A MULTIPLICATIVE CLUSTER EXPANSION for the CORRELATED BASIS FUNCTIONS THEORY

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1. INTRODUCTION

This work deals with the Correlated Basis Functions [1-7] approach to the many body problem in the presence of forces with strong repulsion at short distances. In that approach one has to distingish two steps: the main idea and the technical formalism for the development of the method.

The main idea is to work with a (complete) set of many body states which incorporates dynamical correlations. The simplest realization of that set is obtained by using the Jastrow ansatz

$$/\Psi_p> = \prod_{i<j} f(r_{ij}) \; /p>$$

where the two-body correlation factor satisfies the healing property, and $/p>$ is a generic state of an uncorrelated basis, like e.g. a set of Slater determinants constructed with single particle states of a certain shell model potential. With this set one can write an Euler-Lagrange equation

$$\sum_p \{<\Psi_q/H/\Psi_p>-E<\Psi_q/\Psi_p>\} C_p=0$$

its solution giving the energies and wave functions, $\sum C_p/\Psi_p>$, of the ground and excited states. By choosing appropriately the two-body correlation factor $f(r_{ij})$ [it is not clear what means "appropriately": the usual procedure [7] is to assign a parametric form to f and carry out a variational searching on the g.s. energy for an assumed configuration $/p_{gs}>$] one expects to account through the correlation function for the main structure of the actual nuclear state, so as to be able to limit the uncorrelated set $\{/p>\}$ to a rather small space.

The second step is only a (non trivial) question of technology: how do we compute the matrix elements $\langle \Psi_q / H / \Psi_p \rangle$ and $\langle \Psi_q / \Psi_p \rangle$? These matrix elements involve the evaluation of many body (up to A) operators and, with the exception of very light nuclei, the exact evaluation of that matrix elements is not feasible.

The corresponding problem for diagonal matrix elements, $\langle \Psi_p / H / \Psi_p \rangle$ or $\langle \Psi_p / \Psi_p \rangle$ is solved, in finite nuclei, by means of a cluster expansion. That cluster expansions are ultimately an extrapolation mechanism to obtain the expectation value of a A-body operator in terms of the simpler expectation values of 1, 2, 3 ... n-body operators. The extension of this procedure to the case of non-diagonal matrix elements has been carried out by Clark and coworkers in the frame of the aditive Iwamoto-Yamada cluster expansion (see particularly Ref. [6]). This expansion, however is not the best for the case of finite fermionic systems: numerical studies of various cluster expansions in finite nuclei have shown [8] it not to be stable and the advantage of using multiplicative cluster expansions (particularly the Factor-Aviles-Hartog-Tolhoek, FAHT [10]cluster expansion). The conclusion is the need of deriving a multiplicative cluster expansion for non-diagonal matrix elements: this is the goal of this work.

To this end we generalize the standard FAHT cluster expansion in section 2: in its original form this expansion was only defined for uncorrelated states which are normalized Slater determinants. The generalization of section 2 permits the use of uncorrelated states of a wider class, like e.g. configuration mixing states. In this form one obtains the expectation value of the energy for a general state $f_{ij}\sum C_p / p\rangle$, but the multiplicative character of the expansion prevents for the obtention of an Euler equation. This problem is carefully stated in section 3, and solved in section 4. The main result of our work is given in eq. (27), where a multiplicative cluster expansion for non-diagonal matrix elements of the generalized normalization integral is obtained.

Section 5 analyzes the properties satisfied by this new cluster expansion. Finally, in section 6 several remarks on the whole work are stated. The mathematical development of this work uses various properties of combinatorial numbers which are listed and proved in the Appendix.

