New results in the CBF theory
for medium-heavy nuclei

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Abstract

Momentum distributions, spectroscopic factors and quasi-hole wave functions of medium-heavy doubly closed shell nuclei have been calculated in the framework of the Correlated Basis Function theory, by using the Fermi hypernetted chain resummation techniques. The calculations have been done by using microscopic two-body nucleon-nucleon potentials of Argonne type, together with three-body interactions. Operator dependent correlations, up to the tensor channels, have been used.

1   Introduction

The validity of the non relativistic description of the atomic nuclei has been well established in the last ten years. The idea is to describe the nucleus with a Hamiltonian of the type:

$$H = -\frac{\hbar^2}{2m} \sum_i \nabla^2 + \sum_{i<j} v_{ij} + \sum_{i<j<k} v_{ijk} \ , \tag{1}$$

where the two- and three-body interactions, v_{ij} and v_{ijk} respectively, are fixed to reproduce the properties of the two- and three-body nuclear systems.

About fifteen years ago, we started a project aimed to apply to the description of medium and heavy nuclei the Correlated Basis Function (CBF) theory, successfully used to describe the nuclear and neutron matter properties [1, 2]. We solve the many-body Schrödinger equation by using the variational principle:

$$\delta E[\Psi] = \delta \frac{< \Psi|H|\Psi >}{< \Psi|\Psi >} = 0 \ . \tag{2}$$

The search for the minimum of the energy functional is carried out within a subspace of the full Hilbert space spanned by the A-body wave functions which can be expressed as:

$$\Psi(1, ..., A) = \mathcal{F}(1, ..., A)\Phi(1, ..., A) \ , \tag{3}$$

where $\mathcal{F}(1,...,A)$ is a many-body correlation operator, and $\Phi(1,...,A)$ is a Slater determinant composed by single particle wave functions, $\phi_\alpha(i)$. We use two and three-body interactions of Argonne and Urbana type, and we consider all the interaction channels up to the spin-orbit ones. The complexity of the interaction requires an analogously complex correlation:

$$\mathcal{F} = \mathcal{S} \left(\prod_{i<j=1}^{A} F_{ij} \right) \ , \tag{4}$$

where $\mathcal{S}$ is a symmetrizer operator and F_{ij} has the form:

$$F_{ij} = \sum_{p=1,6} f^p(r_{ij}) O_{ij}^p \ . \tag{5}$$

In the above equation we have adopted the nomenclature commonly used in this field, by defining the operators as:

$$O_{ij}^{p=1,6} = [1, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, S_{ij}] \otimes [1, \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j] \ , \tag{6}$$

where $S_{ij} = (3\hat{\mathbf{r}}_{ij} \cdot \boldsymbol{\sigma}_i \hat{\mathbf{r}}_{ij} \cdot \boldsymbol{\sigma}_j - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)$ is the tensor operator.

The binding energies and the charge distributions of ^{12}C , ^{16}O , ^{40}Ca , ^{48}Ca and ^{208}Pb doubly closed shell nuclei have been obtained by solving the Fermi Hypernetted Chain (FHNC) equations in the Single Operator Chain (SOC) approximation [3]. These calculations have the same accuracy of the best variational calculations done in nuclear and neutron matter [1, 2].

By using this FHNC/SOC computational scheme we have investigated the effects of the correlations on some ground state quantities which are related to observables. A first quantity we have studied is the momentum distribution. It is well known that the short–range correlations enhance by orders of magnitude the high-momentum components of the momentum distribution [4]. We have also studied the spectroscopic factors since, as we have already mentioned, their empirical values are always smaller than the independent particle model (IPM) predictions.

The present study has been done by using the many-body wave functions obtained in Ref. [3]. The Argonne v_8' two-nucleon potential, together with the Urbana XI three-body force has been used.

In the next sections we present the results of our study of the One-Body Density Matrix (OBDM) and of the momentum distribution and we evaluate the spectroscopic factors.

