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V. Sonnad, J. Escher, M. Kruse, R. Baker

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An Informal Overview of the Unitary Group Approach

V. Sonnad[1], J. Escher[1], M. Kruse[1], and R. Baker[2]

[1]*Lawrence Livermore National Laboratory, 7000 East Ave., Livermore, CA 94550*
[2]*Louisiana State University, Department of Physics and Astronomy, Baton Rouge, LA 70803*

Abstract

The Unitary Groups Approach (UGA) is an elegant and conceptually unified approach to quantum structure calculations. It has been widely used in molecular structure calculations, and holds the promise of a single computational approach to structure calculations in a variety of different fields. We explore the possibility of extending the UGA to computations in atomic and nuclear structure as a simpler alternative to traditional Racah algebra based approaches. We provide a simple introduction to the basic UGA and consider some of the issues in using the UGA with spin dependent, multi-body Hamiltonians requiring multi-shell bases adapted to additional symmetries. While the UGA is perfectly capable of dealing with such problems, it is seen that the complexity rises dramatically, and the UGA is not at this time, a simpler alternative to Racah algebra based approaches.

1 Introduction

Computer codes for quantum many-body structure calculations in atomic, nuclear, and molecular physics play important roles and are among the most heavily used in their respective fields. The typical approach to solving such problems is to expand the unknown wave function as a linear combination of known basis functions. The Hamiltonian corresponding to the problem is discretized in these bases and the result is a matrix eigenproblem that is readily solved by accessing linear algebra libraries. Basis functions which are adapted to the symmetry inherent in the problem can result in significantly smaller matrices often leading to dramatic savings in computational effort. The traditional approach with symmetry adapted bases utilizes Racah Algebra (RA) which is highly effective but is notoriously difficult and requires a customized approach for each class of problems.

It would be very desirable to find a simpler alternative to Racah Algebra based approaches. The emphasis on simplicity is not based on aesthetic considerations alone: high performance computation relies heavily on graphics processors, and complex algorithms would not be expected to perform well on these processors without heavy commitments in manpower. In addition, simpler algorithms allow rapid prototyping to test new theories as well as greatly reduced time on code maintenance. The benefits of a relatively simple determinantal approach for atomic calculations has been demonstrated by Ed Hill [12], where the performance penalty as compared to the Racah Algebra approach was minimal for problem sizes of practical interest.

The UGA provides an elegant and unified starting point for quantum structure calculations, and in past decades has been highly successful in quantum molecular computations. The two key ideas in the UGA (which will be described in more detail in sections below) are the expression of the Hamiltonian in terms of generators of the unitary group and the use of Gelfand-Tsetlin (GT) bases. Extending this to other fields such as atomic and nuclear physics requires dealing with

spin dependent Hamiltonians with multi-shell bases; in addition, the GT bases must be adapted to the symmetries of the problem ($SU(2)$, $SU(3)$ etc.). This report is an attempt to provide a reasonably self-contained overview of the basics of the UGA with reference to the literature so that interested readers can readily grasp the basic ideas and appreciate the issues in extending the UGA to fields beyond molecular structure calculations.

2 Description of the problem

In order to provide a basic explanation of the structure problem in quantum mechanics, it is useful to start with a concrete example, and we consider a nonrelativistic problem in atomic structure which is given by

$$\hat{H}\hat{\psi} = \hat{\lambda}\hat{\psi} \tag{1}$$

where $\hat{H}$ is the Hamiltonian corresponding to the Schrödinger equation, $\hat{\psi}$ is the wave function corresponding to a multi-electron atom, and $\hat{\lambda}$ is the eigenvalue corresponding to the energy of the system. The standard approach to transforming this continuum problem into a discrete problem is the Galerkin approach, where the first step is to approximate the wave function by a linear combination of chosen basis functions:

$$\hat{\psi} = \sum_{j=1}^{n} c_j \phi_j \tag{2}$$

where c_j are unknown constants to be determined, and ϕ_j are the chosen basis functions. When this expression for $\hat{\psi}$ is substituted into Eq. (1), the resulting equation is no longer exact and we can define an error as:

$$Error = \hat{H}\sum_{j=1}^{n} c_j \phi_j - \hat{\lambda}\sum_{j=1}^{n} c_j \phi_j \tag{3}$$