2. THE FAHT CLUSTER EXPANSION IN TERMS OF SUBNORMALIZATION INTEGRALS

Our aim is the description of A-body systems in the presence of one-, two-, three- ... body correlations. It is convenient to introduce the quantities, appropriate for the n-body subsystem,

$$F_n = \prod_{\lambda=1}^{n} \prod_{i_1<i_2<..i_\lambda}^{n} f^{(\lambda)}_{i_1 i_2 .. i_\lambda} \tag{1}$$

and

$$r_n = F_n^{\dagger} \exp(\beta H_n) F_n \ , \tag{2}$$

where $H_n = \sum^{n} T_i + \sum^{n} V_{ij}$ is the hamiltonian corresponding to the n-body subsystem. The F_n correspond to the expansion in terms of the number of bodies of the whole correlation function F_A. The explicit form of the first terms clarifies their definition:

$$\begin{aligned} F_1 &= f^{(1)}_1 \\ F_2 &= f^{(1)}_1 f^{(1)}_2 f^{(2)}_{12} \\ F_3 &= f^{(1)}_1 f^{(1)}_2 f^{(1)}_3 f^{(2)}_{12} f^{(2)}_{13} f^{(2)}_{23} f^{(3)}_{123} \end{aligned} \tag{3}$$

where the suffixes of the f's label particle coordinates. In the particular case of $f^{(\lambda)}=1$ for $\lambda \neq 2$ we have the well known Jastrow form.

The FAHT cluster expansion is built up with the help of the above operators through the generalized subnormalization integrals

$$J_n = \frac{\langle \Psi / \ r_n / \Psi \rangle}{\langle \Psi / \Psi \rangle} \quad , \ n=1, \ 2 \ .. \ A \tag{4}$$

where $/\Psi\rangle$ is the A-body model wave function describing the "uncorrelated' system. For future reasons we have not considered that function to be normalized (note however that the whole wave function of the system $F_A/\Psi\rangle$ will not be normalized even if $/\Psi\rangle$ were).

From the subnormalization integrals J_n one defines the cluster integrals Y_n by means of the equations

$$J_n = \prod_{\lambda=1}^{n} Y_\lambda^{(n_\lambda)} \quad , \ n=1, \ 2 \ ... \ A \tag{5}$$

in such a form that J_1 defines Y_1, J_2 defines Y_2 ... and finally J_A defines the cluster integral Y_A. The equation for n=A gives then the

generalized normalization integral J_A in terms of the clusters Y_1, Y_2... Y_A, so that the expectation value of the hamiltonian is obtained from

$$\langle H\rangle = \frac{\partial}{\partial\beta} \ln J_A \Big|_{\beta=0} = \sum_{\lambda=1}^{A} \binom{A}{\lambda} \frac{Y'_\lambda(0)}{Y_\lambda(0)} \tag{6}$$

This equation is simply an identity. However, if one assumes that all cluster integrals Y_{n+1}, Y_{n+2} ... Y_A are exactly 1, then one is lead with an extrapolation formula which gives the matrix element of the A-body operator in terms of matrix elements of up to n-body operators r_λ, $\lambda=1,\dots n$, i.e.

$$J_A(n) = \prod_{\lambda=1}^{n} Y_\lambda^{\binom{A}{\lambda}} \tag{7}$$

where $J_A(n)$ means "the value of J_A at the n-th order of the approximation". Even if there are not yet firmly established properties on the goodness of such approximation mechanism, numerical studies give a strong confidence on this extrapolation method [8,9] and in various cases it has been shown to give very good results already at third order (i.e., at n=3 in eq. (7) above) when only two body correlations are taken into account.

Equations (6) and (7) have an appealing form: each correction appears as a multiplicative factor for the generalized normalization integral eq.(7), or as an aditive correction for the expectation value. However it is convenient to rewrite both equations directly in terms of the sub-normalization integrals J_1,... J_n. In other words, one has to invert the set of eqs. (5). By simple induction one obtains (see, e.g. the J.W.CTark lectures in these Proceedings)

$$Y_\lambda = \prod_{k=1}^{\lambda} J_k^{(-1)^{\lambda-k}\binom{\lambda}{k}} \tag{8}$$

and substituting in (7) it turns out for $J_A(n)$ the result

$$J_A(n) = \prod_{k=1}^{n} J_k^{N(n,k)} \tag{9}$$

where

$$N(n,k) = \sum_{\lambda=k}^{n} (-1)^{\lambda-k} \binom{A}{\lambda} \binom{\lambda}{k} \tag{10}$$

Explicit expressions at various orders follow:

$$J_A(1) = J_1^A$$
$$J_A(2) = J_1^{A-2\binom{A}{2}}\, J_2^{\binom{A}{2}} \qquad (11)$$
$$J_A(3) = J_1^{A-2\binom{A}{2}+3\binom{A}{3}}\, J_2^{\binom{A}{2}-3\binom{A}{3}}\, J_3^{\binom{A}{3}}$$

Certainly, if we compute $J_A(n=A)$ from eq. (9) we obtain the trivial result $J_A(n=A)=J_A$, as it should correspond to an expansion which, at the end, becomes an identity. This result follows from the property (A.4) of the numbers N(n,k) proved in the Appendix.

