AB INITIO CALCULATIONS IN MEDIUM–HEAVY NUCLEI

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A review of recent results obtained within the Correlated Basis Function theory framework in doubly closed shell is presented.

1 Introduction

The Correlated Basis Function (CBF) theory together with the Fermi Hypernetted Chain (FHNC) resummation techniques has been widely applied in the past to describe infinite nuclear systems [1]. In this last decade we have extended, tested and applied the theory to the description of medium-heavy doubly closed shell nuclei [2,3,4].

The aim is the solution of the many-body Schrödinger equation using a realistic hamiltonian. This hamiltonian is built by a two–body interaction constructed to fit the two–nucleon scattering data and the deuteron properties. An additional three–body force is added to this interaction to reproduce the properties of the three-nucleon systems.

The method used is based upon the variational principle where the minimum of the energy functional is searched within a space of states which can be described as:

$$\Psi_0(1,2...A) = G(1,2...A)\Phi_0(1,2...A) \tag{1}$$

where $\Phi_0(1,2...A)$ is a Slater determinant of single particle wave functions in its ground state, i.e. all the levels below the Fermi energy are occupied and those lying above are empty. The correlation function $G(1,2...A)$ is given as product of two-body correlation functions which have an operatorial dependence.

From a study of the various nucleon clusters it turns out that it is possible to sum in a closed form all diagrams having certain topological properties. This leads to the FHNC integral equations. This summation is possible only for purely scalar (Jastrow) correlations. In case of state dependent correlations one has to resort to approximations. Specifically, we used the Single Operator Chain (SOC) approximation consisting in considering diagrams where in the correlation chains the operatorial dependence appears only once per site.

Summarizing, with respect to an exact solution of the many–body Schrödinger equation, our approach has three approximations: the use of the variational principle, the fact that in FHNC some diagrams are not considered and finally the SOC approximation. A test of the various approximations has been done both in nuclear matter [1] and in finite nuclei [2,3,4] and it has been estimated an uncertainty on the binding energy per nucleon of about 1 MeV.

2 Ground state of ^{16}O and ^{40}Ca nuclei

The ground state of the ^{16}O and ^{40}Ca nuclei has been studied [4] by using two potentials of the Argonne family: the V14 and the V18. We used only the first 8 channels of the two potentials, i.e. the four central channels, the tensor and spin orbit channels together with their isospin partners. In the case of the Argonne V18 the truncation has been done by slightly rearranging the parameters of the considered channels in order to take into account the contribution of those which have been neglected. This potential, called Argonne V8', has been used in the Green Function Montecarlo calculations in light nuclei of the Urbana–Argonne group [5]. These two-body potentials have been implemented with the appropriate three-body forces of Urbana type: Urbana VIII for the V14 and the Urbana IX for the V8'.

In tab. 1 we compare the calculated energies with the experimental ones and, for the V8' case, also with nuclear matter estimates. The difference with the experimental value is of the same order of magnitude of that found in the nuclear matter case. There is room for improvement. These calculations

E/A (MeV)	^{16}O	^{40}Ca	n.m.
Exp	-7.97	-8.55	-16.0
A14	-5.11	-6.50	
A8'	-5.48	-6.97	-10.9
A8'*	-5.41	-6.64	

Table 1. Binding enrgies per nucleon in ^{16}O, ^{40}Ca and nuclear matter calculated with the Argonne V14 potential (A14) and with the V8' (A8'). The A8'* results have been obtained with a set of single particle wave functions reproducing the empirical charge densities.

have been done using identical single particle wave functions for protons and neutrons and in ls coupling. Furthermore in our calculations we do not include three-body correlation function.

A test of the quality of the obtained wave functions has been done by calculating the electron scattering elastic cross section which is compared in Fig. 1 with the experimental points. The results of the A14 and A8' calculations are represented by the dotted and the dashed lines. Also in this case the agreement with the data is unsatisfactory. To improve it we have selected a set of single particle waves reproducing at best the charge distributions. With these wave functions we have minimized the energy for the V8' interaction by changing only the correlation function. The cross sections obtained in this case are shown by the continuous lines and the corresponding binding energies are given in tab. 1 by the A8'* row. The set of single particle wave functions are rather different from those used in the A8' calculation. For example, the Woods–Saxon parameters used for ^{16}O are V=-42.0 MeV, R=3.60 fm and a=0.55 fm for A8', against V=-53.0 MeV, R=3.45 fm and a=0.70 fm for A8'*. Analogous differences are found in ^{40}Ca. In spite of this large difference in the single particle basis, the binding energies values do not change much as it is shown in tab. 1. This means that the behaviour of the energy functional around the variational minimum is rather flat and not sufficiently selective to identify unambigously the ground state wave functions.

