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Multiparticle-multihole Gogny energy density functional for low-lying spectroscopy applications

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Abstract. In this work, we present a few spectroscopic results deduced from a multiparticle-multihole Gogny energy density functional. Both pairing correlations in the ground state and low-lying spectroscopy of a few tin isotopes are discussed. All the results have been obtained using the same D1S Gogny interaction in the one-body mean-field and the residual part associated with a two-body and density-dependent Hamiltonian.

1. Introduction
Mean field approaches are one of the most powerful methods to tackle an approximate solution of the nuclear many-body problem. Nowadays, a lot of efforts is applied to go beyond the mean field approximation to account for missing correlations. Special attention is paid to the restoration of broken symmetries in mean field approaches \([1]-[7]\), for example using projection technics. An alternate way is to develop a theory in which the trial wave functions preserve certain symmetries. In particular, this is achieved by multiconfiguration methods widely used in various domains of physics, including atomic physics, molecular physics or condensed matter physics. When the interaction is known, this kind of approach provides a very accurate description of a system. In a previous work, we have proposed a variational and self-consistent derivation of multiconfiguration methods in the nuclear physics context with two-body density-dependent and finite range interaction \([8]\). In section 2, we recall briefly the basics of the method. Results concerning pairing correlations in the ground states and the effect of particle number conservation in tin isotopes are presented in section 3. In section 4, preliminary spectroscopic results for tin isotopes are discussed. All the results are obtained with the D1S Gogny interaction \([9, 10]\). Conclusions and perspective are given in section 5.

2. Multiparticle-multihole configuration mixing formalism
Multiparticle-multihole (MPMH) configuration mixing method aims to unify nuclear long range correlations in a symmetry preserving context. The trial wave function is built as a superposition of Slater determinants, not restricted to a single shell:

\[
|\Psi\rangle = \sum_{\alpha, \alpha_\pi} A_{\alpha, \alpha_\pi} \left[ |\Phi_{\alpha_\nu}\rangle \otimes |\Phi_{\alpha_\pi}\rangle \right]
\] (1)
where \( \{A_{\alpha_\pi, \alpha_\nu}\} \) represents the set of mixing coefficients and \( \{|\Phi_{\alpha_\pi}\}, \{|\Phi_{\alpha_\nu}\}\} \) are proton and neutron Slater determinants, respectively, built on single-particle functions \( \varphi_i \). In this formulation, particle numbers are conserved and Pauli principle is fully respected. Moreover, as the wave function contains a lot of correlations through multiple particle-hole configurations, the total angular momentum may be chosen as a good quantum number.

The mixing coefficients and the single-particle orbitals are the variational parameters. If one defines the energy functional \( F(\rho) \) as
\[
F(\rho) = \langle \Psi | \hat{H}(\rho) | \Psi \rangle - \lambda \langle \Psi | \Psi \rangle,
\]
the variational parameters are determined applying a variational principle:
\[
\frac{\partial F(\rho)}{\partial A^*_{\alpha_\pi, \alpha_\nu}} = 0 \quad \text{and} \quad \frac{\partial F(\rho)}{\partial \varphi_i^*} = 0.
\]
In Eq. (2), the Hamiltonian \( \hat{H}(\rho) = \hat{T} + \hat{V}(\rho) \), where \( \hat{V}(\rho) \) represents the two-body Gogny effective interaction plus the Coulomb term. In addition, \( \hat{T} \) and \( \hat{V}(\rho) \) contain 1 and 2-body center-of-mass corrections, respectively.

