FAHT CLUSTER EXPANSION IN FINITE NUCLEI: FUN WITH PADE APPROXIMANTS

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1. INTRODUCTION

Trustable evaluation of matrix elements of operators between correlated states in finite many-body systems is an ineludible task any variational calculation has to face and which in particular is an important problem when cluster approximation schemes are used in the Jastrow approach.

Different methods available for this evaluation have been extensively discussed in this School [1] . In our contribution we are going to concentrate from a numerical point of view in one of them: the Factor-Aviles-Hartog-Tolhoek (FAHT) cluster expansion.

To gain confidence in the use of a cluster expansion one has to know as much as possible about its convergence properties and, as no general theory exists, we propose to focus on two aspects of the problem:

a) Tests of the cluster expansion in model calculations

b) Improvement of the convergence.

Point a) lead us to use the FAHT cluster expansion to evaluate matrix elements which are exactly known on other grounds so that we can get some insight about the rate of convergence. These so called "model calculations" [2] are reviewed in Section 2.

As far as point b) is concerned we try to apply the Padé approximants technique as a procedure to accelerate the convergence of the cluster algorithm, and this is done in Section 3.

It should be stressed from the very beginning that none of these two points can be considered as rigorous proofs but we believe the numerical results obtained, which are discussed in Section 4, are signi-

ficant enough to justify further work in this direction and may reassure in the use of the FAHT cluster expansion.

2. MODEL CALCULATIONS

We shall consider an A-body fermionic system in a state of the Jastrow type

$$\Psi = F \Phi \tag{1}$$

which is a product of a model state Φ and a correlation factor F.

As we are here interested in a numerically accurate evaluation of certain matrix elements rather than in a realistic description of the system we shall use simple wave functions which allow analytic calculations. Consequently Φ in eq. (1) will be the Slater determinant of single particle states from the harmonic oscillator potential and the Jastrow factor will be taken state-independent

$$F = \prod_{i<j} f(r_{ij}) \tag{2}$$

with

$$f(r) = 1 + a \exp(-b^2 r^2) \tag{3}$$

where $\underline{a}$ and $\underline{b}$ measure respectively the depth and (inverse) range of the correlation.

The general idea behind model calculations is simple: consider matrix elements whose value is exactly known, then test the results of a cluster expansion calculation of them to different orders.

We deal with two types of matrix elements: the first type corresponds to expectation values in the correlated state Ψ of some operators which are directly calculable because of symmetry properties of the model state Φ which are not spoiled by the presence of the correlation factor F. The second type of matrix elements are not expectation values but involve F and some operators in such a way that their values can be exactly predicted and compared with the result of successive approximations of a cluster expansion.

In reference [2] three of these model calculations have been considered:

i) If the system under consideration is saturated in spin-isospin

(as is the case for ^{4}He, ^{16}O and ^{40}Ca nuclei) the model wave function Φ corresponds to the one-dimensional irreducible representation of SU(4) and the same is true for our correlated state Ψ . The expectation values of the Casimir operators of the group are exactly known and we have

$$\langle V_\sigma \rangle = \langle V_\tau \rangle = \frac{1}{3}\langle V_{\sigma\tau} \rangle = -\frac{3}{2} A \qquad (4a)$$

where

$$V_\nu = \sum_{i<j} v_{ij} \qquad (4b)$$

with

$$v_{ij} = \begin{cases} \vec{\sigma}_i \vec{\sigma}_j , & \nu = \sigma , \quad \text{SPIN MODEL} \\ \vec{\tau}_i \vec{\tau}_j , & \nu = \tau , \quad \text{ISOSPIN MODEL} \\ (\vec{\sigma}_i \vec{\sigma}_j)(\vec{\tau}_i \vec{\tau}_j), & \nu = \sigma\tau, \quad \text{SPIN-ISOSPIN MODEL} \end{cases} \qquad (4c)$$

and

$$\langle V \rangle = \frac{\langle \Psi/V/\Psi \rangle}{\langle \Psi/\Psi \rangle} = \frac{\langle \Phi/FVF/\Phi \rangle}{\langle \Phi/F^2/\Phi \rangle} \qquad (5)$$

Observe that V given by (4b),(4c) can be interpreted as the limit of a very smooth and long-ranged spin/isospin dependent potential.