As a further test of our ground state wave functions we have calculated the overlap functions between the nuclei composed by A and A-1 nucleons. This quantity can be investigated in one nucleon emission knock-out reactions like (e,e'p).

In the Independent Particle Model (IPM) the overlap function corresponds to the single particle hole wave function. The presence of correlations

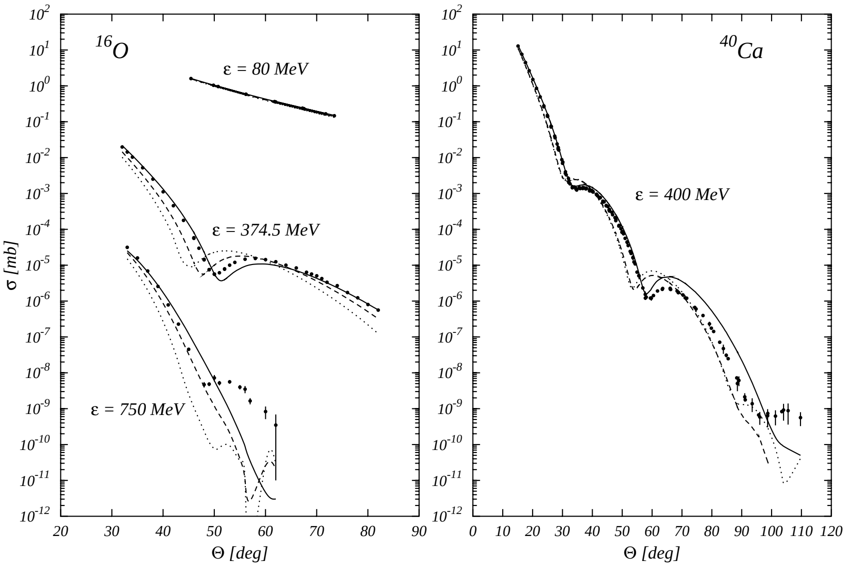

Figure 1. Elastic electron scattering cross sections compared with the exparimental data. Dotted lines A14, dashed lined A8', full lines A8'*.

in our approach modifies the situation. This is evident in fig. 2 where we show the squares of the overlap functions calculated in ^{16}O and ^{40}Ca using the A8'* wave functions. The symbols indicate the IPM results and the FHNC-SOC results are shown by the continuous lines. The dashed lines have been obtained using only the scalar part of the correlation. It is evident that while the Jastrow component of the correlation produces small effects, the tensor ones are extremely important.

The role of the tensor correlations becomes also clear in the spectroscopic factor, which is defined as the integral of the functions shown in fig. 2 weighted by r^2. We obtain for the 1p states of ^{16}O the value of 0.98 for Jastrow correlations while the calculation with the full correlation gives 0.90. An analogous effect is found in ^{40}Ca where the spectroscopic factor of the d levels is 0.97 for Jastrow correlations and it decreases to the value 0.87 in the full calculation.

We should notice that the empirical values of these spectroscopic factors

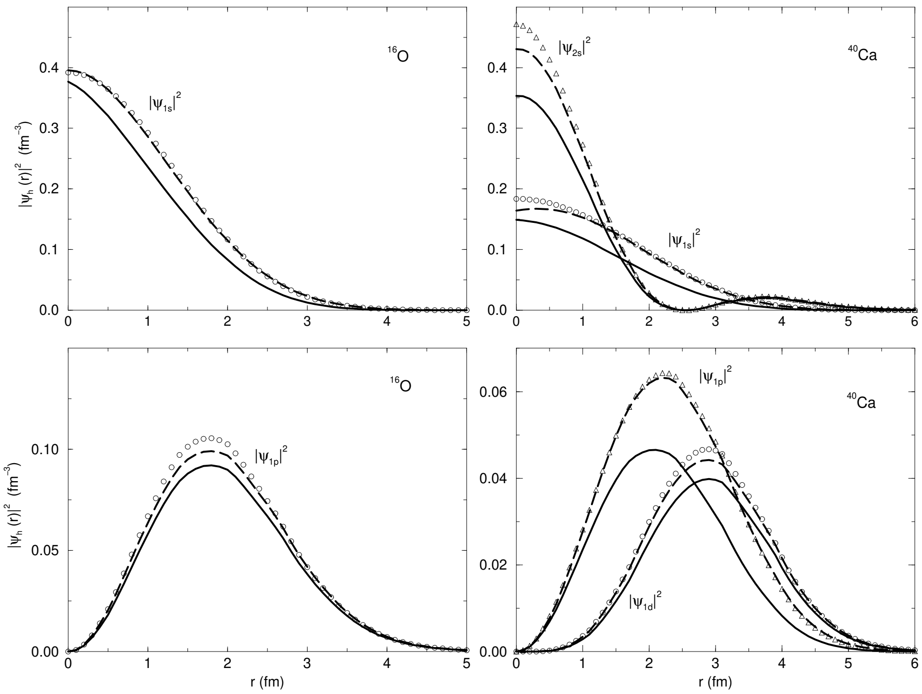

Figure 2. Overlap functions. The symbols indicate the IPM, the full lines the complete calculation and the dashed lines the Jastrow results .