The second step in the Galerkin process is to require that the error be orthogonal to the basis functions, or equivalently, that the projection of the error on to the space spanned by the basis functions is zero. When this condition is imposed on the error we get a set of discrete equations of the form

$$Hc = \lambda c \tag{4}$$

where H is a matrix of size $n \times n$, c is a vector of unknowns of length n, and λ is an eigenvalue. This is a standard eigenproblem and can be solved by calling appropriate libraries. The elements of the matrix H are given by

$$H(i,j) = \langle \phi_i | \hat{H} | \phi_j \rangle \tag{5}$$

3 The role of symmetry

The choice of the basis functions in the discretization of the problem is critical and can greatly affect the difficulty in forming matrix elements as well as the overall computational effort required to solve the problem. One of the most important considerations in the choice of the basis functions is that they reflect the symmetry inherent in the problem. As a starting point, it is customary for quantum structure calculations to use basis functions that are products of single orbital basis functions. The most basic requirement is that the basis functions incorporate antisymmetry under exchange of particles, and this is typically accomplished by expressing basis functions in terms of Slater determinants. Subsequent to this are various additional symmetries that have

to be satisfied: discrete symmetries for molecules and crystals, continuous symmetries ($SU(2)$, $SU(3)$, $Sp(3,\mathbb{R})$, etc.) for atomic and nuclear structure calculations.

The existence of a symmetry implies that the Hamiltonian is invariant under the action of a group operation and hence commutes with the group operators (for a finite group) or with the generators of the group (continuous group).

$$\begin{aligned} H &= GHG^{-1} \\ HG &= GH \end{aligned} \tag{6}$$

If basis functions are chosen such that they are invariant and irreducible under the action of a group, then the action of the group members on the basis functions results in a linear combination of the same basis functions; they form an invariant subspace. Since the group operators commute with the Hamiltonian, the effect of the Hamiltonian on the basis functions preserves the invariant subspaces and hence results in block diagonal matrices [5]. The eigenequation $Hc = \lambda c$ is transformed into a number of smaller independent eigenequations.

$$\left[\begin{array}{c|c|c|c} G_1 & 0 & 0 & 0 \\ \hline 0 & G_2 & 0 & 0 \\ \hline 0 & 0 & G_3 & 0 \\ \hline 0 & 0 & 0 & G_4 \end{array}\right] \left[\begin{array}{c} c_1 \\ \hline c_2 \\ \hline c_3 \\ \hline c_4 \end{array}\right] = \lambda \left[\begin{array}{c} c_1 \\ \hline c_2 \\ \hline c_3 \\ \hline c_4 \end{array}\right]$$

This is the primary benefit of using "symmetry adapted" basis functions, and can often result in dramatic computational savings. Thus there is powerful motivation to find and use basis functions that are adapted to the symmetry of the problem.

4 The Unitary Group Approach

The Unitary Group Approach is an elegant idea that is based on two key concepts. The first is the idea of expressing the Hamiltonian in terms of the generators of the unitary group and the second is the use of Gelfand-Tsetlin basis functions to discretize the Hamiltonian. The credit for introducing a combination of these two as a single approach goes to Moshinsky and the basic ideas ideas are described in [26]. Each of these will be explained below.

4.1 Hamiltonian expressed in terms of the generators of the unitary group

When describing the UGA, it is customary to resort to the language of creation-annihilation operators. While this is a perfectly good approach, we will follow a somewhat more transparent description from [32], which provides one of the best introductions to the UGA even though a majority of the book deals with the symmetric group.

For an atom with N electrons in n orbitals, each basis function is made up of products of N one-electron orbitals $|i_1\rangle|i_2\rangle.....|i_N\rangle$ where orbital i_k is from the entire set of orbitals $|1\rangle.....|n\rangle$. The total number of basis functions is made up of all possible products and the dimension of the

space is n^N. We now define operators

$$\begin{aligned} e^i_{rs} &= |r^i\rangle\langle s^i| \\ E_{rs} &= \sum_{i=1}^{i=N} e^i_{rs} \end{aligned} \tag{7}$$

where $|r^i\rangle$ and $|s^i\rangle$ are single orbital bases corresponding to the i^{th} particle. It can then be shown that the replacement operators E_{rs} have the following commutation relations:

$$[E_{r,s}, E_{t,u}] = \delta_{st}E_{ru} - \delta_{ru}E_{ts} \tag{8}$$

It is of fundamental importance in the UGA that *these commutation relations are the same as those of the generators of the unitary group.*

We will next show how the Hamiltonian can be expressed in terms of these operators. A spin-free Hamiltonian can be written as

$$\hat{H} = \sum_{i=1}^{N} h(i) + \sum_{i=1}^{N}\sum_{j>i}^{N} g(i,j) \tag{9}$$

where $h(i)$ and $g(i,j)$ are one-electron and two-electron operators respectively. Consider the matrix elements of the one-particle operator between two product basis functions:

$$\langle i_1| \dots \langle i_N| \left[\sum_{i=1}^{N} h(i)\right] |j_1\rangle|j_2\rangle \dots |j_N\rangle \tag{10}$$

