14).

(v) The transformation from the spin or space to Euclidian space in the (j,m) scheme, Eq. (4.19) and the form of the non-compact generators in Euclidian space (4.21).
(vi) The group theoretical derivation of the recursion relations for Legendre polynomials, Eqs. (4.25), (4.27) and (4.29) and for Gegenbauer polynomials, Eqs. (4.32), (4.34) and (4.35).

Chapter VI

(i) Realization that the SO(2,2) group is the appropriate dynamical group for the hydrogen atom in a magnetic field.

(ii) The derivation of Eq. (2.10) which turns out to be known in the theory of O(2,1) group representations.

(iii) The conclusion following the equation (2.15) concerning the reduction of the class of the SO(2,1) group representations with respect to the SO(2,1) subgroup.

Chapter VII

(i) The method for diagonalizing the symmetrical matrix by a canonical matrix, Eqs. (3.5) - (3.28), together with the result, Eq. (3.29) and the conclusion of this Chapter.

To achieve a comparatively clear presentation of the material dealt with in this thesis, most of the derivations have been omitted or reduced to essential minima necessary for understanding the methods.

Also due to the differing nature of the various problems involved, no attempt has been made to give a complete literature survey for each case; the references quoted are those on which the research is based or which exemplify the ideas.
SPECIAL MATHEMATICAL METHODS WITH APPLICATIONS