are around 0.6 in both case. The difference with our results seems to indicate that our description of the ground state is missing some important physics effects.

3 Electromagnetic excitations

The study of nuclear excitation mechanisms implies the evaluation of the transition matrix element from the ground to the excited state of the nuclear system. Therefore it is possible to test the description of the ground state also by studying the nuclear excitations.

In our approach we made an ansatz on nuclear final states analogous to that done in eq. (1) for the ground state:

$$|\Psi_n\rangle \;=\; G\,|\Phi_n\rangle \tag{2}$$

where $|\Phi_n\rangle$ is a Slater determinant containing particle–hole excitations. In

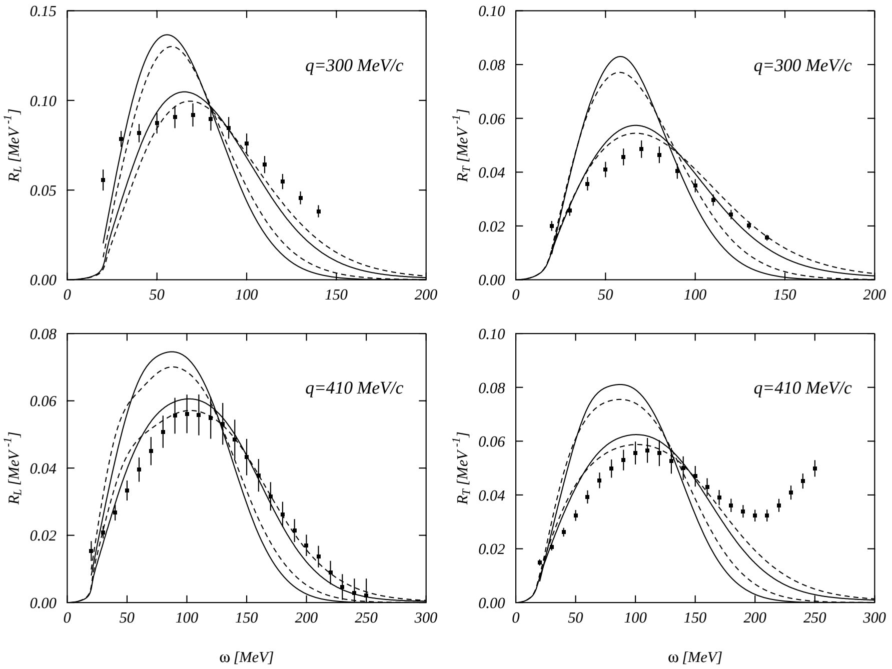

Figure 3. Quasi-elastic responses of ^{40}Ca compared with the data of ref. [10]. Full lines show the A8'* results dashed lines have been obtained with the S3 interaction. The lower lines have been obtained after inserting FSI .

our calculations we restrict ourselves to treat the case of a single particle–hole excitation. The correlation function G is the same as for the ground state.

We calculate the transition matrix element between $|\Psi_0\rangle$ and $|\Psi_n\rangle$ induced by one-body electromagnetic operators by making a cluster expansion. The full expansion has been widely used to study nuclear matter responses [7]. For finite nuclei we use a model which retains only those terms containing a single correlation line [8,9]. This implies the calculation of 4 two-point diagrams and 6 three-point diagrams in addition to the uncorrelated term. This set of diagrams it is necessary to conserve the appropriate normalization of the wave function. In the appropriate limit the contribution of the three-point diagrams cancels that of the two-point leaving the normalization of the uncorrelated term which is correctly constructed [9].

