The Potential Harmonic Expansion Method

M. Fabre de la Ripelle

Division de Physique Théorique*, Institut de Physique Nucléaire
F-91406 ORSAY Cedex

IPNO-TH 82-9

MARCH 1982

* Laboratoire associé au C.N.R.S.

Abstract

Various properties of the hyperspherical potential basis are investigated. The expansion of any two body function, in particular the two body potential, is given. The matrix elements with two and three potential harmonics needed for the construction of the potential matrix are calculated. Useful recurrence formulae are derived. The concept of potential basis is extended to systems with any number of fermions. A method for improving the accuracy in the expansion of the wavefunction in taking more than the two body correlations is suggested.

-CONTENTS-

Introduction

Among the various methods used for solving the Schrödinger equation the Hyperspherical Harmonic (H.H.) expansion method seems to be one of the most efficient. But any method has its own difficulties. Here the large degeneracy of the H.H. basis prevents to take the complete basis into account in the expansion problems. One must therefore select a restricted basis adapted to the investigated problem. It has been shown longtime ago that in chosing the potential basis[1] for the expansion of the wave function one nearly exhaust the effect of the potential leaving only a weak residual interaction.

It is the consequence of the property that, for a two body interaction the potential basis gives a complete description of the two body correlations. Therefore to go beyond it is necessary to introduce the many body correlations which give only small contributions, at least in nuclear bound state problems, because the probability for three particles (or more) to interact at the same time is small.

In this work a method for constructing the potential basis and calculate the related potential matrix is investigated. The so called optimal subset, which is actually the ingredient from which the wavefunction is constructed, is constituted by linear combinations of elements of the potential basis for various pairs of particles adapted to the required symmetry in the exchange of particles. Before going into the subject let us begin with a brief history of the potential basis.

In the first stage of the H.H. expansion method only the three and four body nuclear bound state have been investigated[2,3]. The results was not encouraging because too many coupled equations should have been integrated to obtain a converged solution even with the most simple potentials[4]. Then Simonov [5] constructed a basis introducing the symmetry in the three particles system as a quantum number. This basis is obviously a linear combination of the unsymmetrized complete basis, nevertheless in keeping only the H.H. exhibiting the required symmetry one reduces again the number of components occuring in the expansion of the wavefunction. But even in using this reduced basis the degeneracy was still too large to enables one to treat the three body problem with realistic interactions[6], because a too large number of coupled equations have again to be integrated in order to obtain a good accuracy. Then the potential basis was introduced [1] in order to reduce to the minimum the number of coupled equations in keeping only the equations directly connected to the most important term in the expansion of the wavefunction.

This potential basis is extracted from the product of the potential and the predominant term occuring in the expansion of the wavefunction. The first proof that this procedure leads to a good solution was given in using the optimal subset for solving the trinucleon bound state in the space completely symmetric S state [7,8,9]. Erens et al.[8] expressed the potential basis as suitable linear combinations of the Simonov basis [5] and studied the error made in using exclusively the optimal subset. The potential basis which was in a first step only constructed for central two body potentials has been later on defined for any tensorial

two body operator [10] and in particular for the nuclear tensor force.

Nearly at the same time Efros[11] also derived the equations leading to the potential basis but he did not understand the adequacy of the technic using the kinematic rotation vector[23] as a tool[1] to derive the matrix elements with potential harmonics. The first physical application of the potential basis has been the calculation of the bound state of the trinucleon system and ^4He[8,9,12-19].

To this respect J. Bruinsma et al.[12] who did not use the potential basis for the D state occuring in the triton wavefunction had difficulties to obtain a converged solution because too many harmonics were included in the D component. Since its first introduction all the good realistic calculations [13-19] have been done in using the potential basis. The extension of the calculation to systems with a large number of fermions is difficult because the basis must be defined individualy for each investigated state. A method for treating this problem has been proposed by Gorbatov et al.[20] and applied to the calculation of either the ground state or excited states of light nuclei with the semi realistic GPDT potential [24].

In recent papers [21,22] we presented another method for solving this problem in defining the weight function associated with the harmonic polynomials constituting the potential basis. The concept of potentail basis is so important in the H.H. expansion method that we thought that an extensive analysis of the properties of this particular subset of the complete H.H. basis deserves a publication.

In this work we derive the potential basis from polynomials associated with a weight function. Then one explains how to calculate the H.H. expansion of a two body operator. In the H.H. expansion method the Schrödinger equation is transformed into an infinite set of coupled second order differential equations. In the last part of this work one shows how to obtain the various matrix elements needed for the calculation of the potential matrix occuring in the coupled equations.

Finally, a few simple applications are given in order to illustrate how the H.H. expansion method must be used.

1-The Hyperspherical Harmonics

Let $(\vec{\xi}_1,\ldots,\vec{\xi}_N)$ be a set of linear coordinates. A homonogeneous polynomial of degree L, $H_{[L]}(\vec{\xi}_1,\ldots,\vec{\xi}_N)$, is harmonic when it fulfils Laplace's equation

$$\sum_{i=1}^{N} \nabla_i^2 \, H_{[L]}(\vec{\xi}_1,\ldots,\vec{\xi}_N) = 0 \qquad (1.1)$$

Let us define the hyperradius

$$r = \left[\sum_{i=1}^{N} \xi_i^2\right]^{1/2} \qquad (1.2)$$

The function

$$Y_{[L]}(\Omega) = r^{-L} H_{[L]}(\vec{\xi}) \quad , \quad (\vec{\xi} \text{ is the set } \vec{\xi}_1,\ldots,\vec{\xi}_N), \qquad (1.3)$$

is called hyperspherical harmonics (H.H.). Ω is a set of 3N-1 angular coordinates describing the position of a point at the surface of the unit hypersphere $r = 1$.

[L] is a set of 3N-1 numbers labelling the polynomial. It could be for instance the degree n of each of the linear coordinates $\vec{\xi}$ occuring in the polynomial, subject to the condition $\sum_{i=1}^{3N} n_i = L$. $Y_{[L]}(\Omega)$ is the value of the harmonic polynomial $H_{[L]}(\vec{\xi})$ at the surface of the unit hypersphere $r = 1$. The complete hyperspherical harmonic basis can be calculated by recurrence. For this purpose one uses the property that the H.H.'s constitute a complete basis for functions defined over the surface of the unit hypersphere.

Therefore, if the $H_{[L]}(\xi_1,\ldots,\xi_q)$ constitute a complete set of orthonormalized H.H. for the linear coordinates $(\xi_1,\ldots,\xi_q)$, then the complete set for the coordinates $(\xi_1,\ldots,\xi_q,\xi_{q+1})$ is given by the solution of the equations :

$$\int H_{[L]}(\xi_1,\ldots,\xi_q)\ p_n^{[L]}(\xi_{q+1})\ p_{n'}^{[L']}(\xi_{q+1})\ H_{[L']}(\xi_1,\ldots,\xi_q)\ d\Omega_{q+1} = \delta_{[L],[L']}\,\delta_{n,n'} \qquad (1.4)$$

where the integral is taken over the surface of the unit hypersphere in the q+1 dimensional space and the p's are polynomials.

Using the hyperspherical coordinates

$$\begin{cases} \xi_{q+1} = r\cos\phi_{q+1} \\ \xi_i = r\sin\phi_{q+1}\ \ldots\ \sin\phi_{i+1}\cos\phi_i \\ \xi_1 = r\sin\phi_{q+1}\ \ldots\ \sin\phi_2 \quad (\phi_1 = 0) \end{cases} \qquad (1.5)$$

the surface elements is given by

$$d\Omega_{q+1} = (\sin\phi_{q+1})^{q-1}(\sin\phi_q)^{q-2}\ \ldots\ \sin\phi_3\ d\phi_{q+1}\ldots\ d\phi_2 \qquad (1.6)$$

and the condition (1.4) becomes

$$\int_0^{\pi}(\sin\phi_{q+1})^{2L+q-1}\ p_n^L(\cos\phi_{q+1})\,p_{n'}^L(\cos\phi_{q+1})\ d\phi_{q+1} = \delta_{n,n'} \qquad (1.7)$$

The polynomials $p_n^L(x)$ associated with the weight function

$(1 - x^2)^{L+\frac{q}{2}-1}$ are Gegenbauer polynomials $C_n^{L+\frac{q-1}{2}}(x)$. The basis obtained by recurrence, which is a product of Gegenbauer polynomials is not adapted to the physical problems because it is not covariante in a rotation of any vector $\vec{\xi}_i$ in the 3 dimensional space.

Instead one can define the harmonic polynomials independently for each coordinate $\vec{\xi}_i$. Let $H_L(\vec{\xi}_\alpha, \vec{\xi}_\beta, \ldots)$ and $h_\ell(\vec{\xi}_i, \vec{\xi}_j, \ldots)$ be two harmonic polynomials of degree L and ℓ respectively of two separate sets of coordinates $(\vec{\xi}_\alpha, \vec{\xi}_\beta, \ldots)$ and $(\vec{\xi}_i, \vec{\xi}_j, \ldots)$. The product $H_L(\vec{\xi}_\alpha, \ldots) h_\ell(\vec{\xi}_i, \ldots)$ is also a harmonic polynomial of degree $L + \ell$. This result is an obvious consequence of the linear structure of the Laplace operator

$$\nabla^2 = \sum_{i=1}^{N} \nabla_i^2 \tag{1.8}$$

Let $H_{[L_{N-1}]}(\vec{\xi}_1, \ldots, \vec{\xi}_{N-1})$ be the complete set of harmonic polynomials for the first coordinates $(\vec{\xi}_1, \ldots, \vec{\xi}_{N-1})$, then $H_{[L_{N-1}]}(\vec{\xi}_1, \ldots, \vec{\xi}_{N-1}) \xi_N^{\ell_N} Y_{\ell_N}^{m_N}(\omega_N)$, where ω_N are the spherical coordinates of $\vec{\xi}_N$ and Y_ℓ^m is a spherical harmonic, is again a harmonic polynomial. Using the notation of the Ref.(1)

$$\left[\sum_{i=1}^{N-1} \xi_i^2\right]^{1/2} = r \sin\phi_N \qquad \xi_N = r \cos\phi_N \qquad 0 \leqslant \phi_N \leqslant \frac{\pi}{2} \tag{1.9}$$

Eq.(1.4) becomes :

$$\int_0^{\pi/2} P_n^{L_{N-1}, \ell_N}(\cos\phi_N)\, P_{n'}^{L_{N-1}, \ell_N}(\cos\phi_N) (\sin\phi_N)^{2L_{N-1}+3N-4} (\cos\phi_N)^{2(\ell_N+1)} d\phi_N = \delta_{n,n'} \tag{1.10}$$

The polynomials $p_n^{L_{N-1},\ell_N}$ are generated by the weight function

$$(1 - x)^{L_{N-1}+\frac{3N-5}{2}} (1 + x)^{\ell_N+\frac{1}{2}}, \quad x = \cos 2\phi_N,$$

in the range $-1 \leq x \leq 1$.

They are the Jacobi polynomials

$$P_n^{\nu_{N-1},\ell_N+\frac{1}{2}}(x) \qquad \text{with} \quad \nu_{N-1} = L_{N-1}+\frac{D-5}{2}$$

in the D = 3N dimensional space. To obtain our basis we now apply a recurrence formula, starting from the 3 dimensional space which provides the spherical harmonics $Y^{m_1}_{\ell_1}(\omega_1)$. The hyperspherical coordinates that we use are[25]

$$\Omega(\omega_1; \omega_2, \phi_2; \ldots; \omega_N, \phi_N) \tag{1.11}$$

where ω_i are the two angular coordinates of $\vec{\xi}_i$ and ϕ_i is given by

$$\tan\phi_i = \left(\sum_{j=1}^{i-1} \xi_j^2\right)^{1/2} \xi_i^{-1} \tag{1.12}$$

i.e. by

$$\begin{cases} \xi_N = r \cos\phi_N \\ \xi_i = r \sin\phi_N \ldots \cos\phi_i \\ \xi_1 = r \sin\phi_N \ldots \sin\phi_2 \qquad (\phi_1 = 0) \end{cases} \tag{1.13}$$

Generating the normalized basis by recurrence one obtains[25]

$$Y_{[L]}(\Omega) = Y_{\ell_1}^{m_1}(\omega_1) \prod_{j=2}^{N} Y_{\ell_j}^{m_j}(\omega_j)\, {}^{(j)}P_{L_j}^{\ell_j, L_{j-1}}(\phi_j) \qquad (1.14)$$

where, following the notation of reference (1),

$${}^{(j)}P_{L_j}^{\ell_j, L_{j-1}}(\phi_j) = \left[\frac{2\nu_j \Gamma(\nu_j - n_j) n_j!}{\Gamma(\nu_j - n_j - \ell_j - \frac{1}{2})\Gamma(n_j + \ell_j + \frac{3}{2})}\right]^{1/2} (\cos\phi_j)^{\ell_j} (\sin\phi_j)^{L_{j-1}}$$

$$P_{n_j}^{\nu_{j-1}, \ell_j + \frac{1}{2}}(\cos 2\phi_j) \qquad (1.15)$$

with

$$\nu_j = \nu_{j-1} + 2n_j + \ell_j + \frac{3}{2} = L_j + \frac{3j}{2} - 1 = L_{j-1} + 2n_j + \ell_j + \frac{3j}{2} - 1$$

$P_n^{a,b}$ is a Jacobi polynomial.

The set $[L]$ of the 3N-1 quantum numbers associated with the 3N-1 degrees of freedom (Ω) is constituted by the 2N orbital and azimutal quantum numbers ℓ_j, m_j $(j = 1,\ldots,N)$ and the N-1 hyperspherical quantum numbers L_j $(j = 2,\ldots,N)$ including the grand orbital quantum number $L = L_N$.

L_j is related to the quantum numbers n_i by

$$L_j = \sum_{i=1}^{j} (2n_i + \ell_i) \ , \ (n_1 = 0) \qquad (1.16)$$

The H.H. (1.14) fulfils the relations

$$\int Y^*_{[L]}(\Omega) Y_{[L']}(\Omega)\, d\Omega = \delta_{[L],[L']} \qquad (1.17)$$

where the Kronecker symbol is one where the two sets [L] and [L'] are identical and zero otherwise. The surface element of the unit hypersphere is

$$d\Omega = d\omega_1 \prod_{j=2}^{N} d\omega_j (\sin\phi_j)^{3j-4} \cos^2\phi_j \, d\phi_j \tag{1.18}$$

In particular, we have

$$\int_0^{\pi/2} {}^{(j)}P_{L_j}^{\ell_j, L_{j-1}}(\phi_j) \, {}^{(j)}P_{L_j'}^{\ell_j, L_{j-1}}(\phi_j) (\sin\phi_j)^{3j-4} \tag{1.19}$$

$$\cos^2\phi_j \, d\phi_j = \delta_{L_j, L_j'}$$

The Laplace operator written in hyperspherical coordinates in the D dimensional space becomes

$$\nabla^2 = \sum_{i=1}^{N} \nabla_i^2 = \frac{d^2}{dr^2} + \frac{D-1}{r} \frac{d}{dr} + \frac{L^2(\Omega)}{r^2} \tag{1.20}$$

where $L^2(\Omega)$ is the grand orbital operator. Noting that $r^L Y_{[L]}(\Omega)$ is a harmonic polynomial one obtains the eigenequation fulfilled by the H.H.

$$\{L^2(\Omega) + L(L+D-2)\} \; Y_{[L]}(\Omega) = 0 \tag{1.21}$$

where L, the degree of the polynomial, is called the grand orbital quantum number.

2-The Potential Basis

Let us assume that we intend to expand in H.H. a function $V(\vec{r}_{ij})$ of the coordinates between the particles $\vec{r}_{ij} = \vec{x}_i - \vec{x}_j$. One defines a set of Jacobi coordinates for which

$$\vec{\xi}_N = \vec{r}_{ij} \tag{2.1}$$

$$r^2 = 2 \sum_{i=1}^{A} (\vec{x}_i - \vec{X})^2 = \frac{2}{A} \sum_{k,\ell>k} r_{k\ell}^2 \ , \quad \vec{X} = \frac{1}{A} \sum_{1}^{A} \vec{x}_i$$

$$A = N + 1$$

The H.H basis which is complete for the expansion of $V(\vec{r}_{ij})$ does not contain any function of the coordinates $\vec{\xi}_j$ with $j < N$ and is therefore given by

$$\mathcal{Y}^{\ell,m}_{2K+\ell}(\Omega_{ij}) = Y^{m}_{\ell}(\omega_{ij}) \ {}^{(N)}P^{\ell,0}_{2K+\ell}(\phi_N) \ Y_0(D-3) \tag{2.2}$$

where we have put $\cos\phi_N = \frac{r_{ij}}{r}$, and

$$Y_0(D-3) = \left(\frac{\Gamma(\frac{D-3}{2})}{2\pi^{\frac{D-3}{2}}} \right)^{1/2} \tag{2.3}$$

is the H.H. of order zero in the D-3 dimensional space spanned by the vectors $(\vec{\xi}_{N-1}, \ldots, \vec{\xi}_1)$.