The set of equations in Eq. (3) are equivalent to a set of non-linear secular equations and inhomogeneous Hartree-Fock (HF) equations:
\[
\sum_{\alpha_\pi', \alpha_\nu'} \mathcal{H}_{\alpha_\pi, \alpha_\nu, \alpha_\pi', \alpha_\nu'} A_{\alpha_\pi', \alpha_\nu'} = \lambda A_{\alpha_\pi, \alpha_\nu},
\]
\[
[ h(\rho, \sigma), \rho ] = G(\sigma).
\]
In Eq. (4), \( \mathcal{H} \) contains contributions from \( \hat{H}(\rho) \) and rearrangement terms coming from the density-dependent part of the Gogny interaction. In Eq. (5), \( h \) represents the effective one-body Hamiltonian deduced from \( \hat{H}(\rho) \), and \( \sigma \) is the two-body correlation matrix. The fully self-consistent solution is obtained by the simultaneous solution of systems (4) and (5). Practically, an iterative procedure is applied.

3. Beyond BCS pairing correlations in tin ground states

In this part, we discuss pairing correlations. We have investigated pairing properties of the ground states of tin isotopes using the Hartree-Fock-Bogoliubov approximation and the MPMH configuration mixing approach. In both cases, the D1S Gogny interaction has been used. Before discussing the results, it is important to emphasize that the MPMH configuration mixing approach can be equivalent to a particle number projection before variation. For example, starting from a BCS wave function, it is easy to establish that the BCS wave function projected on good particle number is equivalent to a MPMH wave function restricted to particular configurations [8]. Specifically, one has to introduce only configurations corresponding to excitations of pairs of nucleons, where a pair is understood as two nucleons in time-reversed states. The proton-neutron pairing is not included in the present study.

We discuss mean field properties of selected tin isotopes. Figs. 1-2 display the evolution of the total Hartree-Fock-Bogoliubov energy (arbitrary scale) and the pairing energy, respectively, according to the dimensionless deformation parameter \( \beta \) for \(^{100}\text{Sn} \), \(^{106}\text{Sn} \) and \(^{116}\text{Sn} \) (energies are expressed in MeV). One concludes that the minimum of total energy is found at \( \beta=0 \) for the three isotopes. The potential energy curve is less rigid for \(^{116}\text{Sn} \), where one can also see the appearance of the second minimum at \( \beta > 0 \), than for \(^{100}\text{Sn} \) and \(^{106}\text{Sn} \). Concerning pairing energies, at \( \beta=0 \), no proton pairing is found. However, concerning neutron pairing, one can
Figure 1. Axial potential energy curves for $^{100}$Sn, $^{106}$Sn and $^{116}$Sn in an arbitrary scale (in MeV).

Figure 2. Axial pairing energy curves for $^{100}$Sn, $^{106}$Sn and $^{116}$Sn (in MeV).

say that these three Sn isotopes simulate three pairing regimes: weak, medium and strong, respectively, for $^{100}$Sn ($0$ MeV), $^{106}$Sn ($\sim 10$ MeV) and $^{116}$Sn ($\sim 20$ MeV).

One quantity we have been interested in is the correlation energy $E_{\text{corr}}$. It is taken as the difference between the total energy $E(\Psi) = \langle \Psi | \hat{H} | \Psi \rangle$ of the correlated system and the energy of the simple HF method $E_{\text{HF}}^0 = \langle \Phi_0 | \hat{H} | \Phi_0 \rangle$:

$$E_{\text{corr}} = E(\Psi) - E_{\text{HF}}^0$$

Table 1 summarizes the results obtained solving Eq. (4) of the MPMH configuration mixing method (no renormalization of the single-particle orbitals). The total correlation energy (expressed in MeV) found with the MPMH wave function, as well as the neutron contribution, are indicated. The BCS correlation energy is also shown. One sees that with the MPMH configuration mixing approach, the correlation energy is never vanishes, even for the doubly-magic nucleus $^{100}$Sn for which it is equal to $3.67$ MeV. The contribution due to protons is found similar for the tin isotopes. It is interesting to notice that the correlation energy found with the MPMH wave function is systematically stronger than the one found in the BCS approximation.
The difference between both approaches is much larger when the pairing regime is weak. In other words, from an energy point of view, the BCS approximation can serve as a good approximation in the strong pairing regime. It is no longer the case in medium and weak pairing regimes. This is a well known result in exactly solvable models of the pairing Hamiltonian [11, 12, 13].

