RECENT RESULTS IN CBF THEORY
FOR MEDIUM-HEAVY NUCLEI

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ABSTRACT

We extend the correlated basis functions theory (CBF) for nuclei with \( N \neq Z \) and \( j-j \) coupling scheme. By means of the Fermi hypernetted chain integral equations, in conjunction with the single operator chain approximation (FHNC/SOC), we evaluate the ground state and the one-body densities for \(^{40}\text{Ca},^{48}\text{Ca} \) and \(^{208}\text{Pb} \) nuclei. The realistic Argonne V8’ two-nucleon potentials have been used. We compare the ground-state properties of these nuclei calculated by using correlation functions with \((f_6 \text{ model})\) and without \((f_4 \text{ model})\) tensor components.

The aim of this contribution is to report on the progresses done in the framework of a project \([1] - [5]\) aimed to apply the CBF theory to finite nuclear systems. The starting point of the theory is the variational principle,

\[
\delta E[\Psi] = \delta \left[ \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \right] = 0
\]

with the following ansatz for the expression of the many-body wave functions \( \Psi \):

\[
\Psi(1, 2, ..., A) = G(1, 2, ..., A) \Phi(1, 2, ..., A)
\]

The search of the minumum of the energy functional is done by making variations of the many-body correlation operator \( G(1, 2, ..., A) \) and of the single particle wave functions forming the Slater determinant \( \Phi(1, 2, ..., A) \). The many-body correlation operator is supposed to be described by a product of two-body operators \( F_{ij} \):

\[
G(1, 2, ..., A) = S \prod_{i<j} F_{ij}
\]

where the operator \( S \) symmetrizes the product. The two-body correlations \( F_{ij} \) have an operatorial dependence analogous to that of the modern nucleon-nucleon interactions. We consider \( F_{ij} \) of the form:

\[
F_{ij} = \sum_{p=1,8} f^p(r_{ij}) O_{ij}^p
\]

where the involved operators are:

\[
O_{ij}^{p=1,8} = [1, \sigma_i \cdot \sigma_j, S_{ij}, (L \cdot S)] \otimes [1, \tau_i \cdot \tau_j]
\]
In the above equation $\sigma$ and $\tau$ indicate the usual spin and isospin Pauli matrices, and $S_{ij}$ the tensor operator.

The evaluation of the many-variables integrals necessary to calculate the energy functional (1) is done by using the integral summation technique known as Fermi hypernetted chain (FHNC) [6], originally developed for infinite systems. The FHNC equations allows the sum of a set of infinite classes of Mayer-like diagrams resulting from the cluster expansion of Eq. (1). The use of state dependent correlations, as those of Eq. (4), requires special attention because the various correlation operators do not commute. In our calculations this difficulty is handled by considering, in addition to all the scalar correlations, only those diagrams having chains of correlation functions containing a single operator with $p > 1$. This is the so-called single operator chain (SOC) approximation [7].

|        | $F_4$ | $F_6$ | $F_4$ | $F_6$ | $F_4$ | $F_6$ |
|--------|-------|-------|-------|-------|-------|-------|
| $^{40}$Ca | 40.00 | 40.00 | 40.00 | 40.00 | 40.00 | 40.00 |
| $^{40}$Ca | 40.00 | 40.00 | 40.00 | 40.00 | 40.00 | 40.00 |
| $^{48}$Ca | 48.00 | 48.00 | 48.00 | 48.00 | 48.00 | 48.00 |
| $^{48}$Ca | 48.00 | 48.00 | 48.00 | 48.00 | 48.00 | 48.00 |
| $^{208}$Pb | 208.00 | 208.00 | 208.00 | 208.00 | 208.00 | 208.00 |
| $^{208}$Pb | 208.00 | 208.00 | 208.00 | 208.00 | 208.00 | 208.00 |

Table 1: Contributions to the binding energies per nucleon for the three nuclei considered. All the quantites are expressed in MeV.

In the past, we have applied this theory to describe the ground state of doubly closed shell nuclei by using two-body potentials and correlations containing operator terms up to the tensor components [1, 2, 3, 4], and also a three-body interaction [5]. These calculations have been limited to the $^{16}$O and $^{40}$Ca nuclei since the formalism was developed in $ls$ coupling scheme and for single particle wave functions equal for both protons and neutrons. Formally this situation is very similar to that of the symmetric nuclear matter.

In this report we present the first results obtained by extending the FHNC/SOC scheme for nuclei with different wave functions for protons and neutrons and in $jj$ coupling representation. The results of these calculations have been done by using the realistic $v'_{8}$ Argonne two-body potential, but without any three-body force, which, in any case, will be soon implemented. For this reason, the results we show here, should not be considered fully realistic. In any case, already at this stage, they give interesting informations on the nuclear structure.