The subset $\{\mathcal{Y}^{\ell,m}_{2K+\ell}(\Omega_{ij})\}$ constituted by the H.H. of order $2K+\ell$ which are tensors of rank ℓ in the 3 dimensional space is called the "Potential Basis". It enables one to expand in H.H.

any function of $\vec{r}_{ij}$ and in particular any kind of two body potential $V(\vec{r}_{ij})$. It contains only three quantum numbers : the orbital and azimutal quantum numbers ℓ and m , and the grand orbital $2K+\ell$.

The Potential Harmonics fulfil the relation :

$$\int \mathcal{Y}^{\ell,m*}_{2K+\ell}(\Omega_{ij})\ \mathcal{Y}^{\ell',m'}_{2K'+\ell'}(\Omega_{ij})d\Omega = \delta_{K,K'}\ \delta_{\ell,\ell'}\ \ \delta_{m,m'}$$

In terms of hypergeometric polynomials ${}_2F_1$ the potential H.H. become

$$\mathcal{Y}^{\ell,m}_{2K+\ell}(\Omega_{ij}) = f^{\ell}_{K}\ Y^{m}_{\ell}(\omega_{ij})\left(\frac{r_{ij}}{r}\right)^{\ell}\ {}_2F_1\left[-K, K+\ell+\frac{D}{2}-1; \ell+\frac{3}{2}; \frac{r^2_{ij}}{r^2}\right] \qquad (2.4)$$

$$f^{\ell}_{K} = \frac{(-1)^K}{\Gamma(\ell+\frac{3}{2})}\left\{\frac{\Gamma(D-\frac{3}{2})}{\pi^{\frac{D-3}{2}}} \times \frac{(2K+\ell+\frac{D}{2}-1)\Gamma(K+\ell+\frac{D}{2}-1)}{K!\ \Gamma(K+\frac{D-3}{2})} \times \Gamma(K+\ell+\frac{3}{2})\right\}^{1/2}$$

For a definite pair of particles (i,j) and for fixed (ℓ,m) there is a single H.H for any grand orbital $2K+\ell$.

3- The potential multipoles

Let us write the two body potential

$$V(\vec{r}_{ij}) = \sum_{\ell,m} A^{m}_{\ell}(i,j)\ Y^{m}_{\ell}(\omega_{ij})\ V_{\ell}(r_{ij}) \qquad (3.1)$$

where $A^{m}_{\ell}(i,j)$ is an operator independent of the coordinate $\vec{r}_{ij}$. For instance it could be a spin or isospin operator as for the nuclear potential.

The H.H. expansion of the potential is given by

$$V(\vec{r}_{ij}) = \sum_{K,\ell,m} A_{\ell}^{m}(i,j)\, \mathcal{P}_{2K+\ell}^{\ell,m}(\Omega_{ij})\, V_{K}^{(D,\ell)}(r) \qquad (D = 3N) \tag{3.2}$$

where

$$V_{K}^{(D,\ell)}(r) = \langle \mathcal{P}_{2K+\ell}^{\ell,m}(\Omega_{ij}) | V(r_{ij}) \rangle = \left[Y_0(D-3) \right]^{-1} \int_0^{\pi/2} P_{2K+\ell}^{(N)\ell,0}(\phi)\, V_{\ell}(r\cos\phi)\, (\sin\phi)^{D-4} (\cos\phi)^2 d\phi \tag{3.3}$$

is called a "potential multipole".

Using (2.4) the potential multipoles can also be written :

$$V_{K}^{(D,\ell)}(r) = 2\, \frac{(-1)^K}{\Gamma(\ell+\frac{3}{2})} \left\{ \pi^{\frac{D-3}{2}} \frac{(2K+\ell+\frac{D}{2}-1)\Gamma(K+\ell+\frac{D}{2}-1)\Gamma(K+\ell+\frac{3}{2})}{K!\,\Gamma(\frac{D-3}{2})\Gamma(K+\frac{D-3}{2})} \right\}^{1/2} \int_0^1 V_{\ell}(ur)\, {}_2F_1(-K, K+\ell+\tfrac{D}{2}-1; \ell+\tfrac{3}{2}; u^2)(1-u^2)^{\frac{D-5}{2}} u^{\ell+2}\, du \tag{3.4}$$

Various formulae convenient for the calculation of the multipoles are given in the Appendix. For instance, it is shown that they can be obtained by a recurrence formula in starting from the multipoles calculated either for the D = 5 or the D = 6 dimensional space according to whether D is odd or even.

One should note that the multipoles of a central potential $V(\vec{r}_{ij})$ are $2\sqrt{\pi}\, V_{K}^{(D,0)}(r)$ to take into account the spherical harmonic Y_0^0 included in the definition (3.1).

As an example we give the expansion of a central potential $(r_{ij})^n$:

$$(r_{ij})^n = r^n \sum_{K=0}^{\infty} \mathcal{P}^0_{2K}(\Omega_{ij}) \frac{\sqrt{\pi}\Gamma(n+2)}{2^n \Gamma(\frac{n}{2}+1-K)\Gamma(K+\frac{D+n}{2})} \left\{ \frac{\pi^{\frac{D-1}{2}}}{2^{D-5}} \frac{2K+\frac{D}{2}-1}{\Gamma(\frac{D-3}{2})} \frac{(2K+D-4)!}{(2K+1)!} \right\}^{1/2} \qquad (3.5)$$

When $\ell = 0$ the obvious m=0 is taken out.
Any analytic function of r_{ij} can be expanded by using (3.5). When in the above n is an even positive integer the expansion contains only $\frac{n}{2}+1$ terms ($K = 0,1,\ldots,\frac{n}{2}$). For instance an harmonic oscillator (n=2) has a two terms expansion (K=0,1).

The case $n = -1$ provides the expansion of the Coulomb potential. For $n \leq -2$ it may be convenient to use the relation

$$\frac{\sqrt{\pi}}{2^n} \frac{\Gamma(n+2)}{\Gamma(\frac{n}{2}+1-K)} = \frac{2\Gamma(\frac{n+3}{2})\Gamma(\frac{n}{2}+1)}{\Gamma(\frac{n}{2}+1-K)} = (-1)^K 2\Gamma(\frac{n+3}{2}) \frac{\Gamma(K-\frac{n}{2})}{\Gamma(-\frac{n}{2})}$$

If n is not an even integer, the multipoles of a potential which behaves like $(r_{ij})^n$ for short range are in r^n near the origin. A potential which is an analytical function of $(r_{ij})^2$ (as for a Gaussian potential) has multipoles of order K, which behave like r^{2K} when $r \to 0$, because the terms $n<2K$ (n even integer) in the expansion (3.5) vanish.

Eq.(3.4) provides the assymptotic behaviour of the multipoles by using $ur = x$ and taking the limit for $r \to \infty$:

$$V_K^{(D,\ell)}(r) \xrightarrow[r\to\infty]{} (-1)^K \frac{2}{\Gamma(\ell+\frac{3}{2})} \left\{ \pi^{\frac{D-3}{2}} \frac{(2K+\ell+\frac{D}{2}-1)\Gamma(K+\ell+\frac{D}{2}-1)\Gamma(K+\ell+\frac{3}{2})}{K!\Gamma(\frac{D-3}{2})\ \Gamma(K+\frac{D-3}{2})} \right\}^{1/2}$$

$$r^{-(\ell+3)} \int_0^\infty V_\ell(x)\ x^{\ell+2}\ dx \qquad (3.6)$$

which is valid when the integral

$$\lim_{r\to\infty} \int_0^r V_\ell(x)\ x^{2K} \left(1-\frac{x^2}{r^2}\right)^{\frac{D-5}{2}}\ x^{\ell+2}\ dx$$

is finite

This is true for any potential which can be neglected for $x > x_0$ (i.e. $V_\ell(x) = 0$ for $x > x_0$).

4-The Coupled Equations

The ultimate purpose of the hyperspherical formalism is to provide a method for solving the Schrödinger equation. Let us assume for the sake of simplicity that we have to deal with a system of A identical particles, like nucleons in nuclei, and that we intend to solve the Schrödinger equation

$$\left\{ -\frac{\hbar^2}{2m} \sum_{i=1}^{A} \nabla_{\vec{x}_i}^2 + \sum_{i,j>i} V(\vec{r}_{ij}) - E \right\} \Psi(\vec{x}) = 0 \qquad (4.1)$$

where $(\vec{x})$ stands for the set of coordinates $\vec{x}_i$ of the particles

and $V(\vec{r}_{ij})$ is a two body interaction.

The center of mass can be eliminated by using the Jacobi coordinates

$$\vec{\xi}_i = \sqrt{\frac{2i}{i+1}} \left(\vec{x}_{i+1} - \frac{1}{i} \sum_{j=1}^{i} \vec{x}_j \right) \quad , \; i = 1,\ldots,N = A-1$$

leading to the Schrödinger equation in the center of mass

$$\left\{ -\frac{\hbar^2}{m} \nabla^2 + V(\vec{\xi}) - E \right\} \Psi(\vec{\xi}) = 0 \qquad (4.2)$$

where the set of Jacobi coordinates $\{\vec{\xi}\}$ corresponds to the Laplace operator (1.8). In the hyperspherical formalism, the wave function is expanded on the H.H. basis

$$\Psi(\vec{\xi}) = r^{-\frac{D-1}{2}} \sum_{[L]} Y_{[L]}(\Omega) \; u_{[L]}(r) \qquad (4.3)$$

Then (4.2) is transformed into an infinite set of second order coupled differential equations[1]

$$-\left\{ \frac{\hbar^2}{m} \left[\frac{d^2}{dr^2} - \frac{\mathcal{L}(\mathcal{L}+1)}{r^2} \right] + E \right\} u_{[L]}(r)$$

$$+ \sum_{[L']=0}^{\infty} \langle Y_{[L]}(\Omega) \,|\, V(\vec{\xi}) \,|\, Y_{[L']}(\Omega) \rangle \, u_{[L']}(r) = 0 \qquad (4.4)$$

$$\mathcal{L} = L + \frac{D-3}{2}$$

which is subsequently truncated in order to be treated numerically. The degeneracy of the H.H. basis is so large that without a guide enabling one to choose a suitable subset one could not

solve the Schrödinger equation with accuracy. The guide is provided by the procedure leading to the construction of the so called optimal subset. The idea leading to the concept of the optimal subset proceeds from the assumption that the first term (independent of Ω) in the H.H. expansion of the potential $V(\vec{\xi})$ is largely predominant in such a way that the coupling between the various H.H. components of the wave function, mediated by the potential harmonics, can be considered a perturbation.

The validity of this assumtion has been tested for the ground state of few nucleon systems (trinucleon and ^4He) [7-9,12-19]. One finds that for various potentials the contribution of the first hyperspherical term (K = 0) of the potential expansion to the binding energy amounts to 80% or more of the total contribution of the potential. One finds also that in the wave function the first lowest order H.H. (L = 0) is largely dominant. This result lead us to retain in the wave function only those H.H. directly related by the potential to the first predominant term. The H.H. selected according to this procedure constitute the so called "optimal subset". It is therefore the H.H. subset generated by the potential operator $V(\vec{\xi})$ applied to the H.H. of minimal order contributing to the expansion of the investigated state. Let us give an example.

The lowest order H.H. in the expansion of the ground state of the trinucleon system or ^4He is $Y_0(D)$ (all the nucleons in the 1S state). The optimal subset is therefore generated by

$$V(\vec{\xi})Y_0$$

It is constituted by linear combinations of the potential basis. We have shown in another work[21] that the weight function generating the optimal subset is obtained from the minimal order H.H. included in the expansion of the state being investigated. For boson ground states where all the particles may be in the 1S state the minimal order is L = 0 and the optimal subset is again a combination of the potential basis (2.2).

Let us explain the procedure to obtain the coupled equations in this simple case. It will be extended later to the more difficult case of fermion systems. The wave function describing the ground state of a system of A = N+1 bosons interacting through a two body central potential is written in the scheme of the optimal subset

$$\Psi_{g.s.}(\vec{\xi}) = r^{-\frac{D-1}{2}} \sum_{K=0}^{\infty} \left\{ \sum_{i,j>i} \mathcal{Y}^{00}_{2K}(\Omega_{ij}) \right\} u_K(r) \qquad (4.5)$$

The partial waves u_K are solution of the coupled differential equations (4.4), where the $Y_{[L]}(\Omega)$ are the potential harmonics. One needs however only to introduce the potential H.H. for one single pair (i,j), calculate the solution for this pair in projecting out the Schrödinger equation on the potential basis complete for this pair (i,j), and then symmetrize the solution by summing over all the pair (i,j). One can choose arbitrarily the pair (i,j), let us take (2,1), equation (4.4) then becomes :

$$-\left\{ \frac{\hbar^2}{m} \left[\frac{d^2}{dr^2} - \frac{\ell_K(\ell_K+1)}{r^2} \right] + E \right\} u_K(r)$$
$$+ \sum_{K'=0}^{\infty} \langle \mathcal{Y}^{0}_{2K}(\Omega_{21}) \mid V(\vec{\xi}) \mid \mathcal{Y}^{0}_{2K'}(\Omega_{21}) \rangle u_{K'}(r) = 0 \qquad (4.6)$$

where $\mathcal{L}_K = 2K + \frac{D-3}{2}$, $D = 3N$, $N = A-1$.

For the calculation of the potential matrix $\langle \mathcal{P}^0_{2K} | V(\vec{\xi}) | \mathcal{P}^0_{2K'} \rangle$ one uses the potential expansion (3.2) with $\ell = m = 0$ and $A^0_0 = 1$ Matrix elements with two and three potential H.H. occur for various pair (i,j) of particles. The calculation of these matrix elements can be achieved either by taking into account the relationship between H.H. and harmonic oscillator functions, or by using the kinematic rotation vector as a tool in connection with the H.H. expansion of the plane wave.

This last method, which is more flexible, is used in this work. The choice of the potential basis in the expansion (4.5) eliminates from the full set (4.4) the equations which are not coupled to the first predominant equation (K = 0 in (4.6)). It reduces drastically the number of coupled equations by including only two body correlations generated by the two body potential. For taking more than two body correlations into account, the basis must be enlarged and contains more elements than the potential basis.

