Momentum distributions and spectroscopic factors of doubly-closed shell nuclei in correlated basis function theory

C. Bisconti$^{1,2,3}$, F. Arias de Saavedra$^2$ and G. Co$^1$

$^1$ Dipartimento di Fisica, Università del Salento and I.N.F.N., sezione di Lecce, I-73100 Lecce, Italy
$^2$ Departamento de Física Atómica, Molecular y Nuclear, Universidad de Granada, E-18071 Granada, Spain
$^3$ Dipartimento di Fisica, Università di Pisa, I-56100 Pisa, Italy

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I. INTRODUCTION

One of the major achievements of nuclear structure studies in the last ten years is the consolidation of the validity of the non relativistic many-body approach. The idea is to describe the nucleus with a Hamiltonian of the type:

$$H = -\frac{\hbar^2}{2m} \sum_i A \nabla_i^2 + \sum_{i<j=1}^A v_{ij} + \sum_{i<j<k=1}^A v_{ijk}, \quad (1)$$

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. The Schrödinger equation has been solved without approximations for few body systems [1] and light nuclei [2], up to A=12 [3]. The obtained results provide good descriptions, not only of the energies of these nuclei, but also of other observables.

The difficulties in extending to medium and heavy nuclei the techniques used in few body systems and light nuclei, favored the development of models, and of effective theories. The basic idea of the effective theories is to work in a restricted space of the many-body wave functions. Usually, one works with many-body wave functions which are Slater determinants of single particle wave functions. The idea of single particle wave functions implies the hypothesis of a mean-field where each nucleon move independently from the other ones. This Independent Particle Model (IPM) is quite far from the picture outlined by the microscopic calculations quoted above, describing the nucleus as a many-body system of strongly interacting nucleons. In the Hartree-Fock theory, which provides the microscopic foundation of the IPM, the Hamiltonian is not any more that of Eq. (1), but it is an effective Hamiltonian built to take into account, obviously in an effective manner, the many-body effects that the microscopic calculations explicitly consider. The construction of effective interactions starting from the microscopic ones, covers a wide page of the nuclear physics history, starting from the Brueckner G-matrix effective interactions [4,5], up to the recent $V_{lowk}$ interaction [6,7] and the interaction obtained by applying the unitary correlation operator method [8,9].

The application of the IPM is quite successful, but there are evidences of the intrinsic limitations in its applicability. For example, the measured spectroscopic factors are systematically smaller than one [10,11,12], which is the value predicted by the IPM. The (e,e’)p cross sections in the quasi-elastic region need a consistent reduction of the IPM hole strength to be explained [13,14]. The same holds for the electromagnetic form factors of the low-lying states, especially those having large angular momentum [15,16]. The emission of two like nucleons in photon and electron scattering process cannot be described by the IPM [17,18]. Also the charge density distributions extracted by elastic electron scattering data are, in the nuclear interior, smaller than those predicted by the IPM [19,20]. These examples indicate the presence of physics effects, commonly called correlations, which are not described by the IPM.

It is common practice to distinguish between long- and short-range correlations since they have different physical sources. The long-range correlations are related to collective excitations of the system, such as the giant resonances. The short-range correlations (SRC) are instead connected to the strongly repulsive core of the microscopic nucleon-nucleon interaction. The repulsive core reduces the possibility that two nucleons can approach each other, and this
modifies the IPM picture where, by definition, the motion of each nucleon does not depend on the presence of the other ones.

Even though most of the calculations of medium heavy nuclei are based on the IPM, and on the effective theories, various techniques, aiming to attack the problem by using the microscopic Hamiltonian \( H \), have been developed. The Brueckner-Hartree-Fock approach has been recently applied to the \(^{16}\text{O} \) nucleus \[21\]. No core-shell model calculations have been done for nuclei lighter than \(^{12}\text{C} \) \[22, 23\]. The coupled cluster method has been used to evaluate \(^{16}\text{O} \) properties \[24, 25\].

About fifteen years ago \[26\], 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 \[27, 28\]. We solve the many-body Schrödinger equation by using the variational principle:

\[
\delta E[\Psi] = \delta \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = 0. \tag{2}
\]

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

\[
\Psi(A) = \mathcal{F}(1, \ldots, A) \Phi(1, \ldots, A), \tag{3}
\]

where \( \mathcal{F}(1, \ldots, A) \) is a many-body correlation operator and \( \Phi(1, \ldots, A) \) is a Slater determinant composed by single particle wave functions, \( \phi_\alpha(i) \). In our calculations, we used two-body interactions of Argonne and Urbana type, and we considered all the interaction channels up to the spin-orbit ones. Together with these two-body interactions, we used the appropriated three-body forces of Urbana type. The complexity of the interaction required the use of operator dependent correlations. We consider correlations of the type:

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

where \( S \) is a symmetrizer operator and \( F_{ij} \) is expressed in terms of two-body correlation functions \( f_p \) as:

\[
F_{ij} = \sum_{p=1}^6 f_p(r_{ij}) O_{ij}^p. \tag{5}
\]

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

\[
O_{ij}^{p=1,6} = [1, \sigma_i \cdot \sigma_j, S_{ij}] \otimes [1, \tau_i \cdot \tau_j], \tag{6}
\]

where \( \sigma_i \) and \( \tau_i \) indicate the usual Pauli spin and isospin operators, and \( S_{ij} = (3 \hat{r}_{ij} \cdot \sigma_i \cdot \sigma_j - \sigma_i \cdot \sigma_j) \) is the tensor operator.

We recently succeeded in formulating the Fermi Hypernetted Chain (FHNC) equations, in Single Operator Chain (SOC) approximation, for nuclei non saturated in isospin, and with single particle basis described in a \( jj \) coupling scheme. We presented in Ref. \[29\] the binding energies and the charge distributions of \(^{12}\text{C} \), \(^{16}\text{O} \), \(^{40}\text{Ca} \), \(^{48}\text{Ca} \) and \(^{208}\text{Pb} \) doubly closed shell nuclei obtained by using the minimization procedure \[2\]. These calculations have the same accuracy of the best variational calculations done in nuclear and neutron matter \[27, 28\].

In the present article, we show the results of our study, done in the FHNC/SOC computational scheme, on some ground state quantities related to observables. They are momentum distributions, natural orbits and their occupation numbers, quasi-hole wave functions and spectroscopic factors. We used the many-body wave functions obtained in Ref. \[29\] by solving Eq. \[2\] with the Argonne \( v'_{\text{8}} \) two-nucleon potential, together with the Urbana IX three-body force. We have calculated momentum distributions also with the wave functions produced by another interaction, the Urbana \( v'_{\text{14}} \) truncated up to the spin-orbit terms, implemented with the Urbana VII three-body force. The results obtained with this last interaction do not show relevant differences with those obtained with the \( v'_{\text{8}} \) and UIX interaction, therefore we do not present them.

The paper is organized as follows. In Sect. \[II\] we present the results of the One-Body Density Matrix (OBDM) and of the momentum distribution. In Sect. \[III\] we discuss the natural orbits, i.e. the single particle wave functions forming the basis where the OBDM is diagonal. In Sect. \[IV\] we present our results about the quasi-hole wave functions and in Sect. \[V\] we summarize our results and draw our conclusions.
II. ONE-BODY DENSITY MATRIX AND MOMENTUM DISTRIBUTION

We define the one-body density matrix, (OBDM), of a system of \( A \) nucleons as:

\[
\rho(x_1, x'_1) = \sum_{s,s^t} \rho^{s,s^t}(r_1, r'_1) \chi_s^t(1) \chi_{s^t}(1') \chi_t(1') \chi_t(1)
\]

\[
= \frac{A}{\langle \Psi | \Psi \rangle} \int dx_2 \ldots dx_A \psi^t(x_1, x_2, \ldots, x_A) \psi(x'_1, x_2, \ldots, x_A).
\]

(7)

In the above expression, the variable \( x_i \) indicates the position \((r_i)\) and the third components of the spin \((s_i)\) and of the isospin \((t_i)\) of the single nucleon. The \( \chi(i) \) functions represent the Pauli spinors. With the integral sign we understand that also the sum on spin and isospin third components of all the particles from 2 up to \( A \), is done. In our calculations we are interested in the quantity:

\[
\rho^t(r_1, r'_1) = \sum_{s=\pm 1/2} \left[ \rho^{s,s^t}(r_1, r'_1) + \rho^{s,-s^t}(r_1, r'_1) \right],
\]

(8)

whose diagonal part \((r'_1 = r_1)\) represents the one-body density of neutrons or protons.