The separated treatment of protons and neutrons requires that the correlations should be considered separately in their spin and isospin part:

$$ F_{ij} = \sum_{k=1}^{3} \sum_{l=0}^{1} f_{2k-1+i}(r_{ij})O_{ij}^{2k-1+l} = \sum_{l=0}^{1} (\vec{\sigma}_i \cdot \vec{\sigma}_j)^l \sum_{k=1}^{3} f_{2k-1+i}(r_{ij})P_{ij}$$

(6)

Another, in principle more obvious, consequence, is that the FHNC/SOC equations should be almost triplicated to consider one- and two-body densities of proton-proton, neutron-neutron, and isospin mixed type. In $jj$ coupling these equations should be further extended to distinguish between two different types of statistical correlations, with parallel or antiparallel spin.

As already stated, the calculations have been done by using the $v'_{8}$ reduction of the Argonne $v_{18}$ two-body potential [8]. The operator structure of this potential is given in Eq. (5). The channels up to $p = 6$ have been treated within the FHNC/SOC formalism without any approximation, while the contributions of the two spin-orbit channels have been calculated by using perturbation theory [8, 9].

In the correlations the two spin-orbit channels have been neglected. The results have been obtained by using a fixed set of single particle wave functions and searching for the minimum by modifying the correlations. The two-body
correlation functions, have been generated by solving a set of coupled Euler-Lagrange equations. The search of the minimum has been done by changing only two parameters: the healing distance $d_t$ of the two tensor channels, and another healing distance $d_c$ related to all the other channels. These are the nucleonic relative distances where the various two-body correlation functions reach their asymptotic values, one for $p = 1$ and zero for all the other cases.

We show in Tab. 1 the results obtained for the $^{40}$Ca, $^{48}$Ca and $^{208}$Pb nuclei. The single particle wave functions have been generated by using a Woods-Saxon potentials whose parameters have been taken from the literature [3]. For each nucleus, in addition to the full calculation, whose results are indicated in the $F_6$ columns, we also made calculations by using only the first four central channels of the correlations. These are the results shown by the $F_4$ columns. The rows of the table indicate the contributions of the various terms to the binding energy per nucleon: $T$ is the kinetic energy, $V_8$ the nuclear interaction term, $V_C$ the Coulomb term (here divided by the number of protons), and finally $E_{ee}$ is the contribution of a relevant elementary diagram that should be added to the FHNC/SOC calculations [1] to properly satisfy the various sum rules. All the terms with the $jj$ labels indicate the contribution due to the antiparallel spin densities.

A first remark, is that the $f_4$ calculations produce more binding than the $F_6$ ones. The tensor terms of the correlation reduce the binding as it is shown by the $V_8$ row. The kinetic energies have similar values in all the calculations, and also the Coulomb terms are not affected by the tensor correlation.

![Correlation Functions](image)

Figure 1: The $f^1, f^6$ correlation functions. The $^{40}$Ca, $^{48}$Ca, $^{208}$Pb correlations are indicated with solid, dashed and dotted lines respectively.

In Fig. 1 we compare the correlation functions of the three nuclei considered. In the upper panel the scalar correlation functions, are shown, while in the other panel the tensor-isospin correlation functions, $p = 6$ channel in Eq. 4, are compared. The scalar correlation functions are rather similar for all the three nuclei considered, they heal at 1.4 fm. The tensor-isospin correlations heal at larger distances and show a strong dependence on the nucleus. The healing for the $^{208}$Pb is larger than that for the other two nuclei.
Another interesting remark comes from observing the results obtained by the same type of calculation in the various nuclei. Kinetic energies and nuclear energies clearly show saturation properties while the repulsive Coulomb contribution increases with increasing proton number. The comparison between the Coulomb terms of the two calcium isotopes show a relatively large difference. This is surprising, but it demonstrates that the presence of a different number of neutrons modifies the proton densities, as it is shown in Fig. 2.

A further remark about the results shown in Tab. 1 regards the contribution of the antiparallel spin terms, the $jj$ contributions. In general, these contributions are rather small and, as expected, they become even smaller in $^{40}$Ca where all the spin-orbit partners levels are saturated.

To conclude, we may say that the extension of the FHNC/SOC formalism to treat nuclei with $N \neq Z$ in $jj$ coupling scheme has been successful. This has allowed us to perform calculations of binding energies and density distributions of medium-heavy nuclei with neutron excess such as $^{48}$Ca and $^{208}$Pb, by using a realistic two-body potential. To the best of our knowledge this is the first microscopic calculation for the $^{208}$Pb nucleus. As already mentioned, a fully realistic calculation should include also a three-body interaction. The work in this direction has quite advanced and we plan to obtain results in short time.

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