We call these calculations the spin-, isospin- and spin-isospin-models respectively. They all have the same structure and give the same information so we need only to consider one of them, say for example the isospin-model.

ii) The second model has to do with the well-known Elliot-Skyrme factorization property of the harmonic oscillator shell model wave functions: if $\vec{R}$ denotes the center of mass coordinates and α is the inverse length parameter of the H.O. then if the single particle states are filled up in increasing order of energy we have:

$$\Phi(\vec{r}_1 \ldots \vec{r}_A) = \left\{\frac{A\alpha^2}{\pi}\right\}^{3/4} \exp(-A\alpha^2 \vec{R}^2)\ \Phi(\vec{r}_1 - \vec{R} \ldots \vec{r}_A - \vec{R}) \qquad (6)$$

This relation means that the expectation values of operators depending only on $\vec{R}$ are easy to calculate. In particular for example

$$\langle \vec{R}^2 \rangle = \frac{3A}{2\alpha^2} = \langle \sum r_i^2 + 2 \sum \vec{r}_i \vec{r}_j \rangle \qquad (7)$$

and when the corresponding form of eq. (5) is written we refer to this

case as the R-model.

iii) The last model we consider, which we name the H.O. model, is of the second type specified above: if $h_i = \frac{1}{2m}(\vec{p}_i^{\,2} + \alpha^4 \vec{r}_i^{\,2})$ is the single particle H.O. hamiltonian for the i-th particle then Φ is an eigenfunction of the operator $\sum h_i$ with eigenvalue given by

$$E_o = \hbar\omega \sum N_{nl}(2n + l - \tfrac{1}{2})$$

where N_{nl} is the occupation number of the nl shell and the sum is over the occupied shells.

Then we have the identity

$$\frac{\langle \Phi / F^2 \sum h_i / \Phi \rangle}{\langle \Psi / \Psi \rangle} = E_o \qquad (8)$$

and a corresponding model calculation is obtained when the FAHT cluster expansion is used to evaluate the l.h.s..

Notice that the fact that the models originate from properties of the uncorrelated wave functions means that obviously they are trivially satisfied in the first order approximation when no correlations are included. That they also hold when the full correlation factor is turned on means that if we were able to carry out the cluster expansion to order A the models would be again trivially satisfied. The interesting point is: what happens when we stop the calculation at a lower order? In this respect it is interesting to note a remarkable property of the FAHT cluster expansion which is not shared by other cluster formalisms: the expectation value of the identity operator which is of course unity remains so to all orders when the identity operator is interpreted as the limit of a n-body operator.

We cannot expect this property to hold also for other non-trivial operators like those of the previous models. We should actually expect deviations from the exact relations when the cluster expansion is carried out only up to order $n < A$, and this is what happens. The magnitude of these deviations is a measure of the goodness of the expansion.

The scope and physical content of the above defined models in terms of the two-body distribution function have been analysed in [2]. The main conclusion of this analysis is that the FAHT predictions to third order for ^{40}Ca and up to fourth order for ^{16}O are within 10-15% of the exact results for small values of the parameter $v = \langle \Phi / (1 - f^2) / \Phi \rangle$, a

range which includes the physically interesting cases. So one can conclude that the FAHT is a fairly efficient algorithm.

3. PADEIZATION OF THE FHAT CLUSTER EXPANSION.

There are two considerations that motivate the discussion we are going to present in this section.

Firstly, from a theoretical point of view it is interesting to analize the previous models over a larger range of values of the "wound volume" parameter v than in [2]. The results of this analysis (see figures 1 and 2 in the next section) indicate that as v increases the contibutions from higher orders tend to dominate in such a way that an asymptotic character for the cluster expansion is suggested.

Secondly, in view of the technical difficulties in calculating higher order contributions beyond the third or fourth order the following question becomes important: is it possible to obtain more profit from the information given by the calculation up to an (necessarily low) order n ? Or in other words, is it possible to accelerate the convergence of the expansion ?