5-The kinematic rotation vector

Let $\vec{Z}$ be any linear combination of the $\vec{\xi}_i$

$$\vec{Z} = \sum_{i=1}^{N} a_i \vec{\xi}_i = C \sum_{i=1}^{N} \left(\frac{a_i}{C}\right) \vec{\xi}_i \qquad \text{with } C^2 = \sum_{i=1}^{N} a_i^2 \qquad (5.1)$$

One defines the kinematic rotation vector.

$$\vec{z}(\varphi) = \sum_{i=1}^{N} \sin\varphi_N \sin\varphi_{N-1} \cdots \sin\varphi_{i+1} \cos\varphi_i \vec{\xi}_i \ , \ \varphi_1 = 0 \ ; \quad (5.2)$$

and writes (5.1) in terms of the angular parameters (φ)

$$\vec{Z} = C\vec{z}(\varphi) \qquad \text{with} \quad \cos\varphi_i = \frac{a_i}{\left(\sum_{j=1}^{i} a_j^2\right)^{1/2}} \tag{5.3}$$

For isolated systems it is suitable to eliminate the center of mass motion. For a system of A = N+1 identical mass particles one can use the Jacobi coordinates :

$$\begin{cases} \vec{\xi}_N = \vec{x}_2 - \vec{x}_1 \\ \vec{\xi}_{N-i+1} = \sqrt{2\frac{i+1}{i}}\,(\vec{x}_{i+1} - \vec{X}_{i+1}) = \sqrt{\frac{2i}{i+1}}(\vec{x}_{i+1} - \vec{X}_i) \\ \vec{\xi}_1 = \sqrt{\frac{2A}{A-1}}\,(\vec{x}_A - \vec{X}) \\ \vec{X}_j = \frac{1}{j}\sum_{i=1}^{j} \vec{x}_i \qquad , \; X \text{ is the center of mass.} \end{cases} \tag{5.4}$$

One notices that with the choice (5.4) the hyperradius

$$r = \left[\sum_{i=1}^{N} \xi_i^2\right]^{1/2} = \left[2\sum_{i}^{A} (\vec{x}_i - \vec{X})^2\right]^{1/2} = \left[\frac{2}{A}\sum_{i,j>i} (\vec{x}_i - \vec{x}_j)^2\right]^{1/2}$$

is a function invariante and symmetric in any exchange of the particles. Let us denote by (φ^{ij}) the set of parameters for which

$$\vec{x}_i - \vec{x}_j = \vec{z}(\varphi^{ij}) \tag{5.6}$$

For two coordinates in sequence we have

$$\vec{x}_{i+1} - \vec{x}_i = -\sqrt{\frac{i-1}{2i}}\;\vec{\xi}_{N+2-i} + \sqrt{\frac{i+1}{2i}}\;\vec{\xi}_{N+1-i} \tag{5.7}$$

which corresponds to the set

$$\begin{cases} \varphi_j = \frac{\pi}{2} & j > N+2-i \\ \varphi_k = 0 & k < N+2-i \\ \cos\varphi^{i+1,i}_{N+2-i} = -\sqrt{\frac{i-1}{2i}} & \sin\varphi^{i+1,i}_{N+2-1} = \sqrt{\frac{i+1}{2i}} \end{cases} \qquad (5.8)$$

In table 1 are shown the values of the parameters used in this work for the calculation of the matrix elements.

i	j	$\varphi^{i,j}_N$ cos	$\varphi^{i,j}_N$ sin	$\varphi^{i,j}_{N-1}$ cos	$\varphi^{i,j}_{N-1}$ sin	$\varphi^{i,j}_{N-2}$ cos	$\varphi^{i,j}_{N-2}$ sin	$\varphi^{i,j}_{N-3}$ cos	$\varphi^{i,j}_{N-3}$ sin	$\varphi^{i,j}_{N-4}$ cos
2	1	1								
3	2	$-\frac{1}{2}$	$\frac{\sqrt{3}}{2}$	1						
1	3	$-\frac{1}{2}$	$-\frac{\sqrt{3}}{2}$	1						
4	2	$-\frac{1}{2}$	$\frac{\sqrt{3}}{2}$	$\frac{1}{3}$	$\sqrt{\frac{8}{9}}$	1				
4	3	0	1	$-\frac{1}{\sqrt{3}}$	$\sqrt{\frac{2}{3}}$	1				
5	4	0	1	0	1	$-\sqrt{\frac{3}{8}}$	$\sqrt{\frac{5}{8}}$	1		
6	5	0	1	0	1	0	1	$-\sqrt{\frac{2}{5}}$	$\sqrt{\frac{3}{5}}$	1

The indices (i,j) which refer to the pair $\vec{r}_{ij}=\vec{x}_i-\vec{x}_j$ are in the first column. In the following columns are shown the values of $\cos\varphi^{i,j}_k$ and $\sin\varphi^{i,j}_k$ for k = N,N-1,...etc. When $\cos\varphi=1$ in one column it conserves the same value in the other columns situated at right. For any $\vec{x}_i-\vec{x}_j$ where i>j the parameters are obtained in writting $\vec{x}_i-\vec{x}_j=(\vec{x}_i-\vec{x}_{i-i})+(\vec{x}_{i-1}-\vec{x}_{i-2})+\ldots+(\vec{x}_{j+1}-\vec{x}_j)$ and in using (5.7).

6-The plane wave expansion

The calculation of the matrix elements with potential harmonics is carried out in starting from the plane wave expansion[1]:

$$e^{i\vec{k}.\vec{\xi}} = \frac{(2\pi)^{\frac{D}{2}}}{(kr)^{\frac{D}{2}-1}} \sum_{[L]=0}^{\infty} i^{L} Y^{*}_{[L]}(\Omega_k) Y_{[L]}(\Omega) J_{\ell+\frac{1}{2}}(kr) \qquad (6.1)$$

$$\vec{k}.\vec{\xi} = \sum_{i=1}^{N} \vec{k}_i.\vec{\xi}_i \ , \quad \ell = L + \frac{D-3}{2} \ , \quad D = 3N.$$

J is a Bessel function and (k,Ω_k) are hyperspherical coordinates of $\vec{k}$. The sum is taken over all the quantum numbers [L] for L runing from zero to infinity. Defining by $\vec{k}.\vec{\xi} = kr\cos\alpha$ the angle between the directions of $\vec{k}$ and $\vec{\xi}$ in the D dimensional space, the the plane wave can be expanded in terms of Gegenbauer polynomials

$$e^{i\vec{k}.\vec{\xi}} = \Gamma(\tfrac{D}{2}-1)\left(\frac{2}{kr}\right)^{\frac{D}{2}-1} \sum_{L=0}^{\infty} i^{L}(\ell+\tfrac{1}{2}) C_{L}^{\frac{D}{2}-1}(\cos\alpha) J_{\ell+\frac{1}{2}}(kr) \qquad (6.2)$$

leading to the relation between H.H. of the same order L

$$\sum_{[L]} Y^{*}_{[L]}(\Omega)\, Y_{[L]}(\Omega_k) = \tfrac{1}{2}(\ell+\tfrac{1}{2}) \frac{\Gamma(\frac{D}{2}-1)}{\pi^{D/2}} C_{L}^{\frac{D}{2}-1}(\cos\alpha) \qquad (6.3)$$

which generalizes the well known formula between spherical harmonics and Legendre polynomials $C_{\ell}^{1/2}$ in the 3 dimensional space. Here the sum is taken over all the quantum numbers for the grand orbital L fixed. For $\Omega_k = \Omega$, i.e. $\alpha = 0$, one obtains the addition

theorem for surface harmonics

$$\sum_{[L]} Y^{*}_{[L]}(\Omega) Y_{[L]}(\Omega) = \frac{2\mathcal{L}+1}{4\pi^{D/2}} \frac{\Gamma(\frac{D}{2}-1)\ (L+D-3)!}{L!\ (D-3)!} \tag{6.4}$$

Integrating (6.4) over the surface of the unit hypersphere provides the number of independent H.H. of order L

$$N(L) = \frac{(2L+D-2)\ (L+D-3)!}{L!\,(D-2)!} \tag{6.5}$$

in which we used

$$\int d\Omega = \frac{2\pi^{D/2}}{\Gamma(\frac{D}{2})} = \left[Y_0(D)\right]^{-2} \tag{6.6}$$

where $Y_0(D)$ is the H.H of order zero in the D dimensional space. Let us oriente all the vectors $\vec{k}_i$ in the same direction and write each vector $\vec{k}_i$ in hyperspherical coordinates :

$$\vec{k}_i = \sin\varphi_N \ldots \sin\varphi_{i+1}\cos\varphi_i \vec{k} \tag{6.7}$$

where $\vec{k}$ is a 3 dimensional vector with

$$k^2 = \sum_{i=1}^{N} k_i^2$$

Introducing (6.7) in (6.1) gives

$$e^{i\vec{k}.\vec{z}(\varphi)} = \frac{(2\pi)^{D/2}}{(kr)^{\frac{D}{2}-1}} \sum_{[L]=0}^{\infty} i^{L} Y^{*}_{[L]}(\Omega_z)\, Y_{[L]}(\Omega)\, J_{\mathcal{L}+\frac{1}{2}}(kr) \tag{6.8}$$

which provides the H.H. expansion of the 3 dimensional plane wave in the D dimensional space. The angular set Ω_z is constituted by the set $\{\varphi\}$ and ω_k the angular coordinates of $\vec{k}(k,\omega_k)$, leading to

$$Y_{[L]}(\Omega_z) = Y_{\ell_1}^{m_1}(\omega_k) \prod_{i=2}^{N} Y_{\ell_i}^{m_i}(\omega_k) \; P_{L_i}^{(i)\,\ell_i,L_{i-1}}(\varphi_i) \qquad (6.9)$$

In projecting out (6.8) on the spherical harmonic basis $Y_\ell^m(\omega_k)$ and defining the parametric functions[10]

$$Y_{[L]}^{\ell,m}(\varphi) = \int Y_\ell^m(\omega_k)\, Y_{[L]}^{*}(\Omega_z)\, d\omega_k \qquad (6.10)$$

the plane wave expansion becomes

$$e^{i\vec{k}.\vec{z}(\varphi)} = \frac{(2\pi)^{\frac{D}{2}}}{(kr)^{\frac{D}{2}-1}} \sum_{L,\ell,m} i^L\, Y_\ell^{m*}(\omega_k) \left\{ \sum_{[L]} Y_{[L]}^{\ell,m}(\varphi)\, Y_{[L]}(\Omega) \right\} J_{\ell+\frac{1}{2}}(kr) \qquad (6.11)$$

The sum in braces is taken over all the quantum numbers for L fixed. The expression in braces is a H.H. of order L and a tensor of rank ℓ in the 3 dimensional space. When we have to deal with a function of $\vec{Z}$ (Eq.(5.1) and (5.3)) instead of $\vec{z}$, the formula (6.11) is still valid replacing k by Ck (or alternatively r by Cr) inside the Bessel function and in the denominator. Chosing the set φ_{ij} describing $\vec{r}_{ij}$ one obtains $\vec{r}_{21}$ for $\varphi = 0$ (see Table 1) and finds

$$Y_{[L]}^{\ell,m}(0) = P_L^{(N)\,\ell,0}(0)\; Y_0(D-3) \qquad (6.12)$$

There are only two quantum numbers L and ℓ in (6.12). Let us write $L = 2K+\ell$ then Eq.(6.11) becomes:

$$e^{i\vec{k}.\vec{r}_{21}} = \frac{(2\pi)^{\frac{D}{2}}}{(kr)^{\frac{D}{2}-1}} \sum_{K,\ell,m} (-1)^K i^{\ell} {}^{(N)}P^{\ell,0}_{2K+\ell}(0)\, Y_0(D-3)\, Y^{m^*}_{\ell}(\omega_k)$$

$$\times\ Y^{m}_{\ell}(\omega_{21})\, {}^{(N)}P^{\ell,0}_{2K+\ell}(\phi_N)\, Y_0(D-3)\, J_{\ell+\frac{1}{2}}(kr) \qquad (6.13)$$

One recognizes in the second line the potential harmonic (2.2) for the pair (2,1). Defining the H.H. of order $2K+\ell$ related to the coordinate $\vec{r}_{ij}$

$$\mathcal{P}^{\ell,m}_{2K+\ell}(\Omega_{ij}) = \left[{}^{(N)}P^{\ell,0}_{2K+\ell}(0)\, Y_0(D-3) \right]^{-1} \sum_{[L]} Y^{\ell,m_{ij}}_{[L]}(\varphi^{ij})\, Y_{[L]}(\Omega) \qquad (6.14)$$

where $L = 2K+\ell$, and reminding that $\vec{z}(\varphi^{ij}) = \vec{r}_{ij}$, Eq.(6.11) can be written :

$$e^{i\vec{k}.\vec{r}_{ij}} = \frac{(2\pi)^{\frac{D}{2}}}{(kr)^{\frac{D}{2}-1}} \sum_{K,\ell,m} (-1)^K i^{\ell} {}^{(N)}P^{\ell,0}_{2K+\ell}(0)\, Y_0(D-3)\, Y^{m^*}_{\ell}(\omega_k)$$

$$\times\ \mathcal{P}^{\ell,m}_{2K+\ell}(\Omega_{ij})\, J_{\ell+\frac{1}{2}}(kr) \qquad (6.15)$$

A comparison between (6.15) and (6.13) shows that (6.14) provides an expression of the potential harmonics for the pair (i,j) in terms of the angular parameters $\{\varphi^{ij}\}$ related by (5.6) to the Jacobi

coordinates (5.4). This expression will be used in the calculation of the matrix elements with two and three potential H.H..

7-Matrix elements with potential harmonics

Our purpose in this section is to derive the matrix elements with two and three potential H.H. In the first case we intend to calculate

$$\langle \mathcal{Y}^{\ell,m}_{2K+\ell}(\Omega_{k\ell}) | \mathcal{Y}^{\ell,m}_{2K+\ell}(\Omega_{ij}) \rangle$$

where the braket means an integration over the surface of the unit hypersphere in the D=3N dimensional space.

The other matrix elements disappear because the quantum numbers $L(= 2K+\ell), \ell, m$ are conserved in the rotation in hyperspace which transforms the coordinates $\vec{r}_{ij}$ in $\vec{r}_{k\ell}$, and which obviously preserves the hyperradius

$$r = \left[\frac{2}{A} \sum_{i,j>i} r^2_{ij}\right]^{1/2}$$

There are three possibilities : either the two pairs (i,j) and (k,ℓ) are identical, or they have one common index or both are different. In the matrix element the choice of one pair is arbitrary, let us chose for the sake of simplicity $(k,\ell) \equiv (2,1)$. Using Eq.(2.2) for the pair (2,1) and Eq.(6.14) for the pair (i,j) one finds :

$$\langle \mathcal{D}^{\ell,m}_{2K+\ell}(\Omega_{21}) | \mathcal{D}^{\ell,m}_{2K+\ell}(\Omega_{ij}) \rangle = \frac{P^{(N)\,\ell,0}_{2K+\ell}(\varphi_N^{ij})}{P^{(N)\,\ell,0}_{2K+\ell}(0)} = (\cos\varphi_N^{ij})^{\ell} \frac{P_K^{\frac{D-5}{2},\ell+\frac{1}{2}}(\cos 2\varphi_N^{ij})}{P_K^{\frac{D-5}{2},\ell+\frac{1}{2}}(1)} \tag{7.1}$$

where $\varphi_N^{ij}=0$ for $(i,j)\equiv(2,1)$, $\varphi_N^{ij}=\frac{\pi}{2}$ when i and j are larger than 2 (i.e. no common index) and $\cos\varphi_N^{ij}=\pm\frac{1}{2}$ for particles of equal mass when one of the indices only is larger than 2 (one common index).

From (7.1) it comes out that for i and j>2 the matrix element

$$\langle \mathcal{D}^{\ell,m}_{2K+\ell}(\Omega_{21}) | \mathcal{D}^{\ell,m}_{2K+\ell}(\Omega_{ij}) \rangle = \frac{(-1)^K}{2^{2K}} \frac{(2K+1)!}{K!} \frac{\Gamma(\frac{D-3}{2})}{\Gamma(K+\frac{D-3}{2})} \delta_{\ell} \tag{7.2}$$

vanishes for $\ell \neq 0$ when there are no common indices. Of course, the matrix element (7.1) is one when $(i,j)\equiv(2,1)$. For numerical purposes when i or j≤2 (one common index) Eq.(7.1) can be calculated in using the recurrence relation between Jacobi polynomials with $\cos 2\varphi_N^{ij} = -\frac{1}{2}$ for equal mass particles. When $\ell = 0$ it is convenient to rewrite (7.1) in terms of Gegenbauer polynomials leading to the equivalent expression

$$\langle \mathcal{D}^{0}_{2K}(\Omega_{21}) | \mathcal{D}^{0}_{2K}(\Omega_{ij}) \rangle = \frac{(2K+1)!\,(D-5)!}{(2K+D-4)!} \frac{C^{\frac{D}{2}-2}_{2K+1}(\cos\varphi_N^{ij})}{\cos\varphi_N^{ij}}$$

One notices that $x^{-1}\, C^{\frac{D}{2}-2}_{2K+1}(x)$ is independent of the sign of x because $C_{2K+1}(-x) = -C_{2K+1}(x)$. When $\cos\varphi_N^{ij} = \frac{1}{2}$ it is convenient to use the recurrence formula

$$C^{\frac{D}{2}-2}_{n+1}(\tfrac{1}{2}) = \frac{1}{n+1}\left\{(n+\tfrac{D}{2}-2)\,C^{\frac{D}{2}-2}_{n}(\tfrac{1}{2}) - (n+D-5)\,C^{\frac{D}{2}-2}_{n-1}(\tfrac{1}{2})\right\} \tag{7.4}$$

with $C_0=1$, $C^{\frac{D}{2}-2}_{1}(\tfrac{1}{2})=\tfrac{D}{2}-2$, which for large D leads to the asymptotic expression :

$$C^{\frac{D}{2}-2}_{n}(\tfrac{1}{2}) \xrightarrow[D\to\infty]{} \frac{1}{n!}\,\frac{\Gamma(\frac{D}{2}-1)}{\Gamma\left[\frac{D}{2}-(n+1)\right]} \tag{7.5}$$

Eq(7.5) is exact for any D when n=0,1,2 and valid for D>>n.