2   The momentum distributions

The OBDM, of a system of A nucleons is defined as:

$$\rho^{s,s';t}(\mathbf{r}_1, \mathbf{r}_1') = \frac{A}{<\Psi|\Psi>} \int dx_2 \ldots dx_A$$
$$\Psi^\dagger(x_1, x_2, \ldots, x_A)\chi_t(1)\chi_s(1)\chi_t^\dagger(1')\chi_{s'}^\dagger(1')\Psi(x_1', x_2, \ldots, x_A) \ . \tag{7}$$

In the above expression, the variable x_i indicates the position ($\mathbf{r}_i$) and the third components of the spin (s) and of the isospin (t) of the single nucleon. With the integral sign we understand that also the sum on spin and isospin of all the particles, including $1'$, is performed. The OBDM of eq. (7) is characterized by the quantum numbers relative to the particle 1. In our
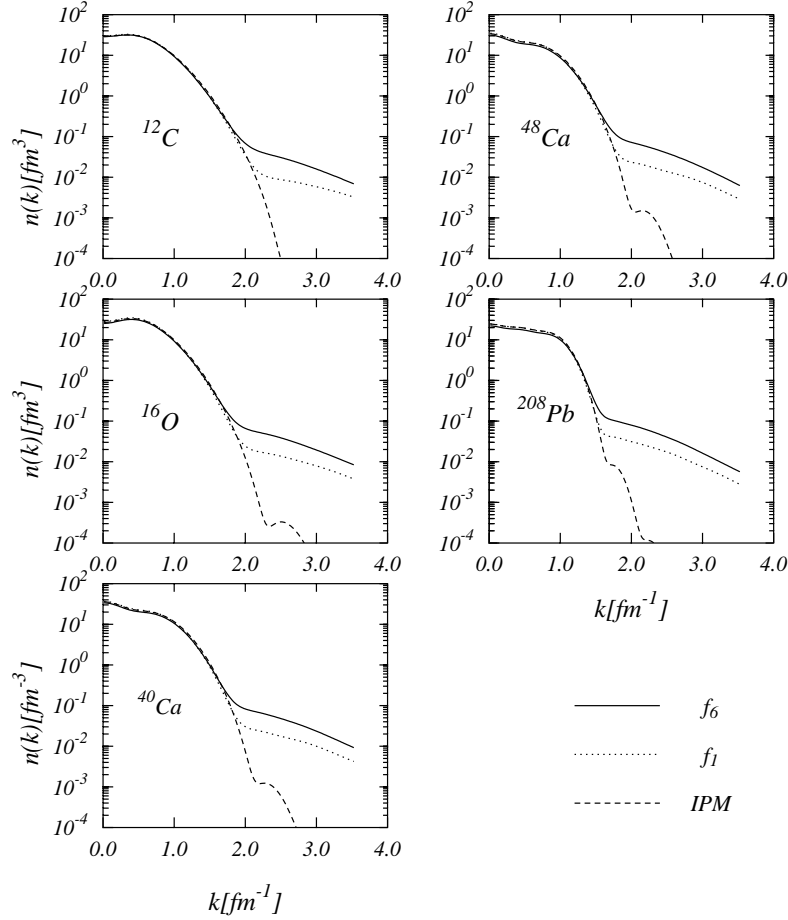
Figure 1: The proton momentum distributions for the ^{12}C , ^{16}O , ^{40}Ca , ^{48}Ca , ^{208}Pb nuclei calculated in the IPM model (dashed lines), by using the scalar correlation only (dotted lines) and the full correlation operator in FHNC/SOC approximation (solid lines).

calculations we are interested in the quantity:

$$\rho^t(\mathbf{r}_1, \mathbf{r}_1') = \sum_{s=\pm 1/2} \left[\rho^{s,s;t}(\mathbf{r}_1, \mathbf{r}_1') + \rho^{s,-s;t}(\mathbf{r}_1, \mathbf{r}_1') \right] \quad , \tag{8}$$

whose diagonal part represents the one-body density of neutrons or protons, this last one is related to the charge density distribution of the nucleus.

