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Computer Oriented Method of Coupling Slater Determinants for the Construction of K-Harmonics*

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A method to construct totally antisymmetric K-harmonics with definite total angular momentum, total spin and total isospin, by coupling Slater determinants, is presented. For light nuclei it can be made by hand but, for heavy nuclei, computers must be used. The notation and presentation of the method is made aiming to such a possibility. Changing the determinants by permanents and taking into account the corresponding symmetry modifications, the method applies as well to totally symmetric K-harmonics for the case of boson systems.

Apresenta-se um método para se construir K-harmônicos totalmente antissimétricos com momento angular, spin e isospin totais e suas terceiras componentes bem definidos. Para núcleos leves seu uso pode ser feito à mão mas, para núcleos pesados, é necessário usar-se computadores. A apresentação do método e a notação usada foram feitos tendo em vista essa possibilidade. O método também se aplica a sistema bosônicos, bastando para tanto trocar os determinantes por permanentes e levar em conta as modificações acarretadas pela npva simetria.

1. INTRODUCTION

A method for obtaining bound state energies and wave functions of a systems of A particles, the K- harmonics methods, was i'ntroduced by Zickendraht[1] and Simonov[2]. The startingpoint of themethod is to

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As pointed out by Simonov[9], the polynomials (2.1) are automatically harmonic when $K=K_{min}$ and $K_{min}+1$. For $K>K_{min}+1$, however, they are neither harmonic nor eigenfunctions of total angular momentum (L), total spin (S) an total isospin (T).

In the following, a method to couple the polynomials (2.1), to produce polynomials with definite values of L, M, S, S_z, T and T_z is developed. As an example, it is applied to obtain the K-harmonics appropriate for describing a-particle states with S= T = 0.

The total angular momentum, in the center of mass frame, $\vec{L}$, is defined as the vector sum of the angular momentum in each *relative Jacobi variable*. In terms of the variables $\vec{x}_i=\vec{r}_i-\vec{R}$ it can be written as

$$\vec{L} = \sum_{k=1}^{A}{}' \vec{L}(\vec{x}_k) = -i\hbar \sum_{k=1}^{A}{}' \vec{x}_k \times \vec{\nabla}_{\vec{x}_k} , \qquad (2.4)$$

where the dash in the sum means that one $\vec{x}_i$ (it can be any one) must be excluded.

From (2.4), and the fact that $\vec{L}$ is a first order linear operator, it follows that the effect of acting with any component of $\vec{L}$ on a polynomial of a vector variable $\vec{x}_i$ is the same as the one obtained acting with this component of $\vec{L}(\vec{x}_i)$, i.e.,

$$L_q \; P(\vec{x}_i) \equiv L_q(\vec{x}_i) \; P(\vec{x}_i) \quad , \qquad (2.5)$$

for any polynomial P in the components of the vector $\vec{x}_i$.

One now uses the properties of the derivative of a determinant, to obtain

$$L_q(\phi_1,\phi_2,\ldots,\phi_A) = (\psi_1,\phi_2,\ldots,\phi_A) + (\phi_1,\psi_2,\phi_3,\ldots,\phi_A) + (\phi_1,\ldots,\phi_{A-1}\psi_A), \qquad (2.6)$$

where

$$\psi_i(j) = L_q \; \phi_i(\vec{x}_j) \equiv L_q(\vec{x}_j)\phi_i(\vec{x}_j) \quad , \qquad (2.7)$$

use being made of (2.5) in the last step.

Consider, then, A independent vectors $\vec{v}_i$ and A functions, one for each vector, with definite angular momentum ℓ_i and z-projection m_i. Denoting (sloppily) these functions by $|\ell_i m_i>_i$, the application of a component of the total angular momentum on a product of such functions gives

$$L_q|\ell_1m_1>_1|\ell_2m_2>_2\dots|\ell_Am_A>_A = [L_q(\vec{v}_1)|\ell_1m_1>_1]|\ell_2m_2>_2\dots|\ell_Am_A>_A$$

$$+|\ell_1m_1>_1[L_q(\vec{v}_2)|\ell_2m_2>_2]|\ell_3m_3>_3\dots|\ell_Am_A>_A+\dots+$$

$$+|\ell_1m_1>_1\dots|\ell_{A-1}m_{A-1}>_{A-1}[L_q(\vec{v}_A)|\ell_Am_A>_A] \ . \qquad (2.8)$$

From this result, it follows the usual rules to couple functions of definite angular momentum to obtain functions with definite <u>total</u> angular momentum L and z-projection M.