The simplest matrix element with three potential H.H. refers to identical pairs

$$\langle \mathcal{D}^{\ell,m}_{2K+\ell}(\Omega_{21}) | \mathcal{D}^{\lambda,\mu}_{2\chi+\lambda}(\Omega_{21}) | \mathcal{D}^{\ell',m'}_{2K'+\ell'}(\Omega_{21}) \rangle = Y_0(D-3)$$

$$\langle \ell m|\lambda\mu;\ell' m'\rangle \langle {}^{(N)}P^{\ell,0}_{2K+\ell} | {}^{(N)}P^{\lambda,0}_{2\chi+\lambda} | {}^{(N)}P^{\ell',0}_{2K'+\ell'} \rangle \tag{7.6}$$

where

$$\langle \ell m|\lambda\mu;\ell' m'\rangle = \int Y^{m*}_{\ell}(\omega)\; Y^{\mu}_{\lambda}(\omega)\; Y^{m'}_{\ell'}(\omega)\,d\omega \tag{7.7}$$

The matrix element

$$\langle {}^{(N)}P^{\ell,0}_{2K+\ell} | {}^{(N)}P^{\lambda,0}_{2\chi+\lambda} | {}^{(N)}P^{\ell',0}_{2K'+\ell'} \rangle = \int_0^{\pi/2} (\sin\phi)^{D-4} \cos^2\phi\; {}^{(N)}P^{\ell,0}_{2K+\ell}(\phi)\; {}^{(N)}P^{\lambda,0}_{2\chi+\lambda}(\phi)\; {}^{(N)}P^{\ell',0}_{2K'+\ell'}(\phi)\,d\phi \tag{7.8}$$

is called "3 P coefficient".

When on pair of particles only is different one obtains :

$$\langle \mathcal{D}^{\ell,m}_{2K+\ell}(\Omega_{21}) | \mathcal{D}^{\lambda,\mu}_{2\chi+\lambda}(\Omega_{ij}) | \mathcal{D}^{\ell',m'}_{2K'+\ell'}(\Omega_{21}) \rangle = \langle \mathcal{D}^{\lambda,\mu}_{2\chi+\lambda}(\Omega_{21}) | \mathcal{D}^{\lambda,\mu}_{2\chi+\lambda}(\Omega_{ij}) \rangle$$

$$\langle \mathcal{D}^{\ell,m}_{2K+\ell}(\Omega_{21}) | \mathcal{D}^{\lambda,\mu}_{2\chi+\lambda}(\Omega_{21}) | \mathcal{D}^{\ell',m'}_{2K'+\ell'}(\Omega_{21}) \rangle \qquad (7.9)$$

where the first matrix element is given by (7.1) while the second is (7.6). In the most general case the pairs of particles are different and we have to calculate

$$\langle \mathcal{D}^{\ell,m}_{2K+\ell}(\Omega_{ij}) | \mathcal{D}^{\lambda,\mu}_{2\chi+\lambda}(\Omega_{21}) | \mathcal{D}^{\ell',m'}_{2K'+\ell'}(\Omega_{k\ell}) \rangle$$

Let q be the value in the set $\{\varphi^{ij}\}$ such that

$$\begin{cases} \varphi^{ij}_m = 0 & \text{for } m \leq q \\ \varphi^{ij}_n \neq 0 & \text{for } n > q \end{cases} \qquad (7.10)$$

The parametric function (6.10) is given by

$$Y^{\ell,m}_{[L]}(\varphi^{ij}) = \langle \ell_N m_N ; \ell_{N-1} m_{N-1} ; \ldots ; \ell_q m_q | \ell m \rangle$$

$$P^{(N)\ \ell_N, L_{N-1}}_{L}(\varphi^{ij}_N) \quad P^{(N-1)\ \ell_{N-1}, L_{N-2}}_{L_{N-1}}(\varphi^{ij}_{N-1}) \ldots P^{(q)\ell_q, 0}_{L_q}(0)\ Y_0(3q-3) \qquad (7.11)$$

with

$$\langle \ell_N m_N ; \ldots ; \ell_q m_q | \ell_m \rangle = \int \left[Y^{m_N}_{\ell_N}(\omega) \ldots Y^{m_q}_{\ell_q}(\omega) \right]^* Y^{m}_{\ell}(\omega)\, d\omega \qquad (7.12)$$

The complex conjugate of (7.12) is denoted by $\langle \ell m | \ell_N m_N ; \ldots ; \ell_q m_q \rangle$

Let k be the largest of the q in the sets $\{\varphi^{ij}\}$ and $\{\varphi^{k\ell}\}$

Using (7.11) the general formula giving the matrix element with three potential H.H. is :

$$\langle \mathcal{P}^{\ell,m}_{L}(\Omega_{ij}) | \mathcal{P}^{\lambda\ \mu}_{\Lambda}(\Omega_{21}) | \mathcal{P}^{\ell',m'}_{L'}(\Omega_{k\ell}) \rangle = \frac{\left[Y_0(3k-3) \right]^2}{Y_0(D-3)\ {}^{(N)}P^{\ell,0}_{L}(0)\ {}^{(N)}P^{\ell',0}_{L'}(0)}$$

$$\sum_{\substack{\ell_N,\ell'_N \\ m_N,m'_N \\ \{L_j,\ell_j,m_j \\ j=N-1,\ldots,k}} \langle \ell_N m_N | \lambda\mu ; \ell'_N m'_N \rangle \langle \ell_N m_N ; \ell_{N-1} m_{N-1} ; \ldots ; \ell_k m_k | \ell m \rangle \langle \ell'_N m'_N ; \ell_{N-1} m_{N-1} ; \ldots \ell_k m_k | \ell' m' \rangle \tag{7.13}$$

$$\langle {}^{(N)}P^{\ell_N,L_{N-1}}_{L} \left| {}^{(N)}P^{\lambda,0}_{\Lambda} \right| {}^{(N)}P^{\ell'_N,L_{N-1}}_{L'} \rangle$$

$$ {}^{(N)}P^{\ell_N,L_{N-1}}_{L}(\varphi^{ij}_N)\ {}^{(N)}P^{\ell'_N,L_{N-1}}_{L'}(\varphi^{k\ell}_N) \prod_{q\neq k}^{N-1} {}^{(q)}P^{\ell_q,L_{q-1}}_{L_q}(\varphi^{ij}_q)\ {}^{(q)}P^{\ell_q,L_{q-1}}_{L_q}(\varphi^{k\ell}_q)$$

The 3P coefficient is defined as in (7.8) but with $L_{N-1} \neq 0$. All the possibilities for the pair (i,j) and (k,ℓ) occuring in Eq.(7.13) can be deduced from the restricted cases reported in table I.

Let us treat the case k = N-1 which refers to one of the indices i,j,k,ℓ equal to 1 or 2 i.e. in which there is at least on common index between the three couples of indices.

In Eq.(7.13) the sum must be taken over the seven quantum numbers $m_N, m'_N, m_{N-1}, \ell_N, \ell'_N, \ell_{N-1}$ and L_{N-1}. The sum over m, the azimutal quantum

numbers , can be performed leading to a matrix element including a quadruple sum :

$$\langle \mathcal{P}^{\ell,m}_{L}(\Omega_{ij}) | \mathcal{P}^{\lambda,\mu}_{\Lambda}(\Omega_{21}) | \mathcal{P}^{\ell',m'}_{L'}(\Omega_{k\ell}) \rangle = \frac{\left[Y_0(D-6)\right]^2}{Y_0(D-3)}$$

$$\frac{(-1)^{m+\lambda}}{{}^{(N)}P^{\ell,0}_{(0)\,L}\;{}^{(N)}P^{\ell',0}_{(0)\,L'}} \left[\frac{(2\ell+1)(2\ell'+1)(2\lambda+1)}{(4\pi)^3}\right]^{1/2} \begin{pmatrix} \ell' & \lambda & \ell \\ m' & \mu & -m \end{pmatrix}$$

$$\sum_{\substack{\ell_N,\ell'_N,\ell_{N-1} \\ L_{N-1}}} (-1)^{\ell_{N-1}} (2\ell_N+1)(2\ell'_N+1)(2\ell_{N-1}+1) \begin{pmatrix} \ell_N & \ell'_N & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_N & \ell_{N-1} & \ell \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell'_N & \ell_{N-1} & \ell \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} \ell' & \lambda & \ell \\ \ell_N & \ell_{N-1} & \ell'_N \end{Bmatrix}$$

$$\langle {}^{(N)}P^{\ell_N,L_{N-1}}_{L} | {}^{(N)}P^{\lambda,0}_{\Lambda} | {}^{(N)}P^{\ell'_N,L_{N-1}}_{L'} \rangle$$

$$\langle {}^{(N)}P^{\ell_N,L_{N-1}}_{L}(\varphi^{ij}_N) | {}^{(N)}P^{\ell'_N,L_{N-1}}_{L'}(\varphi^{k\ell}_N) | {}^{(N)}P^{\ell_{N-1},0}_{(0)\,L_{N-1}} | {}^{(N)}P^{\ell_{N-1},0}_{(\varphi^{k\ell}_{N-1})\,L_{N-1}} \rangle \qquad (7.14)$$

we assumed that one of the indices (i,j) is either 1 or 2. When $\lambda = \mu = 0$, a case which happens with central potentials, the matrix element (7.14) contains only a triple sum and takes the simpler form :

$$\langle \mathcal{P}^{\ell,m}_{L}(\Omega_{ij}) | \mathcal{P}^{0}_{\Lambda}(\Omega_{21}) | \mathcal{P}^{\ell,m}_{L'}(\Omega_{ij}) \rangle = \frac{\left[Y_0(D-6)\right]^2}{Y_0(D-3)} \frac{(4\pi)^{-\frac{3}{2}}}{{}^{(N)}P^{\ell,0}_{(0)\,L}\;{}^{(N)}P^{\ell,0}_{(0)\,L'}}$$

$$\sum_{\ell_N,\ell_{N-1},L_{N-1}} (2\ell_N+1)(2\ell_{N-1}+1) \begin{pmatrix} \ell_N & \ell_{N-1} & \ell \\ 0 & 0 & 0 \end{pmatrix}^2 \langle {}^{(N)}P^{\ell_N,L_{N-1}}_{L} | {}^{(N)}P^{0,0}_{\Lambda} | {}^{(N)}P^{\ell_N,L_{N-1}}_{L'} \rangle$$

$$\times \underset{L}{P}{}^{(N)\ell_N,L_{N-1}}(\varphi_N^{ij}) \quad \underset{L'}{P}{}^{(N)\ell_N,L_{N-1}}(\varphi_N^{k\ell}) \quad \underset{L_{N-1}}{P}{}^{(N-1)\ell_{N-1},0}(0) \quad \underset{L_{N-1}}{P}{}^{(N-1)\ell_{N-1},0}(\varphi_{N-1}^{k\ell}) \qquad (7.15)$$

For matrix elements with only central potential harmonics $\ell = m = 0$, the sum over ℓ_{N-1} vanishes and Eq.(7.15) contains a double sum :

$$\langle \mathcal{P}^0_{2K^{ij}}(\Omega_{ij}) | \mathcal{P}^0_{2\chi}(\Omega_{21}) | \mathcal{P}^0_{2K'}(\Omega_{k\ell}) \rangle = \frac{\left[Y_0(D-6)\right]^2}{Y_0(D-3)} \frac{(4\pi)^{-\frac{3}{2}}}{\underset{2K}{P}{}^{(N)\,00}(0)\ \underset{2K'}{P}{}^{(N)\,00}(0)}$$

$$\sum_{\ell_N, L_{N-1}} (2\ell_N+1) \langle \underset{2K}{P}{}^{(N)\ell_N,L_{N-1}} | \underset{2\chi}{P}{}^{(N)\,00} | \underset{2K'}{P}{}^{(N)\ell_N,L_{N-1}} \rangle$$

$$\underset{2K}{P}{}^{(N)\ell_N,L_{N-1}}(\varphi_N^{ij}) \quad \underset{2K'}{P}{}^{(N)\ell_N,L_{N-1}}(\varphi_N^{k\ell}) \quad \underset{L_{N-1}}{P}{}^{(N-1)\ell_N,0}(0) \quad \underset{L_{N-1}}{P}{}^{(N-1)\ell_N,0}(\varphi_{N-1}^{k\ell}) \qquad (7.16)$$

where $\ell_N \leq L_{N-1} \leq \min\left[2K-\ell_N, 2K'-\ell_N\right]$.

Eqs(7.14), (7.15) and (7.16) can be used when one at least of the indices (that we chose in the pair (i,j)) is 1 or 2 . In the last case that we have to investigate there is no common index between the three pairs (2,1), (i,j) and (k,ℓ). One can chose arbitrarily (i,j) = (4,3) and (k,ℓ) = (6,5). One finds that the matrix element (7.13), which vanishes except when $\ell = \ell' = \lambda = 0$, is given by

$$\langle \mathcal{P}^0_{2K}(\Omega_{43}) | \mathcal{P}^0_{2\chi}(\Omega_{21}) | \mathcal{P}^0_{2K'}(\Omega_{65}) \rangle \quad \frac{\left[Y_0(D-9)\right]^2}{Y_0(D-3)} \frac{(4\pi)^{-\frac{5}{2}}}{\underset{2K}{P}{}^{(N)\,00}(0)\ \underset{2K'}{P}{}^{(N)\,00}(0)}$$

$$\times \sum_{L_{N-1}L_{N-2}} \langle {}^{(N)}P^{0,L_{N-1}}_{2K} | {}^{(N)}P^{00}_{2\chi} | {}^{(N)}P^{0,L_{N-1}}_{2K'} \rangle \; {}^{(N)}P^{0,L_{N-1}}_{2K}(\tfrac{\pi}{2}) \; {}^{(N)}P^{0,L_{N-1}}_{2K'}(\tfrac{\pi}{2}) \rangle$$

$$P^{(N-1)\,0,L_{N-2}}_{L_{N-1}^{N}|}(\varphi^{43}_{N-1}) \; P^{(N-1)\,0,L_{N-2}}_{L_{N-1}}(\tfrac{\pi}{2}) \; P^{(N-2)\,00}_{L_{N-2}}(0) \; P^{(N-2)\,00}_{L_{N-2}}(\pi/2) \qquad (7.17)$$

with $\cos\varphi^{43}_{N-1} = -\frac{1}{\sqrt{3}}$ for equal mass particles. Eq.(7.17) applies to any three potential harmonics where each particle occurs only once.

8-3P coefficients

The matrix elements with two and three H.H. are needed for the calculation of the potential matrix in (4.4). For two H.H. we derived the formula (7.1). For three H.H. if one uses a symmetrized (or antisymmetrized) H.H. basis in the expansion of the wave function, the two body potential occuring between the two H.H. in (4.4) can be chosen for an arbitrary pair of particles (e.g. for the pair (2,1)). Then using a H.H. expansion of the potential, as in (3.2), in the calculation of the potential matrix one finds that the needed matrix elements are of the type (7.13).

But if one takes advantage of the closure of the potential basis in an expansion of any two body functions, the Eq.(4.6) is used and the matrix elements can be calculated for only one definite pair of particles (for instance (2,1)). Then the full potential V (ξ) must be sandwiched between two potential harmonics defined for the

same pair (e.g.(2,1)) leading to an utilisation of the matrix elements (7.9) when the potential is expanded in H.H..

In the first procedure the knowledge of the general matrix elements (7.14) and (7.17) are needed,but when we have to deal with unsymmetrized H.H. only the knowledge of the simpler matrix elements (7.9) is necessary. In any case we have to calculate 3P coefficients but for the last procedure only those which refer to $L_{N-1} = 0$ (see Eq.(7.8)) are used. Moreover for central potentials only 3P coefficients with both ℓ and $L_{N-1} = 0$ are needed. A general formula, reproduced in Appendix, giving the 3P coefficients as a double sum has been derived in ref.(27).

