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THE UNITARY GROUP FORMULATION OF THE MANY-BODY PROBLEM: AN ALTERNATIVE TO SECOND QUANTIZATION

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ABSTRACT

Professor Moshinsky (UNAM) has shown that the fermion unitary group formulation of many-body theory is equivalent to the particle number projected second quantized formulation, and that the freeon unitary group formulation is equivalent to the particle number and spin projected second quantized formulation. Our freeon formulation employs *the generator basis*, an overcomplete, non-orthonormal basis constructed by applying weight lowering (excitations) operators to the highest weight (lowest zero-order energy) state. This basis permits facile matrix elements evaluation. We convert the generator basis to the complete, orthonormal Gel'fand basis by means of the Moshinsky-Nagel construction.

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RESUMEN

El profesor Moshinsky (UNAM) ha demostrado que el formalismo del grupo unitario de fermiones en la teoría de muchos-cuerpos es equivalente al de segunda cuantización proyectando número de partículas, y que el formalismo del grupo unitario de partícula libre es equivalente al de segunda cuantización proyectando número de partículas y espín. Nuestro formalismo de partícula libre usa *la base de generadores*, una base sobrecompleta, no-ortonormal construida mediante la aplicación de operadores (excitaciones) que reducen de peso al estado de máximo peso (mínima energía de orden-cero). Esta base permite la fácil evaluación de elementos de matrices. Nosotros transformamos la base de generadores a la base Gel'fand que es completa y ortonormal mediante la construcción Moshinsky-Nagel.

1. INTRODUCTION

The freeon unitary group formulation of quantum chemistry, is currently being widely used in the theory of atoms, molecules and solids when a spin-free Hamiltonian is applicable[1,2]. In this formulation the configuration state spaces are realized by irreducible representation (irrep) spaces of U(p), where p is the number of freeon orbitals. The most familiar basis is the orthonormal, complete Gel'fand basis $\{|G\rangle\}$. We have introduced the overcomplete, non-orthonormal generator basis $\{|E)\}$[3] which permits facile matrix elements evaluation. We relate these two bases by the Moshinsky-Nagel construction[4]. In section 2, we review the unitary group formulation and introduce the Gel'fand and generator bases; in section 3, we describe the procedure for reducing the degree of generator states. In section 4, we use the Moshinsky-Nagel construction to relate the two bases; in section 5, we construct many-body Gel'fand states, and use them in section 6 to calculate Hamiltonian matrix elements. In section 7, we show the second-quantized Hamiltonian matrix elements to be equivalent to our formulation. Section 8 includes summary and conclusions of the unitary group formulation.

2. THE UNITARY GROUP, ITS IRREDUCIBLE REPRESENTATION SPACE AND ITS ALGEBRAS

The group under consideration is U(p), the group of unitary transformations on a vector space,

$$V(p):\{|r), \ r = 1 \text{ to } p\} \quad , \tag{2.1}$$

spanned by p freeon orthonormal vectors. In the quantum mechanical treatement, these vectors represent orbitals; *i.e.*, one-particle states.

Associated with the unitary group U(p), are two algebras:

i) its Lie algebra

$$\text{LAU}(p) : \{E_{rs};\ r,\ s = 1 \text{ to } p\} \quad , \tag{2.2}$$

where the operators E_{rs} commute according to

$$[E_{rs}, E_{tu}] = \text{delta}\ (s,t)\ E_{ru} - \text{delta}\ (r,u)\ E_{ts} \quad . \tag{2.3}$$

ii) its associative enveloping algebra

$$\text{EALU}(p) : \{I, E_{rs}, E_{rs}E_{tu}, \ldots\} \tag{2.4}$$

The irreducible representation spaces (IRS) of U(p) are labeled by partitions of integers

$$[\lambda_p] = [\lambda_1, \lambda_2, \ldots \lambda_p] \tag{2.5}$$

$$\lambda_1 \geqq \ldots \geqq \lambda_p \geqq 0 \tag{2.6}$$

with

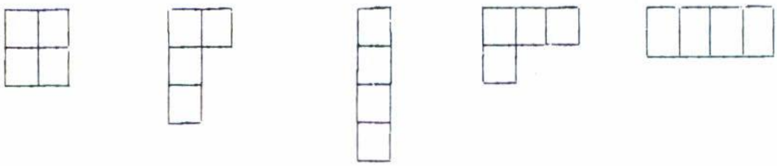
$$\sum_{i=1}^{p} \lambda_i = N \quad , \tag{2.7}$$

where N represents the number of particles. A graphical representation of these partitions consists of Young diagrams $YD[\lambda_p]$, consisting of arrays of N boxes with λ_i boxes in the ith row. For example, when p = 4,

$$[\lambda_4] = [\lambda_1, \lambda_2, \lambda_3, \lambda_4] \tag{2.8}$$

and we can have five possible Young diagrams:

$[2^2]$ $[2, 1^2]$ $[1^4]$ $[3, 1]$ $[4]$



Notice the number of boxes is always 4 (*i.e.* the number of particles), as required by Eq. (2.7). The last two configurations are not of physical significance since these violate the Pauli exclusion principle.