Inserting the identity operator before and after the one-particle operator in the above expression, we have

$$\langle i_1| \dots \langle i_N| \sum_{r=1}^{n}\sum_{s=1}^{n}\sum_{i=1}^{N} \left(|r^i\rangle\langle r^i|h(i)|s^i\rangle\langle s^i|\right) |j_1\rangle|j_2\rangle \dots |j_N\rangle \tag{11}$$

If we denote

$$h_{rs} = \sum_{i=1}^{N} \langle r^i|h(i)|s^i\rangle \tag{12}$$

we can see that the one-particle operator can be expressed as

$$\sum_{i=1}^{N} h(i) = \sum_{r=1}^{n}\sum_{s=1}^{n} h_{rs}E_{rs} \tag{13}$$

Following an identical approach for the two-particle term (with the identity operator inserted twice), we can get an expression in terms of the replacement operator and the Hamiltonian can be written as:

$$\hat{H} = \sum_{r=1}^{n}\sum_{s=1}^{n} h_{rs}E_{rs} + \frac{1}{2}\sum_{r=1}^{n}\sum_{s=1}^{n}\sum_{t=1}^{n}\sum_{u=1}^{n} \left[E_{ru}E_{st} - \delta_{us}E_{rt}\right] g(ru,st) \tag{14}$$

where

$$g(ru,st) = \sum_{i=1}^{N}\sum_{j=1}^{N} \langle r^i|\langle u^i|g(i,j)|s^j\rangle|\ t^j\rangle \tag{15}$$

We see that a variety of different Hamiltonians can be expressed entirely in terms of the generators of the unitary group. This opens up the possibility of developing a single computational technique for structure calculations in a variety of different fields.

4.2 Gelfand-Tsetlin bases

Given that the Hamiltonian is expressed in terms of the generators of the unitary group, it is reasonable to use basis functions that transform "well" under the action of the generators. The Gelfand-Tsetlin (GT) bases are invariant and irreducible under the action of the generators of the unitary group making them an obvious choice.

These bases are a cornerstone of the UGA and would have been lost to researchers outside Russia without the expert knowledge of Moshinsky and the efforts of Baird and Biedenharn in re-deriving and expanding on the results of the original paper. It is very interesting to read some remarks in a paper by Baird and Biedenharn [1]:

> "[T]he paper of Gelfand and Zetlin ... is extremely brief (three pages) and does not appear to have been translated in either the usual Journal translations or the translations on group-theoretical subjects of the American Mathematical Society, or even referred to in the review articles on group theory by Gelfand himself. Moreover, the results are presented without the slightest hint as to the methods employed and contain not a single reference or citation of other work. ... We should like to express our appreciation to Professor Moshinsky for his calling the Gelfand-Zetlin paper to our attention."

One can only speculate as to how Moshinsky was aware of this work. As a student of Wigner's, he had the group theoretical background and training to appreciate the significance of this difficult paper; his parents were from Ukraine and it is possible he was able to read the paper in the original without need of a translation.

The GT bases are difficult to understand because of the extremely compact and powerful notation and are often the first obstacle encountered in attempting to understand the UGA. We will attempt to present the GT bases by informal analogy with the more familiar spherical harmonics Y_{lm}.

The functions Y_{lm} are simultaneous eigenfunctions of the commuting operators L^2 and L_z. Here L^2 is the Casimir operator of the $SO(3)$ group in that it commutes with all the three generators of the group (given by L_x, L_y, L_z). It is useful to think of L_z as the Casimir operator of $SO(2)$. The Y_{lm} are thus adapted to the group chain $SO(3) \supset SO(2)$ each with Casimir operators L^2 and L_z that commute with each other. The values of l and m are directly related to the eigenvalues of the above two operators and serve to completely label the eigenfunctions of these operators. There are limits on the values of m for a given value of l, viz. $-l \leqslant m \leqslant l$. The spherical harmonics Y_{lm} form an invariant irreducible subspace under the action of the generators of the group in that the action of the $SO(3)$ generators on the Y_{lm} results in a linear combination of functions with the same l but differing values of m. Note here that the previous description does not even mention explicit expressions for Y_{lm}, but simply characterizes them by the labels l and m. This would seem to be an inadequate description, but for the purpose of forming matrix elements of $SO(3)$ generators, it is entirely sufficient to know how Y_{lm} transforms under the action of the $SO(3)$ generators and that they are orthogonal; an explicit expression for Y_{lm} is not required. We can look at the labels l and m as a complete and compact way of characterizing spherical harmonics for the purpose of forming matrix elements of the generators of $SO(3)$.