We obtain the momentum distributions of protons \((t=1/2)\) or neutrons \((t=-1/2)\) as:

\[
n^t(k) = \frac{1}{(2\pi)^3 N_t} \int \frac{1}{N_t} \int d\mathbf{r}_1 d\mathbf{r}'_1 \, e^{i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}'_1)} \rho^t(\mathbf{r}_1, \mathbf{r}'_1),
\]

(9)

where we have indicated with \( N_t \) the number of protons or neutrons. The above definitions imply the following normalization of \( n(k) \):

\[
\int d\mathbf{k} n^t(k) = 1.
\]

(10)

We describe doubly closed shell nuclei, with different numbers of proton and neutrons, in a \( jj \) coupling scheme. The most efficient single particle basis to be used is constructed by a set of single particle wave functions expressed as:

\[
\phi_{nljm}^t(\mathbf{r}_i) = R_{nlj}(r_i) \sum_{\mu,s} <l\mu \mid s|jm> Y_{\mu}(\Omega_i) \chi_s(i) \chi_t(i) = R_{nlj}^t(r_i) Y_{lj}^m(\Omega_i) \chi_t(i).
\]

(11)

In the above expression we have indicated with \( Y_{\mu} \) the spherical harmonics, with \(<|>\) the Clebsch-Gordan coefficient, with \( R_{nlj}^t(r_i) \) the radial part of the wave function, and with \( Y_{lj}^m \) the spin spherical harmonics \(30\).

The uncorrelated OBDMs, those of the IPM, are obtained by substituting in Eq. (7) the correlated function \(|\Psi\rangle\) with the Slater determinant \(|\Phi\rangle\) formed by the single particle wave functions (11). We obtain the following expressions:

\[
\rho_o^t(r_1, r'_1) = \sum_s \left[ \rho_o^{s,s^t}(r_1, r'_1) + \rho_o^{s,-s^t}(r_1, r'_1) \right],
\]

(12)

\[
\rho_o^{s,s^t}(r_1, r'_1) = \frac{1}{8\pi} \sum_{nlj} (2j + 1) R_{nlj}^t(r_1) R_{nlj}^t(r'_1) P_l(\cos \theta_{11'}) \sin \theta_{11'},
\]

(13)

\[
\rho_o^{s,-s^t}(r_1, r'_1) = \frac{1}{4\pi} \sum_{nlj} (-1)^{j-l-1/2} R_{nlj}^t(r_1) R_{nlj}^t(r'_1) P_l(\cos \theta_{11'}) \sin \theta_{11'} P_l'(\cos \theta_{11'})
\]

(14)

In the above equations \( \theta_{11'} \) indicates the angle between \( r_1 \) and \( r'_1 \), and \( P_l \) and \( P_l' \) the Legendre polynomials and their first derivative respectively. The presence of the second term of Eq. (12), the antiparallel spin terms given in Eq. (14), is due to the \( jj \) coupling scheme required to describe heavy nuclei.

The correlated OBDM is obtained by using the ansatz (3) in Eq. (7). This calculation is done by using the cluster expansion techniques as indicated in \(31\) and \(32\), where only scalar correlations have been used, and in \(33\), where the state dependent correlations have been used, but in a \( ls \) coupling scheme. We followed the lines of Ref. \(33\) and, in addition, we consider the presence of the antiparallel spin terms and we distinguish proton and neutron contributions.
FIG. 1: The proton one-body density matrix, $\rho(r_1, r'_1)$, for the $^{208}$Pb nucleus in FHNC/SOC approximation, calculated for $\theta_{11'}=0$. The diagonal part $\rho(r_1, r_1)$ is the proton density distribution.

FIG. 2: The difference $\rho_o(r_1, r'_1) - \rho(r_1, r'_1)$, between the proton IPM one-body density matrix of the $^{208}$Pb nucleus, and that obtained with our FHNC/SOC calculations. The two density matrices, have been calculated for $\theta_{11'}=0$. Note that the scale here is ten times larger than that of Fig. 1.

The explicit expression of the OBDM, in terms of FHNC/SOC quantities, such as two-body density distributions, vertex corrections, nodal diagrams etc., is given in Appendix A. The diagonal part of the OBDM is the one-body density, normalized to the number of nucleons. Because of this, the momentum distribution satisfies the following sum rule:

$$S_2^t = \frac{\hbar^2}{2m} \int dk k^2 n^t(k)/T_{FHNC}^t = 1,$$

where we have indicated with $T_{FHNC}^t$ the kinetic energy of the protons or of the neutrons. We have verified the accuracy of our calculations by testing the normalization and the exhaustion of the above sum rule for every $n^t(k)$ calculated. We found that these quantities are always satisfied at the level of few parts on a thousand in a full FHNC/SOC calculation, and even better when only scalar correlations are used. The surface shown in Fig. 1 represents the proton OBDM of the $^{208}$Pb nucleus, for $\theta_{11'}=0$. We have shown in [29] that the SRC lower the one-body proton distribution, and also that of the neutrons, in the nuclear center. In order to highlight the effects of the correlations on the density matrix, we show in Fig. 2 the quantity $\rho_o(r_1, r'_1) - \rho(r_1, r'_1)$. Note that the $z$-axis scale of Fig. 2 is ten times larger than that of Fig. 1. It is interesting to notice that the major differences between the OBDMs are not
in the diagonal part, but just beside it. The consequences of these, small, differences between the OBDMs on the momentum distributions, are shown in Fig. 3. In this figure, we compare the $^{12}$C, $^{16}$O, $^{40}$Ca, $^{48}$Ca and $^{208}$Pb proton momentum distributions calculated in the IPM model, with those obtained by using scalar and operator dependent correlations.

The general behavior of the momentum distributions, is very similar for all the nuclei we have considered. Correlated and IPM distributions almost coincide in the low momentum region up to a precise value, when they start to deviate. The correlated distributions show high momentum tails, which are orders of magnitude larger than the IPM results. The value of $k$ where uncorrelated and correlated momentum distributions start to deviate, is smaller the heavier is the nucleus. It is about 1.9 fm$^{-1}$ for $^{12}$C, and 1.5 fm$^{-1}$ for $^{208}$Pb. We notice that the value of the Fermi momentum of symmetric nuclear matter at the saturation density is 1.36 fm$^{-1}$.

The results presented in Fig. 3 clearly show that the effects of the scalar correlations are smaller than those obtained by including the operator dependent terms. We shall see in the following that this is a common feature of our results.

Since relatively small differences are compressed in logarithmic scale, we use the linear scale in Fig. 4 to show, as
FIG. 4: The proton momentum distributions of the $^{16}$O and $^{208}$Pb nuclei multiplied by $k^2$. The full lines show the IPM results, the dotted lines have been obtained by using scalar correlations only, and the dashed lines with the complete correlation.

examples, the proton momentum distributions for $^{16}$O and $^{208}$Pb nuclei, multiplied by $k^2$. This quantity, multiplied by a factor $4\pi$, is the probability of finding a proton with momentum $k$. We observe that the effects of the SRC on the quantity shown in Fig. 4 are basically two. The first one is the already mentioned enhancement at large values of $k$. This effect is less evident here than in Fig. 3. The second effect, hardly visible in Fig. 3, is a reduction of the maxima which appear approximately at $k=1$ fm$^{-1}$ in both nuclei. These two effects are obviously related, since all the momentum distributions are normalized as indicated by Eq. (10), therefore reductions and increases must compensate.

We found that the proton and neutron momentum distributions for nuclei with $N = Z$ are very similar. For this reason we do not show the neutron momentum distributions of the $^{12}$C, $^{16}$O and $^{40}$Ca nuclei. We compare in the panels (a) and (b) of Fig. 5 the proton and neutron momentum distributions of $^{48}$Ca and $^{208}$Pb. The thicker lines show the results of our FHNC/SOC calculation, the thinner lines the IPM momentum distributions.