Finally the expectation value of the hamiltonian at order n is obtained from the logarithmic derivative of eq. (9) with respect to β at $\beta=0$, with the result

$$E(n)= \sum_{k=1}^{n} N(n,k)\, \frac{\langle \Psi / F_k^\dagger H_k F_k / \Psi \rangle}{\langle \Psi / F_k^\dagger F_k / \Psi \rangle} \qquad (12)$$

The advantages of this formulation of the FAHT cluster expansion with respect to the form of Clark and Westhaus [10] are the following:

1. It is not limited to "uncorrelated"states corresponding to a single Slater determinant.
2. Is given directly in terms of the matrix elements of $F_k^\dagger H_k F_k$ and $F_k^\dagger F_k$, which are the quantities that one has to evaluate in practical applications.

We have put quotes to the word uncorrelated because, according to our formulation, one can include some kind of correlations in the model wave function, like deformations or configuration mixing, as we will do in the next section.

3. CORRELATED BASIS FUNCTIONS APPROACH

As announced at the end of the previous section, we are now going to write a general expression for the model wave function $/\Psi>$

$$/\Psi> = \sum_p C_p /p> \qquad (13)$$

where the states /p> form a complete and orthonormalized set of basis

functions; in particular this set may be the usual shell model basis. The problem we face up is to determine the coefficients $\{C_p\}$ which give the lowest expectation value of the hamiltonian according with the formalism previously sketched. In other words, we would like to find the ground and excites states of the hamiltonian in the non-orthogonal basis

$$/\Psi_p> = F_A/p> \tag{14}$$

where F_A has been defined in eq. (1). This is the so called correlated basis functions approach of Feenberg and col. [1-7]. It is worth mentioning the main characteristics of this approach:

1. One expects the correlated basis to be appropriate for interactions having short range repulsions. In other words, an early truncation of the uncorrelated basis /p> should not have strong effects on the ground state energy.
2. As far as, in most cases, the repulsive core of the interaction is state independent, one may try to account for the state dependence of the correlations through the configuration mixing, while the correlation factor is considered state independent. This procedure avoids the cumbersome symmetrization of the correlation factor in the case of state dependent correlations.
3. As far as an Euler equation should result from the minimization with respect to the constants C_p, this procedure may give also the excited states of the systems.

This third point, however, creates some troubles. If we were able to compute exactly the hamiltonian expectation value

$$E = \frac{<\Psi/F_A^\dagger H_A F_A/\Psi>}{<\Psi/F_A^\dagger F_A/\Psi>} = \frac{\sum C_m^* C_p <m/F_A^\dagger H_A F_A/p>}{\sum C_m^* C_p <m/F_A^\dagger F_A/p>} \tag{15}$$

then the condition of E being stationary under variation of $\{C^*\}$ gives the equation

$$\sum_p <m/F_A^\dagger H_A F_A/p> C_p - \left\{ \frac{\sum_{rq} C_r^* C_q <r/F_A^\dagger H_A F_A/q>}{\sum_{rq} C_r^* C_q <r/F_A^\dagger F_A/q>} \right\} \sum_p <m/F_A^\dagger F_A/p> C_p = 0 \tag{16}$$

This equation is solved with the help of a Lagrange multiplier E, i.e. one solves the pair of equations

$$\sum\{\langle m/F_A^\dagger H_A F_A/p\rangle - \langle m/F_A^\dagger F_A/p\rangle\ E\}\ C_p = 0 \tag{17.a}$$

$$E = \frac{\sum C_r^*\ C_q \langle r/F_A^\dagger H_A F_A/q\rangle}{\sum C_r^*\ C_q \langle r/F_A^\dagger F_A/q\rangle} \tag{17.b}$$

the first being the usual Euler equation in a non-orthogonal basis. It is easily checked that the values of E which make (17.a) solvable,i.e. the solutions of the secular equation

$$\det\{\langle m/F_A^\dagger H_A F_A/p\rangle - E\langle m/F_A^\dagger F_A/p\rangle\} = 0 \tag{18}$$

satisfy the relation (17.b).