It is helpful to look at the GT bases as a (profound!) generalization of the above scheme to the unitary group $U(n)$. While the group $SO(3)$ has 2 generators, the group $U(n)$ has n^2 generators which are conveniently arranged in an array

$$\begin{bmatrix} E_{11} & E_{12} & E_{13} & \dots & E_{1n} \\ E_{21} & E_{22} & E_{23} & \dots & E_{2n} \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ E_{n1} & E_{n2} & E_{n3} & \dots & E_{nn} \end{bmatrix}$$

Gelfand and Tsetlin were able to construct a total of n Casimir operators (termed Gelfand Invariants) for the Lie algebra of $U(n)$ in terms of the above generators. Explicit expressions for these invariants are presented in [32]. It follows that there are $n, n-1, n-2 \dots 2, 1$ Gelfand Invariants corresponding to each of the the groups $U(n), U(n-1), U(n-2) \dots U(2), U(1)$. Just as the Y_{lm} are based on the group chain $SO(3) \supset SO(2)$, the Gelfand bases are based on the following group chain:

$$U(n) \supset U(n-1) \supset U(n-2) \cdots \supset U(2) \supset U(1) \tag{16}$$

For the above chain, there are a total of $n(n+1)/2$ invariants each of which commutes with all other invariants. The simultaneous eigenfunctions of these invariants are the Gelfand bases which are uniquely labelled by a set of $n(n+1)/2$ integers that are directly related to the eigenvalues of the invariants. This is analogous to looking at the spherical harmonics as simultaneous eigenfunctions of the 2 commuting operators L^2 and L_z; they are uniquely labelled by two integers l and m that are directly related to the eigenvalues of the commuting Casimir operators. The set of $n(n+1)/2$ integers that label a Gelfand basis is conveniently arranged in a Gelfand pattern as shown below:

$$\begin{array}{ccccccccccc} m_{1,n} & & m_{2,n} & & \dots & & m_{n-1,n} & & m_{n,n} \\ & m_{1,n-1} & & m_{2,n-1} & & \dots & & m_{n-1,n-1} & \\ & & \ddots & & \vdots & & \iddots & & \\ & & & m_{1,2} & & m_{2,2} & & & \\ & & & & m_{1,1} & & & & \end{array}$$

These integers satisfy the following conditions:

1) For the topmost row: $m_{1n} \geqslant m_{2,n} \geqslant \cdots \geqslant m_{n,n}$
2) For the subsequent rows: $m_{i,j+1} \geqslant m_{i,j} \geqslant m_{i+1,j+1}$

These $n(n+1)/2$ labels are a generalization of the l, m labels for the Y_{lm} and the "in-between" conditions are generalizations of the simpler conditions on the values of m for a given value of l, (viz. $-l \leqslant m \leqslant l$). The uppermost row in the Gelfand pattern identifies the irrep of $U(n)$ just as the value of l idenitifies the irrep for $SO(3)$. The subsequent rows in the Gelfand pattern identify the specific bases that belong to that irrep, just as the value of m identifies the specific Y_{lm}. Because of the in-between conditions, specifying the uppermost row allows one to fill in all the numbers in the numbers of the subsequent rows. It is thus possible to construct a complete set of basis functions corresponding to an irrep of $U(n)$ each of which is completely labelled by a Gelfand pattern.

The GT bases are a tour-de-force of compactness and abstraction and explicit expressions for these bases are not easy to obtain. However, as mentioned in the description of the Y_{lm}, it is not necessary to have explicit expressions for the basis functions in the construction of matrix elements as long as we are able to determine the action of the generators on the basis functions. Gelfand and Tsetlin provide techniques for obtaining matrix elements of some of the generators of $U(n)$ using GT bases with the rest obtained by recursion relations.

4.2.1 Electronic Gelfand Bases

The section above gave a description of GT bases for a completely general case where the triangular pattern can contain any integers that satisfy the "in-between" conditions. The expressions and technique derived by Gelfand and Tsetlin for the action of the generators of $U(n)$ on the general GT bases are extremely involved and impractical to implement in a code. This was a major reason why the UGA did not make immediate headway after it was introduced by Moshinsky.

Paldus [27] made an important observation that for electronic computations, the highest possible number in the uppermost row of the Gelfand pattern was 2, (based on the Pauli principle). Then using the constraints on the numbers, it was possible to generate the rest of the Gelfand pattern. With this insight, Paldus was able to define an array that contained information equivalent to that in the Gelfand pattern using just $3n$ numbers instead of $n(n+1)/2$ numbers in the Gelfand pattern. Given a Gelfand pattern, one can count the number of *2's 1's* and *0's* in each row i and denote them by a_i, b_i, c_i and this is the Paldus array. Paldus was able to re-derive the general expressions of Gelfand and Tsetlin for the restricted case and they are considerably more tractable. This led to an explosion of interest in the UGA and was an important factor in driving subsequent research in the UGA. The papers on UGA by Paldus and his associates track most of the major developments in the UGA and merit careful study.