The figure shows that, in our calculations, the differences between protons and neutrons momentum distributions are more related to the different single particle structure than to the correlation effects. The main differences in the two distributions is in the zone where the $n(k)$ values drops of orders of magnitudes. This corresponds to the discontinuity region of the momentum distribution in the infinite systems, which is related to the Fermi momentum. In a finite system, the larger number of neutrons implies that the neutron Fermi energy is larger than that of the protons, and, consequently, the effective Fermi momentum. For this reason, the neutrons momentum distributions drops at larger values of $k$ than the proton distributions. In the panels (c) and (d) of Fig. 5 we show the quantity

$$\Delta = \frac{n^t_0(k) - n^t(k)}{n^t_0(k) + n^t(k)},$$

(16)

where $n^t_0(k)$ indicates the uncorrelated momentum distribution. This quantity is useful to point out the effects of
correlations. We see that in the low $k$ region $\Delta$ is almost zero. After the discontinuity region $\Delta$ reaches an almost constant value around minus one. This behavior indicates that in the low $k$ region the momentum distribution is dominated by single particle dynamics. The differences between protons and neutrons at low $k$ are due to different single particle wave functions. In the higher $k$ region the correlation plays an important role. We observe that protons and neutrons $\Delta$ are very similar, and this indicate that the effect of the SRC is essentially the same for both kinds of nucleons. Our results are in agreement with the findings of Ref. [34], where $n(k)$ of asymmetric nuclear matter is presented. There is however a disagreement with the results of Ref. [35], where, always in asymmetric nuclear matter, correlations effects between protons were found to be stronger than those between neutrons.

The increase of the momentum distribution at large $k$ values, induced by the SRC is a well known result in the literature, see for example the review of Ref. [36]. The momentum distributions of medium-heavy nuclei, have been usually obtained by using approximated descriptions of the cluster expansion, which is instead considered at all orders in our treatment. The importance of a complete description of the cluster expansion is exemplified in Fig. 6, where, together with our results, we also show the results of Ref. [37], obtained by truncating the cluster expansion to the first order in the correlation lines. In both calculations the same correlation functions and single particle basis, those...
the nodal functions \( N_\omega \) as defined as in Ref. [29], have been used. The results obtained with the first order approximation, provide only a qualitative description of the correlation effects. They show high-momentum enhancements which, however, underestimate the correct results by orders of magnitude.

III. NATURAL ORBITS

The natural orbits are defined as those single particle wave functions forming the basis where the OBDM is diagonal:

\[
\rho^t(r_1, r'_1) = \sum_{nlj} c^t_{nlj} \phi^{t,NO}_{nlj}(r_1) \phi^{t,NO}_{nlj}(r'_1). \tag{17}
\]

In the above equation the \( c^t_{nlj} \) coefficients, called occupation numbers, are real numbers. In the IPM, the natural orbits correspond to the mean-field wave functions of Eq. (11), and the \( c^t_{nlj} \) numbers are 1, for the states below the Fermi surface, and 0 for those above it.

In order to obtain the natural orbits, we found convenient to express the OBDM of Eq. (17) as:

\[
\rho^t(r_1, r'_1) = A^t(r_1, r'_1) \rho^t_0(r_1, r'_1) + B^t(r_1, r'_1), \tag{18}
\]

where \( \rho^t_0(r_1, r'_1) \) is the uncorrelated OBDM of Eq. (12), and the other two quantities are defined as:

\[
A^t(r_1, r'_1) = 2C^t_{\omega, SOC}(r_1)C^t_{\omega, SOC}(r'_1) \exp[N^t_{\omega, \omega, p}(r_1, r'_1)] + 2C^t_{\omega}(r_1)C^t_{\omega, SOC}(r'_1) \exp[N^t_{\omega, \omega, p}(r_1, r'_1)] \sum_{p>1} A^k \Delta^k N^t_{\omega, \omega, p}(r_1, r'_1), \tag{19}
\]

\[
B^t(r_1, r'_1) = -2C^t_{\omega, SOC}(r_1)C^t_{\omega, SOC}(r'_1) \exp[N^t_{\omega, \omega, p}(r_1, r'_1)] N^t_{\omega, \omega, p}(r_1, r'_1) - 2C^t_{\omega}(r_1)C^t_{\omega, SOC}(r'_1) \exp[N^t_{\omega, \omega, p}(r_1, r'_1)] \times \sum_{p>1} A^k \Delta^k \left( N^t_{\omega, \omega, p}(r_1, r'_1) N^t_{\omega, \omega, p}(r_1, r'_1) + N^t_{\omega, \omega, p}(r_1, r'_1) \right). \tag{20}
\]

The meaning of the \( \omega, \omega_{\omega}, \omega_{\omega} \) labels used in the above equations have been defined in [33] where the index \( k \) has been defined as \( p = 2k + l - 1 \) with \( l = 0, 1 \) and \( p = 1, \ldots, 6 \). The detailed expressions of the vertex corrections \( C \) and of the nodal functions \( N \) are given in Appendix A.

We expand the OBDM on a basis of spin spherical harmonics \( Y^m_{lj} \), Eq. (11):

\[
\rho^t(r_1, r'_1) = \sum_{ljm} \frac{1}{2j + 1} \left[ A^t_{lj}(r_1, r'_1) + B^t_{lj}(r_1, r'_1) \right] Y^m_{lj}(\Omega_1) Y^m_{lj}(\Omega'_1). \tag{21}
\]
where $\Omega_1$ and $\Omega_1'$ indicate the polar angles identifying $\mathbf{r}_1$ and $\mathbf{r}_1'$. The explicit expressions of the $A$ and $B$ coefficients are:

$$
A_{lj}^t(r_1, r_1') = (2l + 1) \sum_{n2l_2j_2\ell} (2l_2 + 1)(2j_2 + 1) \left\{ \begin{array}{ccc} l & l_1 & l_2 \\ 0 & 0 & 2j_2 \end{array} \right\}^2 \left\{ \begin{array}{ccc} j_2 & l_1 & j \\ l & 1/2 & l_2 \end{array} \right\}^2 R_{n2l_2j_2}(r_1) R_{n2l_2j_2}(r_2) A_{lj}^t(r_1, r_1')
$$
(22)

with

$$
A_{lj}^t(r_1, r_1') = \frac{2}{2l + 1} \int d\Omega_A^t(r_1, r_1') P_l(\cos \theta_{11'})
$$
(23)

and

$$
B_{lj}^t(r_1, r_1') = \frac{4\pi}{2l + 1} \int d(\cos \theta_{11'}) B_{lj}^t(r_1, r_1') P_l(\cos \theta_{11'})
$$
(24)

In the above equations we have used the 3j and 6j Wigner symbols [30]. The term $A$ depends on both orbital and total angular momenta of the single particle, $l$ and $j$ respectively, and the term $B$ depends only on the orbital angular momentum $l$.

As it has been done in Refs. [38] and [39] we identify the various natural orbit with a number, $\alpha$, ordering them with respect to the decreasing value of the occupation probability. The general behavior of our results is analogous to that described in Ref. [38] where a system of $^3$He drops composed by 70 atoms have been studied. The orbits corresponding to states below the Fermi level in the IPM picture, have occupation numbers very close to unity for $\alpha = 1$, and very small in all the other cases. As example of our results, we show in Figs. 7 and 8 the proton and neutron occupation numbers for the natural orbits with $\alpha = 1$ of the $^{48}$Ca nucleus. In the figures, the IPM results are indicated by the dashed lines. The black bars show the values obtained by using scalar correlations only, the gray bars those obtained with the complete operator dependent correlations.

The correlated occupation numbers are smaller than one for orbits below the Fermi surface, and larger than zero for those orbits above the Fermi level. This effect is enhanced by the operator dependent correlations. We observe that, for the states above the Fermi surface, the gray bars are larger than the black ones, indicating that also for these states the operator dependent correlations, produce larger effects than the scalar ones.