Equations (2.6) and (2.8) are formally identical. One, then, can use the usual rules of coupling angular momenta to obtain, from (2.1), totally antisymmetric polynomials with definite angular momentum L and z-projection M. Denoting, by $\phi_{n_i\ell_im_i}(\vec{x}_j)$, the functions (2.2) with spatial part given by (2.3), a possible coupling could be

$$\sum_{\text{all } m\text{'s}} <\ell_1m_1\ell_2m_2|\ell_{12}m_{12}><\ell_{12}m_{12}\ell_3m_3|\ell_{123}m_{123}>\dots$$

$$\dots<\ell_{12\dots(A-1)}m_{12\dots(A-1)}\ell_Am_A|LM>(\phi_{n_1\ell_1m_1},\phi_{n_2\ell_2m_2},\dots,\phi_{n_A\ell_Am_A}), \quad (2.9)$$

giving a polynomial with definite angular momentum L and z-projection M.

The same arguments hold in the couplings of spin and isospin and the three couplings are evidently independent.

expand the wave function of the system in terms of a complete set of angular functions over the unity sphere of the $3(A-1)$-dimensional vector space of relative coordinates of the A particles. Such angular functions, whose construction is essential to the method, are known as K-harmonics and are a $3(A-1)$-dimensional generalization of the usual spherical harmonics. They are the angular part of homogeneous and harmonic polynomials in the space variables, whose coefficients are functions of spin and isospin variables.

To enforce the Pauli principle, such K-harmonics must be totally antisymmetric or symmetric in space, spin and isospin variables, according to whether one is dealing with a system of fermions or bosons, respectively. One way of obtaining such totally antisymmetric (symmetric) K-harmonics is to construct spatial polynomials with definite permutational symmetry and couple them with spin-isospin functions of the appropriate permutational symmetry, in order to have functions of the desired symmetry (symmetric or antisymmetric under the exchange of particles) [We quote in Refs. 3-7 some papers in this line.]. Another way is to construct Slater determinants (or permanents) with single particle functions of space, spin and isospin variables. To obtain functions with definite total angular momentum, total spin, total isospin and their z-components, out of these Slater determinants (or permanents), projection techniques are used[8].

It is presented, in this paper, an alternative way to obtain functions with definite quantum numbers, out of Slater determinants (or permanents), just by coupling them in a way similar to the coupling of angular momenta, in which the symmetries of determinants (or permanents) are fully exploited. To allow for the application of such a coupling scheme to heavy nuclei, a non-standard notation, which enables one to translate it in any high level programming language is introduced. The method is developed in terms of Slater determinants, the adaptation for permanents being straightforward.

In Section 2, a method to couple Slater determinants is presented which, in Section 3, is applied to describe the $S=T=0$ states of the alpha particle. In Section 4, the effect of the Laplacian over coupled polynomials is exhibited, while in Section 5 the possibility of applying the method to heavier nuclei is examined.

2. METHOD OF SLATER DETERMINANTS COUPLING

Let us denote by $(\phi_1, \phi_2,\ldots,\phi_A)$ the Slater determinant

$$(\phi_1, \phi_2,\ldots \phi_A) = \begin{vmatrix} \phi_1(1) & \phi_1(2)\ldots & \phi_1(A) \\ \phi_2(1) & \phi_2(2)\ldots & \phi_2(A) \\ \ldots & \ldots & \ldots \\ \phi_A(1) & \phi_A(2)\ldots & \phi_A(A) \end{vmatrix}, \qquad (2.1)$$

constructed from the single-particle functions

$$\phi_i(j) = f_i(\vec{x}_j)\sigma_i(j)\tau_i(j), \qquad (2.2)$$

where $f_i(x_j)$, $\sigma_i(j)$ and $\tau_i(j)$ are, respectively, the spatial, spin and isospin part of the wave function of particle j. The relative spatial coordinate $\vec{x}_j$ is referred to the center of mass, to assure translational invariance to $(\phi_1, \phi_2,\ldots,\phi_A)$.