Now the problem comes in when we are forced to use an approximate value for the energy expectation value, as for example eq. (12). In this case the energy expectation value at order n-th is given by

$$E(n) = \sum_{k=1}^{n} N(n,k)\ \frac{\sum C_m^* C_p \langle m/F_k^\dagger H_k F_k/p\rangle}{\sum C_m^* C_p \langle m/F_k^\dagger F_k/p\rangle} \tag{19}$$

and variations on the constants C_m^* give for C_p the equations

$$\sum_{k=1}^{n} N(n,k)\left\{\frac{\sum\langle m/F_k^\dagger H_k F_k/p\rangle C_p}{\sum\langle r/F_k^\dagger F_k/q\rangle C_r^* C_q} - \frac{\sum\langle r/F_k^\dagger H_k F_k/q\rangle C_r^* C_q}{\left[\sum\langle r/F_k^\dagger F_k/q\rangle C_r^* C_q\right]^2}\ \sum\langle m/F_k^\dagger F_k/p\rangle C_p\right\} = 0 \tag{20}$$

This is no longer an Euler equation. Moreover, the attempt to solve it by means of the introduction of n Lagrange multipliers is unsuccesful.

The reason of that trouble is that the expectation value of the Hamiltonian and the normalization integral are no longer quadratic forms on the constants C_p. Certainly one may still attempt to solve eq. (19) by means of a direct multiparameter search of the minimum, this being still a workable task as far as the uncorrelated basis is truncated. quite early. Analogously, the search of other sets of parameters which make E(n) stationary will give the excited states. This is, certainly, a cumbersome procedure of limited application, so that the next task is to obtain Euler equations from equation (19), and we will do that in the next section.

4. A MULTIPLICATIVE CLUSTER EXPANSION FOR NON-DIAGONAL MATRIX ELEMENTS

In order to obtain an Euler equation to determine the mixing amplitudes C and the eigenvalues of the hamiltonian we have to rewrite eq.(19) in a form analogous to eq. (15), i.e. as a quotient of quadratic forms. Moreover, this task has to be carried out at each order of the cluster expansion.

To this end it is important to realize that the fact that eq. (19) is not the quotient of two quadratic forms is a direct consequence of the non linearity of eq. (9): if we write $/\Psi>$ according to eq. (13) the cluster expansion for the generalized normalization integral reads

$$J_A(n) = \prod_{k=1}^{n} \left\{ \frac{\sum C_p^* C_q <p/r_k/q>}{\sum C_q^* C_q} \right\}^{N(n,k)} \qquad (21)$$

and this expression must be transformed into

$$J_A(n) = \frac{\sum C_p^* C_q <p/r_A(n)/q>}{\sum C_q^* C_q} \qquad (22)$$

in order to have the standard form for the energy expectation value after computing the logarithmic derivative of $J_A(n)$ with respect to β. In eq. (22) we have defined a set of new quantities, $<p/r_A(n)/q>$: this symbol represents the n-th order approximation to the non diagonal matrix element $<p/r_A/q>$, and should not be confused with $<p/r_n/q>$ which is the matrix element of the n-body operator r_n. The values of the n-th order approximation to the non diagonal matrix elements of the full operator r_A are obtained by means of the identification of eqs. (21) and (22). This identification cannot be exact, because of the very different dependence of both equations on the mixing amplitudes C_p, but as far as the FAHT cluster expansion is a good approximation to the exact value for diagonal matrix elements, it is expected to obtain from this mechanism also a good approximation for non-diagonal matrix elements.

To proceed further let us state the hypothesis to be used :

1. At a given order n we assume the equality

$$\frac{\sum C^*_p C_q \langle p/r_A(n)/q\rangle}{\sum C^*_p C_p} = \prod_{k=1}^{n} \left\{ \frac{\sum C^*_p C_q \langle p/r_k/q\rangle}{\sum C^*_p C_p} \right\}^{N(n,k)} \qquad (23)$$

at order $C^*_p C_p$, $C^*_q C_q$ and $C^*_p C_q$.