We show in Fig. 9 some $\alpha = 1$ natural orbits for three neutron states in $^{48}$Ca. In this figure, we compare the IPM results (full lines) with those obtained with scalar correlation only (dotted lines), and with the full operator dependent correlation (dashed lines). The effect of the correlations is a lowering of the peak and a small widening of the function. Despite the small effect, it is interesting to point out that this is the only case where we found that the inclusion of operator dependent terms diminishes the effect of the scalar correlation. This fact is coherent with the results on the density distributions shown in Ref. [29]. In Tab. 1 we show the occupation numbers of the $^{16}$O protons and neutrons natural orbits also for $\alpha > 1$, and we make a direct comparison with the results of Ref. [39]. As already said in the discussion of the $^{48}$Ca results, the inclusion of the state dependent correlations increases the

![Image](image_url)
FIG. 8: The same as Fig. 7 for the occupation numbers of the neutron natural orbits of the $^{48}\text{Ca}$ nucleus.

TABLE I: Protons (p) and neutrons (n) natural orbits occupation numbers for $^{16}\text{O}$. The PMD values are those of Ref. [39].

| State | $\alpha = 1$ | $\alpha = 2$ | $\alpha = 3$ |
|-------|--------------|--------------|--------------|
|       | $f_1$ | $f_0$ | PMD | $f_1$ | $f_0$ | PMD | $f_1$ | $f_0$ | PMD |
| $1s_{1/2}$ (p) | 0.956 | 0.873 | 0.921 | 0.011 | 0.038 | 0.013 | 0.002 | 0.007 | 0.002 |
| (n) | 0.957 | 0.873 | 0.921 | 0.012 | 0.039 | 0.007 | 0.003 | 0.008 | 0.001 |
| $1p_{3/2}$ (p) | 0.973 | 0.921 | 0.947 | 0.004 | 0.013 | 0.007 | 0.001 | 0.003 | 0.001 |
| (n) | 0.973 | 0.924 | 0.947 | 0.004 | 0.014 | 0.007 | 0.001 | 0.003 | 0.004 |
| $1p_{1/2}$ (p) | 0.970 | 0.923 | 0.930 | 0.003 | 0.012 | 0.008 | 0.001 | 0.003 | 0.002 |
| (n) | 0.970 | 0.922 | 0.930 | 0.004 | 0.013 | 0.008 | 0.002 | 0.003 | 0.002 |
| $1d_{5/2}$ (p) | 0.001 | 0.005 | 0.016 | 0.013 | 0.003 | 0.003 | 0.000 | 0.000 | 0.000 |
| (n) | 0.001 | 0.005 | 0.016 | 0.004 | 0.003 | 0.003 | 0.000 | 0.000 | 0.000 |
| $1d_{3/2}$ (p) | 0.002 | 0.005 | 0.019 | 0.001 | 0.003 | 0.005 | 0.000 | 0.000 | 0.001 |
| (n) | 0.002 | 0.005 | 0.019 | 0.001 | 0.003 | 0.005 | 0.000 | 0.000 | 0.000 |

IV. QUASI-HOLE WAVE FUNCTIONS AND THE SPECTROSCOPIC FACTORS

The quasi-hole wave function is defined as:

$$
\psi_{nljm}^A(x) = \sqrt{A} \frac{<\Psi_{nljm}(A-1)|\delta(x-x_A)P_A^f|\Psi(A)>}{[<\Psi_{nljm}(A-1)|\Psi_{nljm}(A-1)>]^1/2},
$$

(25)

where $|\Psi_{nljm}(1,\ldots,A-1)>$ and $|\Psi(1,\ldots,A)>$ are the states of the nuclei formed by $A-1$ and $A$ nucleons respectively, and $P_A^f$ is the isospin projector. In analogy to the ansatz [6], we assume that the state of the nucleus with $A-1$ nucleons can be described as:

$$
\Psi_{nljm}(A-1) = F(1,\ldots,A-1)\Phi_{nljm}(1,\ldots,A-1),
$$

(26)

where $\Phi_{nljm}(1,\ldots,A-1)$ is the Slater determinant obtained by removing from $\Phi(1,\ldots,A)$ a particle characterized by the quantum numbers $nljm$, and the correlation function $F$ is formed, as indicated in Eq. [6], by the two-body correlation functions $f_p$ obtained by minimizing the $A$ nucleon system. In an uncorrelated system the quasi-hole wave functions coincide with the hole mean-field wave functions [11].

We are interested in the radial part of the quasi-hole wave function. We obtain this quantity first by multiplying equation (25) by the vector spherical harmonics $Y_{ij}^m(\Omega)$, then, by integrating over the angular coordinate $\Omega$, and,
finally, by summing over \( m \). It is useful to rewrite the radial part of the quasi-hole wave function as \(^{28}\): 
\[
\psi_{nlj}^t(r) = \frac{1}{2j+1} \sum_m \int d\Omega \, Y_{lj}^m(\Omega) \psi_{nljm}^t(x) = \frac{1}{2j+1} \sum_m \mathcal{X}_{nljm}^t(r)[\mathcal{N}_{nljm}^t]^{1/2},
\]  
where we have defined: 
\[
\mathcal{X}_{nljm}^t(r) = \sqrt{\frac{\langle \psi_{nljm}^t(A-1)|Y_{lj}^m(\Omega)\delta(r-r_A)P_A^d|\psi^t(A)\rangle}{\langle \psi_{nljm}^t(A-1)|\psi_{nljm}^t(A-1)\rangle}},
\]
and 
\[
\mathcal{N}_{nljm}^t = \frac{\langle \psi_{nljm}^t(A-1)|\psi_{nljm}^t(A-1)\rangle}{\langle \psi^t(A)|\psi^t(A)\rangle}.
\]

| \( nlj \) | \( ^{12}\text{C} \) | \( ^{16}\text{O} \) | \( ^{40}\text{Ca} \) | \( ^{48}\text{Ca} \) | \( ^{208}\text{Pb} \) |
|-------|-------|-------|-------|-------|-------|
|      | \( f_1 \) | \( f_4 \) | \( f_6 \) | \( f_1 \) | \( f_4 \) | \( f_6 \) | \( f_1 \) | \( f_4 \) | \( f_6 \) | \( f_1 \) | \( f_4 \) | \( f_6 \) |
| \( 1s_{1/2} \) | 0.96 | 0.95 | 0.91 | 0.95 | 0.90 | 0.85 | 0.93 | 0.84 | 0.78 | 0.94 | 0.85 | 0.78 |
| \( 1p_{3/2} \) | 0.96 | 0.96 | 0.94 | 0.96 | 0.93 | 0.89 | 0.95 | 0.87 | 0.82 | 0.95 | 0.87 | 0.81 |
| \( 1p_{1/2} \) | 0.96 | 0.93 | 0.89 | 0.95 | 0.87 | 0.81 | 0.95 | 0.83 | 0.80 | 0.94 | 0.83 | 0.77 |
| \( 1d_{5/2} \) | 0.96 | 0.90 | 0.86 | 0.96 | 0.90 | 0.85 | 0.94 | 0.84 | 0.79 | 0.94 | 0.84 | 0.79 |
| \( 2s_{1/2} \) | 0.96 | 0.92 | 0.87 | 0.94 | 0.92 | 0.86 | 0.94 | 0.86 | 0.80 | 0.94 | 0.84 | 0.79 |
| \( 1d_{3/2} \) | 0.95 | 0.90 | 0.85 | 0.96 | 0.90 | 0.84 | 0.94 | 0.86 | 0.81 | 0.94 | 0.86 | 0.81 |
| \( 1f_{7/2} \) | 0.95 | 0.87 | 0.82 | 0.95 | 0.87 | 0.81 | 0.95 | 0.83 | 0.77 | 0.94 | 0.83 | 0.77 |
| \( 2p_{3/2} \) | 0.95 | 0.88 | 0.83 | 0.95 | 0.88 | 0.83 | 0.95 | 0.84 | 0.79 | 0.94 | 0.84 | 0.79 |
| \( 1f_{5/2} \) | 0.95 | 0.86 | 0.80 | 0.95 | 0.87 | 0.82 | 0.95 | 0.83 | 0.77 | 0.94 | 0.83 | 0.77 |
| \( 2p_{1/2} \) | 0.95 | 0.87 | 0.82 | 0.95 | 0.88 | 0.83 | 0.95 | 0.84 | 0.79 | 0.94 | 0.84 | 0.79 |
| \( 1g_{9/2} \) | 0.95 | 0.88 | 0.83 | 0.95 | 0.88 | 0.83 | 0.95 | 0.84 | 0.79 | 0.94 | 0.84 | 0.79 |
| \( 1g_{7/2} \) | 0.95 | 0.88 | 0.83 | 0.95 | 0.88 | 0.83 | 0.95 | 0.84 | 0.79 | 0.94 | 0.84 | 0.79 |
| \( 2d_{5/2} \) | 0.95 | 0.89 | 0.83 | 0.95 | 0.89 | 0.83 | 0.95 | 0.84 | 0.79 | 0.94 | 0.84 | 0.79 |
| \( 1h_{11/2} \) | 0.94 | 0.90 | 0.86 | 0.94 | 0.90 | 0.86 | 0.94 | 0.86 | 0.80 | 0.94 | 0.86 | 0.80 |
| \( 2d_{3/2} \) | 0.95 | 0.89 | 0.83 | 0.95 | 0.89 | 0.83 | 0.95 | 0.85 | 0.79 | 0.94 | 0.85 | 0.79 |
| \( 3s_{1/2} \) | 0.95 | 0.90 | 0.85 | 0.95 | 0.90 | 0.85 | 0.95 | 0.86 | 0.80 | 0.94 | 0.86 | 0.80 |