4.2.2 Gelfand Patterns and Weyl tableau

The Gelfand pattern with the appropriate numbers in the various rows uniquely specifies a GT basis function. It turns out that a Gelfand pattern can be uniquely associated with a Weyl tableau (a modification of Young tableau where numbers are allowed to repeat), and there are well defined rules for constructing a Weyl tableau from a given Gelfand Pattern [32]. This also holds for the Paldus array where it is shown that the Paldus array corresponds to Weyl tableau with at most two columns. The benefit of being able to specify a GT basis with Weyl tableau is that it is possible to directly construct a tableau given a configuration of electrons; furthermore it is possible to calculate several quantities directly from the tableau, and we will provide examples of this in subsequent sections. An example of the equivalence of a Gelfand Pattern and Weyl Tableau is given below:

$$\begin{array}{ccccccccc} 2 & & 2 & & 0 & & 0 \\ & 2 & & 0 & & 0 & \\ & & 2 & & 0 & & \\ & & & 0 & & & \end{array} \tag{17}$$

$$\begin{array}{|c|c|}\hline 2 & 2 \\ \hline 4 & 4 \\ \hline \end{array} \tag{18}$$

4.3 Symmetry in the Unitary Group Approach

We note here that the role of symmetry in the UGA is different from that seen in problems where the Hamiltonian commutes with the generators of a group. In the UGA, the Hamiltonian itself is expressed in terms of the generators of the unitary group and does *not* commute with the generators of the unitary group. The UGA is an example of a Spectrum Generating Algebra with dynamic symmetry [13]. Block diagonalization occurs because the basis functions form an invariant irreducible subspaces under the action of the generators and is independent of any kind of physical symmetry (except for permutational symmetry which is always present for fermions).

However in many problems it is necessary take into account additional physical symmetries – we would like symmetry-adapted GT bases. The approach that is adopted is similar to the approach used to derive the GT bases themselves. The idea is to work with the Casimir operators of the Lie algebra of the group corresponding to the desired symmetry, and form matrices of these operators with the appropriate GT bases. Since the Casimir operators commute with each other, we can find a set of eigenvectors that are common to all the Casimir operators. These common eigenvectors are linear combinations of GT bases, and are symmetry adapted to the appropriate group, in that they form an invariant irreducible subspace under the action of the generators of the desired group. These eigenvectors can then be used to form matrix elements of the Hamiltonian and result in matrices that are appropriately block diagonal.

An equivalent approach to finding the symmetry adapted GT bases is to use ladder operators. For the $SO(3)$ group, this approach has been adopted by Drake, Kent and Schlesinger [6, 14, 34].

4.4 The appeal of the Unitary Group Approach and issues with extending to other fields

Based on the descriptions above, we see that the UGA offers a conceptually unified approach to structure calculations in a variety of different fields. Regardless of the field of origin, the quantum Hamiltonian is expressed in terms of generators of the unitary group. The GT bases are tailored to match the generators, and techniques are available to calculate the matrix elements of the generators using GT bases. Finally, we can adapt GT bases to the required symmetry by calculating eigenfunctions of Casimir operators of the Lie algebra of the appropriate symmetry group. These eigenfunctions can then be used to calculate matrix elements of the Hamiltonian, and the resultant matrices are blocked in accordance with the symmetry of the Hamiltonian.

While we have not yet explained the implementation of the UGA, it is useful to provide here an example of the benefits of using the UGA for a spin-free Hamiltonian [9]. For a four-electron system with seven spatial orbitals there are 1001 Slater determinants. The unitary group decomposition of this set of determinants into sets of states with well defined S and M_s gives 196 singlet states, 630 triplet states, and 175 quintet states. Thus the matrix is block diagonalized into blocks of size 196, 630 and 175 corresponding to $S = 0, S = 1, S = 2$ respectively. There is additional block diagonalization: within each of these blocks, there there are $2S + 1$ diagonal blocks corresponding to the values of M_s. Thus the $S = 0$ is a singe block, the $S = 1$ block has 3 sub-blocks of size 210 each, and the $S = 1$ block has 5 blocks of size 35 each. Furthermore, the sub-blocks within each block are the same. Thus the solution of a problem of size 1001 has been reduced to the solution of 3 problems of size 196, 210 and 35. This explains the attraction of the UGA for spin-free Hamiltonians. However as explained in the same reference [9], for Hamiltonians with spin terms, the blocks are no longer diagonal but are block-tridiagonal. This means that the problem has not been reduced in size (it's still of size 1001), although it may be simpler to solve than the original problem because of the block tridiagonal nature.

