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High-spin intruder states in the *fp*-shell nuclei and isoscalar proton-neutron correlations

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We perform a systematic theoretical analysis of fully-aligned, high-spin $f^n_{7/2}$ seniority isomers and $d^{-1}_{3/2}f^{n+1}_{7/2}$ intruder states in the $A \sim 44$ nuclei from the lower-*fp* shell. The configuration-interaction calculations, based on the nuclear shell model, are performed in the full *sdfp* configuration space allowing $1p$-$1h$ cross-shell excitations. The density functional theory calculations are carried out within the self-consistent Hartree-Fock approach with the Skyrme energy functional that reproduces empirical Landau parameters. While there is a nice agreement between experimental and theoretical relative energies of fully-aligned states in $N > Z$ nuclei, this is no longer the case for the $N = Z$ systems. The remaining deviation from the data is attributed to the isoscalar proton-neutron correlations. It is also demonstrated that the Coulomb corrections at high spins noticeably depend on the choice of the energy density functional.

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There are two major theoretical approaches to the structure of complex heavy nuclei. In the interacting shell model (SM) [1], which is a variant of the configuration-interaction method known from quantum chemistry, the effective Hamiltonian of an A-body system is diagonalized in a subspace of Slater determinants involving a limited number of valence protons and neutrons moving in several single-particle orbits. The remaining nucleons belong to a fixed core. The main advantage of this method is the proper treatment of many-nucleon correlations within the valence configuration space. The resulting wave functions are eigenstates of the symmetry invariants of the SM Hamiltonian (angular momentum, parity, and particle number).

For heavy systems having many valence particles, the dimension of the SM Hilbert space becomes intractable, and the tool of choice is the nuclear density functional theory (DFT) [2] in the formulation of Kohn and Sham [3]. Here, the main ingredient is the energy density functional (EDF) that depends on densities and currents representing distributions of nucleonic matter, spins, momentum, and kinetic energy, as well as their derivatives (gradient terms). There are three aspects of the nuclear DFT that make it different from the standard electronic DFT: (i) two kinds of fermionic species; (ii) short-ranged interaction; and (iii) the lack of the confining external field (nuclei are self-bound systems). Standard Skyrme functionals employed in self-consistent mean-field (MF) calculations are parametrized by means of about ten coupling constants that are adjusted to basic properties of nuclear matter and to selected data on finite nuclei. The functionals are augmented by the pairing term which describes nuclear superfluidity [4]. A significant part of many-body correlations can be included by considering symmetry-breaking intrinsic states. However, like in electron DFT, correlations beyond mean field are important as nuclei are finite quantum systems.

From a theoretical standpoint, the *sdfp*-shell nuclei are particularly good candidates to study the competition between collective and single-particle excitations. The large-scale SM calculations [5–8] have been spectacularly successful in describing spectroscopic features of these medium-mass systems. Since the associated configuration spaces are not prohibitively large for SM calculations, and, at the same time, the number of valence particles (and holes) is large enough to create substantial collectivity, these systems form a crucial playground to confront the spherical SM with collective approaches based on DFT [9,10].

In spite of the success of the SM description, there are still many open questions and challenges in this region of the nuclear chart that offer many opportunities for new physics. In particular, studies of mirror-symmetric nuclei and precise measurements of the Coulomb energy displacement shed light on isospin-breaking effects [11,12]. Another frontier is investigations of unnatural-parity intruder states in $A \sim 44$ nuclei from the lower-*fp* shell associated with cross-shell excitations across the $N = Z = 20$ magic gap that give rise to shape coexistence effects and emergence of collective rotational excitations [13–15]. A simple SM interpretation of the excitation energy of the $d_{3/2}$ hole states was given in the mid-sixties in terms of the Bansal-French-Zamick (BFZ) mechanism [16], in which the key element is the isospin-dependent part of the SM effective interaction.