Table 1. Total and neutron correlation energies (in MeV) obtained from the MPMH configuration mixing for $^{100}$Sn, $^{106}$Sn and $^{116}$Sn. The last column indicates the correlation energy deduced from a BCS approximation.

| Nucleus | $E_{\text{total}}^{\text{corr}}$ | $E_{\text{neutron}}^{\text{corr}}$ | $E_{\text{BCS}}^{\text{corr}}$ |
|---------|-----------------|-----------------|-----------------|
| $^{100}$Sn | 3.67 | 1.90 | 0.00 |
| $^{106}$Sn | 4.62 | 2.88 | 1.37 |
| $^{116}$Sn | 5.44 | 3.74 | 3.25 |

It is also instructing to discuss the content of the wave function. In order to have a measure of the amount of correlations in the MPMH wave function $|\Psi\rangle$, we define the quantity $T(i, j)$:

$$T(i, j) = \sum_{\alpha, \alpha'} |A_{\alpha\alpha'}|^{2}$$

The first and second arguments of $T$ stand for the number of excited proton and neutron pairs included in $|\Psi\rangle$, respectively. Results are presented in Table 2. No renormalization of single-particle orbitals have been taken into account in those results. In the case of $^{100}$Sn, the HF approximation is good in the sense that 90% of the wave function correspond to the HF component. Configurations corresponding to the excitation of one pair of nucleons constitute the rest of the wave function. Among those configurations, none are dominant. The dissymmetry between proton and neutron configurations comes from the Coulomb term. $^{106}$Sn and $^{116}$Sn nuclei are much more correlated. The HF component is now contributing to only $\sim$66% of the wave function. In the case of $^{106}$Sn, there is a dominant configuration corresponding to the diffusion of one neutron pair from the 2d$_{5/2}$ shell toward the 1g$_{7/2}$ shell. In the case of $^{116}$Sn, there are two dominant configurations corresponding to the diffusion of the pair contained in 3s$_{1/2}$ toward the 2d$_{3/2}$ and 1h$_{11/2}$ shells. For $^{106}$Sn and $^{116}$Sn, the actual wave function is far from the HF approximation.

Table 2. Components of ground state wave functions for $^{100}$Sn, $^{106}$Sn and $^{116}$Sn without single particle renormalization.

| Nucleus | $T(0,0)$ | $T(0,1)$ | $T(1,0)$ | $T(0,2)$ | $T(1,1)$ | $T(2,0)$ |
|---------|---------|---------|---------|---------|---------|---------|
| $^{100}$Sn | 90.85 | 5.02 | 3.70 | 0.16 | 0.18 | 0.09 |
| $^{106}$Sn | 67.44 | 25.29 | 3.63 | 2.54 | 0.99 | 0.11 |
| $^{116}$Sn | 65.38 | 26.04 | 4.50 | 2.68 | 1.23 | 0.17 |
Finally, we discuss possible effects coming from the renormalization of single particle orbitals. In order to partly account for it, we solved Eq. (5) in an approximate way, by neglecting terms associated with the two-body correlation matrix $\sigma$. Doing so, a non-negligible gain for the correlation energy has been obtained, as expected. What is more interesting is the effect on correlated wave functions. The results are summarized in Table 3. One sees that for $^{100}$Sn and $^{106}$Sn, no striking effect is obtained. However, this is completely different for $^{116}$Sn. In particular, the main contribution to the correlated wave function comes from configurations corresponding to the excitation of one neutron pair. The HF component is now provides to 42% of the wave function. This huge change comes from a $\sim$400keV reduction of the neutron gap between the $1d_{3/2}$ and $1h_{11/2}$ shells. The renormalization by correlations of single-particle orbitals is a very important effect, in particular for the prediction of the ground state spins in odd-$A$ nuclei. For example, it is known that a single-particle spectrum obtained with the D1S Gogny interaction in the context of Hartree-Fock-Bogoliubov calculation using self-consistent blocking is unable to provide the right spin for $^{121}$Sn, $^{129}$Sn and $^{131}$Sn.