Clearly the benefits of using the GT bases are important. However, there are obstacles in carrying out the above steps when dealing with multi-shell problems for Hamiltonians with spin. When considering multiple shells the expressions become more complex and the formation of matrix elements becomes more involved. With the addition of spin terms in the Hamiltonian, the difficulty goes up significantly, and when we have a combination of multi-shell and spin, the expressions are formidable and the derivations very difficult to follow. All of this is for problems where we employ ls coupling; there has been very little work on solving problems in jj coupling and that is yet another issue that is not easily resolved.

We will briefly present the main steps in the implementation of the UGA. Some of the topics are difficult, and we can only give a brief description of the main concept and point to the appropriate reference for details.

5 Decomposition of basis functions into orbital and spin parts

The first step in the implementation of the UGA is the separation of the basis functions into spin and angular momentum components [27]. For N electrons occupying $2n$ spin-orbitals, the set of determinantal bases forms an irreducible subspace of $U(2n)$. Each determinantal basis function can be decomposed into a product of basis functions that depend on the orbital angular momentum and spin separately. This decomposition (denoted as $U(2n) \supset U(n) \otimes U(2)$) must be such that the overall product is antisymmetric. If the Hamiltonian is spin-free, the spin part of the basis functions does not play a direct role in the formation of the matrix elements; the matrix elements needed are of the form $\langle p|E_{i,j}|q\rangle$ where $E_{i,j}$is a generator of $U(n)$ and p and q are GT bases associated with $U(n)$.

6 Matrix elements of the generators of $U(n)$

There are several methods for determining the matrix elements. We give below brief descriptions of some of the major approaches.

6.1 Basic approach

6.1.1 Using the Paldus Table

The Paldus table for N particles occupying n orbitals with total spin S can be constructed as follows:

$$\begin{aligned} a_n + b_n + c_n &= n \\ b_n &= 2S \\ 2a_n + b_n &= N \end{aligned} \tag{19}$$

where $a_i + b_i + c_i = i$ for each row [28]. Given two GT basis fuctions described by Paldus tables p and q, we need to be able to form matrix elements $\langle p|E_{i,j}|q\rangle$ where $E_{i,j}$ is a generator of $U(n)$. There are several different cases to consider:

- when $i = j$: $\langle p|E_{i,i}|q\rangle = n_i$ where n_i is the occupation number of orbital i.
- when $i \neq j$:
  - A raising generator $i > j$: The first step is to form $\langle p|E_{i,i+1}|q\rangle$ and Paldus provides explicit expressions for $\langle p|E_{i,i+1}|q\rangle$. This is followed by the use of a recursion relation $[E_{i,i+1}, E_{i+1,i+2}] = E_{i,i+2}$ based on the commutation relation of the generators.

– A lowering generator $i < j$: Here we simply utilize the fact that $E_{j,i} = E_{i,j}^{\dagger}$

6.1.2 Using Weyl Tableau

Corresponding to a Paldus table, there is a well defined scheme to construct a Weyl tableau [32]. Harter and Patterson in a series of publications [10,11,31] have used the Weyl tableau to determine the matrix elements. As with the Paldus table approach, the first step is to get expressions for the matrix element $\langle p|E_{i,i+1}|q\rangle$. They provide "jawbone" formulas for the matrix elements of $\langle p|E_{i,i+1}|q\rangle$ in terms of the "city block" distance between two orbitals in a tableau. The other matrix elements are obtained by the same recursion as used above, viz. $[E_{i,i+1}, E_{i+1,i+2}] = E_{i,i+2}$. The tremendous value of tableau is that they provide a visual depiction of the problem and are a good approach from small scale calculations.

In an interesting continuation of the above work, Lin and Cao [24, 25] used the tableau approach to obtain matrix elements $\langle p|E_{i,j}|q\rangle$ without having to use a recursion relationship. The required matrix element is obtained as a product of factors with each factor being calculated with the formula of Harter and Patterson. While not the most efficient approach, this is quite possibly the simplest way to calculate matrix elements in the UGA.

6.2 Graphical Unitary Group Approach

The key insights in the Graphical Unitary Group Approach (GUGA) are due to Shavitt [35–37] who pointed out that the the Paldus array has considerable duplication in the numbers and proposed a "distinct row table" which incorporates the information in several Paldus arrays at once and contains a significantly smaller number of elements as compared to the Paldus arrays. A critical step following this is to represent the information in the distinct row table by a directed graph where each Paldus array is represented by a directed walk. Each walk is numbered and is assigned a weight. The graph is a very compact way of representing all the information about several Paldus arrays at once.