Recently, a systematic MF analysis of maximum-spin states (also referred to as terminating states or seniority isomers) has been performed within the Skyrme-Hartree-Fock (SHF) approach [17,18] for the $[f^n_{7/2}]_{I_{\rm max}}$ and $[d^{-1}_{3/2}f^{n+1}_{7/2}]_{I_{\rm max}}$ configurations (n denotes the number of valence particles outside the ^{40}Ca core). Those fully-aligned states, experimentally known in a number of $20 \leqslant Z < N \leqslant 24$ nuclei, have fairly simple SM configurations, and they provide an excellent testing ground for the SM effective interaction and the time-odd densities and fields that appear in the MF description. In this context, the energy difference between the excitation energies of the terminating states,

$$\Delta E = E\left(\left[d^{-1}_{3/2}\, f^{n+1}_{7/2}\right]_{I_{\rm max}}\right) - E\left(\left[f^{n}_{7/2}\right]_{I_{\rm max}}\right), \qquad (1)$$

is a sensitive probe of time-odd spin couplings and the strength of the spin-orbit term in the EDF. In particular, it was demonstrated [17,18] that by constraining the Skyrme EDF to the empirical spin-isospin Landau parameters and by slightly reducing the spin-orbit strength, good agreement with the data could be obtained. This result, based on high-spin data for terminating states, is consistent with conclusions of previous works [19,20] based on different theoretical methodology and experimental input (such as giant resonances, beta decays, and moments of inertia).

The DFT studies of Refs. [17,22] rely on the assumption that, for the terminating states, the correlation term in the EDF is small, i.e., those states are excellent examples of unperturbed single-particle motion. This further implies that ΔE, unlike the absolute excitation energies $E([d_{3/2}^{-1} f_{7/2}^{n+1}]_{I_{\max}})$ and $E([f_{7/2}^{n}]_{I_{\max}})$, mainly depends on properties of the underlying MF: the energy of the cross-shell excitation and symmetry-breaking effects. The main objective of the present work is to (i) via SM analysis, study the role of dynamical correlations on ΔE; (ii) investigate the origin of large deviations between MF results and experimental data for $N = Z$ nuclei; and (iii) through studies of hole states test the isospin effects present in the SM scheme. Preliminary results of this analysis were published in Refs. [23,24].

Our SM calculations were carried out using the code ANTOINE [9] in the *sdfp* configuration space limited to 1*p*-1*h* cross-shell excitation from the *sd* shell to the *fp* shell. In the *fp*-shell SM space we took the FPD6 interaction [25]. The remaining matrix elements are those of Ref. [26]. As compared to the earlier work [10], the mass scaling of the SM matrix elements was done here consistently, thus reducing the *sd* interaction channel by ∼4%. As seen in Fig. 1, excellent agreement was obtained between the SM and experiment for the absolute excitation energies of terminating states for both $E([f_{7/2}^{n}]_{I_{\max}})$ and $E([d_{3/2}^{-1} f_{7/2}^{n+1}]_{I_{\max}})$ configurations.

The calculated SM and SHF energy differences ΔE are shown in Fig. 2 relative to experimental values. We note that while Fig. 1 suggests a similar level of agreement between

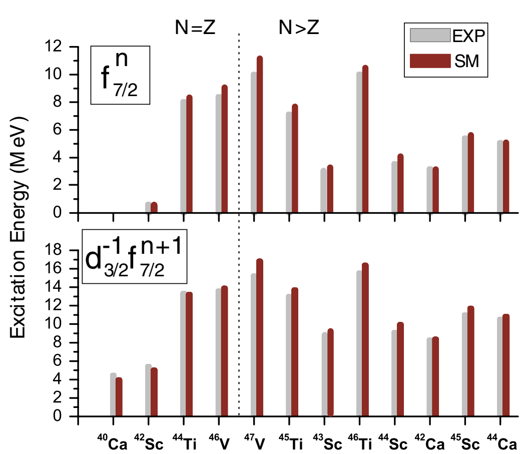

FIG. 1. (Color online) Experimental (gray bars) and shell model (black bars) excitation energies of maximum-spin states of $f_{7/2}^{n}$ (top) and $d_{3/2}^{-1} f_{7/2}^{n+1}$ (bottom) configurations in $N = Z$ (left) and $N > Z$ (right) *fp*-shell nuclei. Experimental data are taken from Refs. [17,21].