We define the momentum distributions of protons or neutrons as:

$$n^t(k) = \frac{1}{\mathcal{N}_t} \int d\mathbf{r}_1 d\mathbf{r}_1' \, e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_1')} \rho^t(\mathbf{r}_1, \mathbf{r}_1') \quad , \tag{9}$$

where we have indicated with $\mathcal{N}_t$ the number of protons or neutrons. We describe doubly closed shell nuclei, with different numbers of proton and neutrons, in a jj coupling scheme. The correlated OBDM is obtained by using the ansatz (3) in Eq. (7). The calculation is done by following the lines indicated in Ref. [5] and considering, in addition, the presence of the antiparallel spin terms and distinguishing proton and neutron contributions. The diagonal part of the OBDM

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is the one-body density, normalized to the number of nucleons. We present in Fig.1 the proton momentum distributions, for the ^{12}C , ^{16}O , ^{40}Ca , ^{48}Ca and ^{208}Pb nuclei. The dashed lines show the results obtained in the IPM model, the dotted lines those results calculated by using the scalar correlations only and, finally, the solid lines indicate the momentum distributions obtained by using the full operator dependent correlations. The high momentum components of the correlated distributions are orders of magnitude larger than those produced by the IPM. The operator dependent terms of the correlations further increase this behavior.

3   The spectroscopic factors

The quasi-hole wave function is defined as:

$$\psi^t_{nljm}(x) = \sqrt{A}\frac{<\Psi_{nljm}(A-1)|\delta(x-x_A)P^t_A|\Psi(A)>}{<\Psi_{nljm}(A-1)|\Psi_{nljm}(A-1)>^{1/2}<\Psi(A)|\Psi(A)>^{1/2}} \quad , \tag{10}$$

where we have indicated with $\Psi_{nljm}(A-1)$ and $\Psi(A)$ the wave functions describing the nuclei formed by $A-1$ and A nucleons respectively, and with P^t_A the isospin projector. The subindexes $nljm$ designate the quantum numbers of the odd-even nucleus.

We describe the wave function of the nucleus with $A-1$ nucleons by using an ansatz analogous to that of Eq. (3):

$$\Psi_{nljm}(A-1) = F(1,...,A-1)\,\Phi_{nljm}(1,...,A-1) \quad , \tag{11}$$

where $\Phi_{nljm}(1,...,A-1)$ indicates a Slater determinant obtained by removing from the Slater determinant $\Phi(1,...,A)$ a single state characterized by the quantum numbers $nljm$. In the IPM the quasi-hole wave functions coincide with the mean-field wave functions.

In order to obtain the radial part of the quasi-hole wave function we multiply equation (10) by $<jm|$, we integrate over the angular coordinate Ω, and sum on the spin coordinates [5]:

$$\psi^t_{nlj}(r) = \sum_{\mu,s} <l\mu 1/2s|jm> \int d\Omega\, Y^*_{l\mu}(\Omega)\chi^\dagger_s\, \psi^t_{nljm}(x) = \mathcal{X}^t_{nlj}(r)[\mathcal{N}^t_{nlj}]^{1/2} \quad . \tag{12}$$

From the knowledge of the quasi-hole functions we obtain the spectroscopic factors as:

$$S^t_{nlj} = \int dr\, r_1^2\, |\psi^t_{nlj}(r)|^2 \quad . \tag{13}$$

In Fig. 2 we compare the theoretical spectroscopic factors calculated for the proton bound states of the ^{208}Pb nucleus with the experimental data of Ref. [6]. In abscissa we give the separation energies defined as the difference between the energy of a A-nucleon system and that of the $A-1$-nucleon system obtained by removing the $nljm$ state. The agreement between theory and experiment is better for the deeply bound shells than for those levels closer to the Fermi surface. This could be due to the strong coupling between the quasi-hole wave function and the low-lying surface vibrations. The effects of this coupling, usually called long-range correlations, not explicitly treated by our theory, are expected to be larger for the external shells than for the internal ones.

