FHNC/SOC calculations in finite nuclei*

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In this contribution we include in the description of the doubly closed nuclei with Fermi HyperNetted Chain equations the effect of three–body forces and we also make an estimation of the momentum dependent terms in the two–nucleon potential. The comparison with Monte Carlo results shows again the validity of these techniques.

1 Introduction

The knowledge of the physical properties of a many–body system starting from the interaction among its constituents is one of the main goals of many–body theories. Probably, the system that received more attention from the many–body theoreticians is the atomic nucleus. This is a system composed by Z protons and N neutrons. If electromagnetic interaction is neglected both particles can be considered as two states of the nucleon, therefore the nucleus can be treated as a system of $A = N + Z$ nucleons. One of the greatest difficulties in the description of this system, is due to the fact that it has not been possible to extract from first principles the form of the interactions among the nucleons. A first approximation consists in assuming that it is a two–nucleon interaction. Here, we shall make use of the so called realisitic potentials, i. e. potentials builded by fitting the deuteron properties and the nucleon–nucleon scattering data below the pion production threshold. Specifically, in the present contribution we shall make use of the Urbana [1] and Argonne [2] v_{14} potentials built during the eighties. Since in this decade new scattering data become available, the Argonne potential has been updated [3] and a new parametrization (Av_{18}) with 18 channels has been proposed where four channels takes into account the breaking of the isospin symmetry.

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However, it is a known fact that these two–body interactions underbind light nuclei and predict charge radii that are too large, and at the same time overbind infinite nuclear matter and overestimate the value of the saturation density. The straightforward extension of the theory consits in the inclusion of a three–nucleon potential. In our calculations we shall use three-body forces of the Urbana model [4]: the parameters pf those forces are fixed to reproduce to the binding energy of ^{3}He and the saturation density of nuclear matter. We shall combine the parameterizations with two–nucleon potentials: the UV [4] with Urbana Uv_{14} potential, the UVII [5] with Argonne Av_{14} and the UIX [6] for Av_{18}.

The calculations with these combination of potentials were first performed for infinite system (mainly, symmetrical nuclear matter [7] and pure neutron matter [5]) using the extension of Fermi HyperNetted Chain (FHNC) equations to treat operatorial correlations with the so called Single Operator Chain (SOC) approximation [8]. More recently these interactions have been used in finite nuclei; for ^{16}O with Variational Monte Carlo techniques [9] and with Green Function Monte Carlo (GFMC) calculations for nuclei with up to 7 nucleons [10].

The FHNC equations were extended by Fantoni and Rosati in 1979 [11] to treat finite system with central correlations by Fantoni and Rosati but they have not been used to describe the ground state of doubly closed shell nuclei until the nineties. The first application of the FHNC computational scheme was done to study the energy and momentum distribution of light and medium double closed shell nuclei in ls coupling [12,13] with scalar correlations and semi–realistic interactions. After that the FHNC equations were generalized to the case of jj coupling with central correlations and correlations dependening on the third component of the isospin [14]. Since calculations with realistic interactions requires the use of state–dependent correlations, the next step has been the inclusion in both interaction and correlation of the spin and tensor channels with and without the isospin channel [15] for ls coupling. Some of the main results obtained with these calculations will be discussed in the present contribution.

To complete the work we have to include the remaining channels of the two–nucleon interaction and the three–nucleon potential. Also the correlation should become more elaborated, and it would require, at least, additional spin–orbit dependent terms.

These steps, in particular the last one, are not so straightforward since the correlation operator acts on the uncorrelated state. **I do not understand what is your point here.**

Some results obtained by including the three–nucleon potential and first estimates of the magnitude of the other effects will be presented in the following.