Taking the functions $f_i(\vec{x}_j)$, in (2.2), as homgeneous polynomials of degrea λ_i, the function (2.1) turns out to be a homgeneous polynomial of degree $K = \Sigma\lambda_i$ in the spatial variables, as required by the K-harmonics rnethod. For a given A, K assumes the values $K= K_{min}$, $K_{min}+1,\ldots$, where K_{min} is a function of A. Following Simonov[9], we will take for the functions $f_i(\vec{x}_j)$ the polynomials

$$f_i(x_j) \equiv f_{n_i\ell_i m_i}(x_j) = (\vec{x}_j^2)^{n_i}\mathcal{Y}^{l_i}_{m_i}(\vec{x}_j), \qquad (2.3)$$

since these polynomials constitute a basis for homgeneous polynomials, of degree $\lambda_i = 2n_i + \ell_i$, in the spatial coordinates. They have the advantage of having definite angular mmentum ℓ_i and z-projection m_i, For a given nucleus, the spin-isospin couplings can be performed once for all, for all degrees K of the spatial part of (2.1). Let us illustrate this point with the K-harmonics which appear in constructing the a-particle states with $S=T=0$.

3. ANTISYMMETRIC POLYNOMIALS FOR A SYSTEM OF TWO PROTONS AND TWO NEUTRONS (ALPHA PARTICLE) WITH S = T = 0

The coupling of four 1/2 spins, to total spin 0, gives rise to two states:

$$
\begin{aligned}
|00\rangle_1 = \frac{1}{2\sqrt{3}} \Big[& 2|1/2\ 1/2\rangle_1 |1/2\ 1/2\rangle_2 |1/2 -1/2\rangle_3 |1/2 -1/2\rangle_4 - \\
& -|1/2\ 1/2\rangle_1 |1/2 -1/2\rangle_2 |1/2\ 1/2\rangle_3 |1/2 -1/2\rangle_4 - \\
& -|1/2 -1/2\rangle_1 |1/2\ 1/2\rangle_2 |1/2\ 1/2\rangle_3 |1/2 -1/2\rangle_4 - \\
& -|1/2\ 1/2\rangle_1 |1/2 -1/2\rangle_2 |1/2 -1/2\rangle_3 |1/2\ 1/2\rangle_4 - \\
& -|1/2 -1/2\rangle_1 |1/2\ 1/2\rangle_2 |1/2 -1/2\rangle_3 |1/2\ 1/2\rangle_4 + \\
& +2|1/2 -1/2\rangle_1 |1/2 -1/2\rangle_2 |1/2\ 1/2\rangle_3 |1/2\ 1/2\rangle_4 \Big]
\end{aligned}
\tag{3.1}
$$

$$
\begin{aligned}
|00\rangle_2 = \frac{1}{2} \Big[& |1/2\ 1/2\rangle_1 |1/2 -1/2\rangle_2 |1/2\ 1/2\rangle_3 |1/2 -1/2\rangle_4 - \\
& -|1/2 -1/2\rangle_1 |1/2\ 1/2\rangle_2 |1/2\ 1/2\rangle_3 |1/2 -1/2\rangle_4 - \\
& -|1/2\ 1/2\rangle_1 |1/2 -1/2\rangle_2 |1/2 -1/2\rangle_3 |1/2\ 1/2\rangle_4 + \\
& +|1/2 -1/2\rangle_1 |1/2\ 1/2\rangle_2 |1/2 -1/2\rangle_3 |1/2\ 1/2\rangle_4 \Big]
\end{aligned}
$$