2. At a given order n-th we assume the equality

$$\langle q/r_A(n)/q\rangle = \prod_{k=1}^{n} (\langle q/r_k/q\rangle)^{N(n,k)} \qquad (24)$$

This hypothesis is just to assume that the FAHT cluster expansion is valid for diagonal matrix elements.

3. Finally, we consider that the only non-negligible matrix elements $\langle p/r_A(n)/q\rangle$ correspond to states /p> and /q> differing in a small number of single particle orbitals, much less than the number of particles A. According to this statement we assume that the following equalities hold

$$\langle p/r_A(n)/p\rangle = \langle q/r_A(n)/q\rangle = \sqrt{\langle p/r_A(n)/p\rangle\langle q/r_A(n)/q\rangle} \qquad (25)$$

This approximation is expected to be valid in order 1/A. Note that this hypothesis is neccessary in order to obtain a hermitian value for the non diagonal matrix elements.

We will also extend this approximation to the n-body matrix elements $\langle p/r_n/p\rangle$ and $\langle q/r_n/q\rangle$.

Apart from these hypothesis it is also important to stress the importance of the uncorrelated basis being orthonormal. If not, we would not have had such a simple form for the denominators in eq.(23).

According to our hypothesis we may transform the basic eq.(23) into

$$\sqrt{\langle p/r_A(n)/p\rangle\langle q/r_A(n)/q\rangle} + \frac{C^*_p C_q}{|C_p|^2 + |C_q|^2} \langle p/r_A(n)/q\rangle + c.c. =$$

$$= \prod_{k=1}^{n} \left\{ \sqrt{\langle p/r_k/p\rangle\langle q/r_k/q\rangle} + \frac{C^*_p C_q}{|C_p|^2 + |C_q|^2} \langle p/r_k/q\rangle + c.c. \right\}^{N(n,k)} . \qquad (26)$$

where, given that we are interested in the matrix element $\langle p/r_A(n)/q\rangle$ we have limited the configuration mixing to only two generic states.

Expanding the r.h.s. up to first degree on $C_p^* C_q$ and equating the coefficients (after use of eq. (24)) we obtain the value of the non-diagonal matrix elements at order n

$$\langle p/\Gamma_A(n)/q\rangle = \prod_{k=1}^{n} \left\{\langle p/\Gamma_k/p\rangle\langle q/\Gamma_k/q\rangle\right\}^{\frac{1}{2}N(n,k)} \sum_{r=1}^{n} N(n,r) \frac{\langle p/\Gamma_r/q\rangle}{\sqrt{\langle p/\Gamma_r/p\rangle\langle q/\Gamma_r/q\rangle}} \qquad (27)$$

This equation is the bulk of our work. It corresponds to the generalization of the standard FAHT cluster expansion to non-diagonal matrix elements. From here we can obtain the physically interesting matrix elements $\langle p/F_A^\dagger F_A/q\rangle$, which correspond to the normalization, and $\langle p/F_A^\dagger H_A F_A/q\rangle$ which is the matrix element of the hamiltonian, by putting $\beta=0$ and by taking the derivative with respect to β at $\beta=0$, respectively. In this form one obtains:

Matrix elements of the identity ($p\neq q$)

$$\langle p/F_A^\dagger F_A/q\rangle_n = \prod_{k=1}^{n} \left(\langle p_k/p_k\rangle\langle q_k/q_k\rangle\right)^{\frac{1}{2}n(n,k)} \sum_{r=1}^{n} N(n,r) \frac{\langle p_r/q_r\rangle}{\sqrt{\langle p_r/p_r\rangle\langle q_r/q_r\rangle}} \qquad (28)$$