2 FHNC/SOC theory for finite systems

Our work is carried out in the framework of the non relativistic description of the atomic nucleus with hamiltonians of the type:

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

The two- and three-nucleon potentials, v_{ij} and v_{ijk}, are determined at large interparticle distances by meson exchange processes. The intermediate and short distances regime is treated in a semi-microscopic or purely phenomenological fashion in the cases presented in the introduction. The first 14 channels for these two–nucleon interactions have the following parametrization

$$v_{14,ij} = \sum_{p=1,14} v^p(r_{ij}) O_{ij}^p, \tag{2}$$

with

$$O_{ij}^{p=1,14} = \left[1, \sigma_i \cdot \sigma_j, S_{ij}, (\mathbf{L}\cdot\mathbf{S})_{ij}, L^2, L^2 \sigma_i \cdot \sigma_j, (\mathbf{L}\cdot\mathbf{S})_{ij}^2\right] \otimes \left[1, \tau_i \cdot \tau_j\right], \tag{3}$$

$S_{ij} = (3\hat{r}_{ij} \cdot \sigma_i \hat{r}_{ij} \cdot \sigma_j - \sigma_i \cdot \sigma_j)$ being the usual tensor operator.

We shall carry out variational calculations of the energy of the ground state using a correlated A-body trial wave function given by:

$$\Psi(1, 2...A) = \left(\mathcal{S} \prod_{i<j} F_{i,j}\right) \Phi(1, 2...A), \tag{4}$$

where a symmetrized product of two-body correlation operators, F_{ij}, acts on the mean field state, $\Phi(1, 2...A)$, taken as a Slater determinant of single particle wave functions $\phi_\alpha(i)$. The single particle wave functions are generated by a mean field potential which may have or not spin–orbit term. In the first case we shall use a jj coupling scheme and in the second the ls coupling. The expression of the two-body correlation F_{ij} is chosen consistently with the form of the nucleon–nucleon interaction:

$$F_{ij} = \sum_{p=1}^{N} f^p(r_{ij}) O^p_{ij}. \tag{5}$$

FHNC calculations for the energy and momentum distribution the doubly closed–shell nuclei ^{16}O and ^{40}Ca within ls coupling [12,13] and, in jj coupling [14], also for the ^{12}C, ^{48}Ca and ^{208}Pb nuclei are available for the case $N = 1$. The ground state of ^{16}O has been studied within the FHNC/SOC approximation [15] and $N = 6$ as well as with Cluster Monte Carlo techniques [9] for $N = 8$. Only FHNC/SOC calculations [15] with $N = 6$ are available for ^{40}Ca.

The evaluation of the ground state mean value if the hamiltonian, $\langle H \rangle$, is done by using the Jackson-Feenberg identity [16] for the kinetic energy. Details of the calculations done with two–body potential v_{ik} can be found in [12,13,14,15]. The contribution of $< v_{ijk} >$ can be generalized from the nuclear matter expression [4] and will be given in a future publication [17].

It is possible to produce FHNC/SOC equations which can be expressed in terms of the one- and two-body densities and only, defined respectively as:

$$\rho_1(\mathbf{r}_1) = \langle \sum_i \delta(\mathbf{r}_1 - \mathbf{r}_i) \rangle \tag{6}$$

and

$$\rho^p_2(\mathbf{r}_1, \mathbf{r}_2) = \langle \sum_{i \neq j} \delta(\mathbf{r}_1 - \mathbf{r}_i) \delta(\mathbf{r}_2 - \mathbf{r}_j) O^p_{ij} \rangle. \tag{7}$$

Their explicit expressions within the FHNC/SOC approximation can be found in [15].

In order to show the differences between the treatment of infinite and finite system and the use of state–independent or dependent correlations, we compare the various expressions for the one–body density. In the case of infinite homogeneus system, like nuclear matter, the one–body density $\rho_1(r)$ is constant. The one–body density of an uncorrelated finite system is given by the traditional shell– model expression:

$$\rho_1(\mathbf{r}_1) = \rho_0(\mathbf{r}_1) = \sum_{\alpha=1}^{A} |\phi_\alpha(\mathbf{r}_1)|^2. \tag{8}$$

In a correlated system new terms appear in the density. If the correlation is a purely scalar function, $N = 1$ in eq. 5, the uncorrelated density (8) is modified by the direct $U_d(\mathbf{r})$ and exchange $U_e(\mathbf{r})$ vertex corrections which are calculated with FHNC tecniques. The only approximations done in this calculations is the exclusion of the so-called elementary diagrams. The validity of this approximation has been studied in [12]. The one–body density assumes the following expression:

$$\rho_1(\mathbf{r}_1) = \rho_1^c(\mathbf{r}_1) = [\rho_0(\mathbf{r}_1) + U_e^c(\mathbf{r}_1)] \exp(U_d(\mathbf{r}_1)), \tag{9}$$