Here we intend to give simple recurrence formulae enabling one to calculate the matrix elements (7.8) for central and tensor forces i.e. when ℓ, λ and ℓ' are either 0 or 2.Refering to (7.9) and (3.2) for a central potential, one must calculate the potential matrix

$$<\mathcal{P}^0_{2K}(\Omega_{21})|\ V(r_{ij})|\mathcal{P}^0_{2K'}(\Omega_{21})> =$$

$$\sum_{\chi} <\mathcal{P}^0_{2K}(\Omega_{21})|\mathcal{P}^0_{2\chi}(\Omega_{21})|\mathcal{P}^0_{2K'}(\Omega_{21})><\mathcal{P}^0_{2}(\Omega_{21})|\mathcal{P}^0_{2\chi}(\Omega_{ij})>\ V^{(D,0)}_{\chi}(r) \tag{8.1}$$

where the last matrix element is given by (7.3). The first matrix element is (7.6) with $\ell = \lambda = \ell' = 0$. In order to calculate the 3P coefficients (7.8) one derives two different expressions for $P^{(N)}$. First one uses the relation between Jacobi $P_n^{a,\frac{1}{2}}(\cos 2\phi)$ and Gegenbauer $C^{a+\frac{1}{2}}_{2n+1}(\cos\phi)$ polynomials[28] to write :

$$P^{(N)\ 0,L_{N-1}}_{2K+L_{N-1}}(\phi) = g(\nu,K)\ \frac{(\sin\phi)^{L_{N-1}}}{\cos\phi}\ C^{\nu}_{2K+1}(\cos\phi) \qquad (8.2)$$

where

$$g(\nu,K) = 2^{\nu-\frac{1}{2}}\Gamma(\nu)\left[\frac{2}{\pi}\ \frac{(2K+\nu+1)(2K+1)!}{[2(K+\nu)]!}\right]^{1/2}$$

$$\nu = L_{N-1}+\frac{D}{2} - 2 \qquad (29)$$

Then one utilizes the relation between Jacobi polynomials

$$(n+\nu)\ P^{\nu-\frac{1}{2},\frac{1}{2}}_{n}(x) + (n+\nu-\tfrac{1}{2})P^{\nu-\frac{1}{2},\frac{1}{2}}_{n-1}(x) = (2n+\nu)\ P^{\nu-\frac{1}{2},-\frac{1}{2}}_{n}(x)$$

to find the relation between two contiguous $^{(N)}P$ functions :

$$P^{(N)\ 0,L_{N-1}}_{2K+L_{N-1}}(\phi) + \left[\frac{2K+\nu+1}{2K+\nu-1}\quad\frac{2K+2\nu-1}{K+\nu}\quad\frac{K}{2K+1}\right]^{1/2} P^{(N)\ 0,L_{N-1}}_{2(K-1)+L_{N-1}}(\phi)$$

$$= 2\ \frac{2K+\nu}{2K+1}\ g(\nu,K)\ (\sin\phi)^{L_{N-1}}\ C^{\nu}_{2K}(\cos\phi) \qquad (8.3)$$

Introducing twice (8.2) and once (8.3) into Eq.(7.8) for $\ell=\ell'=\lambda=0$ one obtains the recurrence formula

$$\langle P^{(N)\ 0,0}_{2K}\ |\ .\ P^{(N)\ 0,0}_{2\chi}\ |\ P^{(N)\ 0,0}_{2K'}\rangle$$

$$+\left[\frac{2\chi+\nu+1}{2\chi+\nu-1}\ .\ \frac{2\chi+2\nu-1}{\chi+\nu}\ .\ \frac{\chi}{2\chi+1}\right]^{1/2} \langle P^{(N)\ 0,0}_{2K}\ |\ P^{(N)\ 0,0}_{2(\chi-1)}\ |\ P^{(N)\ 0,0}_{2K'}\rangle$$

$$= \frac{2\chi+\nu}{2\chi+1}\ g(\nu,K)\ g(\nu,K')\ g(\nu,\chi)\ D_1(\nu,2K+1,2K'+1,2\chi) \qquad (8.4)$$

where D_1, the integral calculated by Hsü [30], is given in terms of binomial coefficients by

$$D_1(\nu,2K+1,2K'+1,2\chi) = \frac{\pi}{2^{2\nu-1}} \binom{S-2K+\nu-1}{\nu-1} \binom{S-2K'+\nu-1}{\nu-1}$$

$$\binom{S-2\chi+\nu}{\nu-1}\binom{S+2\nu}{\nu-1} \qquad (8.5)$$

where $S = K+K'+\chi$. D_1 vanishes when χ is out of the range

$$|K-K'| \leq \chi \leq K+K'+1$$

On the other hand K, and K' in (7.8) must fulfil the triangle inequalities for $\ell = \lambda = \ell' = 0$ to provide a non vanishing 3P coefficient.

For applying the recurrence formula (8.4) one can either start from the minimal value $\chi_m = |K-K'|$ and generate higher order matrix elements or begin with the maximal value $\chi_m = K+K'+1$ for which the first term in (8.4) vanishes and generate lower order matrix elements. In this last case the first matrix element is

$$\langle {}^{(N)}P^{0,0}_{2K} \,|\, {}^{(N)}P^{0,0}_{2(K+K')} \,|\, {}^{(N)}P^{0,0}_{2K'} \rangle = \frac{\pi}{2^{2\nu-1}} \binom{2K+\nu}{\nu-1}\binom{2K'+\nu}{\nu-1}$$

$$\binom{2(K+K'+\nu)+1}{\nu-1}\left[\frac{2(K+K')+\nu+1}{2(K+K')+\nu+3} \cdot \frac{K+K'+\nu+1}{2(K+K'+\nu)+1} \cdot \frac{2(K+K')+3}{K+K'+1}\right]^{1/2} \qquad (8.6)$$

When we have to deal with a tensor force $V_T(r_{ij})\, S_{ij}$.

where the tensor operator

$$S_{ij} = 3\frac{(\vec{\sigma}_i \vec{r}_{ij})(\vec{\sigma}_j \vec{r}_{ij})}{r_{ij}^2} - (\vec{\sigma}_i \vec{\sigma}_j) = \left(\frac{24\pi}{5}\right)^{1/2} \left(S^{(2)} . Y(\omega_{ij})\right)$$

is the inner product of two tensor operators, we have to compute the 3P coefficients (7.8) either for $\ell=\ell'=2$ and $\lambda=0$ or for $\ell=\ell'=\lambda=2$ in order to calculate the potential matrix. This can be achieved in using a recurrence formula relating ${}^{(N)}P^{2,0}_{2K}$ and ${}^{(N)}P^{00}_{2K}$. Using the properties of the Jacobi polynomials one writes both ${}^{(N)}P$ in terms of the Jacobi polynomials $P_n^{\frac{D-5}{2},\frac{3}{2}}(\cos 2\phi)$:

$$ {}^{(N)}P^{00}_{2K}(\phi) = \left[\frac{2\Gamma(K+\nu+1)K!}{(2K+\nu+1)\Gamma(K+\nu+\frac{1}{2})\Gamma(K+\frac{3}{2})}\right]^{1/2}$$

$$(K+\nu+1)\, P^{\nu-\frac{1}{2},\frac{3}{2}}_{2K}(\cos 2\phi) + (K+\nu-\tfrac{1}{2})\, P^{\nu-\frac{1}{2},\frac{3}{2}}_{K-1}(\cos 2\phi) \qquad (8.7)$$

$$ {}^{(N)}P^{2,0}_{2K}(\phi) = \left[\frac{2\Gamma(K+\nu+2)(K-1)!}{(2K+\nu+1)\Gamma(K+\nu-\frac{1}{2})\Gamma(K+\frac{5}{2})}\right]^{1/2}$$

$$\left[K\, P^{\nu-\frac{1}{2},\frac{3}{2}}_{K}(\cos 2\phi) + (K+\tfrac{3}{2})\, P^{\nu-\frac{1}{2},\frac{3}{2}}_{K-1}(\cos 2\phi)\right] \qquad (8.8)$$

When Eqs(8.7) and (8.8) are written for two consecutive K and K-1 one obtains four linear equations with only three independent polynomials. One eliminates P_K between the first set and P_{K-2} between the second set of two equations, then equating the two expressions obtained for $P^{\nu-\frac{1}{2},\frac{3}{2}}_{K-1}$ provides the following relation :

$$\left[(2K+3)(K+\nu+1)(2K+\nu-1)\right]^{1/2}\ {}^{(N)}P^{2,0}_{(\phi)\,2K}$$

$$+\left[(K-1)(2K+\nu+1)(2K+2\nu-3)\right]^{1/2}\ {}^{(N)}P^{2,0}_{(\phi)\,2(K-1)}$$

$$=\left[K(2K+2\nu-1)(2K+\nu-1)\right]^{1/2}\ {}^{(N)}P^{00}_{(\phi)\,2K}$$

$$+\left[(2K+1)(2K+\nu+1)(K+\nu)\right]^{1/2}\ {}^{(N)}P^{00}_{(\phi)\,2(K-1)} \qquad (8.9)$$

Eq.(8.9) is used to calculate the needed 3P coefficients by recurrence in starting from the 3P coefficients for $\ell=\ell'=\lambda=0$ previously calculated with Eqs(8.4) and (8.6). First the coefficients $\langle {}^{(N)}P^{2,0}_{2K} \mid {}^{(N)}P^{0,0}_{2\chi} \mid {}^{(N)}P^{0,0}_{2K'} \rangle$ are computed. Then starting from these coefficients and using again (8.9) one calculate the set

$$\langle {}^{(N)}P^{2,0}_{2K} \mid {}^{(N)}P^{0,0}_{2\chi} \mid {}^{(N)}P^{2,0}_{2K'} \rangle$$

and finally applying again the recurrence formula one obtains the set

$$\langle {}^{(N)}P^{2,0}_{2K} \mid {}^{(N)}P^{2,0}_{2\chi} \mid {}^{(N)}P^{2,0}_{2K'} \rangle$$

9-A Few Applications

As extensive applications are not in the scope of this article we intend to illustrate this work in giving only simple examples which may provide a kind of instruction for use.

The simplest one refers to the ground state of a system of A = N+1 identical interacting bosons. A two body central potential is assumed. The wave function completelly symmetric in any exchange of particles contains a sum over all pairs of particles :

$$\Psi(r,\Omega) = r^{-\frac{D-1}{2}} \sum_{K=0} \left[\sum_{i,j>i} \mathcal{P}^0_{2K}(\Omega_{ij}) \right] u_K(r) \qquad (9.1)$$

The partial waves $u_K(r)$ are eigenfunctions of the coupled equations (4.6). One notices that in (9.1) the potential H.H. $\mathcal{P}^0_{2K}(\Omega_{ij})$ are normalized but not the symmetrical combination, therefore in order to expand Ψ in terms of normalized H.H. one introduces the symmetrized basis :

$$B^{(s)}_{2K}(\Omega) = C_K \sum_{i,j>i} \mathcal{P}^0_{2K}(\Omega_{ij}) \qquad \langle B^{(s)}_{2K}(\Omega) | B^{(s)}_{2K'}(\Omega) \rangle = \delta_{K,K'} \qquad (9.2)$$

where

$$C_K^{-2} = \sum_{\substack{i,j>i \\ k,\ell>k}} \langle \mathcal{P}^0_{2K}(\Omega_{ij}) | \mathcal{P}^0_{2K}(\Omega_{k\ell}) \rangle$$

Then Eq.(9.1) becomes :

$$\Psi(r,\Omega) = r^{-\frac{D-1}{2}} \sum_{k=0}^{\infty} B^{(s)}_{2K}(\Omega)\ \phi_K(r) \qquad \phi_K = C_K^{-1} u_K \qquad (9.3)$$

where Ψ is normalized when

$$\sum_{K=0}^{\infty} \int_0^{\infty} (\phi_K(r))^2 dr = \sum_{K=0}^{\infty} C_K^{-2} \int_0^{\infty} (u_K(r))^2 dr = 1 \qquad (9.4)$$

According to (7.3) the normalization constante C_K is given by

$$C_K^{-2} = \frac{A(A-1)}{2} \langle \mathcal{D}^0_{2K}(\Omega_{21}) | \sum_{i,j>i} \mathcal{D}^0_{2K}(\Omega_{ij}) \rangle \qquad (9.5)$$

where

$$\langle \mathcal{D}^0_{2K}(\Omega_{21}) | \sum_{i,j>i} \mathcal{D}^0_{2K}(\Omega_{ij}) \rangle = 1+4(N-1)\frac{(2K+1)!\,(D-5)!}{(2K+D-4)!}\, C^{\frac{D}{2}-2}_{2K+1}(1/2) \qquad (9.6)$$

$$+ \frac{(-1)^K}{2^{2K+1}}(N-1)(N-2)\frac{(2K+1)!}{K!}\,\frac{\Gamma(\frac{D-3}{2})}{\Gamma(K+\frac{D-3}{2})}$$

For A large the approximate value (7.5) can be used. Then performing in (9.6) a reduction in the ratio of the Γ functions in terms of powers of D leads to the approximate formula :

$$\langle \mathcal{D}^0_{2K}(\Omega_{21}) | \sum_{i,j>i} \mathcal{D}^0_{2K}(\Omega_{ij}) \rangle \xrightarrow[D \to \infty]{} \frac{(N+2)(N-1)}{2}\ \delta_{K,0} + \frac{5}{6}\,\delta_{K,2}$$

$$+ 1 + \frac{N-1}{2^{2K-1}}\left[\frac{(D-2K-4)^2}{(D+K-3)(D+K-2)}\right]^K \delta_{K>1} \qquad (9.7)$$

where the Kronecker symbol $\delta_{K>1} = \begin{cases} 0 \text{ for } K \leq 1 \\ 1 \text{ for } K > 1 \end{cases}$. The accuracy of (9.7) has been tested for N = 100, 200 and 400. The result is shown in table 2 (for K = 0 (9.7) is exact and for K = 1 $B_2^{(s)}(\Omega)$ does not exist).

N	K	2	3	4	5	6	7
100	(9.7)	13.01	3.50	1.536	1.110	1.021	1.004
	Exact	12.96	3.45	1.521	1.104	1.019	1.003
200	(9.7)	25.48	6.59	2.296	1.294	1.065	1.014
	Exact	25.46	6.57	2.288	1.290	1.064	1.0137
400	(9.7)	50.47	12.83	3.847	1.678	1.160	1.0374
	Exact	50.46	12.82	3.843	1.676	1.159	1.0370

Table 2

The matrix element (9.7) goes quickly to one for increasing K because for two different pairs (i,j) and (k,ℓ) the potential harmonics become orthogonal for rather small K values. Coming back to Eqs(8.1), (7.9) and (7.6) the potential matrix occuring in (4.6) is given by

$$\langle \mathcal{D}^0_{2K}(\Omega_{21}) | \sum_{i,j>i} V(r_{ij}) | \mathcal{D}^0_{2K}(\Omega_{21}) = \frac{1}{\sqrt{4\pi}} Y_0^{(D-3)} \qquad (9.8)$$

$$\sum_{\chi} \langle P^{(N)\,00}_{2K} | P^{(N)\,00}_{2\chi} | P^{(N)\,00}_{2K'} \rangle \langle \mathcal{D}^0_{2\chi}(\Omega_{21}) | \sum_{i,j>i} \mathcal{D}^0_{2\chi}(\Omega_{ij}) \rangle V^{D,0}_{\chi}(r)$$

where the 3P coefficients are calculate with the recurrence formula (8.4). The calculation of (9.8) can be simplified in computing separately the matrix element for $V(r_{21})$.

Then the matrix elements which refer to $V(r_{ij})$ for $(i,j)\neq(2,1)$ whose contribution vanishes rapidely for rather small χ, can be calculated only for the first few values of χ(e.g. for $\chi\leq 7$ in the cases of Table 2). The matrix element for $V(r_{21})$ in (9.8) is calculated in using the relation between the spherical harmonics $Y^m_\ell(\Theta,\varphi) = \Theta^m_\ell(\Theta)\frac{e^{im\varphi}}{\sqrt{2\pi}}$ and the $P^{(N)}_L(\phi)$ functions :

$$\Theta_{\ell}^{\nu_{N-1}} = (-1)^{\nu_{N-1}} \left[\frac{(\ell+\frac{1}{2})(\ell-\nu_{N-1})!}{(\ell+\nu_{N-1})!}\right]^{1/2} P_{\ell}^{\nu_{N-1}}(\cos\phi)$$

$$= \frac{1}{\sqrt{2}}(\sin\phi)^{\frac{D-5}{2}} \cos\phi \; {}^{(N)}P_{L}^{0,L_{N-1}}(\phi)$$

$$\ell = L + \frac{D-3}{2} \; , \; \nu_{N-1} = L_{N-1} + \frac{D-5}{2} \qquad (9.9)$$

where $P_n^m(\cos\phi)$ is an associated Legendre function of the first kind.