The same result applies to isospin. So, for <u>fixed</u> spatial parts of the ϕ_i's, there are, at most, four possible antisymmetric polynomials with

$S = T = 0$. Adopting the following enumeration of the spin and isospin functions,

$$
\begin{aligned}
p &= \text{proton with spin up} \leftrightarrow 1\ , \\
\bar{p} &= \text{proton with spin down} \leftrightarrow 2\ , \\
n &= \text{neutron with spin up} \leftrightarrow 3\ , \\
\bar{n} &= \text{neutron with spin down} \leftrightarrow 4\ ,
\end{aligned}
\tag{3.2}
$$

and omitting (for the moment), in the RHS, the spatial parts, these polynomials are written (neglecting overall multiplicative constants) as

$$
\begin{aligned}
P(f,g,h,u)_I = \Big[&(1234)+(1243)+(1324)+(1342)+(2134)+(2143) + \\
&+(2413)+(2431)+(3124)+(3142)+(3412)+(3421) + \\
&+(4213)+(4231)+(4312)+(4321) -2(2233)-(2323) - \\
&-(2332)-(3223)-(3232)-2(3322)-2(1144)-(1414) - \\
&-(1441)-(4114)-(4141)-2(4411)\Big] \ ,
\end{aligned}
$$

$$
\begin{aligned}
P(f,g,h,u)_{II} = \Big[&(1234)+(1243)+(1324)+(1342)-(1423)-(1432) + \\
&+(2134)+(2143)-(2314)-(2341)+(2413)+(2431) + \\
&+(3124)+(3142)-(3214)-(3241)+(3412)+(3421) - \\
&-(4123)-(4132)+(4213)+(4231)+(4312)+(4321) - \\
&-2(2233)-2(3322)-2(1144)-2(4411)\Big] \ ,
\end{aligned}
\tag{3.3}
$$

$$
\begin{aligned}
P(f,g,h,u)_{III} = \Big[&(1234)-(1243)+(1324)-(1342)-(2134)+(2143) + \\
&+(2413)-(2431)+(3412)-(3421)-(3124)+(3142) -
\end{aligned}
$$

$$-(4312)+(4321)-(4213)+(4231)-(2323)+(2332)+$$

$$+(3223)-(3232)-(1414)+(1441)+(4114)-(4141)\Big],$$

$$P(f,g,h,u)_{IV} = \Big[(1234)-(1243)-(1324)+(1342)+(1423)-(1432)-$$

$$-(2134)+(2143)+(2314)-(2341)-(2413)+(2431)+$$

$$+(3124)-(3142)-(3214)+(3241)+(3412)-(3421)+$$

$$+(4132)-(4123)+(4213)-(4231)-(4312)+(4321)\ .$$

In the above expressions, any of the terms (a b c d), on the RHS's, are Slater determinants (2.1), all of them having the same spatial parts ϕ_i given by $f_1=f, f_2=g$, $f_3=h, f_4=u$. The digits 1 to 4, showing up inside parentheses, refer to spin and isospin values, in accordance with conventions (3.2).

When some of the functions f,g,h,u are equal, one can use the symmetries of the Slater determinant to simplify (and, eventually, annihilate) the polynomials (3.3).

Taking into account that the spatial functions in (a b c d) are of the form (2.3), further simplifications occur when some of them, q in number say, have the same quantum numbers, n_i and ℓ_i, differing only be the quantum number m_i. In this case, we make in (3.3) the coupling of the spatial parts, coupling together those q functions. In this way, each term (a b c d), in (3.3), leads to an spatially coupled polynomial with definite L and M, hereby denoted by $\{a\ b\ c\ d\}$. Such coupled polynomials have the additional property that the interchange of two of the numbers $a,b,c,d,$ associated to any two of these q functions, simply multiplies $\{a\ b\ c\ d\}$ by a (-1) factor, if the coupling is symmetric, or leaves it unchanged when antisymmetric. For example,

$$\sum_m (-)^m (\mathcal{Y}^1_m p,\ \mathcal{Y}^1_m \bar{p}, n, \bar{n}) = -\sum_m (-)^m (\mathcal{Y}^1_m \bar{p}\ ,\ \mathcal{Y}^1_m p, n, \bar{n})\ . \qquad (3.4)$$