TABLE II: Proton spectroscopic factors of the \(^{12}\text{C} \), \(^{16}\text{O} \), \(^{40}\text{Ca} \), \(^{48}\text{Ca} \) and \(^{208}\text{Pb} \) nuclei. We present the results obtained by using the scalar correlation only \((f_1)\), the first four operator channels of the correlation \((f_4)\) and the full correlation operator \((f_6)\).

Following the procedure outlined in Ref. \(^{33}\), we consider separately the cluster expansions of the two terms \( \mathcal{N}^t_\alpha \) and \( \mathcal{X}^t_\alpha \), where we have indicated with \( \alpha \) the set of the \( nljm \) quantum numbers. We obtain for \( \mathcal{X}^t_\alpha \) the expression: 
\[
\mathcal{X}^t_\alpha(r) = C_{\omega, SOC}^{t,\alpha}(r) \left( R_{nlj}^t(r) + \int d^3r_1 R_{nlj}^t(r_1) R_1(\cos \theta) \right)
\times \left\{ d_{\omega,d}^{t,\alpha}(r, r_1) C_{d,pq}^{t,\alpha}(r_1) \left[ -\rho^{t,\alpha}_\omega(r, r_1) + N^{t,\alpha}_{\omega, \omega}(r, r_1) \right] \right.
\left. + \rho^{t,\alpha}_\omega(r, r_1) - N^{t,\alpha}_{\omega, \omega}(r, r_1) - N^{t,\alpha}_{pp}(r, r_1) + \mathcal{X}_{SOC}^{t,\alpha}(r, r_1) \right\},
\]  
and for \( \mathcal{N}^t_\alpha \) the expression: 
\[
\left[ \mathcal{N}^t_\alpha \right]^{-1} = \int d^3r C_{d,pq}^{t,\alpha}(r) \left| \phi^{t,\alpha}_\alpha(r) \right|^2 + \int d^3r_1 \phi^{t,\alpha}_\alpha(r) \phi^{t,\alpha}_\alpha(r_1)
\times 2 \left\{ d_{dd}^{t,\alpha}(r, r_1) C_{d,pq}^{t,\alpha}(r_1) \left[ -\rho^{t,\alpha}_\omega(r, r_1) + N^{t,\alpha}_{\omega, \omega}(r, r_1) \right] \right.
\left. + \rho^{t,\alpha}_\omega(r, r_1) - N^{t,\alpha}_{\omega, \omega}(r, r_1) - N^{t,\alpha}_{pp}(r, r_1) + \mathcal{N}_{SOC}^{t,\alpha}(r, r_1) \right\},
\]  

### Table III: The same as Tab. II for neutron states.

The expressions of the functions \( \mathcal{N}_{SOC}^{t_2}(\mathbf{r}, \mathbf{r}_1) \), \( \mathcal{X}_{SOC}^{t_2}(\mathbf{r}, \mathbf{r}_1) \), are:

\[
\mathcal{X}_{SOC}^{t_2}(\mathbf{r}, \mathbf{r}_1) = \sum_{k=1}^{3} \sum_{t_z=p,n} A^k \left[ (1 - \delta_{k,1}) \mathcal{X}_{2k-1,2k-1}^{t_z}(\mathbf{r}, \mathbf{r}_1) + \chi_1^{t_z} \left( \mathcal{X}_{2k-1,2k}^{t_z}(\mathbf{r}, \mathbf{r}_1) + \mathcal{X}_{2k,2k}^{t_z}(\mathbf{r}, \mathbf{r}_1) \right) + \chi_2^{t_z} \mathcal{X}_{2k,2k}^{t_z}(\mathbf{r}, \mathbf{r}_1) \right],
\]

\[
\mathcal{N}_{SOC}^{t_2}(\mathbf{r}, \mathbf{r}_1) = \sum_{k=1}^{3} \sum_{t_z=p,n} A^k \left[ (1 - \delta_{k,1}) \mathcal{N}_{2k-1,2k-1}^{t_z}(\mathbf{r}, \mathbf{r}_1) + \chi_1^{t_z} \left( \mathcal{N}_{2k-1,2k}^{t_z}(\mathbf{r}, \mathbf{r}_1) + \mathcal{N}_{2k,2k}^{t_z}(\mathbf{r}, \mathbf{r}_1) \right) + \chi_2^{t_z} \mathcal{N}_{2k,2k}^{t_z}(\mathbf{r}, \mathbf{r}_1) \right],
\]

where the indexes \( t \) refer to the isospin, and we have defined:

\[
\mathcal{X}_{pq}^{t_1 t_2}(\mathbf{r}, \mathbf{r}_1) = \frac{1}{2} \left[ h_{d,p}^{t_1 t_2,\alpha}(\mathbf{r}, \mathbf{r}_1) g_{ad}^{t_1 t_2,\alpha}(\mathbf{r}, \mathbf{r}_1) C_{d}^{t_2,\alpha}(\mathbf{r}_1) \left( - \rho_{\alpha}^{t_2,\alpha}(\mathbf{r}, \mathbf{r}_1) + N_{\omega_c}^{t_2,\alpha}(\mathbf{r}, \mathbf{r}_1) \right) \right]
\]

\[
+ g_{ad}^{t_1 t_2,\alpha}(\mathbf{r}, \mathbf{r}_1) C_{d}^{t_2,\alpha}(\mathbf{r}_1) N_{\omega_c}^{t_2,\alpha}(\mathbf{r}, \mathbf{r}_1) \mathcal{X}_{pq}^{t_2}(\mathbf{r}, \mathbf{r}_1) \Delta k_2,
\]

\[
\mathcal{N}_{pq}^{t_1 t_2}(\mathbf{r}, \mathbf{r}_1) = \left[ h_{d,p}^{t_1 t_2,\alpha}(\mathbf{r}, \mathbf{r}_1) g_{ad}^{t_1 t_2,\alpha}(\mathbf{r}, \mathbf{r}_1) C_{d}^{t_2,\alpha}(\mathbf{r}_1) \left( - \rho_{\alpha}^{t_2,\alpha}(\mathbf{r}, \mathbf{r}_1) + N_{\omega_c}^{t_2,\alpha}(\mathbf{r}, \mathbf{r}_1) \right) \right] \Delta k_2,
\]

where \( k_2 = 1, 2, 3 \) for \( q = 1, 3, 5 \). The expressions of the other terms are given in Appendix B. All the quantities used in the above expressions depend on the set of quantum numbers \( \alpha \) characterizing the quasi-hole state, since we have written the various equations by using (30):

\[
\rho_{\alpha}^{t_2,\alpha}(\mathbf{r}, \mathbf{r}_1) = \rho_{\alpha}^{t_2}(\mathbf{r}, \mathbf{r}_1) - \phi_{\alpha}^{t_2}(\mathbf{r}) \phi_{\alpha}^{t_2}(\mathbf{r}_1).
\]

The knowledge of the quasi-hole functions allows us to calculate the spectroscopic factors:

\[
S_{nlj}^{t_2} = \int dr r^2 |\psi_{nlj}^{t_2}(r)|^2.
\]
FIG. 9: Natural orbits for some neutron states in $^{48}$Ca. The full lines show the IPM orbits, the dotted lines those obtained with scalar correlations only and the dashed lines those obtained with the complete operator dependent correlation.