It can be used when ν_{N-1} and ℓ are integers i.e. when D = 3N is odd (A=N+1 even).Then the potential V(rcosϕ) is expanded in terms of Legendre polynomials $P_n(\cos\phi)$ leading to the matrix element :

$$\langle \mathcal{P}_{2K}^{0}(\Omega_{21}) | V(r_{21}) | \mathcal{P}_{2K'}^{0}(\Omega_{21}) \rangle = (-1)^{\nu_{N-1}} \sum_{n \text{ even}} (2n+1)$$

$$\left[(2\ell+1)(2\ell'+1)\right]^{1/2} \begin{pmatrix} \ell & n & \ell' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell & n & \ell' \\ \nu_{N-1} & 0 & -\nu_{N-1} \end{pmatrix} \int_0^1 V(rx) \, P_n(x) \, dx$$

$$\nu_{N-1} = \frac{D-5}{2}, \ell = 2K + \frac{D-3}{2} \; , \qquad (9.10)$$

where the parenthesis stand for 3j coefficients. The integral is calculated once forever for a potential V, only the 3j coefficients have to be changed according to the number of particles.

Eq.(9.10) can also be used to generate the potential multipoles (3.3) in taking K' = 0 :

$$V_K^{D,0}(r) = \left[Y_0(D)\right]^{-1} \langle \mathcal{P}_{2K}^{0}(\Omega_{21}) | V(r_{21}) | \mathcal{P}_{0}^{0} \rangle = (-1)^{\frac{D-5}{2}}$$

$$\times\left[Y_0(D)\right]^{-1}\left[4K+(D-2)\right]^{1/2}(D-2)^{1/2}$$

$$\sum_{n\ \text{even}}^{(2n+1)} \begin{pmatrix} 2K+\frac{D-3}{2} & n & \frac{D-3}{2} \\ \frac{D-5}{2} & 0 & -\frac{D-5}{2} \end{pmatrix} \begin{pmatrix} 2K+\frac{D-3}{2} & n & \frac{D-3}{2} \\ 0 & 0 & x \end{pmatrix}$$

$$\int_0^1 V(rx)\, P_n(x)\, dx \qquad (9.11)$$

An accurate numerical calculation of the potential multipoles is time consuming therefore Eq.(9.11) provides a very economic procedure for generating the potential multipoles when we have to deal with various A, because only integrals with the Legendre polynomials are needed.

Now let us write explicitely as an example the coupled equations describing the ground state of three identical bosons. According to (8.4) and (8.5) with $N = 2$ and $\nu = 1$ the 3P coefficients are

$$\left\langle {}^{(2)}_{2K}{}^{00}_{P} \middle| {}^{(2)}_{2\chi}{}^{00}_{P} \middle| {}^{(2)}_{2K'}{}^{00}_{P} \right\rangle = \frac{4}{\sqrt{\pi}} \quad \text{for } K+K'+\chi \text{ even} \qquad (9.12)$$

and zero otherwise.

The matrix element (7.3) for two different pairs $(i,j) \neq (2,1)$ is

$$\left\langle \mathfrak{D}^0_{2K}(\Omega_{21}) \middle| \mathfrak{D}^0_{2K}(\Omega_{ij}) \right\rangle = \frac{1}{K+1}\, C^1_{2K+1}(1/2) \qquad (i,j) \neq (2,1)$$

where

$$C^1_{2K+1}(1/2) = \frac{\sin 2(K+1)\pi/3}{\sin \pi/3} = \begin{cases} 1 \text{ for } K = 3n \\ -1 \text{ for } K = 3n+1 \\ 0 \text{ for } K = 3n+2 \end{cases} \qquad (9.13)$$

n integer

Using $P^{(2)}_{2K}(\cos 2\theta) = \frac{2}{\sqrt{\pi}} C^{1}_{2K+1}(\cos\theta)/\cos\theta$ and $Y_0(3) = \frac{1}{2\sqrt{\pi}}$

the central potential multipoles become

$$V_K(r) = \sqrt{4\pi}\, V^{(6,0)}_K(r) = 8\sqrt{\pi}\int_0^{\pi/2} V(r\cos\theta)\, \sin 2(K+1)\theta\, \sin\theta\cos\theta d\theta$$

$$= \sqrt{\pi}\int_0^{\pi}\left[\cos K\varphi - \cos(K+2)\varphi\right] V(r\cos\tfrac{\varphi}{2})\, d\varphi \qquad (9.14)$$

The coupled equations (4.6) are

$$-\frac{\hbar^2}{m}\left[\frac{d^2}{dr^2} - \frac{\ell_K(\ell_K+1)}{r^2}\right] u_K(r) + \sum_{K'} U^{K'}_K(r)\, u_{K'}(r) = 0$$

$$\ell_K = 2K + \frac{3}{2} \qquad (9.15)$$

with the potential matrix

$$U^{K'}_K(r) = \frac{1}{\pi}\left\{\frac{W(r)}{|K-K'|} - \frac{W(r)}{K+K'+2} + 2\sum_{Q=0}^{Q_m} \frac{C^{1}(1/2)}{\frac{2K''+1}{K''+1}}\,(W(r)-W(r))^{K''}_{K''+2}\right\}$$

where

$$K'' = |K-K'|+2Q, \qquad Q_m = \tfrac{1}{2}(K+K' - |K-K'|)$$

$$W_Q(r) = \int_0^{\pi} \cos Q\varphi\, V(r\cos\tfrac{\varphi}{2})\, d\varphi$$

The hyperspherical expansion method is a variational method which fulfils the Ritz principle because on one hand only a limited number of coupled equations can be computed numericallly and on the other hand instead of the complete H.H. basis only the optimal

subset is retained in the expansion of the wave function.

The quality of this approximation has been previously investigated[8]. It has also been proved[31,9] that the trend of the convergence of the binding energy toward the exact value as a function of K_m, the number of integrated coupled equations, is determined only by the shape of the two body interaction. In order to illustrate this theorem we chose to study the increase of binding energy in the space completely symmetric S state of the trinucleon system and ^{4}He in the ground state in term of K_m for two kinds of interactions :

i) For potentials constituted by a sum of Gaussian[32-35] for which the binding energy decreases as the inverse of an exponential

ii) For Yukawa potentials[36,45] for which the binding energy decreases as K_m^{-4}. We retained for K_m the values 3,6,9,12 in order to eliminate the fluctuations in the trend of convergence generated by $C^1_{2K+1}(1/2)$ in (9.16) which takes in sequence the values 1,-1 and 0.

In Fig.1, the increase of binding $\Delta E_{K_m} = E_{K_m} - E_{K_m+3}$ is plotted in terms of K_m on a semi-logarithmic scale. The numerical values are are those of ref.(8,9).The points are along a straight line as it should be. The norms of the partial waves in (9.3)

$$N_K = \int_0^\infty (\phi_K(r))^2 dr$$

decrease as $e^{-\alpha K}$ (see ref.(27,37)) where α is a constant specific of the investigated potential.

In fig.2 is plotted $(E_{K_m} - E_{K_m+3})^{-1/4}$ versus K_m for Yukawa potentials Once again the points obtained using the data of ref.(8) are along straight lines as it should be.

The knowledge of the trend of the convergence enables one to obtain a good extrapolated binding energy in starting from a limited number of integrated coupled equations (9.15). Besides the space symmetric S state there are still two other states contributing in the ground state of the trinucleon systems and ^{4}He : the mixed symmetry S' and D states. These states are generated by the spin-isospin dependence of the nuclear interaction acting on $Y_0(D)$ A(s,t), the lowest order H.H. in the expansion of the wave function, where A(s,t) is the completely antisymmetric spin-isospin combination.

Therefore the structure of the wave function is more complicated for fermions than for bosons systems. There is no room enough in this article too fully develop the expansion method for fermion systems, therefore only the case of the ground state with central potentials will be investigated.

10-The Potential Basis for Fermions :

In section 1 we derived the potential basis in starting from $Y_0(D)$ the lowest order H.H.. The lowest order H.H. occuring in the expansion of the wave function of a fermion system cannot be of order zero because the Pauli principle prevent fermions to be in the same state and in particular no more than two fermions can be in the 1S state. We have given in a previous work[38] a method for constructing low order H.H. for fermion systems.

Let us assume that $D_{[L_m]}(\vec{\xi}_1,\ldots,\vec{\xi}_N)$ is a homogeneous polynomial of minimal degree L_m antisymmetric in any exchange of two fermions, where the symbol $D_{[L_m]}(\vec{\xi})$ has been chosen to recall that antisymmetric polynomials can be written as a sum of determinants. It is obviously a harmonic polynomial because the Laplace operator applied to a homogeneous polynomial decreases by two the degree of this polynomial without changing its symmetry, therefore it gives zero when acting on a homogeneous polynomial of minimal degree :

$$\nabla^2 D_{[L_m]}(\vec{\xi}) = 0$$

We assume for the sake of simplicity that $D_{[L_m]}(\vec{\xi})$ is not degenerated, i.e., that it does not exist another harmonic polynomial $D_{[L'_m]}(\vec{\xi})$ of the same degree $L'_m = L_m$ for which

$$\int D^*_{[L'_m]}(\vec{\xi}) \sum_{i,j>i} V(\vec{r}_{ij}) D_{[L_m]}(\vec{\xi})\, d\Omega \neq 0 \qquad (10.1)$$

Let us choose $\vec{\xi}_N = \vec{r}_{ij}$ and $\xi_N = r\cos\phi_N$ as in (2.1). The central

potential $V(\xi_N)$ acting on $D_{[L_m]}(\vec{\xi})$ generates harmonic polynomials of degree L_m+2K (parity $(-1)^{L_m}$) :

$$D_{[L_m]+2K}(\vec{\xi}) = p_K(\xi_N)\, D_{[L_m]}(\vec{\xi}) \qquad (10.2)$$

completely determined by the quantum numbers $[L_m]$ and K which specifies the degree L_m+2K of the polynomial. These polynomials must fulful the equation similar to (7.4) :

$$\int_{(r=1)} D^*_{[L_m]}(\vec{\xi})\; p_K^{[L_m]}(\xi_N)\; p_{K'}^{[L_m]}(\xi_N)\; D_{[L_m]}(\vec{\xi})\; d\Omega = \delta_{K,K'} \qquad (10.3)$$

where the integral is taken over the surface of the unit hypersphere r = 1 in the D = 3N dimensional space.

Let us separate the coordinate $\vec{\xi}_N$ out of the set $(\vec{\xi})$ and let us introduce the hyperspherical coordinates (ρ,Ω_ρ) of the set $(\vec{\xi}_1,\ldots,\vec{\xi}_{N-1})$ in such a way that the hyperspherical coordinates (Ω) be given by $(\Omega_\rho;\omega_N,\phi_N)$ where ω_N are the angular coordinates of $\vec{\xi}_N$ and

$$\rho = r\sin\phi_N\ ,\quad \xi_N = r\cos\phi_N\ . \qquad (10.4)$$

Integrating $|D_{[L_m]}(\Omega)|^2$ over the coordinates Ω_ρ generates the homogeneous polynomial :

$$\int |D_{[L_m]}(\vec{\xi})|^2\, d\Omega_\rho = \sum_{n,\ell} \langle [L_m] | n,\ell\rangle\, Y^0_\ell(\omega_N)\; \xi_N^{2n+\ell}\; \rho^{2L_m-2n-\ell} \qquad (10.5)$$

where ℓ is even and $\langle [L_m] \,|\, n,\ell \rangle$ are geometrical coefficients[38].

When the associated H.H.

$$\underset{[L_m]}{D(\Omega)} = r^{-L_m} \underset{[L_m]}{D(\hat{\xi})}$$

is normalized, the coefficients in (10.5) fulfil the relation :

$$\int \left| \underset{[L_m]}{D(\Omega)} \right|^2 d\Omega = \int \left| \underset{[L_m]}{D(\Omega)} \right|^2 d\Omega_\rho d\omega_N$$

$$(\sin\phi_N)^{D-4} (\cos\phi_N)^2 d\phi_N$$

$$= \frac{\sqrt{\pi}}{\Gamma(L_m+\frac{D}{2})} \sum_n \langle [L_m] \,|\, n,\ell \rangle \Gamma(n+\tfrac{3}{2}) \Gamma(L_m+\tfrac{D-3}{2}-n) = 1 \qquad (10.6)$$

Using (10.5) the condition (10.3), with $x = \cos 2\phi_N$, becomes :

$$\int_{-1}^{1} \underset{K}{P^{[L_m]}(x)} \; \underset{K'}{P^{[L_m]}(x)} \; \underset{[L_m]}{W(x)} \, dx = \delta_{K,K'} \qquad (10.7)$$

where

$$\underset{[L_m]}{W(x)} = \sqrt{\pi} 2^{-(L_m+\frac{D}{2}-1)} \sum_n \langle [L_m] \,|\, n,0 \rangle (1+x)^{n+\frac{1}{2}} (1-x)^{L_m+\frac{D-5}{2}-n}$$

is the weight function associated with the polynomials $\underset{K}{P^{[L_m]}(x)}$.

Eq.(10.7) determines completely the polynomials generating the potential basis

$$D(\Omega_{ij}) \approx \mathcal{D}^{[L_m]}_{K}(\Omega_{ij})\ D(\Omega) \qquad (10.8)$$
$$[L_m]\neq 2K \qquad\qquad [L_m]$$

associated with the lowest order H.H. $D(\Omega)$, where
$[L_m]$

$\mathcal{D}^{[L_m]}_{K}(\Omega_{ij}) = P^{[L_m]}_{K}(\cos 2\phi_N)$ with $\cos\phi_N = r_{ij}/r$.

The basis (10.8) is complete for an expansion of any function of r_{ij} and in particular for the central potential $V(r_{ij})$.

Obviously for $L_m=n=0$ the weight gunctions (10.7) is associated with the Jacobi polynomials $P^{\frac{D-5}{2},\frac{1}{2}}_{K}(x)$ constituting (except for a normalization constant) the potential basis $\mathcal{D}^{0}_{2K}(\Omega_{ij})$ (see Eq.(2.2)).

The procedure to calculate the coefficients $\langle [L_m] | n,\ell \rangle$ enabling one to construct the weight function (10.7) generated by $D(\Omega)$ has been explained in ref.(22).
$[L_m]$

Assuming that the weight function $W(x)$ and the associated normalized polynomials $P_K(x)$ are known, we can apply the general theorems for expansion problems with orthogonal pclynomials.
$[L_m]$ $[L_m]$

In particular the expansion of the potential is given by

$$V(r_{ij}) = \sum_K \mathcal{D}^{[L_m]}_{K}(\Omega_{ij})\ V^{[L_m]}_{K}(r) \qquad (10.9)$$

where the multipoles are

$$V^{[L_m]}_{K}(r) = \int_{-1}^{1} V(rx)\ P^{[L_m]}_{K}(x)\ W_{[L_m]}(x)\ dx \qquad (10.10)$$

To calculate the matrix elements with potential harmonics for two pairs (2,1) and (i,j) we use as in section 6 the kinematic rotation vector as a tool and find

$$\langle D^{[L_m]+2K}(\Omega_{12}) \mid D^{[L_m]+2K}(\Omega_{ij}) \rangle = \frac{P_K^{[L_m]}(\cos 2\varphi_N^{ij})}{P_K^{[L_m]}(1)} \tag{10.11}$$

which reproduces (7.1) when $L_m = \ell = 0$.

The expansion of the wavefunction in terms of potential harmonics becomes

$$\Psi(r,\Omega) = r^{-\frac{D-1}{2}} D^{[L_m]}(\Omega) \sum_K \left\{ \sum_{i,j>i} \mathcal{P}_K^{[L_m]}(\Omega_{ij}) \right\} u_K(r) \tag{10.12}$$

The partial waves $u_K(r)$ are solution of the system of coupled equations

$$-\left\{ \frac{\hbar^2}{m} \left[\frac{d^2}{dr^2} - \frac{(\ell_m+2K)(\ell_m+2K+1)}{r^2} \right] + E \right\} u_K(r) + \sum_{K'} U_K^{K'}(r)\, u_{K'}(r) = 0 \tag{10.13}$$

where

$$U_{K'}^{K}(r) = \langle D^{[L_m]+2K}(\Omega_{21}) \mid \sum_{i,j>i} V(r_{ij}) \mid D^{[L_m]+2K}(\Omega_{21}) \rangle \tag{10.14}$$

The potential matrix $U_K^{K'}$ is calculated in using (10.9) and (10.11) :

$$U_K^{K'}(r) = \sum_\chi \langle D^{[L_m]+2K} \left| P_\chi^{[L_m]} \right| D^{[L_m]+2K'} \rangle \left[P_\chi^{[L_m]}(1) \right]^{-1} \left[\sum_{i,j>i} P_\chi^{[L_m]}(\cos 2\varphi_N^{ij}) \right] V_\chi^{[L_m]}(r) \tag{10.15}$$

where the matrix elements

$$\langle D^{[L_m]+2K} \left| P_\chi^{[L_m]} \right| D^{[L_m]+2K'} \rangle = \int_{-1}^{1} P_K^{[L_m]}(x)\, P_{K'}^{[L_m]}(x)\, P_\chi^{[L_m]}(x)\, W^{[L_m]}(x)\, dx \tag{10.16}$$

generalize the 3P coefficients (7.8) when $L_m \neq 0$.