An irreducible representation space is spanned by orthonormal Gel'fand states denoted $|G\rangle$ chosen so as to be symmetry-adapted to the canonical chain

$$U(p) \supset U(p-1) \supset \ldots \supset U(k) \supset \ldots \supset U(1) \tag{2.9}$$

and labeled by Gel'fand arrays

$$A_G = \left\backslash \begin{array}{c} [\lambda_p] \\ \cdots \\ [\lambda_k] \\ [\lambda_1] \end{array} \right/ \quad , \tag{2.10}$$

where

$$[\lambda_k] = [\lambda_{1k} \ \cdots \ \lambda_{Jk} \ \cdots \ \lambda_{kk}] \tag{2.11}$$

labels the $[\lambda_k$ th] irreducible representation space of U(k), identifies the highest weight state of that space and satisfies the betweenness condition:

$$\lambda_{Jk} \geqq \lambda_{J\ k-1} \geqq \lambda_{J-1\ k} \quad . \tag{2.12}$$

Again in the p = 4 case, such an array would look like

$$A_G = \left\backslash \begin{array}{ccccccc} \lambda_{14} & & \lambda_{24} & & \lambda_{34} & & \lambda_{44} \\ & \lambda_{13} & & \lambda_{23} & & \lambda_{33} & \\ & & \lambda_{12} & & \lambda_{22} & & \\ & & & \lambda_{11} & & & \end{array} \right/ \qquad \left\backslash \begin{array}{ccccccc} 2 & & 2 & & 0 & & 0 \\ & 2 & & 2 & & 0 & \\ & & 2 & & 2 & & \\ & & & 2 & & & \end{array} \right/ \tag{2.13}$$

which satisfies Eq. (2.12) as required.

Yet another useful way of representing $|G>$ is with a Gel'fand-Weyl tableu (T_G), constructed by inserting N of the orbitals into YD[λ] in non-descending order along rows and ascending order down columns. By listing in the form of A_G the partitions remaining after the p, then the (p-1)th, etc. integers have been successively removed, one obtains a unique relationship between an A_G and a T_G:

$$T_G = \begin{array}{|c|c|} \hline 1 & 1 \\ \hline 2 & \multicolumn{1}{c}{} \\ \cline{1-1} 4 & \multicolumn{1}{c}{} \\ \cline{1-1} \end{array} \qquad A_G = \left\backslash \begin{array}{ccccccc} 2 & & 1 & & 1 & & 0 \\ & 2 & & 1 & & 0 & \\ & & 2 & & 1 & & \\ & & & 2 & & & \end{array} \right/ \tag{2.14}$$

$$T_G = \begin{array}{|c|c|} \hline 1 & 1 \\ \hline 2 & 2 \\ \hline \end{array} \qquad A_G = \left\backslash \begin{array}{ccccccc} 2 & & 2 & & 0 & & 0 \\ & 2 & & 2 & & 0 & \\ & & 2 & & 2 & & \\ & & & 2 & & & \end{array} \right/ \tag{2.15}$$

As a consequence of the symmetry adaptation, each Gel'fand state is an eigenvector to the diagonal generator (E_{JJ}, J = 1 to p); *i.e.*

$$E_{JJ} \; |G> = wG_J \; |G> \quad , \tag{2.16}$$

where wG_J is the jth component of the weight

$$wG = \{wG_1, \ldots, wG_p\} \tag{2.17}$$

of $|G\rangle$. In terms of the Gel'fand arrays A_G,

$$wG_J = \sum_{i=1}^{j} \lambda_{iJ} - \sum_{i=1}^{j-1} \lambda_{i\ J-1} \tag{2.18}$$

$|G\rangle$ is said to be of higher weight than $|G'\rangle$ if $w_1 > w_1'$ or if $w_1 = w_1'$ then $w_2 > w_2'$, etc. For each $Vp[\lambda]$ there exists a unique highest weight state denoted $|0\rangle$. For the p = 4 singlet case (multiplicity m = # boxes in row 1 - # boxes in row 2 + 1), $|G\rangle = \begin{array}{|c|c|}\hline 1 & 1 \\ \hline 2 & 2 \\ \hline\end{array}$ has higher weight than $|G'\rangle = \begin{array}{|c|c|}\hline 1 & 1 \\ \hline 2 & 3 \\ \hline\end{array}$; writing the A_G for $|G'\rangle$ and recalling Eqs. (2.13) and (2.15):

$$T_G = \begin{array}{|c|c|}\hline 1 & 1 \\ \hline 2 & 3 \\ \hline\end{array} \qquad\qquad A_G = \begin{array}{ccccccc} 2 & & 2 & & 0 & & 0 \\ & 2 & & 2 & & 0 & \\ & & 2 & & 1 & & \\ & & & 2 & & & \end{array} \quad , \tag{2.19}$$