The proton and neutron spectroscopic factors for the $^{12}$C, $^{16}$O, $^{40}$Ca, $^{48}$Ca and $^{208}$Pb nuclei are given in Tabs. II and III for each single hole state. In these tables we compare the results obtained by using scalar correlations ($f_1$), with those obtained with the four central channels ($f_4$) and with the full correlation ($f_6$). The inclusion of the correlations produce spectroscopic factors smaller than one, the mean-field value. The $f_6$ results are smaller than those of $f_4$, which are smaller than those obtained with $f_1$.

We found that the effect of the correlations becomes larger the more bound is the state. This fact emerges by observing that for a fixed set of $l_j$ quantum numbers the spectroscopic factors increase with $n$, and, at the same time, that the values of the spectroscopic factors become larger when $n$ and the $l_j$ values increase.

The values of the spectroscopic factors depend on the choice of the single particle basis. As we have already said in the introduction, our results have been obtained by using the Woods-Saxon single particle bases given in Ref. [29]. This basis has been chosen in order to reproduce the single particle energies around the Fermi surface and the charge distribution of each nucleus considered. The correlation function has been fixed by the minimization procedure [2]. We tested the sensitivity of our results to different single particle basis, by calculating $^{16}$O and $^{40}$Ca spectroscopic factors by using with the Harmonic Oscillator and Woods-Saxon single particle wave functions of Ref. [41], fixed by a global minimization of the energy. Despite the remarkable differences between the various single particle basis, we found that the maximum variations in the values of the spectroscopic factors is of about the 5%. This value is smaller than the variations produced by the different terms of the correlations, shown in Tabs. II and III. This indicates that our results are more sensitive to the SRC than to the choice of the single particle basis.

As example of correlation effects on the quasi-hole wave functions, we show in Fig. 10 the squares of the proton $3s_{1/2}$ and neutron $3p_{1/2}$ quasi-hole wave functions for the $^{208}$Pb nucleus. The correlations lower the wave function in the nuclear interior. Also in this case, the effect of the correlations increases together with the number of operator
FIG. 10: Proton 3s$_{1/2}$ and neutron 3p$_{1/2}$ quasi-hole functions, squared, of the $^{208}$Pb nucleus. The various lines show the results obtained by using different type of correlations.

channels considered.

In Fig. 11 we show with a gray band the difference between the empirical charge distributions of $^{206}$Pb and $^{205}$Tl [19]. The dashed dotted line, labeled as IPM, has been obtained by considering that the difference between the two charge distributions can be described as a single 3s$_{1/2}$ proton hole in the core of the lead nucleus. This curve has been obtained by folding the IPM result of Fig. 10 with the electric proton form factor in its dipole form. In a slightly more elaborated picture, the ground state of the $^{205}$Tl is composed by the 3s$_{1/2}$ proton hole in the $^{206}$Pb ground state, plus the coupling of the 2d$_{5/2}$ and 2d$_{3/2}$ proton levels with the first 2$_{+}^{+}$ excited state of $^{206}$Pb [42, 43]. This description of the $^{205}$Tl charge distribution, shown by the dotted line in the figure, is still within the IPM framework. The dashed line has been obtained by adding to the dotted line the core polarization effects produced by long-range correlations. These effects have been calculated by following the Random Phase Approximation approach of Refs. [44, 45]. The full line has been obtained when our SRC effects are also included.

The various effects presented in Fig. 11 have been obtained in different theoretical frameworks, and the final result does not have any pretense of being a well grounded and coherent description of the empirical charge differences. The point we want to make by showing this figure is that the effects of the SRC are of the same order of magnitude of those commonly considered in traditional nuclear structure calculations.

V. SUMMARY AND CONCLUSIONS

In this work we have extended the FHNC/SOC scheme in order to calculate the OBDM’s, the natural orbits and the quasi-hole wave functions of finite nuclear systems non saturated in isospin, and in $jj$ coupling representation of the single particle wave function basis. Our results have been obtained by using the many-body wave functions obtained by minimizing the nuclear hamiltonian with the two-body realistic interaction Argonne $v'_{8}$ and the associated
three-body interaction Urbana IX. The calculations have been done by using operator dependent correlations which include terms up to the tensor ones.

We found that the correlations enhance by orders of magnitude the high-energy tail of the nucleon momentum distribution. The occupation numbers of the natural orbits below the Fermi level, are depleted, and the opposite happens for those above the Fermi level. Also the values of the spectroscopic factors are depleted with respect to the IPM. A reliable comparison between our spectroscopic factors with the empirical ones requires the description of the reactions used to extract them, and this is part of our future projects.

We have shown that the results of models considering expansions up to the first order correlation lines, provide only qualitative descriptions of the SRC effects. In the description of the charge density difference between $^{206}$Pb and $^{205}$Tl, the SRC effects are of comparable size of those commonly considered in traditional nuclear structure calculations based on effective theories.

A general outcome of our study, is that the effects of the correlations increase with the complexity of the correlation function. This means that operator dependent correlations enhance the effects produced by the scalar correlations. This not obvious result, is valid in general, not always. We have shown in Ref. [29], that scalar and operator dependent correlations have destructive interference effects on the density distributions. We found in the present study an analogous behavior regarding the natural orbits. These quantities are related to the density distributions. It seems that the effects of the SRC are rather straightforward on quantities which involve two-nucleons, while they are more difficult to predict on quantities related to single nucleon dynamics. On these last quantities, however, these SRC effects are very small, usually negligible.

In our calculations the nuclear interaction acts only in defining the many-body wave functions by means of the variational principle [2], more specifically, in selecting the correlation function [3]. It is therefore difficult to disentangle the role played by the various parts of the interaction, e.g. the tensor part of the three-body force, on the quantities we have studied in this article. We have instead evaluated the effects of the various parts of the correlation function.

In this work, we have highlighted a set of effects that cannot be described by mean field based effective theories. The description of the nucleus in kinematics regimes where these effects are relevant, requires the use of microscopic theories.

VI. ACKNOWLEDGMENTS

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APPENDIX A

For sake of completeness, we give in this appendix the detailed expression of the OBDM for finite nuclear systems not saturated in isospin, and in jj coupling scheme of the single particle wave function basis \([11]\). The notation for the nodal functions \(N\) and for the vertex corrections \(C\) is that used in Ref. \([33]\). The indexes \(t_1, t_2, t_3\) indicate protons and neutrons, and the subscript \(j\) is related to the antiparallel spin states.