In this way, when one couples the spatial parts of the Slater determinants in (3.3), substantial simplifications occur in the following cases:

1) When two spatial functions have the same labels n_i ℓ_i and are coupled symmetrically, P_I and P_{II} vanish identically while P_{III} and P_{IV} become[10]

$$P\{f,g,(h,h)^S\}_{III} = \{1234\}+\{1324\}+\{2143\}+\{2413\}+\{3412\}+\{3142\} + $$
$$+ \{4321\}+\{4231\}+\{2332\}+\{3223\}+\{1441\}+\{4114\} ,$$
$$P\{f,g,(h,h)^S\}_{IV} = \{1234\}+\{1423\}+\{1342\}+\{2143\}+\{2314\}+\{2431\} + \tag{3.5}$$
$$+ \{3412\}+\{3241\}+\{3124\}+\{4321\}+\{4132\}+\{4213\} .$$

2) When two spatial functions have the same labels n_i ℓ_i, and are coupled antisymmetrically, P_{III} and P_{IV} vanish identically, while P_I and P_{II} become

$$P\{f,g(h,h)^A\}_I = \{1234\}+\{1324\}+\{2134\}+\{2413\}+\{3124\}+\{3412\} +$$
$$+ \{4213\}+\{4312\}-\{2233\}-\{2332\}-\{3223\}-\{3322\} -$$
$$- \{1144\}-\{1441\}-\{4114\}-\{4411\} ,$$
$$P\{f,g,(h,h)^A\}_{II} =\{1234\}+\{1324\}-\{1423\}+\{2134\}-\{2314\}+\{2413\} + \tag{3.6}$$
$$+\{3124\}-\{3214\}+\{3412\}-\{4123\}+\{4213\}+\{4321\} -$$
$$-\{2233\}-\{3322\}-\{1144\}-\{4411\} .$$

3) When two pairs of spatial functions have the same n_i, ℓ_i, and each pair is coupled symmetrically, we have a particular case of (3.5) and the resulting polynomials are

$$P\{(f,f)^S,(g,g)^S\}_{III} = \{1234\}+\{1324\}+\{2413\}+\{3412\}+\{2332\}+\{1441\} , \tag{3.7}$$

$$P\{(f,f)^S,(g,g)^S\}_{IV} = \{1234\}+\{1423\}+\{1342\}+\{2314\}+\{2431\}+\{3412\} .$$

4) In the situation of item 3, but with an antisymmetric coupling in each pair, one is left once again with only two polynomials:

$$P\{(f,f)^A,(g,g)^A\}_I = 2\{1234\}+2\{1324\}+2\{2413\}+2\{3412\}-2\{2332\}$$
$$-2\{1441\}-\{2233\}-\{3322\}-\{1144\}-\{4411\} ,$$
$$(3.8)$$
$$P\{(f,f)^A,(g,g)^A\}_{II} = 2\{1234\}+2\{1324\}-2\{1423\}-2\{2314\}+2\{2413\} +$$
$$+2\{3412\}-\{2233\}-\{3322\}-\{1144\}-\{4411\} .$$

5) When one pair is coupled symmetrically and the other antisymmetrically, all polynomials (3.3) vanish identically.

6) When thi-ee spatial functions have the same n_i, ℓ_i, and are coupled symmetrically, we have a particular case of (3.5) with $P_{III} \equiv 0$, and one is left with only one polynomial

$$P\{f,(g,g,g)^S\}_{IV} = \{1234\}+\{2143\}+\{3124\}+\{4132\} . \qquad (3.9)$$

7) When three spatial functions have the same n_i, ℓ_i, and are coupled antisymmetrically, one has a particular case of (3.6) with $P_I \propto P_{II}$, so one is left with only one polynomial, namely,

$$P\{f,(g,g,g)^A\}_I = \{1234\}+\{2134\}+\{3124\}+\{4123\}-\{2233\} -$$
$$-\{3322\}-\{1144\}-\{4411\} . \qquad (3.10)$$