The matrix elements of the generators are expressed as a product of factors where each factor is dependent on the shape of the walks representing the bra and ket vectors. The work of Siegbahn [38] has resulted in further refinement of the GUGA for direct CI calculations where the matrix is never formed and the desired eigenvalues are obtained by iterative techniques that use matrix vector multiplication. An excellent review of developments in this area is given in [33]. The GUGA is the method of choice for large scale computations in quantum chemistry.

6.3 Clifford Algebra Unitary Group Approach

The Clifford Algebra Unitary Group Approach (CAUGA) [29,30] was developed much later than the other approaches described above. Even though it has not been adopted in any large scale calculations, we include it here because it a particularly interesting approach.

The basic concept of the CAUGA is to re-express the generators of the group $U(n)$ in terms of the generators of the group $U(2^n)$ so that the Hamiltonian is made up of these new generators. The GT bases are also re-expressed in terms of basis functions adapted to the group $U(2^n)$. These bases are numbered according to a scheme related to the pattern of elements of Clifford algebra (although there is absolutely no relation of the bases themselves to Clifford algebra). With this numbering scheme, the new basis functions are given by Weyl tableau consisting of just two boxes which are denoted by $[p|q]$. If we use the notation F_{ij} to denote a generator of the group $U(2^n)$, then the action of this generator on the bases is given by:

$$F_{ij}[p|q] = \delta_{jp}\epsilon_{iq}[i|q] + \delta_{jq}\epsilon_{ip}[i|p] \tag{20}$$

where $\epsilon_{rs} = \sqrt{1+\delta_{rs}}$. Matrix elements can be calculated by a dot product of this ket with the appropriate bra which is also in the two-box form $[i|p]$. This is an amazingly simple recipe for calculating matrix elements between the appropriate basis. The entire implementation is dependent upon being able to express $U(n)$ quantities in terms of $U(2^n)$ quantities. A paper by Li and Paldus [21] gives explicit expressions for expanding GT bases in terms of these two-box bases.

We feel that this method has considerable promise but has not been adequately explored perhaps because of the dominance of the GUGA.

7 Matrix elements of products of generators

One-particle operators are expressed as linear combinations of generators of the unitary group. Multi-particle operators result in products of generators and it is necessary to find expressions for the matrix elements using GT bases.

In a series of two papers Lian-Rong and Fen provide explicit expressions for the matrix elements of one and two-body operators between GT bases. In the first paper [22], the Wigner-Eckhart Theorem is used to evaluate the matrix elements of one and two-body operators between general GT bases and the expressions are formidable. In the second paper [23], the matrix elements are given directly in terms of the elements of the Paldus array which makes for convenient implementation. However it is not entirely clear how one would proceed to derive expressions for an arbitrary number of products of generators.

In a series of papers that preceded the papers by Lian-Rong and Fen, Kent and Schlesinger [17–19] have developed an approach that is general, in that they can address an arbitrary number of products of generators. They recast the generator products into higher rank tensors and use graphical methods of angular momentum to show that multigenerator reduced matrix elements can be written as products of *diagonal* matrices.

8 Matrix elements for multi-shell problems

There appears to be two different approaches to dealing with the problem of multi-shell bases functions. The first one due to Kent and Schlesinger [14] use multi-shell Gelfand bases and they mention that, "[I]t is an indication of the power of the unitary group approach that the computer program is the same for single shell and multi-shell problems".

A second approach pioneered by Patterson and Harter [31] starts with the Gelfand-Tsetlin basis for $U(n)$ and then uses the following decomposition.

$$U(n) \supset U(n_1) \otimes U(n_2) \otimes U(n_3) \otimes \cdots \otimes U(n_k) \tag{21}$$

where the total number of orbitals is a sum of the number of orbitals in each of the k shells, $n = n_1 + n_2 + \cdots + n_k$. In effect this decomposes the Gelfand bases corresponding to all orbitals into a sum of products of Gelfand bases corresponding to each shell. Kent and Schlesinger [14] showed that the subduction coefficients that are necessary to effect this decomposition are related to the 3-j symbols. It would appear that this approach has some advantages over the approach of using multi-shell Gelfand bases, because all subsequent development has been along the lines of splitting the Gelfand bases for all orbitals into sums of products of Gelfand bases limited to a single shell.

While there have been several papers dealing with multi-shell GT bases, we will mention a series of two papers due to Gould and Paldus [7, 8] which use a general and powerful approach.

They show that a vector operator can be expanded in terms of shift operators whose action on the GT bases is very well defined; e.g. when the GT bases are represented by a Paldus table, the shift operators change one row of the table by a specified amount. Gould and Paldus have been able to define the action of the shift operators on multi-shell configurations; in particular they show that the intershell shift operators can be resolved into a sum of shift operators with a very simple action on the multi-shell configurations, and thus are able to form matrix operators of vector operators between multi-shell configurations with an arbitrary number of shells. This is a rigorous approach to the multi-shell problem and the concept of shift operators is important: they play a role in the GT bases that is comparable to the role played by ladder operators for the Y_{lm}.