Comments and conclusion

The concept of optimal subset proceeds from the basic idea that the wavefunction is well described when the two body correlations are included and that the probability for more than two particles to interact at the same time is small.

If these assumptions are fulfilled the wavefunction can be written :

$$\Psi(\vec{x}) = \left\{ \sum_{i,j>i} F(r_{ij},r) \right\} D_{L_m}(\Omega)\psi(r) \qquad (11.1)$$

$F(r_{ij},r)$ is calculated through a H.H. expansion using the potential basis complete for any two body function :

$$F(r_{ij},r) = \sum_K \mathcal{Y}^0_{2K}(\Omega_{ij})\ f_K(r) \qquad (11.2)$$

The numerical calculations[7-9] have shown that this approximation is good. We may wonder why such a drastic simplification leads to a so accurate result. Let us assume that the term $D_{L_m}(\Omega)\ \psi(r)$ solution of (10·13) for K=K'=0 and $\Psi = r^{-\frac{D-1}{2}} u_0(r)$ is already a rather good approximation of the wavefunction, in such a way to be in a situation favorable to apply a perturbation calculation. Here the perturbation is the angular dependent part of the potential:

$$\delta V = \sum_{K\neq 0} \left[\sum_{i,j>i} \mathcal{Y}^{[L_m]}_{2K}(\Omega_{ij}) \right] V^{[L_m]}_K(r)$$

According to previous analysis [38-40] a harmonic oscillator (H.O.)

basis is convenient for the expansion of the radial functions.

Let us denote by $|K,n\rangle$ the H.O. state

$$|K,n\rangle = \left\{ \sum_{i,j>i} D_{L_m+2K}(\Omega_{ij}) \right\} \psi^{H,0}_{L_m+2K,n}(r)$$

constructed with the potential H.H. and the H.O. radial wave $\psi^{H,0}_{L,n}(r)$ (38) where n is the number of nodes of the radial wave. In starting from the unperturbed state $|0\rangle$ the contribution brought by the third-order perturbation which contains the product of matrix elements

$$\langle 0|\delta V|K_1 n_1\rangle\langle K_1 n_1|\delta V|K_2 n_2\rangle\langle K_2 n_2|\delta V|0\rangle$$

can be exactly calculated with the exclusive use of the potential basis, because any H.H. orthogonal to the potential basis cancel this product. The error made in taking only the optimal subset into account in the expansion of the wavefunction is therefore of the fourth-order when the angular part of the potential is treated perturbatively. This fourth-order correction seems very small for the investigated problems.

For solving the expansion problem a large number of coupled equations (10.13) have to be integrated. This procedure, which is generally difficult, can be simplified in using the Adiabatic Approximation method[41,42]. Instead of a H.H. expansion one uses an angular basis B_λ defined as eigenfunction of the angular differential equation:

$$\left\{ -\frac{\hbar^2}{m}\frac{\mathcal{L}^2(\Omega)}{r^2} + V(r,\Omega) \right\} B_\lambda(r,\Omega) = U_\lambda(r)\, B_\lambda(r,\Omega)$$

$$\mathcal{L}^2(\Omega) = L^2(\Omega) - (D-1)(D-3)/4 \qquad (11.3)$$

where r is a parameter.

For solving this equation one expands B_λ in potential harmonics converting (11.3) in a matrix equation which can be solved easily with standard computational programs . The basis B_λ decouple the equations (10.13) when the variation with r of B_λ is neglected Then we have to integrate either one equation or three coupled equations according as we use the Uncoupled[43] or the Coupled Adiabatic Approximation[44] which takes the variation of B_λ with r into account.

In this paper we have shown how to introduce the two-body correlations in the wavefunction. Let us now explain briefly how to improve our solution by including more than the two-body correlations. According to the previous discussion our solution is limited to a third-order perturbation accuracy because the potential basis is not sufficient to describe completely the product $\delta V\, \mathcal{Y}^0_{2K}(\Omega_{ij})$ of a two body potential and a potential harmonic, which contains the product for different pairs of two potential harmonics. In order to enlarge our basis one proceeds like in section 2 for introducing the three-body correlations : one constructs a basis complete for the two Jacobi coordinates :

$$\vec{\xi}_N = \vec{x}_i - \vec{x}_j = \vec{r}_{ij} \ , \ \vec{\xi}_{N-1} = \sqrt{3}(\vec{x}_k - \vec{X}_{ijk}) = \sqrt{3}\,\vec{r}_k$$

where $\vec{X}_{ijk} = \frac{1}{3}(\vec{x}_i+\vec{x}_j+\vec{x}_k)$ is the center of mass of the three particles system. It is obtained in writting that this basis does not depend on the Jacobi coordinates $\vec{\xi}_i$ for $i<N-1$

$$P^{\ell,m}_{L,\Lambda,\ell_{ij},\ell_k}(\Omega_{ijk}) = Y_0(D-6) \sum_{m_1,m_2} \langle \ell_{ij},\ell_k;m_1,m_2|\ell,m\rangle \; Y^{m_1}_{\ell_{ij}}(\omega_{ij}) \; Y^{m_2}_{\ell_k}(\omega_k)$$

$$P^{(N)\ \ell_{ij},\Lambda}_{L}(\phi_N) \qquad P^{(N-1)\ \ell_k,0}_{\Lambda}(\phi_{N-1}) \tag{11.4}$$

where $\omega_{ij}(\omega_k)$ is the spherical coordinates of $\vec{r}_{ij}(\vec{r}_k)$ and $\cos\phi_N = r_{ij}/r$, $\cos\phi_{N-1} = \sqrt{3}\, r_k/[r^2-r_j^2]^{1/2}$. $\langle \ell_{ij},\ell_k:m_1,m_2|\ell\, m\rangle$ is a Clebsh-Gordan coefficient. When $\Lambda = 0$ one finds again the potential basis (2.2). In order to describe only the three- body correlations one must take out the two-body correlations leading to the basis :

$$\mathcal{P}^{\ell,m}_{L,\Lambda,\ell_{ij},\ell_k}(\Omega_{ijk}) = C(L,\Lambda,\ell_{ij},\ell_k)$$

$$\times \left\{ P^{\ell,m}_{L,\Lambda,\ell_{ij},\ell_k}(\Omega_{ijk}) - \sum_{\alpha,\beta>\alpha} \langle \mathcal{P}^{\ell,m}_{L}(\Omega_{\alpha\beta}) | P^{\ell,m}_{L,\Lambda,\ell_{ij},\ell_k}(\Omega_{ijk}) \rangle \mathcal{P}^{\ell,m}_{L}(\Omega_{\alpha\beta}) \right\} \tag{11.5}$$

where C is a normalization constante.

This basis, orthogonal to the potential basis, describes only three-body correlations. It is not our purpose in this paper to study how the coupled equations must be completed in order to improve the solution obtained with the potential harmonics therefore the properties of the three-body basis (11.5) will not be further investigated, but we must keep in mind that the next improvement

of our solution is obtained in taking the three-body correlations into account.

In this work we have shown how to extend the method used in our early paper[1] to any many-body problem by constructing the potential basis enabling one to describe the two-body correlations.

We have seen that contrary to the allegations of Efros[11] the use of the kinematic rotation vector as a tool is not "too artifical" but is very well adapted to the calculation of the matrix elements with potential harmonics. We must notice to this respect that in our early works[1,7] on trinucleon and ^{4}He bound states the mixed symmetry S state was already included as a suitable linear combination of potential harmonics and that the method to expand any two body operator sketched in ref.[10] has been applied with realistic potentials[16]. Our results are of course in agreement with those of Efros[11] for the cases considered by him. The matrix elements with two and three potential harmonics have been explicitely calculated when the lowest order H.H. occuring in the expansion of the wavefunction is of order zero (i.e. $Y_0(D)$). Recurrence relations leading to an easy numerical calculation of the needed matrix elements have been given.

But for fermion systems we have seen that in each case the potential basis must be constructed from the weight function generated by the lowest order H.H. occuring in the expansion of the investigated state. The potential harmonic expansion method which has been applied successfully to the calculation of few nucleon bound states with realistic interactions [13-18] and in a simplified version to light nuclei[20] seems to open one of the

most accurate and promising possibilities of solving the Schrödinger equation by introducing consistently the two-body correlations generated by the interaction.

- Appendix -

-I Expression of the grand orbital operator $L^2(\Omega)$ for the choice of hyperspherical coordinates (1.11).

The operator is obtained from the recurrence formula [1]:

$$L_i^2(\Omega_i) = \frac{\partial^2}{\partial\phi_i^2} + \left[3(i-2)\ \mathrm{cotan}\phi_i + 2(\mathrm{cotan}\phi_i - \tan\phi_i)\right]\frac{\partial}{\partial\phi_i} + \frac{\ell^2(\omega_i)}{\cos^2\phi_i} + \frac{L_{i-1}^2(\Omega_{i-1})}{\sin^2\phi_i}$$

$$= 4(1-z_i^2)\frac{\partial^2}{\partial z_i^2} + 6\left[2-i(1+z_i)\right]\frac{\partial}{\partial z_i} + 2\frac{\ell^2(\omega_i)}{1+z_i} + 2\frac{L_{i-1}(\Omega_{i-1})}{1-z_i}$$

$$z_i = \cos 2\phi_i \qquad \Omega_i(\omega_1,\omega_2,\phi_2,\ldots;\omega_i,\phi_i)$$

$$L^2(\Omega) = L_N^2(\Omega_N),\ \Omega_N = \Omega,\ L^2(\Omega_1) = \ell^2(\omega_1),\ [\ell^2(\omega) + \ell(\ell+1)]\,Y_\ell^m(\omega) = 0 \qquad (I.1)$$

-II Potential multipoles

Other expressions equivalent to (3.3) can be obtained

a) in terms of the Jacobi polynomials $P_K^{a,b}$:

$$V_K^{D,\ell}(r) = \left\{\frac{\pi^{\frac{D-3}{2}}(2K+\ell+\frac{D}{2}-1)\Gamma(K+\ell+\frac{D}{2}-1)K!}{2^{D+\ell-2}\,\Gamma(\frac{D-3}{2})\Gamma(K+\frac{D-3}{2})\Gamma(K+\ell+\frac{3}{2})}\right\}^{1/2}$$

$$\int_{-1}^{1} V(r\sqrt{\tfrac{1+x}{2}})\ P_K^{\frac{D-5}{2},\ell+\frac{1}{2}}(x)\ (1-x)^{\frac{D-5}{2}}\ (1+x)^{\frac{\ell+1}{2}}\ dx \qquad (II.1)$$

b) in terms of the Fourier transform. Let

$$\vec{v}(k) = \sum_{\ell,m} (-i)^\ell\ A_\ell^m(i,j)\ Y_\ell^m(\omega_k)\ v_\ell(k)$$

be the Fourier transform of (3.1) where

$$v_\ell(k) = \frac{1}{2\pi^2} \int_0^\infty j_\ell(kr_{ij})\, V_\ell(r_{ij})\, r_{ij}^2\, dr_{ij}$$

The potential multipoles occuring in (3.2) are given by

$$V_K^{D,\ell}(r) = (-1)^K \left\{ \frac{2^D\, \pi^{\frac{D+3}{2}} (2K+\ell+\frac{D}{2}-1)\Gamma(K+\ell+\frac{D}{2}-1)\Gamma(K+\frac{D-3}{2})}{K!\,\Gamma(\frac{D-3}{2})\Gamma(K+\ell+\frac{3}{2})} \right\}^{1/2} \int_0^\infty v_\ell(k)\, J_{2K+\ell+\frac{D}{2}-1}(kr)\, \frac{k^2\,dk}{(kr)^{\frac{D}{2}-1}} \qquad \text{(II.2)}$$

-III Recurrence formula for the potential multipoles.

The relation between Jacobi polynomials

$$(K+\tfrac{\alpha+\beta}{2}+1)(1-x)\, P_K^{\alpha+1,\beta}(x) = (K+\alpha+1)P_K^{\alpha,\beta}(x) - (K+1)\, P_{K+1}^{\alpha,\beta}(x)$$

applied to the expression (II.1) provides the recurrence formula

$$V_K^{D+2,\ell}(r) = \left[\frac{2\pi}{(2K+\ell+\frac{D}{2})(D-3)}\right]^{1/2} \left\{ \left[\frac{(K+\ell+\frac{D}{2}-1)(K+\frac{D-3}{2})}{2K+\ell+\frac{D}{2}-1}\right]^{1/2} V_K^{D,\ell}(r) - \left[\frac{(K+1)(K+\ell+\frac{3}{2})}{2K+\ell+\frac{D}{2}+1}\right]^{1/2} V_{K+1}^{D,\ell}(r) \right\}$$

-IV Formula for the 3P coefficients :

$$\int_{-1}^{1} (1-x)^{\alpha} (1+x)^{\ell+\frac{1}{2}}\, P_K^{\alpha,\ell+\frac{1}{2}}(x)\, P_{K_1}^{\alpha_1,\ell_1+\frac{1}{2}}(x)\, P_{K_2}^{\alpha_2,\ell_2+\frac{1}{2}}(x)\, dx$$

$$= 2^{\alpha+\ell+\frac{3}{2}}\, \Gamma(K+\ell+\tfrac{3}{2})\, \frac{\Gamma(\alpha_1+K_1+1)\Gamma(\alpha_2+K_2+1)}{K_1!\,K_2!\,\Gamma(\alpha_1+K_1+\ell_1+\frac{3}{2})\Gamma(\alpha_2+K_2+\ell_2+\frac{3}{2})}$$

$$\sum_{q=K}^{K_1+K_2} (-1)^{q+K} \binom{q}{K} \frac{\Gamma(\alpha+q+1)}{\Gamma(\alpha+K+\ell+q+\frac{5}{2})} \sum_{p=\max(0,q-K_2)}^{\min(K_1,q)} \binom{K_2}{q-p}\binom{K_1}{p} \frac{\Gamma(\alpha_1+K_1+\ell_1+q-p+\frac{3}{2})\Gamma(\alpha_2+K_2+\ell_2+p+\frac{3}{2})}{\Gamma(\alpha_1+q-p+1)\Gamma(\alpha_2+p+1)}$$

References

(1) M. Fabre de la Ripelle, Proceedings of the International School on Nuclear Theoretical Physics (Predeal 1969), Ed.A. Corciovei Inst. Atom. Phys., Bucarest; Rev.Roumaine Phys. 14(1969) 1215.

(2) W. Zickendrath, Ann. Phys. 53(1965) 18; Phys. Rev. 159(1967) 1448.

(3) A.J. Dragt, J. Math. Phys. 6(1965) 533.

(4) M. Banville and P.D. Kung, Canad. J. Phys. 44(1966) 2095.

(5) Yu.A. Simonov, Yad. Fiz. 3(1966) 630.

(6) G. Erens, J.L. Visschers and R. van Wageningen, "The Three Body Problem", Ed. J.S.C. McKee and P.M. Rolph,North-Holland (1969) p.291.

(7) M. Fabre de la Ripelle, Proc. of the Second Symposium on Nuclear Physics Problems, Novosibirsk, June 12-19 1970 ; M. Beiner and M. Fabre de la Ripelle, Nuovo Cimento Letters 1(1971) 584.

(8) G. Erens, J.L. Visschers and R. van Wageningen, Ann. Phys. (N.Y.) 67(1971) 461.

(9) J.L. Ballot, M. Beiner and M. Fabre de la Ripelle in "The Nuclear Many Body Problem", (F. Calogero and Y.C. Ciofi degli Atti Eds) Vol.1, Bologna 1973).

(10) M. Fabre de la Ripelle, C.R. Acad. Sc. Paris, A273(1971) 1007.

(11) V.D. Efros, Yad. Fiz. 15(1972) 226.

(12) J. Bruinsma, R. van Wageningen and J.L. Wisschers in "Few Particle Problems in Nuclear Interaction", (I. Slaus Ed.) p.368, North-Holland Amsterdam 1973.

(13) V.F. Demin, Yu.E. Pokrovsky and V.D. Efros, Phys. Lett. B44(1973) 227

(14) V.F. Demin and Yu.E. Pokrovsky, Phys. Lett. B47(1973)394 .