8) In the situation of item 7 but with an antisymmetric coupling, only one polinomial remains:

$$P\{(f,f,f,f)^{S \text{ or } A}\} = \{1234\} . \qquad (3.11)$$

It is possible, making use of formulas (3.5)-(3.11), to construct all homogeneous polynomials of any degree K which are used to describe the states of the alpha particle, with $S = T = 0$, and any $L \leq K$. To this end, one first finds all the partitions of K in four non negative integers, and for each partition, one selects all possible functions (2.3) that can be coupled to the desired L value. One, then, simply cheks each possibility, to see in what of cases 1) to 8) it applies.

4. THE EFFECT OF THE LAPLACIAN OPERATOR ON THE COUPLED POLYNOMIALS

Once the coupled polynomials, with definite values of L, M, S, S_z, T, T_z have been constructed, one has to take linear combinations of them in order to obtain *harmonic* polynomials, as required by the K-harmonics method. To this purpose, it is necessary to know the effect of the Laplacian operator on these polynomials. Since they are expressed in the variables $\vec{x}_j$, referred to the center of mass, it is helpful to have the Laplacian in these variables, namely,

$$\nabla^2 f(\vec{x}_1,\ldots,\vec{x}_A) = \frac{1}{A}\left[(A-1)\sum_{k=1}^{A}{}' \nabla^2_{\vec{x}_k} - 2\sum_{k<k'=1}^{N}{}' \vec{\nabla}_{\vec{x}_k}\cdot\vec{\nabla}_{\vec{x}_{k'}}\right] f , \qquad (4.1)$$

where the dashes in the sums mean that one terrn (*it can be anyone*) is missing, and in f, the $\vec{x}$ corresponding to the missing index should be replaced, using the relation

$$\vec{x}_1 + \vec{x}_2 + \ldots + \vec{x}_A = 0 . \qquad (4.2)$$

Another useful formula is

$$(\vec{\nabla} f)\cdot(\vec{\nabla} g) = \frac{1}{A}\left[(A-1)\sum_{k=1}^{A}{}' (\vec{\nabla}_{\vec{x}_k} f)\cdot(\vec{\nabla}_{\vec{x}_{k}} g) - \sum_{k\neq k'=1}^{A}{}' (\vec{\nabla}_{\vec{x}_k} f)\cdot(\vec{\nabla}_{\vec{x}_{k'}} g)\right]. \qquad (4.3)$$

The Laplacian of each polynomial (3.3), of some degree K, being a homogeneous polynomial of degree $K-2$, is expressible as a linear combination of *harmonic* polynomials of type (3.3) with degrees $K-2, K-4, \ldots$, the coefficients of the linear combination being proportional to ρ, ρ^2, $\rho^4, \ldots$, where ρ is the hyperdistance in the $3(A-1)$-dimensional vector space spanned by the relative Jacobi variables [See Ref. 7 for the proof.]. This is a powerful check to the calculationç.

As a warning, it should be mentioned that the polynomials obtained from (3.5) to (3.11) may not be linearly independent, due to the linear dependence among the $\vec{x}_i$'s expressed in Eq. (4.2).

5. APPLICATION TO HEAVIER NUCLEI

In Section 3, one has seen how our method works in describing the $S = T = 0$ states of the alpha particle. It is evident that the method can be applied to describe other states of the alpha particle and of heavier nuclei as well. All we have to do is to obtain the analogs of Eqs. (3.5) to (3.11). For heavier nuclei, this task is, of course, humanly impossible, but at this point one can call the computers to one's rescue. The method has a very rich structure which allows for an easy codification of computer programs to do the job. It was having such a codification in mind that the non-standard notations of Sections 2 and 3 were introduced.

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10. In Eqs. (3.5) to (3.11), the notation $(h,h)^S$ means that two functions, with same values of n_i, ℓ_i, are coupled to a resultant R, the coupling being a symmetric one. Mutandis for $(h,h)^A$, etc... .