The effect of the correlations on the quasi-hole wave functions is presented in Fig. 3 where we have shown the squared quasi-hole $3s_{1/2}$ proton wave function calculated with increasing complexity in the correlation function. The full line indicates the IPM result, the other lines have been obtained by using only scalar correlations, f_1, operatorial correlations without the
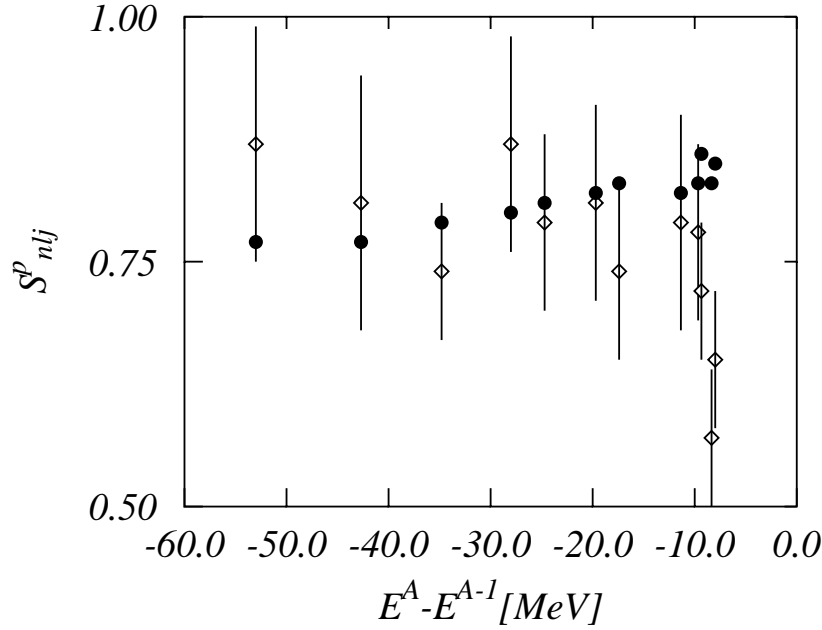
Figure 2: Comparison between the theoretical, black points, and the experimental, empty diamonds, spectroscopic factors for some proton states of ^{208}Pb. In the x axis we indicate the separation energies.

tensor channels, f_4, and correlations which include also the tensor dependent terms, f_6. The presence of the correlations produces a lowering of the quasi-hole wave function in the nuclear center. There is a consistent trend of the correlations effects: the more elaborated is the correlations the larger is the decreasing at the center of the nucleus.

4 Summary and conclusions

In this work momentum distributions, spectroscopic factors and quasi-hole wave functions of medium-heavy doubly closed shell nuclei have been calculated by extending the FHNC/SOC computational scheme. The calculations have been done considering the different number of proton and neutrons and the single particle basis are given in a jj coupling scheme. A microscopic two-body interaction of Argonne type, implemented with the appropriated three-body force of Urbana type, have been used. The calculations have been done with operator dependent correlations which include, in addition to the four central channels, also tensor correlations.

The comparison between our results with those obtained in the IPM highlights the correlations effects. The correlated momentum distributions have high momentum tails which are orders of magnitude larger than the IPM results. The spectroscopic factors are always smaller than one, the IPM value, and in a reasonable agreement with the experimental values, especially for the more bounded states. The quasi-hole wave functions are depleted in the nuclear center by the correlations. We have found that the operator dependent terms emphasize the correlations effects.
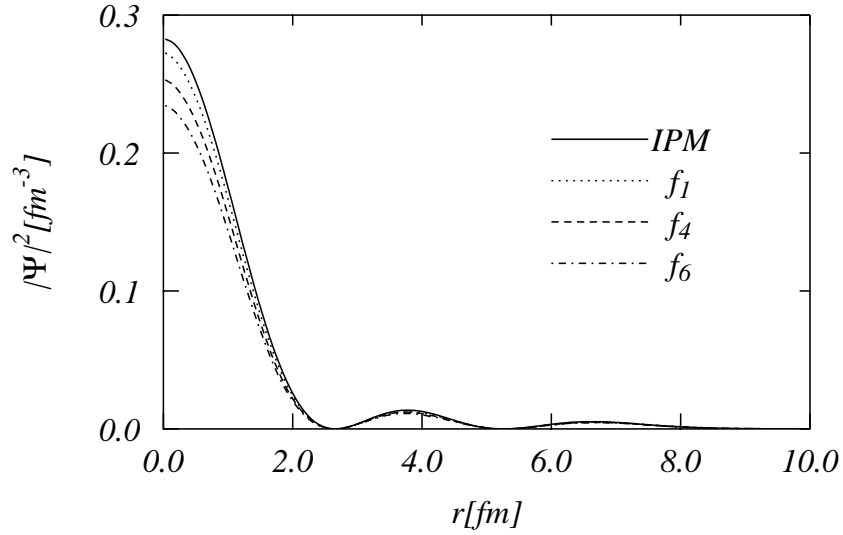
Figure 3: The square of the quasi-hole wave function for the $3s_{1/2}$ proton state of the ^{208}Pb . The labels *unc*, *Jas*, f^4 and f^6 indicate the IPM,Jastrow, f^4 and f^6 models respectively.

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