A standard procedure in many branches of Mathematics and Physics when facing situations like these is to fill as far as possible the Padé table [3] : usually some subfamily of it gives better results than the original algorithm. This is what we do with the FAHT cluster expansion. Although much has been already said in this School about this expansion [4] for the sake of completeness it seems appropiate to recall here a few expressions.

To calculate the expectation value of an operator V with one-body and two-body parts, $V^{(1)}$ and $V^{(2)}$ respectively, in the correlated state Ψ the basic ingredients are the quantities

$$V^{(n)} = \sum_{i}^{n} V_i^{(1)} + \sum_{i<j}^{n} V_{ij}^{(2)} \qquad n \leq A$$

$$F^{(n)} = \prod_{i<j}^{n} f_{ij} \tag{9}$$

$$I_n(\beta) = \langle \Phi / F^{(n)} \exp[\beta V^{(n)}] F^{(n)} / \Phi \rangle$$

and finally

$$I_n(\beta) = \prod_{k=1}^{n} [Y_k(\beta)]^{\binom{n}{k}}$$

where the last equation gives the recursive definition of the cluster integrals $Y_k(\beta)$ as a function of the auxiliar parameter β.

To carry out the calculation up to order n means to take by force $Y_k(\beta) = 1$ for k>n. The expectation value we are looking for is then given by the logarithmic derivative

$$\langle V \rangle_{(n)} = \sum_{k=1}^{n} \binom{A}{k} \frac{Y_k'(0)}{Y_k(0)} \qquad (10)$$

In an analogous way the square of the norm of the correlated state Ψ obviously is

$$\langle \Psi / \Psi \rangle = I_A(0)$$

and to order n we have

$$\ln I_A^{(n)}(0) = \sum_{k=2}^{n} \binom{A}{k} \ln Y_k(0) \qquad (11)$$

Equations (10) and (11) are the expansions whose convergence we want to accelerate by the use of Padé approximants. This procedure is mainly applied to series of the form $S(x) = \sum a_n x^n$ which are slowly convergent or asymptotic. From this point of view the situation we have looks different because, as is clear from eqs. (10) and (11), in evaluating the expectation value $\langle V \rangle$ or the norm of Ψ for a finite many body system we have a finite sum and not properly a series. Certainly the same quantities could be expressed as infinite series in some variable but we do not know exactly how to choose this variable in such a way that somehow the process generates the cluster expansion.

Due to this fact the considerations in this section have to be taken as rather heuristic. The idea is to treat eqs. (10) and (11) as the n-th partial sums of a larger expansion and to construct with the lower order terms the Padé approximants. In all but the few exceptional cases quoted below we deal only with the [1/1] approximant. In terms of the partial sums S_0, S_1, S_2 of the series S it has the simple expresion

$$[1/1]_S = \frac{S_o S_2 - S_1^2}{S_o + S_2 - 2S_1}$$

As a matter of fact higher (non-diagonal) Padé approximants can be constructed for the case of ^{16}O where we have one more term at our disposal because in this nucleus the fourth order calculation has also been carried out. Nevertheless we consider only the [1/1] Padé approximant for the model calculations both in ^{16}O and ^{40}Ca.

In many applications the diagonal of the Padé table gives a sequence with good convergence properties. In our case to go one step farther in the diagonal Padé sequence , i.e. to be able to calculate the [2/2] approximant, we need information up to the fifth order. There exists a case where the cluster expansion has been carried out to this order. This is the analysis [5] of the normalization integral in ^{16}O. Notice however that this is not a model calculation in the sense given above because the norm of the correlated state is not known. In this situation, as pointed out in ref. [5], to get an idea of the goodness of a cluster expansion one has to relie on stability criteria. It is proved there that the FAHT expansion has better performances than other compiting cluster expansions being impressively stable in a fair range of the wound volume v. For larger values of this parameter the asymptotic-like character shows up again. This suggest also the application of the padeization algorithm.

4. RESULTS

In this section we present the results of the padeization of the model calculations for ^{16}O and ^{40}Ca and of the normalization integral for ^{16}O.