therefore

$$wG_1 = \lambda G_{11} = 2 \quad ,$$

$$wG'_1 = \lambda G'_{11} = 2 \quad ,$$

$$wG_2 = \lambda G_{12} + \lambda G_{22} - \lambda G_{11} = 2 + 2 - 2 = 2 \quad ,$$

$$wG'_2 = \lambda G'_{12} + \lambda G'_{22} - \lambda G'_{11} = 2 + 1 - 2 = 1 \quad ,$$

and we see that $w_1 = w_1'$, but $w_2 > w_2'$ as required to have $|G\rangle$ of higher weight than $|G'\rangle$.

$Vp[\lambda]$ is also spanned by canonical states

$$Vp[\lambda] : \{|E) = E|0>\} \quad , \tag{2.20}$$

where

$$E = E_{rs}\ E_{tu}\ E_{vw}\ .\ .\ . \tag{2.21}$$

with

$$r > s,\ t > u,\ v > w,\ .\ .\ . \tag{2.22}$$

$$r \leqq t \leqq v\ .\ .\ . \tag{2.22}$$

$$\text{if } r = t \text{ then } s \leqq u\ .\ .\ .$$

is a product of generators. Noncanonical generator states can be expressed as linear combinations of canonical generator states by repeated application of the commutation rule (Eq. (2.3)). For example if $t > s > r$, $E_{tr}|0>$ and $E_{sr}E_{ts}|0>$ are canonical, whereas $E_{ts}E_{sr}|0>$ is not but

$$\begin{aligned} E_{ts}E_{sr}|0> &= E_{sr}E_{ts}|0> + [E_{ts}, E_{sr}]\,|0> \\ &= E_{sr}E_{ts}|0> + E_{tr}|0> \quad . \end{aligned} \tag{2.23}$$

3. THE REDUCTION PROCEDURE

We define the degree of a generator state as the number of excitations needed to get from the highest weight state (ground state) to the desired state. The degree of a generator state is frequently reducible. To accomplish this reduction, we apply Eq. 2.3 successively to move the weight-raising operators (operators of the form E_{sr}, $r > s$) to the right, where they vanish when applied to $|0>$ according to the following rules: there exists an occupation number w_i, $i = 1$ to p, for each of the orbitals in $|0>$. Then starting with the occupation numbers of the ground state, the action of E_{rs} on $|0>$ increases w_r by one and decreases w_s by one. The application of a generator E_{rs} to $|0>$ where $w_r = 2$ is identically zero, *i.e.* we may not put a third particle into a doubly occupied orbital. The application of E_{rs} to $|0\rangle$ where $w_s = 0$ vanishes identically since we cannot remove an electron from an empty orbital. For example:

For $$|0\rangle = \begin{array}{|c|c|}\hline 1 & 1 \\ \hline 2 & 2 \\ \hline \end{array} \qquad w_1 = w_2 = 2$$

$$E_{21}|0\rangle = 0 \quad \text{because } w_1 = 1,\ w_2 = 3$$

and

$$E_{31}E_{31}E_{41}|0\rangle = 0 \quad \text{because } w_1 = -1 \quad .$$

In addition, for a given Gel'fand tableu, we define the number of rows with 2 boxes by f; this is the maximum number of doubly occupied orbitals allowed. For a particular state, if the number of w_i's, $i = 1$ to p, equal to 2 is greater than f then the state is zero.
For example,

$$|0\rangle = \begin{array}{|c|c|}\hline 1 & 1 \\ \hline 2 & 2 \\ \hline 3 \\ \cline{1-1} 4 \\ \cline{1-1} \end{array} \qquad f = 2$$

and

$$E_{34}|0\rangle = 0 \quad \text{since} \quad w_1 = w_2 = w_3 = 2 \quad .$$

The generator states are also eigenvectors to the diagonal (number) operators thus (applying eq. 2.3 successively),

$$E_{JJ}|E) = E_{JJ}E_{rs}E_{tu} \cdots |0\rangle \tag{3.1}$$

$$= wE_{J}E_{rs}E_{tu} \cdots |0\rangle \tag{3.2}$$

where

$$wE_{J} = w0_{J} + \text{delta}(j,r) + \text{delta}(j,t) + \ldots$$

$$- \text{delta}(j,s) - \text{delta}(j,u) \ldots \tag{3.3}$$

Note that generator states with different weights are orthogonal. Canonical generator states of equal weight are not generally linearly independent; however, the dependence can be recognized by diagonalizing the Gramm matrix and then removed by an algebraic reduction method:

i) Construct a zero canonical generator vector $|E) = 0$

ii) Apply a weight-raising operator on the left

iii) Reduce the degree of the generator vector

For example, in the $p = 4$ case:

$$|0\rangle = \begin{array}{|c|c|}\hline 1 & 1 \\ \hline 2 & 2 \\ \hline\end{array}$$

$$|E) = E_{21}E_{31}E_{31}|0\rangle = 0 \tag{3.4}$$

Now apply E_{12} on the left (this raises the weight since it takes a particle out of orbital 2 and puts it in orbital 1), and we get

$$0 = E_{12}E_{21}E_{31}E_{31}|0\rangle$$

$$= (E_{21}E_{12} + [E_{12}, E_{21}])\ E_{31}E_{31}|0\rangle$$

$$= E_{21}(E_{31}E_{12} - E_{32})\ E_{31}|0\rangle - 2\ E_{31}E_{31}|0\rangle$$

$$= E_{21}E_{31}\,(E_{31}E_{12} - E_{32})\,|\,0> - E_{21}E_{32}E_{31}|0> - 2\,E_{31}E_{31}$$

$$= (-E_{21}E_{31}E_{32} - E_{21}E_{32}E_{31} - 2\,E_{31}E_{31})\;|0> \qquad (3.5)$$

$$= -2\,E_{21}E_{31}E_{32}|0> - 2\,E_{31}E_{31}|0>$$

$$\Longrightarrow$$

$$E_{31}E_{31}|0> \;=\; -\,E_{21}E_{31}E_{32}|0> \quad .$$

4. THE MOSHINSKY-NAGEL CONSTRUCTION

In the Moshinsky-Nagel transformation, Gel'fand states are constructed from canonical generator states; we can write this as

$$|G> \;=\; \sum_{E} |E)\;(E|G> \qquad (4.1)$$

$$= N_G \prod_{m\geq n\geq 1} L_{mn}^{a_{mn}}|0> \qquad (4.2)$$

where N_G is the normalization constant such that if $<0|0> = 1$ then

$$<G|G> \;=\; <0|G^{+}G|0> \;=\; 1 \qquad (4.3)$$

(where the bracket is evaluated by the reduction process of section 3), a_{mn} is given in terms of A_G by

$$a_{mn} = \lambda_{nm} - \lambda_{n\;m-1} \qquad (4.4)$$

and where

$$L_{mn}^{a_{mn}} = \sum_{E} E\;(E|mn) \qquad (4.5)$$

is a weight lowering operator symmetry-adapted to the chain (Eq. 2.9) by requiring that

$$E_{r\;r+1}L_{mn} = 0 \qquad \text{for} \qquad 1 \leq r \leq n-1 \quad . \qquad (4.6)$$

The coefficients $(E|mn)$ involve products of the eigenvalues of the diagonal operators

$$X_{rs} = E_{rr} - E_{ss} - r + s \quad . \tag{4.7}$$

Examples of this transformation (for the $p = 4$ case) follow, where the L's in Eq. (4.2) have been converted to E's (as in Eq. (4.5)) using Table I from the appendix.

From Eq. (4.2) we get for the general form of a Gel'fand state for U(4)

$$|G\rangle = N_G\, L_{21}^{a_{21}}\, L_{31}^{a_{31}}\, L_{32}^{a_{32}}\, L_{41}^{a_{41}}\, L_{42}^{a_{42}}\, L_{43}^{a_{43}}|0\rangle \tag{4.8}$$

then we have

i)

$$|G\rangle = \begin{array}{|c|c|}\hline 1 & 1 \\ \hline 2 & 3 \\ \hline \end{array} \qquad = \qquad \left\backslash \begin{array}{ccccccc} 2 & & 2 & & 0 & & 0 \\ & 2 & & 2 & & 0 & \\ & & 2 & & 1 & & \\ & & & 2 & & & \end{array} \right/$$

or

$$|G\rangle = N_G\, L_{32}|0\rangle$$

so

$$|G\rangle = N_G\, E_{32}|0\rangle$$

this cannot be reduced, so normalizing

$$\begin{aligned} 1 = \langle G|G\rangle &= N_G^2 \langle 0|E_{23}E_{32}|0\rangle \\ &= N_G^2 \langle 0|\ (E_{32}E_{23} + E_{22} - E_{33})|0\rangle \\ &= 2\ N_G^2 \langle 0|0\rangle \end{aligned}$$

therefore

$$|G\rangle = \frac{1}{\sqrt{2}} E_{32}|0\rangle$$

ii)

$$|G\rangle = \begin{array}{|c|c|} \hline 1 & 1 \\ \hline 3 & 3 \\ \hline \end{array} = \left\backslash \begin{array}{ccccccc} 2 & & 2 & & 0 & & 0 \\ & 2 & & 2 & & 0 & \\ & & 2 & & 0 & & \\ & & & 2 & & & \end{array} \right/$$