Matrix elements of the hamiltonian ($p\neq q$)

$$\langle p/F_A^\dagger H_A F_A/q\rangle_n = \prod_{k=1}^{n} \left(\langle p_k/p_k\rangle\langle q_k/q_k\rangle\right)^{\frac{1}{2}N(n,k)} \qquad (29)$$

$$\left\{\left\{\frac{1}{2}\sum_{r=1}^{n} N(n,r)\left\{\frac{\langle p_r/H_r/p_r\rangle}{\langle p_r/p_r\rangle} + \frac{\langle q_r/H_r/q_r\rangle}{\langle q_r/q_r\rangle}\right\}\right\}\left\{\sum_{s=1}^{n} N(n,s) \frac{\langle p_s/q_s\rangle}{\sqrt{\langle p_s/p_s\rangle\langle q_s/q_s\rangle}}\right\}\right.$$

$$\left. + \sum_{s=1}^{n} \frac{N(n,s)}{\sqrt{\langle p_s/p_s\rangle\langle q_s/q_s\rangle}}\left\{\langle p_s/H_s/q_s\rangle - \frac{1}{2}\langle p_s/q_s\rangle\left\{\frac{\langle p_s/H_s/p_s\rangle}{\langle p_s/p_s\rangle} + \frac{\langle q_s/H_s/q_s\rangle}{\langle q_s/q_s\rangle}\right\}\right\}\right\}$$

In the above equations we have used the shorthand notation

$$/p_s\rangle = F_s/p\rangle \ . \qquad (30)$$

These equations do not apply to the case p=q. That diagonal matrix elements should be computed with the standard formulae of the FAHT cluster expansion, and for the shake of completeness are included below:

Diagonal matrix elements of the identity

$$\langle p/F_A^\dagger F_A/p\rangle_n = \prod_{k=1}^{n} [\langle p_k/p_k\rangle]^{N(n,k)} \qquad (31)$$

Diagonal matrix elements of the hamiltonian

$$\langle p/F_A^\dagger H_A F_A/p\rangle_n = \prod_{k=1}^{n} [\langle p_k/p_k\rangle]^{N(n,k)} \sum_{r=1}^{n} N(n,r) \frac{\langle p_r/H_r/p_r\rangle}{\langle p_r/p_r\rangle} \qquad (32)$$

In all formulae (28)-(32), the subscript n on the l.h.s. means "value of the matrix element computed at order n-th".

All that equations may be simplified if one starts from normalized correlated states, defined as

$$/P\rangle = \frac{F_A/p\rangle}{\sqrt{\langle p/F_A^\dagger F_A/p\rangle}} \qquad (33)$$

as in Ref. [5]. In this case the equations read the same without the multiplicative factor in front.

It is appealing the unexpected form of the non diagonal matrix elements of the hamiltonian, particularly the presence in eq. (29) of the diagonal quantities $\langle p_r/H_r/p_r\rangle$. Latter on we will shown that all these quantities cancel exactly when the non-diagonal matrix elements are computed at order n=A. It should be pointed out that the presence of such unexpected quantities may be the clue for good convergence properties (I am grateful to J.W. Clark for pointing me that fact). Moreover it is also important to note that in the Iwamoto-Yamada form of the correlated basis functions theory these quantities are also present (see for example eq. II.21 of Ref. [3]).

5. PROPERTIES OF THE NON-DIAGONAL FAHT CLUSTER EXPANSION

The cluster expansion given by eq. (27) satisfies a very important property: at n=A the expansion is an identity. Before proceeding to the proof it is interesting to state the importance of this theorem. We have to remember that to arrive to eq. (27) we have used two kinds of hypothesis: hypothesis 1 and 2 simply say that the FAHT cluster expansion is a good expansion for diagonal matrix elements, and, as we have already stated in section 2, this cluster expansion for diagonal matrix elements is a chain of identities. Of course, the validity of the FAHT as an approximation mechanism to compute the expectation value of the A-body operator r_A does not result from this chain-of-identities character (actually, all cluster expansions are chains of identities), but if the

A-th order were different from the exact result, the cluster expansion should be ruled out. From this comment we conclude that, with regard to hypothesis 1 and 2 it is not surprising to get for our new cluster expansion also an identity at the A-th order.

On the contrary, we have also assumed the exact validity of relations which are correct only in order 1/A (hypothesis 3). The property we are going to prove means that this 1/A approximation has been restored in the way of obtaining the cluster expansion: in other words, this theorem establishes both the validity of the expansion for finite nuclei and the correct cluster expansion character.