A few comments concerning the actual implementation of the padeization procedure are in order. For purely two-body operators the lowest order in the cluster expansion is not defined (i.e. one cannot define $V^{(1)}$ in eqs. (9)). Here the zero-th order contribution has been taken as the expectation value of the operator when no correlation is present and this has been seen to be a good starting point.

In the evaluation of the Padé approximant for the case (like the

R-model) where we have contributions from both one- and two-body terms we can either treat them separately or not. It turns out numerically that the former is a better alternative.An indication to proceed in this way is given by the observation that the one-body part of the operator (which is $\sum r_i^2$) is not well dealt with by the FAHT cluster expansion which when stopped at low orders can even predict completely unreasonable values for the expectation value while this situation is avoided when the Padé algorithm is used.

In the results presented here the value of the range parameter b in the correlation function given by eq. (3) has been kept fixed and the wound volume $v = \langle\Phi/(1-f^2)/\Phi\rangle$ has been varied over a wide range, which means different values of the depth parameter a.

Figures 1a-c show the results of the Isospin-, R- and H.O.-models for ^{16}O. The FAHT predictions to second, third and fourth order and the [1/1] Padé approximant are plotted versus the wound volume over a very wide range of values of this parameter (consider that the energy minimum for simple gaussian potentials is found for $v \sim .02-.03$). The corresponding results for ^{40}Ca are shown in Fig. 2a-c including only the FAHT predictions up to third order.

For low values of v, the FAHT cluster expansion for the model quantities up to third (^{40}Ca) or fourth (^{16}O) order give quite reasonable agreement with the exact values. The agreement is better for those quantities like the H.O. model involving only the direct part of the distribution function.

When v increases these predictions are getting worse. Then the [1/1] Padé approximant works extremely well compared to the third order. For the Isospin- and R-models it gives values which are, over the whole range of v, closer to the exact result than the second and third order. For the H.O.-model and low values of v the FAHT cluster expansion is clearly convergent and the [1/1] Padé approximant gives (not very much) worse results than the expansion up to third order. However at large values of the wound volume the expansion is asymptotic-like and the Padé result is again much closer to the exact result. This is valid both for ^{16}O an ^{40}Ca.

All this means that the [1/1] Padé approximant, requiring the same computational effort than the third order, is in general preferable to

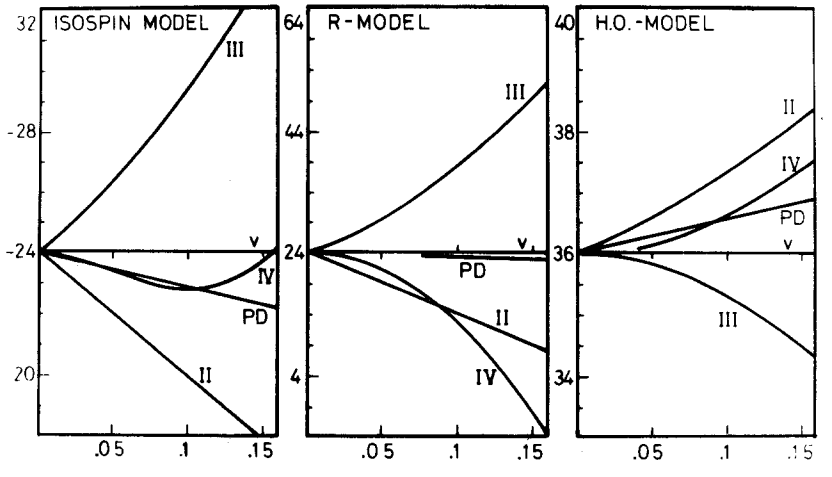

Figure 1. MODEL CALCULATIONS IN ^{16}O: a) Isospin Model, b) R-model, and c) H.O. model. The corresponding model is plotted versus the wound volume $\underline{v}$. II, III and IV refer to second, third and fourth order in the FAHT cluster expansion, and PD to the [1/1] Padé approximant. The horizontal line is the exact value of the model. Note that the vertical scales are different in each figure.