so

$$|G\rangle = N_G E_{32}^2|0\rangle$$

$$= N_G E_{32}E_{32}|0\rangle$$

and normalizing

$$1 = \langle G|G\rangle = N_G^2 \langle 0|E_{23}E_{23}E_{32}E_{32}|0\rangle$$

$$= N_G^2 \langle 0|E_{23}(E_{32}E_{23} + E_{22} - E_{33})E_{32}|0\rangle$$

$$= N_G^2 \langle 0|E_{23}E_{32}(E_{32}E_{23} + E_{22} - E_{33})|0\rangle$$

$$= 2N_G^2 \langle 0|E_{23}E_{32}|0\rangle$$

$$= 4N_G^2 \langle 0|0\rangle$$

therefore

$$|G\rangle = \frac{1}{2} E_{32}E_{32}|0\rangle$$

iii)

$$|G\rangle = \begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 & 4 \\ \hline\end{array} \qquad = \qquad \left\backslash \begin{array}{ccccccc} 2 & & 2 & & 0 & & 0 \\ & 2 & & 1 & & 0 & \\ & & 2 & & 0 & & \\ & & & 1 & & & \end{array} \right/$$

or

$$|G\rangle = N_G\ L_{21}L_{32}L_{42}|0\rangle$$

so

$$|G\rangle = N_G\ E_{21}E_{32}(E_{42}(E_{22} - E_{44} + 2) + E_{32}E_{43})|0\rangle$$

$$= 4N_G\ E_{21}E_{32}E_{42}|0\rangle$$

$$= N_G\ (E_{32}E_{21} - E_{31})E_{42}|0\rangle \qquad \text{(absorbing the 4 into } N_G\text{)}$$

$$= N_G\ [E_{32}(E_{42}E_{21} - E_{41}) - E_{31}E_{42}]|0\rangle$$

$$= N_G\ (E_{32}E_{41} + E_{31}E_{42})|0\rangle$$

and normalizing

$$1 = \langle G|G\rangle = N_G^2\ \langle 0|(E_{24}E_{13} + E_{14}E_{23})\ (E_{32}E_{41} + E_{31}E_{42})|0\rangle$$

$$= 4N_G^2\ \langle 0|0\rangle$$

therefore

$$|G\rangle = \frac{1}{2}\ \ (E_{31}E_{42} + E_{32}E_{41})|0\rangle$$

In Table III in the appendix, we include all 20 singlet states for U(4). The reduction and normalization for these states was carried out by hand

and then checked with our MACSYMA program.

5. MANY-BODY GEL'FAND STATES

The generator states are true many-body states since they are independent of both the number of particles (N), and the number of orbitals (p). The Moshinsky-Nagel construction forms Gel'fand states from generator states; if again we do not specify N and p, these Gel'fand states are true many-body states in which we take $p_e = N_e = 2m$ (where m is the degree of excitation), as the effective number of orbitals and effective number of particles respectively. The associated Gel'fand-Weyl tableu will contain $N_e = 2m$ boxes. Below, we provide examples of this many-body representation for singlet states (the extension to higher multiplicities is straightforward and will not be included here for simplicity).

$$|0\rangle = \begin{array}{|c|c|} \hline h_1 & h_1 \\ \hline \vdots & \vdots \\ \hline h_i & h_i \\ \hline \vdots & \vdots \\ \hline h_f & h_f \\ \hline \end{array} \qquad f = N_e/2 \quad .$$

For a single excitation (m = 1), we have:

$$\frac{1}{\sqrt{2}}\,|ph) = \frac{1}{\sqrt{2}}\,E_{ph}\,|0\rangle = \begin{array}{|c|c|} \hline h_1 & h_1 \\ \hline \vdots & \vdots \\ \hline h_i & h_{i+1} \\ \hline \vdots & \vdots \\ \hline h_f & h_p \\ \hline \end{array} = \begin{array}{|c|c|} \hline h & p \\ \hline \end{array}$$

where $h = h_i$ for $1 \leq i \leq f$.

For a double excitation $(m = 2)$:

$$\frac{1}{2}\ |phph) = \frac{1}{2}\ E_{ph}E_{ph}\ |0> = \begin{array}{|c|c|}\hline h_1 & h_1 \\ \hline \vdots & \vdots \\ \hline h_{i-1} & h_{i-1} \\ \hline h_{i+1} & h_{i+1} \\ \hline \vdots & \vdots \\ \hline h_f & h_f \\ \hline h_p & h_p \\ \hline \end{array} = \begin{array}{|c|c|}\hline h & h \\ \hline p & p \\ \hline \end{array}$$

where $h = h_i$ for $1 \leq i \leq f$

$$\frac{1}{2}\ |php'h') = \frac{1}{2}\ E_{ph}\ E_{p'h'}\ |0> = \begin{array}{|c|c|}\hline h_1 & h_1 \\ \hline \vdots & \vdots \\ \hline h_i & h_{i+1} \\ \hline \vdots & \vdots \\ \hline h_j & h_{j+1} \\ \hline \vdots & \vdots \\ \hline h_f & h_f \\ \hline p & p' \\ \hline \end{array} = \begin{array}{|c|c|}\hline h & h' \\ \hline p & p' \\ \hline \end{array}$$

where

$$\left.\begin{array}{ll} h = h_i & 1 \leq i \leq f \\ h' = h_j & 1 \leq j \leq f \end{array}\right\}\quad i \neq f$$