For the correlated OBDM we obtain the expression:

\[
\rho'(\mathbf{r}_1, \mathbf{r}'_1) = 2C_{\omega, SOC}(\mathbf{r}_1)C_{\omega, SOC}(\mathbf{r}'_1)e^{N_{\omega,\omega}(\mathbf{r}_1, \mathbf{r}'_1)} \left[ \rho'_0(\mathbf{r}_1, \mathbf{r}'_1) - N_{\omega,\omega}(\mathbf{r}_1, \mathbf{r}'_1) \right] + 2C_{\omega, SOC}(\mathbf{r}_1)C_{\omega, SOC}(\mathbf{r}'_1)e^{N_{\omega,\omega}(\mathbf{r}_1, \mathbf{r}'_1)} \times \sum_{p>1} A^k \Delta_k \left\{ N_{\omega,\omega,p}(\mathbf{r}_1, \mathbf{r}'_1) \left[ \rho'_0(\mathbf{r}_1, \mathbf{r}'_1) - N_{\omega,\omega}(\mathbf{r}_1, \mathbf{r}'_1) \right] - N_{\omega,\omega,p}(\mathbf{r}_1, \mathbf{r}'_1) \right\}. \tag{A1}
\]

In the above equation, \(k\) has been defined as in Eq. \([20]\), and we have used \(\Delta_k=1,2,3 = 1 - \delta_k,3,\) and \(A^k=1,2,3 = 1, 3, 6.\)

In the following we shall calculate the expectation value of the isospin operator sequence:

\[
\chi^{t_1 t_2}_n = \chi^*_{t_1}(1)\chi^*_{t_2}(2) (\mathbf{r}_1 \cdot \mathbf{r}_2)^n \chi_{t_1}(1)\chi_{t_2}(2),
\]

by considering that

\[
(\mathbf{r}_i \cdot \mathbf{r}_j)^n = a_n + (1 - a_n)\mathbf{r}_i \cdot \mathbf{r}_j,
\]

with

\[
a_{n+1} = 3(1 - a_n) \quad \text{and} \quad a_0 = 1.
\]

By using the above equations we have that:

\[
\chi^{t_1 t_2}_0 = 1, \quad \chi^{t_1 t_2}_1 = 2\delta_{t_1 t_2} - 1 \quad \text{and} \quad \chi^{t_1 t_2}_n = 2a_n - 1 + 2(1 - a_n)\delta_{t_1 t_2}.
\]

The expressions of the vertex corrections are:

\[
C_{\omega, SOC}(\mathbf{r}_1) = C_{\omega, SOC}^{t_1}(\mathbf{r}_1) \left[ 1 + U_{\omega, SOC}^{t_1}(\mathbf{r}_1) \right], \tag{A2}
\]

\[
U_{\omega, SOC}^{t_1}(\mathbf{r}_1) = \sum_{k=1}^3 A^k \sum_{t_2=p,n} \left[ (1 - \delta_{k,3})U_{\omega,2k-1,2k-1}(\mathbf{r}_1) + \chi^{t_1 t_2}_{t_2}(U_{\omega,2k-1,2k-1}(\mathbf{r}_1) + U_{\omega,2k-1,2k-1}(\mathbf{r}_1)) + \chi^{t_1 t_2}_{t_2}U_{\omega,2k-2k}(\mathbf{r}_1) \right], \tag{A3}
\]

where we have defined

\[
U_{\omega,pq}(\mathbf{r}_1) = \int d\mathbf{r}_2 h_{\omega,pq}(\mathbf{r}_1, \mathbf{r}_2) \left\{ \left[ g_{\omega d}(\mathbf{r}_1, \mathbf{r}_2)N_{\omega d, pq}(\mathbf{r}_1, \mathbf{r}_2) + g_{\omega e}(\mathbf{r}_1, \mathbf{r}_2)N_{\omega e, pq}(\mathbf{r}_1, \mathbf{r}_2) \right] + g_{\omega d}(\mathbf{r}_1, \mathbf{r}_2)N_{\omega d, pq}(\mathbf{r}_1, \mathbf{r}_2) \right\}, \tag{A4}
\]

\[
h_{\omega,pq}(\mathbf{r}_1, \mathbf{r}_2) = \frac{f_p(\mathbf{r}_1)}{f_1(\mathbf{r}_2)} + (1 - \delta_{p,1})N_{\omega d, pq}(\mathbf{r}_1, \mathbf{r}_2). \tag{A5}
\]

The expressions of the two-body distribution functions for \(p > 1\) are:

\[
g_{\omega d}(\mathbf{r}_1, \mathbf{r}_2) = g_{\omega d}(\mathbf{r}_1, \mathbf{r}_2)N_{\omega d, pq}(\mathbf{r}_1, \mathbf{r}_2), \tag{A6}
\]

\[
g_{\omega e}(\mathbf{r}_1, \mathbf{r}_2) = h_{\omega, pq}(\mathbf{r}_1, \mathbf{r}_2)g_{\omega d}(\mathbf{r}_1, \mathbf{r}_2)
\]

\[
= N_{\omega d, pq}(\mathbf{r}_1, \mathbf{r}_2) + X_{\omega d, pq}(\mathbf{r}_1, \mathbf{r}_2), \tag{A7}
\]

\[
g_{\omega e}(\mathbf{r}_1, \mathbf{r}_2) = h_{\omega, pq}(\mathbf{r}_1, \mathbf{r}_2)g_{\omega e}(\mathbf{r}_1, \mathbf{r}_2) + g_{\omega d}(\mathbf{r}_1, \mathbf{r}_2)N_{\omega d, pq}(\mathbf{r}_1, \mathbf{r}_2)
\]

\[
= X_{\omega d, pq}(\mathbf{r}_1, \mathbf{r}_2) + N_{\omega d, pq}(\mathbf{r}_1, \mathbf{r}_2), \tag{A8}
\]

\[
g_{\omega e}(\mathbf{r}_1, \mathbf{r}_2) = h_{\omega, pq}(\mathbf{r}_1, \mathbf{r}_2)g_{\omega e}(\mathbf{r}_1, \mathbf{r}_2) + g_{\omega d}(\mathbf{r}_1, \mathbf{r}_2)N_{\omega d, pq}(\mathbf{r}_1, \mathbf{r}_2)
\]

\[
= X_{\omega d, pq}(\mathbf{r}_1, \mathbf{r}_2) + N_{\omega d, pq}(\mathbf{r}_1, \mathbf{r}_2). \tag{A9}
\]
Finally the nodals functions are expressed as:

$$N_{mn,2k_1-1}(1,1') = \sum_{k_2,k_3=1}^3 \sum_{t_3=p,n} \left[ N_{t_1} t_3^m m,2k_1-1,2k_2-1,2k_3-1(1,1') + \chi_1^t t_3 \left[ N_{t_1} t_3^m m,2k_1,2k_2,2k_3(1,1') \right] \right],$$

(A11)

$$N_{o\omega,n,2k_1-1}(1,1') = \sum_{k_2,k_3=1}^3 \sum_{t_3=p,n} \chi_1^t t_3 N_{o\omega,n,2k_1-1,2k_2,2k_3}(1,1'),$$

(A12)

$$N_{o\omega,n,2k_1}(1,2) = \sum_{k_2,k_3=1}^3 \sum_{t_3=p,n} \left[ N_{t_1} t_3^o \omega,n,2k_1-1,2k_2-1,2k_3-1(1,2) + \chi_1^t t_3 N_{t_1} t_3^o \omega,n,2k_1,2k_2,2k_3(1,2) \right],$$

(A13)

$$N_{o\omega,c,j,2k_1-1}(1,2) = \sum_{k_2,k_3=1}^3 \sum_{t_3=p,n} \left[ N_{t_1} t_3^o \omega,c,j,2k_1-1,2k_2,2k_3-1(1,2) + \chi_1^t t_3 N_{t_1} t_3^o \omega,c,j,2k_1-1,2k_2-1,2k_3(1,2) \right],$$

(A14)

$$N_{o\omega,c,j,2k_1}(1,2) = \sum_{k_2,k_3=1}^3 \sum_{t_3=p,n} N_{o\omega,c,j,2k_1-1,2k_2,2k_3}(1,2),$$

(A15)

$$N_{\omega,c,j,2k_1}(1,2) = \sum_{k_2,k_3=1}^3 \sum_{t_3=p,n} N_{\omega,c,j,2k_1-1,2k_2,2k_3}(1,2).$$

(A16)

with $m = w, w_c$ and $n = d, e$. In the following equations we have that $m, n = c, w_c$.

$$N_{\omega,\omega,pqr}(r_1, r_1') = \left[ X_{t_1} t_3^\omega (r_1, r_2) s_{112}^{k_2 k_3 k_1} C_{t_1} t_3^\omega (r_2) X_{t_1} t_3^\omega (r_2, r_1') + N_{t_1} t_3^\omega (r_2, r_1') \right],$$

(A17)

$$N_{\omega,\omega,pqr}(r_1, r_2) = \left[ X_{\omega,\omega}(r_1, r_2) s_{112}^{k_2 k_3 k_1} C_{t_1} t_3^\omega (r_2) X_{\omega,\omega}(r_2, r_1') \right],$$