The proof starts by putting in eq. (27) the value n=A:

$$<p/r_A(A)/q> = \prod_{k=1}^{A} [<p/r_k/p><q/r_k/q>]^{\frac{1}{2}N(A,k)} \sum_{r=1}^{A} N(A,r) \frac{<p/r_r/q>}{\sqrt{<p/r_r/p><q/r_r/q>}} \tag{34}$$

Then, according with eq. (A.4) of the appendix, $N(A,k)=\delta_{A,k}$, one simply arrives to

$$<p/r_A(A)/q> = <p/r_A/q> \tag{35}$$

The property is then proved. Note that the r.h.s. is the exact value of the generalized normalization integral, whereas the l.h.s. is the A-th order approximation to this quantity.

A secon property is that <u>the non-diagonal cluster expansion satisfies the normalization condition at each order</u>. It is neccessary to specify the meaning of "normalization condition": assume we are going to use the cluster expansion to calculate the expectation value of a μ-body operator H

$$H_A = \sum_{i_1<i_2\ldots<i_\mu}^{A} V_{i_1 i_2 \ldots i_\mu} \tag{36}$$

with V symmetric in all indices. In the limit

$$V_{i_1 i_2 .. i_\mu} \to 1 \tag{37}$$

we have $H_A=\binom{A}{\mu}$ and we say that the normalization condition is satisfied at n-th order if the following obvious relation is fulfilled

$$<p/F_A^\dagger H_A F_A/q>_n = \binom{A}{\mu} <p/F_A^\dagger F_A/q>_n \tag{38}$$

As in the previous case it is also important here to stress the

importance of the validity of eq. (38), this task being accomplished by remembering that, among the usual diagonal cluster expansions valid for finite nuclei, only the FAHT satisfies that property. Moreover, if eq. (38) were not satisfied, the evaluation of expectation values of long range operators would be certainly erroneus.

To prove eq. (38) we must introduce in eq. (29) the appropriate value for H_r and H_s, namely

$$H_r = \sum_{i_1<i_2\ldots<i_\mu}^{s} V_{i_1 i_2 \ldots i_\mu} \rightarrow \binom{s}{\mu} \quad \text{for} \quad \mu \leq s$$

$$\rightarrow \quad 0 \quad \text{for} \quad \mu > s$$

so that we have for eq. (29) the value

$$\langle p/F_A^\dagger H_A F_A/q\rangle_n = \prod_{k=1}^{n} [\langle p_k/p_k\rangle\langle q_k/q_k\rangle]^{\frac{1}{2}N(n,k)}$$

$$\left(\sum_{r=\mu}^{n} N(n,r)\binom{r}{\mu}\right)\left(\sum_{s=1}^{n} N(n,s)\frac{\langle p_s/q_s\rangle}{\sqrt{\langle p_s/p_s\rangle\langle q_s/q_s\rangle}}\right)$$

the second term in the big curly bracket of eq. (29) being exactly null. The first sum has the value $\binom{A}{\mu}$, see eq. (A.5) so that we arrive to the desired result eq.(38).

It is also worth mentioning another property which is not satisfied: this formalism is not invariant under a unitary change of the uncorrelated basis at n-th order of approximation. If this property were satisfied we should have, for any of the eqs. (28)-(32) the transformation law

$$/p\rangle = \sum A_{p\pi} /\pi\rangle \rightarrow \langle p/F_A^\dagger F_A/r\rangle_n = \sum A^*_{p\pi} A_{q\rho} \langle \pi/F_A^\dagger F_A/\rho\rangle_n$$

this relation being not satisfied because of the non-linearity of that equations on the matrix elements $\langle p_r/q_r\rangle$ and $\langle p_r/H_r/q_r\rangle$. This property is, however, satisfied at order n=A. From the practical point of view this means that the set of eigenvalues depends upon the uncorrelated basis used, and this fact is certainly disappointing. Nevertheless, if the n-th order gives a good value of the exact matrix elements, this dependence should be harmless. Let us finally note that this non-invariance should not be confused with the invariance under a unitary transformation of the single particle states used to construct the uncorrelated basis. This last property is obviously satisfied: in all

equations there appear only the A-particle states /p>, /q> ... so that any transformation of the single particle states which leaves the A-particle states unchanged does not alter the value of eqs. (28)-(32).