$p \leq p'$

$4p = p'$ then $h < h'$

6. HAMILTONIAN MATIX ELEMENTS

The freeon unitary group Hamiltonian is

$$H = H_0 + V_1 + V_2 \tag{6.1}$$

where

$$H_0 = \sum_r E_r E_{rr} \tag{6.2}$$

$$V_1 = \sum_r \sum_s [rs]\, E_{rs} \tag{6.3}$$

$$V_2 = \frac{1}{2} \sum_r \sum_s \sum_t \sum_u [rs|tu]\, E_{rs} E_{tu} \quad . \tag{6.4}$$

As examples of hamiltonian matrix elements consider (as in section 5 we will assume singlets for simplicity, but the extension to higher multiplicities is not difficult),

i) the energy of the ground state:

$$E(0) = \langle 0|H|0\rangle$$

$$= 2 \sum_h E_h - \sum_h [hh] + 2 \sum_{h_1} \sum_{h_2} [h_1h_1|h_2h_2]$$

$$+ \sum_f \sum_h [hp|ph]$$

ii) energy of a singly excited state:

$$<|h|p|\,|H|\,|p|h|> = (hp|H|ph) = \frac{1}{2} <0|E_{hp} H E_{ph}|0>$$

$$= 2 \sum_{h_1} E_{h_1} + E_p - E_h$$

$$- \sum_{h_1} [h_1h_1] + (1/2) [hh] - (1/2) [pp]$$

$$+ 2\sum_{h_1} \sum_{h_2} [h_1h_1|h_2h_2] - \sum_{h_1} [h_1h_1|hh]$$

$$- \sum_{h_1} [hh|h_1h_1] - (1/2) [hh|hh]$$

$$+ \sum_{h_1} [h_1h_1|pp] + \sum_{h_1} [pp|h_1h_1]$$

$$+ [pp|pp] + [hp|ph] + [ph|hp] \quad .$$

7. SECOND-QUANTIZED CALCULATION OF HAMILTONIAN MATRIX ELEMENTS

The second quantized hamiltonian is

$$H = H_0 + V_1 + V_2 \tag{7.1}$$

where

$$H_0 = \sum_R E_R a_{R+} a_R \tag{7.2}$$

$$V_1 = \sum_R \sum_S [RS] a_{R+} a_S \tag{7.3}$$

$$V_2 = \sum_R \sum_S \sum_T \sum_U [RS|TU] a_{R+} a_{T+} a_U a_S \tag{7.4}$$

and where we have used capital letters to label fermion orbitals which are products of freeon orbitals and spin orbitals, *i.e.*

$$|R - 1> = |r> |\alpha> \tag{7.5}$$

$$|R> \quad = |r> |\beta>$$

with

$$R = 2\ r \quad .$$

For a spin-free Hamiltonian,

$$E_{R-1} = E_R = E_r \tag{7.6}$$

$$[R\ S\text{-}1] = [R\text{-}1\ S] = [r\ s] \tag{7.7}$$

$$\begin{aligned}[R\ S\text{-}1|T\ U\text{-}1] &= [R\ S\text{-}1|T\text{-}1\ U] = [R\text{-}1\ S|T\ U\text{-}1] \\ &= [R\text{-}1\ S|T\text{-}1\ U] = [r\ s|t\ u]\end{aligned} \tag{7.8}$$

$$\begin{aligned}[R\ S|T\ U] &= [R\ S|T\text{-}1\ U\text{-}1] = [R\text{-}1\ S\text{-}1|T\ U] \\ &= [R\text{-}1\ S\text{-}1|T\text{-}1\ U\text{-}1] = 0 \quad .\end{aligned} \tag{7.9}$$

The zero order ground state is

$$|o\rangle = \prod_H a_{H^+}\ a_{H-1}|\rangle \tag{7.10}$$

where $|\ \rangle$ is the vacuum state.