(A18)

$$N_{\omega,\omega,pqr}(r_1, r_2) = \left[ X_{\omega,\omega}(r_1, r_3) s_{112}^{k_2 k_3 k_1} C_{t_1} t_3^\omega (r_3) X_{\omega,\omega}(r_3, r_2) + N_{t_1} t_3^\omega (r_3, r_2) \right],$$

(A19)

also in the above equations we used $n = d, e$. In the following equations we have that $m, n = c, w_c$.

$$N_{m,nn,2k_1-1;X,2k_1-1}(1,2) = \left[ X_{t_1} t_3 c_{m,nn}(1,3) s_{112}^{k_2 k_3 k_1} \frac{\Delta k_1}{2} c_{t_1} t_3^c (3) X_{t_1} t_3 (3,2) + N_{t_1} t_3 (3,2) + N_{t_1} t_3 (3,2) \right] +$$

$$+ (1 - \delta_{r,1}) \times$$

$$\left[ X_{t_1} t_3 c_{m,nn}(1,3) s_{112}^{k_2 k_3 k_1} \frac{\Delta k_2}{2} \right] c_{t_1} t_3^c (3) X_{t_1} t_3 (3,2) + N_{t_1} t_3 (3,2) + N_{t_1} t_3 (3,2) -$$

$$\left[ X_{t_1} t_3 c_{m,nn}(1,3) s_{112}^{k_2 k_3 k_1} \frac{\Delta k_1}{2} \right] c_{t_1} t_3^c (3) X_{t_1} t_3 (3,2) + N_{t_1} t_3 (3,2) + N_{t_1} t_3 (3,2)$$

$$+ (1 - \delta_{r,1}) \left[ X_{t_1} t_3 c_{m,nn}(1,3) s_{112}^{k_2 k_3 k_1} \frac{\Delta k_2}{2} \right] c_{t_1} t_3^c (3) X_{t_1} t_3 (3,2) + N_{t_1} t_3 (3,2) + N_{t_1} t_3 (3,2) \right],$$

(A20)
\[
N_{mpq}^{t_1t_3}(1,2) = \left[ X_{mcq}^{t_1}(1,3) \xi_{132}^{k_1 k_2 k_3} \frac{\Delta k_3}{2} C_{cqr}^{t_3}(3) \rho_o^{t_3}(3,2) + N_{cp}^{t_3}(3,2) + N_{r_3}(3,2) \right] \\
+ (1 - \delta_{r,1}) \left[ X_{mcq}^{t_1}(1,3) \xi_{132}^{k_1 k_2 k_3} \frac{\Delta k_2}{2} C_{cqr}^{t_3}(3) | N_{cp}^{t_3}(3,2) + N_{r_3}(3,2) \right] \\
- \delta_{k_1,1} \delta_{k_2,1} \delta_{k_3,1} \left\{ \left[ X_{mcq}^{t_1}(1,3) \frac{1}{2} C_{cqr}^{t_3}(3) \rho_o^{t_3}(3,2) + N_{cp}^{t_3}(3,2) + N_{r_3}(3,2) \right] \\
+ (1 - \delta_{r,1}) \left[ X_{mcq}^{t_1}(1,3) \frac{1}{2} C_{cqr}^{t_3}(3) | N_{cp}^{t_3}(3,2) + N_{r_3}(3,2) \right] \right\}, \tag{A21}
\]

\[
N_{\rho pq}^{t_1t_3}(1,2) = -\left[ \rho_0^{t_1}(1,3) \xi_{132}^{k_1 k_2 k_3} \frac{\Delta k_2}{2} C_{cqr}^{t_3}(3) | N_{cp}^{t_3}(3,2) \right] \\
- \left[ \rho_0^{t_1}(1,3) \xi_{132}^{k_1 k_2 k_3} \frac{\Delta k_3}{2} C_{cqr}^{t_3}(3) (1) | N_{cp}^{t_3}(3,2) - \delta_{r,1} \rho_o^{t_3}(3,2) \right] \\
+ \delta_{k_1,1} \delta_{k_2,1} \delta_{k_3,1} \left\{ \left[ \rho_0^{t_1}(1,3) \frac{1}{2} C_{cqr}^{t_3}(3) | N_{cp}^{t_3}(3,2) \right] \\
+ \left[ \rho_0^{t_1}(1,3) \frac{1}{2} C_{cqr}^{t_3}(3) (1) | N_{cp}^{t_3}(3,2) - \delta_{r,1} \rho_o^{t_3}(3,2) \right] \right\}, \tag{A22}
\]

\[
N_{\rho pq}^{t_1t_3}(1,2) = \left[ X_{mcq}^{t_1}(1,3) \xi_{132}^{k_1 k_2 k_3} \frac{\Delta k_3}{2} C_{cqr}^{t_3}(3) | X_{cnj}^{t_3}(3,2) + N_{cnj}^{t_3}(3,2) + N_{r_3}(3,2) \right] \\
+ (1 - \delta_{r,1}) \left[ X_{mcq}^{t_1}(1,3) \frac{1}{2} C_{cqr}^{t_3}(3) | X_{cnj}^{t_3}(3,2) + N_{cnj}^{t_3}(3,2) + N_{r_3}(3,2) \right] \\
+ \delta_{k_1,1} \delta_{k_2,1} \delta_{k_3,1} \left\{ \left[ X_{mcq}^{t_1}(1,3) \frac{1}{2} C_{cqr}^{t_3}(3) | X_{cnj}^{t_3}(3,2) + N_{cnj}^{t_3}(3,2) + N_{r_3}(3,2) \right] \\
+ (1 - \delta_{r,1}) \left[ X_{mcq}^{t_1}(1,3) \frac{1}{2} C_{cqr}^{t_3}(3) | X_{cnj}^{t_3}(3,2) + N_{cnj}^{t_3}(3,2) + N_{r_3}(3,2) \right] \right\}, \tag{A23}
\]

\[
N_{\rho q_3}^{t_1t_3}(1,2) = \delta_{k_1,1} \delta_{k_2,1} \delta_{k_3,1} \left\{ \left[ X_{mcq}^{t_1}(1,3) \frac{1}{2} C_{cqr}^{t_3}(3) | \rho_o^{t_3}(3,2) + N_{cp}^{t_3}(3,2) + N_{r_3}(3,2) \right] \\
+ (1 - \delta_{r,1}) \left[ X_{mcq}^{t_1}(1,3) \frac{1}{2} C_{cqr}^{t_3}(3) | N_{cp}^{t_3}(3,2) + N_{r_3}(3,2) \right] \\
+ \left[ X_{mcq}^{t_1}(1,3) \frac{1}{2} C_{cqr}^{t_3}(3) - \rho_o^{t_3}(3,2) + N_{cp}^{t_3}(3,2) + N_{r_3}(3,2) \right] \\
+ (1 - \delta_{r,1}) \left[ X_{mcq}^{t_1}(1,3) \frac{1}{2} C_{cqr}^{t_3}(3) | N_{cp}^{t_3}(3,2) + N_{r_3}(3,2) \right] \right\}, \tag{A24}
\]

\[
N_{\rho q_3}^{t_1t_3}(1,2) = -\delta_{k_1,1} \delta_{k_2,1} \delta_{k_3,1} \left\{ \left[ \rho_0^{t_1}(1,3) \frac{1}{2} C_{cqr}^{t_3}(3) | N_{cp}^{t_3}(3,2) \right] \\
+ \left[ \rho_0^{t_1}(1,3) \frac{1}{2} C_{cqr}^{t_3}(3) | N_{cp}^{t_3}(3,2) - \delta_{r,1} \rho_o^{t_3}(3,2) \right] \\
+ \left[ \rho_0^{t_1}(1,3) \frac{1}{2} C_{cqr}^{t_3}(3) | N_{cp}^{t_3}(3,2) - \delta_{r,1} \rho_o^{t_3}(3,2) \right] \right\}. \tag{A25}
\]

The values of the $\xi_{ijk}^{k_1 k_2 k_3}$ coefficients are given in Ref. [46].

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