5. FINAL COMMENTS

In this work we have faced up two problems:

1. The generalization of the FAHT cluster expansion [10] to the general case of uncorrelated states which cannot be expressed as a single Slater determinant
2. The construction of a multiplicative cluster expansion, analogous to the FAHT, for the computation of the non-diagonal matrix elements appearing in the Correlated Basis Functions theory.

The generalization of the FAHT cluster expansion opens a wide field of applicability of this cluster expansion. In its original form it could only be applied to closed-shell nuclei (plus/minus a particle), and with this generalization one can also study open-shell or even deformed nuclei.

The non-diagonal FAHT cluster expansion, on the other hand, does not add anything to the Correlated Basis Functions theory. However, we expect it will improve the applications of this theory because of their expected good convergence properties. Let us however note that in practical applications one has to face up still the formidable problem of evaluating matrix elements of many body operators, as in the case of aditive cluster expansions.

There is a close analogy between our method of obtaining the cluster expansion and the method of Clark and Westhaus [3], even if formally both procedures seem to be very different. In [3] the cluster expansion is obtained from a super-generalized normalization integral $I(\alpha_1\alpha_2..;\beta)$ depending on a parameter β which plays the same rôle that our β used in eq. (2), namely to switch the interaction, and several parameters α_1,α_2 ... for switching the single particle states above the Fermi surface. The technique of computing the first derivatives with respect to some α_i at $\alpha_1=\alpha_2=...=0$ is equivalent to the expansion of eq. (26) in first order in $C_p^* C_q$. Our approach is, I think, less cumbersome.

APPENDIX : PROPERTIES OF N(n,k)

The numbers N(n,k) have been defined in eq. (10) as

$$N(n,k) = \sum_{\lambda=k}^{n} (-1)^{\lambda-k} \binom{A}{\lambda} \binom{\lambda}{k} \quad , \quad k=1,2\ldots n \qquad (A.1)$$

where A is the mass number of the nucleus. Explicit values of these number are the following

$$\begin{aligned} N(1,1) &= \binom{A}{1} = A \\ N(2,1) &= A - 2\binom{A}{2} \\ N(2,2) &= \binom{A}{2} \\ N(3,1) &= A - 2\binom{A}{2} + 3\binom{A}{3} \\ N(3,2) &= \binom{A}{2} - 3\binom{A}{3} \\ N(3,3) &= \binom{A}{3} \end{aligned} \qquad (A.2)$$

These values have been used explicitely in eq. (11). In general one can write

$$N(n,n) = \binom{A}{n} \qquad (A.3)$$

An interesting value corresponds to n=A, i.e. to N(A,k):

$$N(A,k) = \delta_{A,k} \qquad (A.4)$$

Proof: Start from the expansion

$$\frac{1}{k!}(1-x)^A = \frac{1}{k!} \sum_{\lambda=0}^{A} (-1)^{\lambda} \binom{A}{\lambda} x^{\lambda}$$

and compute the k-th derivative of both sides ($k \leq A$)

$$\binom{A}{k} (-1)^k (1-x)^{A-k} = \sum_{\lambda=k}^{A} (-1)^{\lambda} \binom{\lambda}{k} \binom{A}{\lambda} x^{\lambda-k}$$

Then, at x=1 the l.h.s. is $(-1)^k \delta_{A,k}$, whereas the r.h.s. is $(-1)^k N(A,k)$ so that eq. (A.4) is proved.

Another relation of interest is

$$\binom{A}{p} = \sum_{k=p}^{n} N(n,k) \binom{k}{p} \qquad (A.5)$$

Proof: Writing in the r.h.s. of (A.5) the explicit value of N(n,k) and reordering the sums on k and λ we obtain

$$\sum_{k=p}^{n} N(n,k) \binom{k}{p} = \sum_{\lambda=p}^{n} \binom{A}{\lambda} (-1)^{\lambda-p} \sum_{k=p}^{\lambda} (-1)^{k-p} \binom{\lambda}{k} \binom{k}{p}$$

The second sum of the r.h.s. is $\delta_{\lambda,p}$ (is the same property of eq. (A.4) for A=λ), so that eq. (A.5) is proved.

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