The use of state–dependent correlations, $N > 1$ in eq. 5, cannot be straightforwardly implemented in the FHNC computational scheme due to the non commutativity of the various operators. Contrary to the case of the state–independent correlations, it not possible to sum all the diagrams of a certain type in a closed form, therefore the calculation is done using additional approximations. In our calculations we use the Single Operator Chain (SOC) approximation consisting in considering all, and only, chain diagrams containing a single operator with $N > 1$. The expression we obtain for the one–body density is:

$$\rho_1(\mathbf{r}_1) = \rho_1^c(\mathbf{r}_1) \, [1 + U_d^{op}(\mathbf{r}_1)] + U_e^{op}(\mathbf{r}_1) \exp(U_d(\mathbf{r}_1)). \tag{10}$$

We control the validity of our approximations by testing how well the following sum rules are are fullfilled:

$$S_1 = \int d\mathbf{r}_1 \rho_1(\mathbf{r}_1) = A \tag{11}$$

$$S_2 = \frac{1}{A(A-1)} \int d\mathbf{r}_1 \int d\mathbf{r}_2 \rho_2^{c,p=1}(\mathbf{r}_1, \mathbf{r}_2) = 1 \tag{12}$$

$$S_\tau = \frac{1}{3A} \int d\mathbf{r}_1 \int d\mathbf{r}_2 \rho_2^{\tau,p=2}(\mathbf{r}_1, \mathbf{r}_2) = -1 \tag{13}$$

3 Results

The state–dependent correlations($N = 6$) we used in our FHNC/SOC calculations are obtained by minimizing the energy evaluated at first order cluster expansion as described in [15]. As example we compare in Figure 1 the correlations obtained in ^{40}Ca with those obtained in nuclear matter at saturation density. We notice the great similarity between these two correlations especially in the long ranged tensor terms.

We verified the validity of our calculations by cross checking our results with those obtained with Cluster Monte Carlo techniques for the nucleus

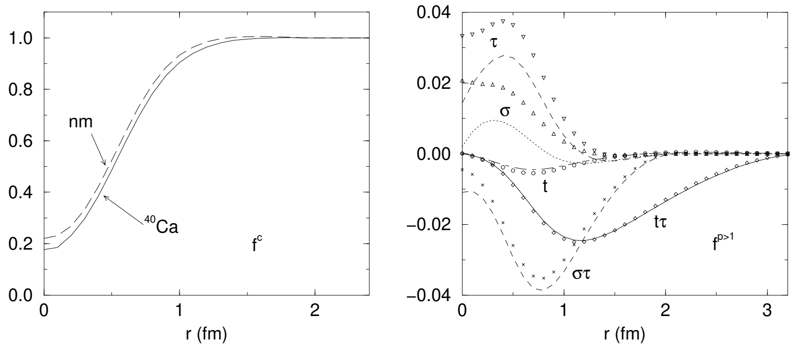

Figure 1. Correlation functions obtained for ^{40}Ca and nuclear matter. The lines stand for Calcium and the simbols for nuclear matter.

^{16}O. The ground state energy obtained with a FHNC/SOC calculation done with an interaction formed by the first six channels of Urbana potential is -4.33 MeV/nucleon to be compared with the value of -4.59 ± 0.1 obtained with Cluster Monte Carlo. The comparison for the Urbana V three–nucleon potential is shown in Table 1 where we have presented the results for the two attractive parts of the potential, the anticommuting ($< v_A^{2\pi} >$) and the commuting ones ($< v_C^{2\pi} >$), and the repulsive term $< v^{rep} >$. The agreement between the results of the two calculations indicates that the approximations used in the FHNC/SOC calculations are well under control.