One particle excitations ($m = 1$) from the ground state and their spin projections follow:

$$\begin{aligned}|G_1\rangle &= |P\text{-}1\ H\text{-}1\rangle \\ &= a_{P-1^+}\ a_{H-1}\ |0\rangle \\ &= \left|\begin{matrix}(p\ h) \\ (\alpha\ \beta)\end{matrix}\right\rangle\end{aligned}$$

$$|G_2\rangle = |P\,H\rangle$$

$$= a_P{}^{+}\,a_H\,|0\rangle$$

$$= \left|\begin{matrix}(p\ h)\\ (\alpha\ \beta)\end{matrix}\right\rangle$$

The projections of these two states give the singlet and triplet one particle excitation states, *i.e.*

$$|ph;\ S\rangle = \frac{1}{\sqrt{2}}\,(|G_1\rangle + |G_2\rangle) \tag{7.11}$$

$$|ph;\ T\rangle = \frac{1}{\sqrt{2}}\,(|G_1\rangle - |G_2\rangle) \tag{7.12}$$

and these states correspond to the singlet and triplet obtained with generator states, *i.e.*

$$|ph;\ S\rangle = \boxed{p\,|\,h} = \frac{1}{\sqrt{2}}\ E_{ph}|0\rangle \qquad |0\rangle = \boxed{h\,|\,h} \tag{7.13}$$

$$|ph;\ T\rangle = \begin{array}{|c|}\hline h\\ \hline p\\ \hline\end{array} = E_{ph}|0\rangle \qquad |0\rangle = \begin{array}{|c|}\hline h_1\\ \hline h\\ \hline\end{array} \tag{7.14}$$

Moreover, since not only the states are equivalent, but the Hamiltonians are also analogous (compare Eqs. (7.1)-(7.4) with (6.1)-(6.4), then the matrix elements are the same and the two formulations are equivalent.

8. SUMMARY AND CONCLUSIONS

We have seen how the unitary group formulation can be used as a many-body theory. We use the overcomplete, nonorthonormal particle-hole canonical generator basis formed by applying weight-lowering generators to the highest-weight state. We transform this basis to the complete, orthonormal many-body Gel'fand basis by the Moshinsky-Nagel construction. Matrix elements over the Gel'fand basis are calculated by first expanding in terms of the canonical basis and then evaluating Lie-algebraically using the reduction procedure of section 3. The algebraic reduction is straight-forward, but tedious even for small p and N systems, thus we have developed a symbolic manipulation program using MACSYMA to perform the Moshinsky-Nagel transformation and the evaluation of matrix elements.

The many-body Gel'fand basis offers an alternative to the spin-projected second quantized approach to spin-free many-body theories; *e.g.* perturbation and coupled cluster theories and direct configuration calculations.

Appendix: Table I

Weight Lowering Operators

$$L_{21} = E_{21}$$

$$L_{32} = E_{32}$$

$$L_{31} = E_{31}X_{12} + E_{21}E_{32}$$

$$L_{43} = E_{43}$$

$$L_{42} = E_{42}X_{23} + E_{32}E_{43}$$

$$L_{41} = E_{41}X_{12}X_{13} + E_{31}E_{43}X_{12} + E_{21}E_{42}X_{13} + E_{21}E_{32}E_{43}$$

$$L_{54} = E_{54}$$

$$L_{53} = E_{53}X_{34} + E_{43}E_{54}$$

$$L_{52} = E_{52}X_{23}X_{24} + E_{42}E_{54}X_{23} + E_{32}E_{53}X_{24} + E_{32}E_{43}E_{54}$$

$$\begin{aligned} L_{51} = {} & E_{51}X_{12}X_{13}X_{14} + E_{41}E_{54}X_{12}X_{13} \\ & + E_{31}E_{53}X_{12}X_{14} + E_{21}E_{52}X_{13}X_{14} \\ & + E_{31}E_{43}E_{54}X_{12} + E_{21}E_{42}E_{54}X_{13} \\ & + E_{21}E_{32}E_{53}X_{14} + E_{21}E_{32}E_{43}E_{54} \end{aligned}$$

where

$$X_{rs} = E_{rr} - E_{ss} - r + s \ .$$

Appendix: Table II

General Form for Weight Lowering Operators

$$L_{n+1\ n} = E_{n+1\ n}$$

$$L_{n+2\ n} = E_{n+2\ n} X_{n\ n+1} + E_{n+1\ n} E_{n+2\ n+1}$$

$$\begin{aligned} L_{n+3\ n} &= E_{n+3\ n} X_{n\ n+1} X_{n\ n+2} + E_{n+2\ n} E_{n+3\ n} X_{n\ n+1} \\ &+ E_{n+1\ n} E_{n+3\ n+1} X_{n\ n+2} + E_{n+1\ n} E_{n+2\ n+1} E_{n+3\ n+2} \end{aligned}$$

$$\begin{aligned} L_{n+4\ n} &= E_{n+4\ n} X_{n\ n+1} X_{n\ n+2} X_{n\ n+3} \\ &+ E_{n+3\ n} E_{n+4\ n+3} X_{n\ n+1} X_{n\ n+2} \\ &+ E_{n+2\ n} E_{n+4\ n+2} X_{n\ n+1} X_{n\ n+3} \\ &+ E_{n+1\ n} E_{n+4\ n+1} X_{n\ n+2} X_{n\ n+3} \\ &+ E_{n+2\ n} E_{n+3\ n+2} E_{n+4\ n+3} X_{n\ n+1} \\ &+ E_{n+1\ n} E_{n+3\ n+1} E_{n+4\ n+3} X_{n\ n+2} \\ &+ E_{n+1\ n} E_{n+2\ n+1} E_{n+4\ n+2} X_{n\ n+3} \\ &+ E_{n+1\ n} E_{n+2\ n+1} E_{n+3\ n+2} E_{n+4\ n+3} \end{aligned}$$