We have tested the validity of our approximation by comparing nuclear matter charge responses in the quasi-elastic region calculated with the full

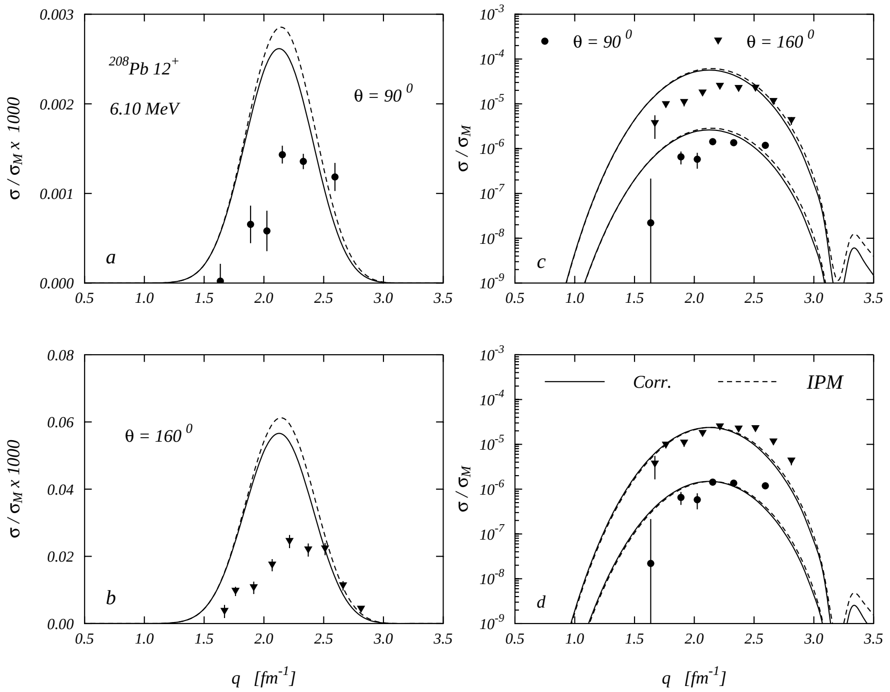

Figure 4. Excitation of the 12^+ state in ^{208}Pb [12]. The dashed line are the IPM results the full lines have been obtained with Jastrow correlations. The right panels show the results in a semilog scale. In the d panels the curves have been multiplied by quenching factors.

expansion and with our model [8]. The agreement is extremely good and makes us confident that the model is adequate to describe electromagnetic excitations, at least those induced by one-body operators.

We show in fig. 3 the ^{40}Ca responses calculated with the A8'* wave functions described in the previous sections. These are the full lines well above the MIT data [10]. The dashed lines, always well above the data, have been calculated by using a semi-realistic interaction, the S3 of Afnan and Tang. In both calculations only the Jastrow part of the correlations have been used. In spite of the possible claims on the effects of the tensor correlations it appears clear the difficulty of our calculations to reproduce the data. Only the inclusion of Final State Interactions (FSI) effects can bring the lines to a reasonable agreement with the data. This is shown in each panel by the two lower lines obtained by simulating the FSI with a phenomenological model.

From this calculation one may conclude that what is lacking in our calculations is the treatment of FSI produced by the re-interaction of the emitted nucleon with the rest nucleus. To test this hypothesis we performed calculations for the excitation of discrete states where the FSI problem is not present [11]. Since our approach cannot describe collective excitations we searched in the literature for those states candidate to be described as pure one-particle one-hole (1p-1h) transition. We analyzed 30 states in ^{16}O, ^{40}Ca, ^{48}Ca and ^{208}Pb nuclei by means of a discrete Random Phase Approximation (RPA) calculations with two different effective interactions. We retained only those states having X amplitude values larger than 0.9 in both calculations. Only 18 states remained: 1 in ^{16}O, 6 in ^{48}Ca and 11 in ^{208}Pb. For each of these states we calculated the electro-excitation in the IPM and including Jastrow correlations.

A typical result of our findings is shown in fig. 4 for the 12^+ case of ^{208}Pb at 6.10 MeV. The correlation lowers the IPM results but the calculations are still largely above the data of ref, [12]. This show that there is some physical effect beyond the correct treatment of FSI that the theory is unable to treat.

This fact is also confirmed by recent calculations of (e,e'p) cross sections [13] which overestimate the data even after the use of an optical potential which is supposed to describe the FSI of the emitted nucleon.

4 Conclusions

From what we have presented we draw three main conclusions:

- *Ab initio* calculations in medium-heavy nuclei are now available. So far these calculations have been done only for few-body systems and nuclear matter. This achievement allows a unified description of all nuclear systems based on the same microscopic hamiltonian. Clearly the status of the art of the calculations in medium-heavy nuclei is not yet comparable with that acheived in the other systems. Work to improve these calculations is in progress as well as the application to other hadronic systems like hypernuclei [14].

- We found that the energy functional has a very flat behaviour around the minimum. This limits the capability of the variational principle to select the many-body wave function of the nuclear ground state.

- From the comparison with the experimental data it appears clear that our approach is still missing some important physical effect.

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