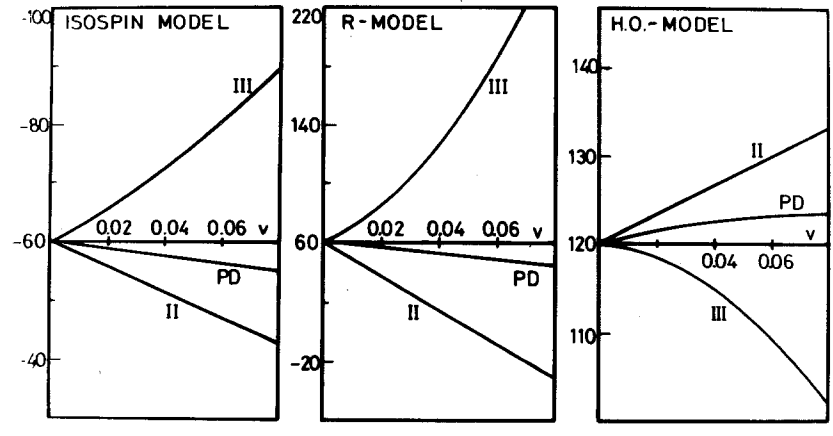

Figure 2. MODEL CALCULATIONS IN ^{40}Ca. See Fig. 1 for caption. Note that the fourth order in the FAHT cluster expansion has not been calculated for this nucleus.

the later.

The conclusion of a comparison between the Padé approximant and the fourth order in ^{16}O is not so compelling: for the R-model the [1/1] approximant is definitely better than the fourth order and the same is true for the H.O.-model if v >.1. On the contrary for the Isospin-model the fourth order prediction is in general better than the Padé approximant.

As pointed out in the previous section the study of the normalization integral in ^{16}O allows the construction of a larger part of the Padé table. Two types of comparison are possible in this case.

One can, on the one hand, calculate directly the I_5 integral ($I_5(0)$ in the notation of eqs. (9)) and compare its value with both the prediction from the fourth order and the [1/1] approximant. If this is done one reaches a conclusion similar to the one state above for the comparison between the fourth order and the Padé approximant in the case of the model calculations.

On the other hand, we can predict the full (squared) norm of the correlated state from the calculated contribution in fifth order and from the padeization procedure. Here it has to be emphasized once more that we do not know the exact value to compare with. The only thing we can say is that for large values of v the FAHT predictions become highly unstable while on the contrary a much higher stability is obtained from the Padé array. By this we mean that if all the approximants which can be reached from the knowledge of $I_1, I_2 \ldots$ up to I_5 are constructed then pretty stable values are obtained. This is shown in an extreme case in Table I.

TABLE I.-The [N/M] Padé table for the normalization integral in ^{16}O. In this case $f^2 = 1 - 0.9 \exp(-0.1r^2)$ which corresponds to a very large wound volume v=0.44. The first column, [N/0], is the FAHT series expansion. In brackets are given the powers of ten.

	0	1	2	3
1	1.83 (-22)	3.36 (-16)	3.72 (-17)	2.92 (-17)
2	1.15 (-13)	2.98 (-17)	2.83 (-17)	
3	1.01 (-19)	2.84 (-17)		
4	1.30 (-15)			

5. CONCLUSIONS

In this work we have tried to point out the interest of analysing a cluster expansion formalism by the method of Padé approximants.

As a first approach to the problem we have presented some numerology. The main conclusion from it is that as a general trend the [1/1] Padé approximant gives better values for the matrix elements considered that the corresponding third order in the cluster expansion and the improvement is progressively impressing as we move towards the asymptotic region of the wound volume parameter.

From a more practical point of view we have checked that when the padeization is applied to the variational determination of the energy neither the value nor the position of the minima are essentially modified. Nevertheless to apply the variational method safely it is necessary to know as accurately as possible the expectation values in a large range of the variational parameters and this is afforded by the Padé approximant.

In conclusion the results presented here seem interesting enough to indicate that it could be worthwhile to study more fundamental questions from the perspective advanced here. A deeper insight into the analytic structure of cluster expansions could emerge from that study.

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