Table 3. Components of ground state wave functions for $^{100}$Sn, $^{106}$Sn and $^{116}$Sn with single particle renormalization.

| Nucleus | $T(0,0)$ | $T(0,1)$ | $T(1,0)$ | $T(0,2)$ | $T(1,1)$ | $T(2,0)$ |
|---------|----------|----------|----------|----------|----------|----------|
| $^{100}$Sn | 88.19 | 6.36 | 4.74 | 0.27 | 0.29 | 0.15 |
| $^{106}$Sn | 62.90 | 28.65 | 3.54 | 3.62 | 1.17 | 0.11 |
| $^{116}$Sn | 42.09 | 44.28 | 3.00 | 8.43 | 2.09 | 0.11 |

4. Low-lying spectroscopy of a few silicon isotopes
In this section, we report very preliminary results that are analyzed and completed in a forthcoming publication [14]. They concern the low-lying spectroscopy of a few silicon isotopes using the MPMH configuration mixing approach combined with the D1S Gogny interaction. From the mean-field and beyond mean-field analysis, silicon isotopes display strong deformation effects [7, 15]. In Table 4, we show the energies of a few excited states in $^{26}$Si and $^{28}$Si. We compare experimental energies with those calculated from the MPMH configuration mixing and from a 5 dimensional collective Hamiltonian approach (5DCH) [7]. For MPMH configuration mixing results, the mixing has been restricted to the $sd$-shell. All the configurations characterized by a given total spin and a given parity are included in the correlated wave function. The renormalization of single-particle orbitals is not taken into account and is not discussed in this contribution. The equations are solved using an harmonic oscillator basis with eleven major shells. With this size, the excitation energies are converged.

One sees that the excitation energies calculated with the MPMH configuration mixing are in a good agreement with experimental values. For those two isotopes, results are better within the MPMH configuration mixing than within the 5DCH approach. This indicates clearly that correlations more general than the quadrupole ones are important to explain the structure of these nuclei. Moreover, the coupling to intrinsic degrees of freedom that exist in the MPMH configuration mixing is important. The deficiency of the 5DCH approach already noticed in [7] is also exhibited here if one considers the $0^+_2$ states.
Table 4. Excitation energies of the lowest states in $^{26}\text{Si}$ and $^{28}\text{Si}$. Experimental energies as well as those deduced from the MPMH configuration mixing (MPMH) and collective Hamiltonian (5DCH) are indicated.

| Nucleus | States | Experiment | MPMH | 5DCH |
|---------|--------|------------|------|------|
| $^{26}\text{Si}$ | $2_1^+$ | 1.795 | 1.502 | 2.426 |
|          | $2_2^+$ | 2.783 | 2.567 | 5.124 |
|          | $0_2^+$ | 3.332 | 3.740 | 8.146 |
| $^{28}\text{Si}$ | $2_1^+$ | 1.779 | 1.993 | 2.469 |
|          | $4_1^+$ | 4.618 | 5.372 | 6.446 |
|          | $0_2^+$ | 4.980 | 4.409 | 10.591 |

5. Conclusion and perspectives
In conclusion, we have firstly discussed a realistic description of pairing correlations in various pairing regimes in the context of multiparticle-multihole configuration mixing approach. In this study, the ground states of a few even-even tin isotopes have been investigated. We have demonstrated that correlations beyond the BCS approximation are important. The renormalization of single-particle orbitals by those correlations can produce strong variations in correlated wave functions and hence in calculated observables. A natural extension of this study would be for odd-$A$ isotopes in order to provide the odd-even mass differences that is an observable directly connected with pairing properties in nuclei. Secondly, we have presented a few results concerning the low-lying spectroscopy of silicon isotopes. The encouraging results indicate the need to perform a precise analysis of the structure of correlated wave functions as well as the $T = 0$ residual channel of the Gogny interaction.

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