where

$$X_{rs} = E_{rr} - E_{ss} - r + s \ .$$

For a more general case, the recursion relationship between lowering operators is useful,

$$L_{mn} = [E_{m\ m-1}, L_{m-1\ n}] X_{n\ m-1} + L_{m-1\ n} E_{m\ m-1}$$

Appendix: Table III

Irreducible, normalized representation of Gel'fand states for

$p = 4$

$$\begin{array}{|c|c|}\hline 1 & 1 \\ \hline 2 & 2 \\ \hline\end{array} = |0\rangle$$

$$\begin{array}{|c|c|}\hline 1 & 1 \\ \hline 2 & 3 \\ \hline\end{array} = \frac{1}{\sqrt{2}} E_{32}|0\rangle$$

$$\begin{array}{|c|c|}\hline 1 & 1 \\ \hline 2 & 4 \\ \hline\end{array} = \frac{1}{\sqrt{2}} E_{42}|0\rangle$$

$$\begin{array}{|c|c|}\hline 1 & 1 \\ \hline 3 & 3 \\ \hline\end{array} = \frac{1}{2} E_{32}E_{32}|0\rangle$$

$$\begin{array}{|c|c|}\hline 1 & 1 \\ \hline 3 & 4 \\ \hline\end{array} = \frac{1}{\sqrt{2}} E_{32}E_{42}|0\rangle$$

$$\begin{array}{|c|c|}\hline 1 & 1 \\ \hline 4 & 4 \\ \hline\end{array} = \frac{1}{2} E_{42}E_{42}|0\rangle$$

$$\begin{array}{|c|c|}\hline 1 & 2 \\ \hline 4 & 4 \\ \hline\end{array} = \frac{1}{\sqrt{2}} E_{41}E_{42}|0\rangle$$

$$\begin{array}{|c|c|}\hline 1 & 3 \\ \hline 2 & 4 \\ \hline\end{array} = \frac{1}{\sqrt{12}} (E_{31}E_{42} - E_{32}E_{41})|0\rangle$$

$$\begin{array}{|c|c|}\hline 1 & 3 \\ \hline 3 & 4 \\ \hline\end{array} = \frac{1}{\sqrt{2}} E_{31}E_{32}E_{42}|0\rangle$$

$$\begin{array}{|c|c|}\hline 1 & 3 \\ \hline 4 & 4 \\ \hline\end{array} = \frac{1}{\sqrt{8}} E_{31}E_{42}E_{42}|0\rangle$$

$$\begin{array}{|c|c|}\hline 2 & 2 \\ \hline 3 & 3 \\ \hline\end{array} = \frac{1}{2} E_{31}E_{31}|0\rangle$$

$$\begin{array}{|c|c|}\hline 2 & 2 \\ \hline 3 & 4 \\ \hline\end{array} = \frac{1}{\sqrt{2}} E_{31}E_{41}|0\rangle$$

$$\begin{array}{|c|c|}\hline 1 & 2 \\ \hline 2 & 3 \\ \hline\end{array} = \frac{1}{\sqrt{2}} E_{31}|0\rangle$$

$$\begin{array}{|c|c|}\hline 1 & 2 \\ \hline 2 & 4 \\ \hline\end{array} = \frac{1}{\sqrt{2}} E_{41}|0\rangle$$

$$\begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 & 3 \\ \hline\end{array} = \frac{1}{\sqrt{2}} E_{31}E_{32}|0\rangle$$

$$\begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 & 4 \\ \hline\end{array} = \frac{1}{2} (E_{31}E_{42} + E_{32}E_{41})|0\rangle$$

$$\begin{array}{|c|c|}\hline 2 & 2 \\ \hline 4 & 4 \\ \hline\end{array} = \frac{1}{2} E_{41}E_{41}|0\rangle$$

$$\begin{array}{|c|c|}\hline 2 & 3 \\ \hline 3 & 4 \\ \hline\end{array} = \frac{1}{\sqrt{8}} E_{31}E_{31}E_{42}|0\rangle$$

$$\begin{array}{|c|c|}\hline 2 & 3 \\ \hline 4 & 4 \\ \hline\end{array} = \frac{1}{\sqrt{2}} E_{31}E_{41}E_{42}|0\rangle$$

$$\begin{array}{|c|c|}\hline 3 & 3 \\ \hline 4 & 4 \\ \hline\end{array} = \frac{1}{4} E_{31}E_{31}E_{42}E_{42}|0\rangle$$

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