	^{16}O				^{40}Ca
	f^c	CMC(f^c)	f^6	CMC(f^6)	f^6
$< v_A^{2\pi} >$	0.74	0.70	-0.39	-0.44	-0.26
$< v_C^{2\pi} >$	-0.17	-0.16	-0.90	-0.86	-1.50
$< v^{rep} >$	1.33	1.28	1.65	1.57	3.20
$< v_3 >$	1.90	1.82	0.36	0.27	1.45

Table 1. Comparison of the mean values of the three–nucleon Urbana V potential obtained with FHNC/SOC and CMC calculations

In our calculations the contributions of all the channels up to the tensor–isospin ($p = 6$) for the two–body interaction and correlation are explicitly considered. The effect of the inclusion of the other channels ($p > 6$) has been evaluated by calculating the contribution of these terms in nuclear matter at various densities, $\Delta E^{NM}(\rho)$, and inserting in finite systems by means of the local density approximation:

$$\Delta E = \frac{1}{A} \int d\mathbf{r} \rho_1(r) \Delta E^{NM}[\rho_1(r)] \tag{14}$$

	A14+UVII		A18+UIX
	WS+nm	Op (HO+nm)	HO+nm
$< T >$	39.4	31.2	24.8
$< v_2 >$	-44.5	-37.5	-29.4
$< v_3 >$	-1.0	-0.4	0.3
$< v_c >$	0.8	0.8	0.8
ΔE	0.2	-0.02	-1.6
E	-5.1	-5.9	-5.1

Table 2. ^{16}O ground state energies calculated in the FHNC/SOC camputational scheme with two different nucleon–nucleon interactions.

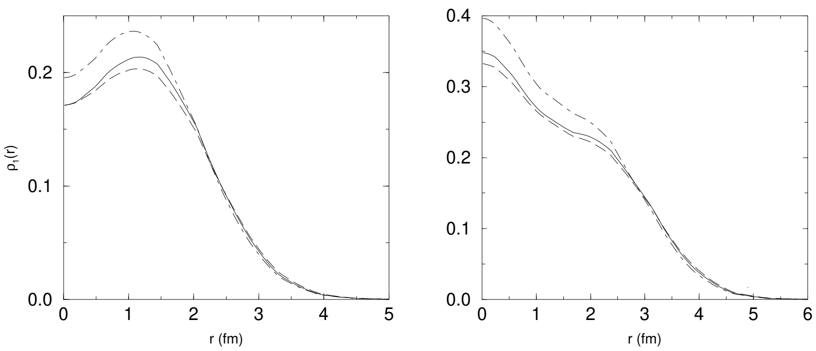

Figure 2. One–body density for ^{16}O and ^{40}Ca. The solid lines includes state–dependent correlations, the dashed line only state–independent ones and the dot–dashed line is the uncorrelated density.

In Table 2 we show the ^{16}O ground state energies, per nucleon, obtained with two different nucleon–nucleon interactions. In this table we show explicitly the contributions of the kinetic energy, $< T >$, two- and three-body potentials, $< v_2 > < v_3 >$, Coulomb interaction, $< v_c >$ and the correction given by the $p > 6$ channels ΔE. The calculations have been done with two different sets of single particle wave functions generated by Woods–Saxon (WS) and harmonic oscillator (HO) potential well. Given the similarity between the nuclear matter and finite nucleus correlations we used the correlation function whose parameters have been optimised in nuclear matter calculations. The results of the calculations with the A14+UVII interaction and HO wave funtions have been obtained by changing the oscillator parameter to minimize the energy. The effect of this optimization is almost 1 MeV/nucleon.

In Figure 2 we show the ^{16}O and ^{40}Ca one–body densities calculated with state dependent correlations (full lines) and with state independent correlations (dashed lines). These densities are compared with the uncorrelated one–body densities. It is interesting to notice that the most important contribution of the correlation is coming from the scalar terms. The inclusion of the other state–dependent terms of the correlations does not modify sensitively the densities. This should be compared with the fact that calculations with realistic potentials but only with scalar correlations do not produce nuclear bound states [15].

4 Summary

We have extended the FHNC/SOC equations to treat three–nucleon potentials in the doubly closed–shell nuclei. The comparison with Monte Carlo results shows that the approximations done in the FHNC/SOC computational scheme are well under control. We made an estimation of the effect of momentum–dependent channels in the two–nucleon interaction and we found that they are relatively small.

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