(15) J. Bruinsma and R. van Wagemingen, Phys. Lett. B44(1973) 221

(16) J.L. Ballot and M. Fabre de la Ripelle, Ann. Phys. (N.Y.) 127(1980) 62.

(17) V.F. Demin, Yu.E. Pokrovsky and V.D. Efros
Phys. Lett. B44(1973) 227.

(18) B.A. Fomin, V.D. Efros, Phys.Lett. B98(1981) 389.

(19) J.L. Ballot, Z. Phys. A302(1981) 347.

(20) A.M. Gorbatov, Yu. N. Krylov and A.B. Solovie
Yad. Fiz. 29(1979) 866, 30(1979)944, 30(1979)1487.

(21) M. Fabre de la Ripelle,
C.R. Acad. Sc. Paris 292 Série II (1981) 275.

(22) M. Fabre de la Ripelle, H. Fiedeldey and G. Wiechers,
Ann. Phys. (N.Y.) 138(1982) 275.

(23) F.T. Smith, Phys. Rev. 120(1960) 1058.

(24) D. Gogny, P. Pires and R. de Tourreil,
Phys. Lett. B32(1970) 591.

(25) F. Zernike and H.C. Brinkman,
Proc. Kon. Ned. Acad. Wensch 33(1935) 3.

(26) Higher Transcendental Functions TII McGraw-Hill, p.175.

(27) M. Fabre de la Ripelle, The Hyperspherical Harmonic
Expansion Method, Weissman preprint WIS 5-80/11/Mar-ph.

(28) Ref.(26), p.176

(29) Ref.(26), p.173.

(30) H. Hsü, Duke Math. J. 4(1938) 374.

(31) T.K. Schneider, Phys. Lett B40(1972) 439.

(32) G.A. Backer, J.L. Gammel, B.J. Hill and J.G. Wills,
Phys. Rev. 125(1966) 1754.

(33) A.B. Volkov, Nucl. Phys. 74(1965) 33.

(34) I.R. Afnan and Y.C. Tang, Phys. Rev. 175(1968) 1337.

(35) H. Eikemeier and H.H. Hackenbroich,
Z. Phys. 195(1966) 412.

(36) D.H. Belland, L.M. Delves, Nucl. Phys. A146(1970)497.
R.A Malflict and J.A. Tjon, Nucl. Phys. A127(1969) 161.

(37) M. Fabre de la Ripelle, Revista Brasileira de Fisica,
Vol.Especial, Maio 1980.

(38) M. Fabre de la Ripelle and J. Navarro,
Ann. Phys. (N.Y.) 123(1979) 185.

(39) G. Erens, Thesis Vrije Universiteit Amsterdam.

(40) H.T. Coelho, T.K. Das and M. Vallieres, Rev. Brasileira Fisica 7(1977) 237.

(41) J.H. Macek, J. Phys. B1(1968) 831.

(42) M. Fabre de la Ripelle, C.R. Acad. Sc. Paris, 274(1972) 104.

(43) T.K. Das, H.T. Coelho and M. Fabre de la Ripelle Phys. Rev. C (in press).

(44) J.L. Ballot, J.S. Levinger and M. Fabre de la Ripelle, submitted to Phys. Rev.C.

Figure Captions

Fig.1 : Increases of binding energy in MeV vs. K_m the number of integrated coupled equations for a) the Triton, b) ^{4}He. The potentials are sum of Gaussians.
E_{K_m} is the binding energy obtained by integrating the K_m first coupled equations using the potentials V_K [9], GPDT [24], B [32], V [33], A-T or S3 [34], E-H or S4 [35].

Fig.2 : Increase of binding energy vs. K_m for the Yukawa potentials Y (Bell-Delves) and MVI (Malfliet-Tjon) [36]. One uses the numbers of ref. [8] and [19].

Fig.3 : Percentage of the partial waves $\phi_K(r)$ in Eq.(9.3) for the ground state of ^{4}He obtained by integrating fourteen coupled equations (K_m = 14) with the Gaussian potentials [19].

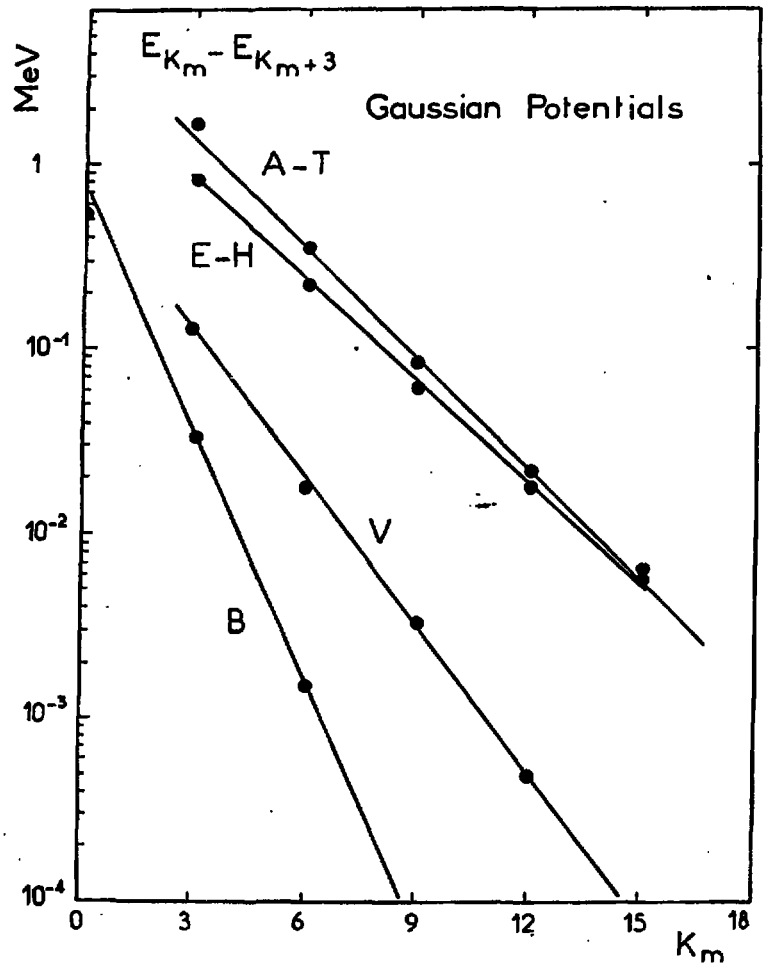
$E_{K_m} - E_{K_{m+3}}$
Gaussian Potentials
MeV
1
10^{-1}
10^{-2}
10^{-3}
10^{-4}
A-T
E-H
V
B
0
3
6
9
12
15
18
K_m

Fig.1a

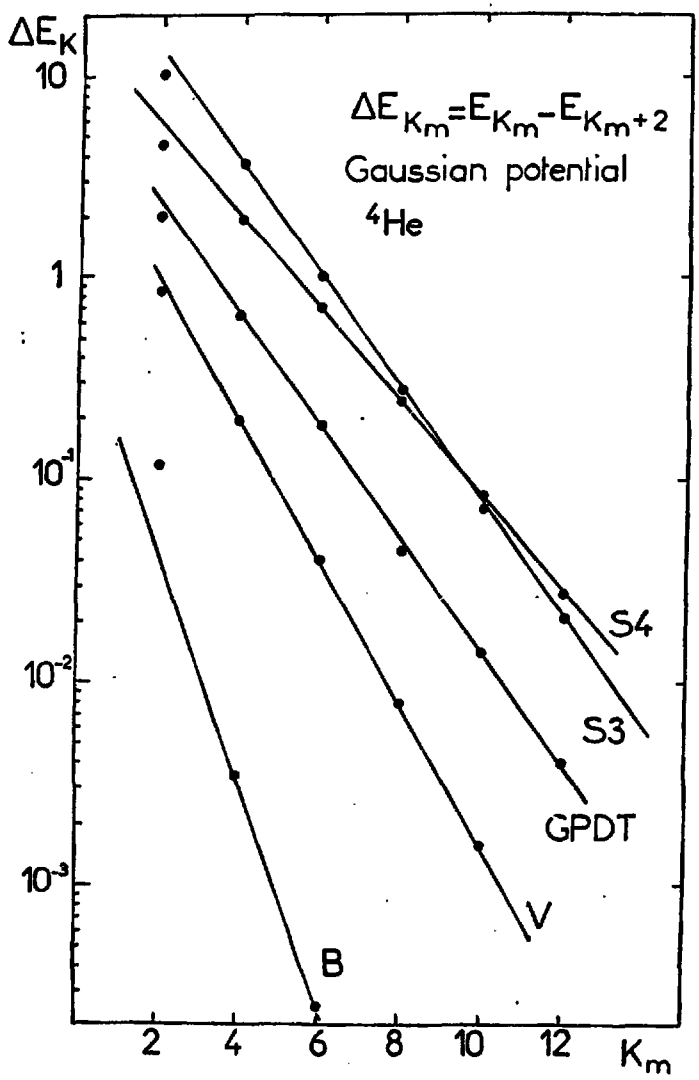
ΔE_K
10
1
10^-1
10^-2
10^-3
ΔE_Km=E_Km-E_Km+2
Gaussian potential
4He
S4
S3
GPDT
V
B
2
4
6
8
10
12
K_m

Fig.1b

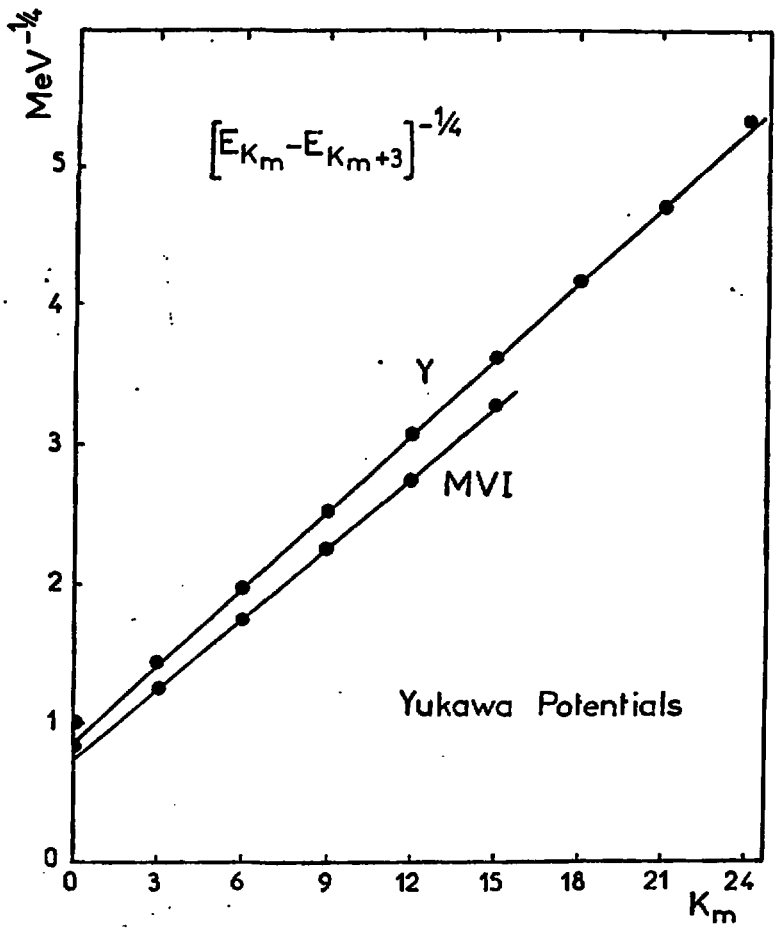
MeV^-¼
[E_Km - E_Km+3]^-¼
Y
MVI
Yukawa Potentials
0
1
2
3
4
5
0
3
6
9
12
15
18
21
24
K_m

Fig.2a

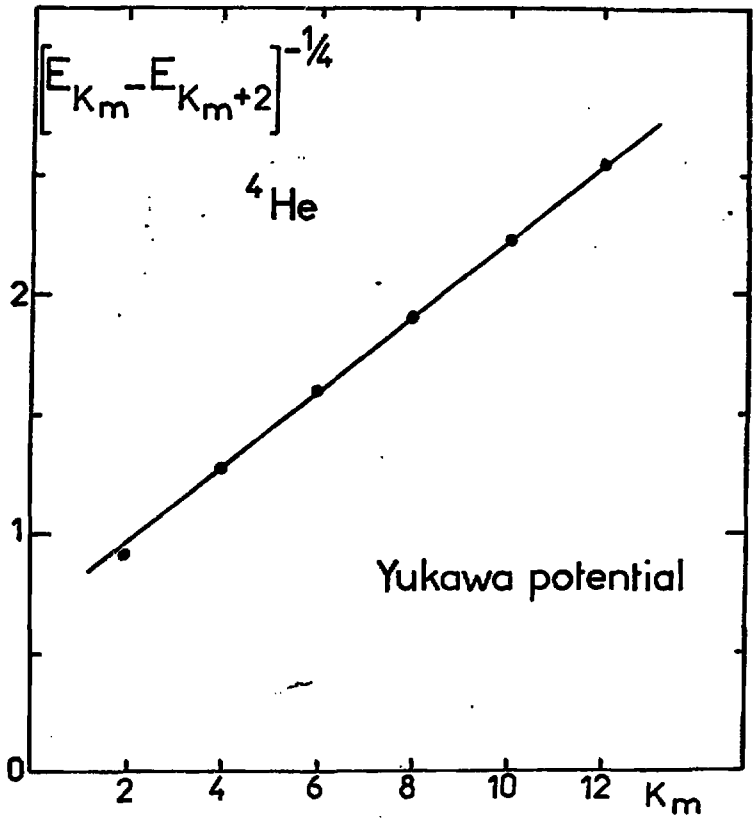

Fig.2b

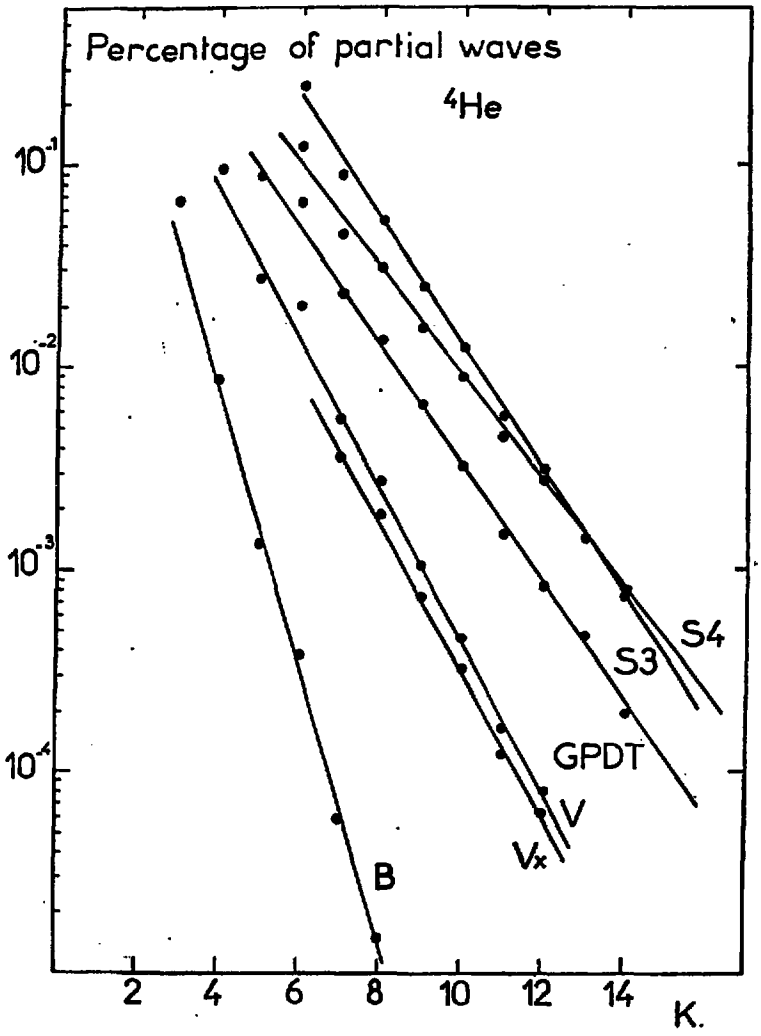
Percentage of partial waves
4He
10-1
10-2
10-3
10-4
S4
S3
GPDT
V
Vx
B
2
4
6
8
10
12
14
K.

Fig.3