9 Matrix elements for Hamiltonians with spin

The most difficult problem faced by the UGA is to form matrix elements for Hamiltonians containing spin terms (especially for multi-shell configurations). The spin terms cannot be expressed in terms of generators of $U(n)$ but are expressed in terms of generators of $U(2n)$. Harter suggests that the simplest approach to take with $U(2n)$ generators is to recast the GT bases in terms of determinants and form the matrix elements of generators with determinants. This can be tedious and there have two different approaches proposed to solve this problem.

The first approach due to Kent and Schlesinger [15, 16, 20] recasts the generators of $U(2n)$ as products of generators of $U(n+1)$, and then uses the techniques previously established by them for dealing with products of generators [17–19], to calculate the necessary matrix elements. This is certainly a viable approach but gets increasingly difficult for multi-particle spin terms in that a 2-particle spin operator of $U(2n)$ would get translated into a product of 4 generators of $U(n+1)$.

The second approach is described in a series of three papers by Burton and Gould [2–4] and utilizes the concept of an adjoint tensor. The matrix elements of the $U(2n)$ generators are determined by the matrix elements of a single $U(n)$ adjoint tensor operator which is a 2nd degree polynomial in the $U(n)$ generators. These papers combine the spin-dependent problem with the multi-shell problem and use an approach that combines shift operators and adjoint tensors to provide a complete solution to the problem of matrix elements of a spin-dependent Hamiltonian in a multi-shell basis.

10 Racah Algebra

The methods pioneered by Giulio Racah immediately after WWII revolutionized the fields of atomic and nuclear spectroscopy and have been the methods of choice in these fields for over sixty years. These methods are based in group theory, but avoid explicit mention of group theory by using an algebraic approach that is termed Racah Algebra; (an excellent explanation of these methods is given in [39]). The central concept in the Racah algebra is that of irreducible tensor operators (ITO). These are a set of operators that are invariant and irreducible under the action of the generators of the group. In the case of SU(2) for example, the ITO transform in the same fashion as the Y_{lm} functions under the action of the generators. The benefit of using irreducible tensor operators is that it becomes possible to apply the power of the Wigner-Eckhart Theorem in the calculation of the matrix elements. The matrix elements of an ITO between coupled basis functions is given by a product of a "reduced matrix element" that is dependent only on l, and a coupling coefficient; this is a highly efficient approach to forming matrix elements.

It is useful to compare UGA and RA: in the UGA the Hamiltonian is expressed in terms of the generators of the unitary group; in RA, the Hamiltonian is expressed in terms of irreducible tensor operators. In the UGA, the basis functions are the GT bases while in RA, the basis functions are obtained by coupling single particle orbitals to give a coupled basis set. The basic UGA does not change with the problem being considered. However, when we need to take advantage of symmetry, the GT bases need to be adapted to the appropriate symmetry. With RA it is necessary to generate the ITO for every different symmetry and the bases corresponding to that symmetry. It is certainly possible to combine these two approaches; e.g. the ITO can be expressed in terms of the generators of the unitary group and coupled bases can be expressed as linear combinations of GT bases. This has been done by Harter and Patterson [10, 11, 31]

11 Conclusions

The UGA provides a conceptually unified approach for quantum structure calculations. Hamiltonians arising in different fields are re-expressed in terms of the generators of the unitary group. Gelfand-Tsetlin bases form a set of invariant irreducible bases with respect to these operators. The first step in the implementation of the UGA decomposes the determinantal bases into a product of GT bases dependent only on orbital angular momentum and GT bases dependent only on spin, (expressed as $U(2n) \supset U(n) \otimes U(2)$). For spin-free matrix Hamiltonians, the matrix elements between the above bases are not very difficult to form, and there are significant advantages over a purely determinantal approach.

However when dealing with Hamiltonians with spin terms, the generators are now of the group $U(2n)$ and these are not entirely compatible with the $U(n) \otimes U(2)$ bases. The difficulty of forming matrix elements with this combination can be appreciated by noting that separate groups spent over a decade each in coming up with final expressions for this problem (that includes multi-shell bases). Clearly the problem of forming matrix elements of Hamiltonians with spin is feasible with the UGA. However it is not easy.

For the reasons outlined above, we conclude that the UGA does not at this time provide a simpler alternative to Racah Algebra when multi-shell problems with spin are encountered. At various stages in the development of the UGA, there have been important conceptual simplifications. It is our belief that such simplifications will continue, and this pleasing and elegant method will live up to its promise over time.

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