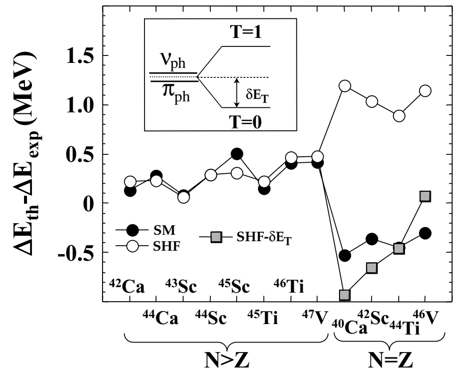

FIG. 2. Difference $\Delta E_{\rm th} - \Delta E_{\rm exp}$ between experimental and theoretical values of ΔE (1) in $A \sim 44$ mass region. Dots denote the SM results. Circles denote the SHF results based on the modified SkO parametrization (see text). The SHF calculations for the $[d_{3/2}^{-1} f_{7/2}^{n+1}]_{I_{\max}}$ intruders in $N = Z$ nuclei yield two nearly degenerate states associated with proton ($\pi_{\rm ph}$) and neutron ($\nu_{\rm ph}$) cross-shell excitations. As shown in the inset, the physical $T = 0$ state in the laboratory frame is shifted down in energy by δE_T (isospin correlation energy). Squares denote the SHF results for $N = Z$ nuclei with the isospin correction added. The SHF results were shifted by 480 keV in order to facilitate the comparison with SM.

experiment and the SM in $N = Z$ and $N > Z$ nuclei, the energy differences tell a different story. Indeed, in $N > Z$ nuclei the SM systematically overestimates the experimental data by ∼280 keV. On the contrary, in $N = Z$ nuclei the SM systematically underestimates the data by ∼410 keV. This clearly suggests that important correlations related to isospin and cross-shell excitations are missing in the present SM implementation.

The SM results are further compared to the SHF calculations based on the SkO [27] parametrization slightly modified along the prescription given in Refs. [17,22]. Without entering into details, we recall that the modifications concern coupling constants related to the time-odd spin fields $C_t^s \boldsymbol{s}^2$ and $C_t^{\Delta s} \boldsymbol{s} \cdot \Delta \boldsymbol{s}$ where $t = 0, 1$ labels isoscalar and isovector terms, respectively. Moreover, the strength of the spin-orbit interaction was reduced by 5% compared to the original SkO value.

In contrast to the SM, the SHF underestimates experimental values of ΔE in $N > Z$ nuclei by ∼200 keV giving rise to an average offset of ∼480 keV between the two models. In order to facilitate the comparison, this average difference was removed by shifting up the HF results in Fig. 2. (It is to be noted that an overall shift in ΔE can easily be accounted for by varying the size of the $N = Z = 20$ gap in SM or by changing the magnitude of the spin-orbit term in SHF.) It is striking to see that SHF calculations follow SM results in $N > Z$ nuclei extremely well, reproducing details of isotopic and isotonic dependence. This result appears to be fairly general. Indeed, as seen in Fig. 3, similar agreement was obtained for SHF calculations based on the SLy4 parametrization [28], modified according to Ref. [17]. These results strongly support our assumption that the maximally-aligned states in $N > Z$ nuclei are excellent examples of an almost unperturbed single-particle motion and that dynamical correlations beyond

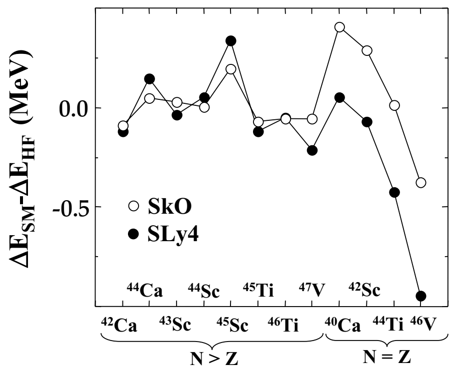

FIG. 3. Difference between SM and SHF values of ΔE. Two Skyrme parametrizations are used: SkO (dots) and SLy4 (circles), modified according to Ref. [17]. As in Fig. 2, the SHF results were shifted by 480 keV.

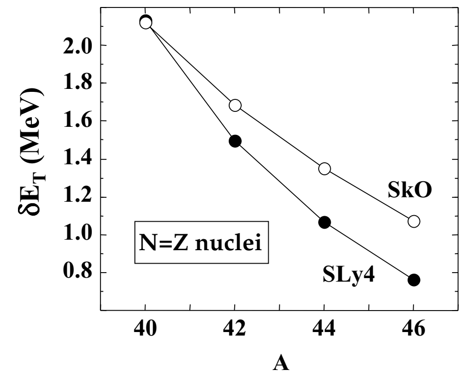

FIG. 4. Phenomenological estimates of the isospin energy correction, $\delta E_T(A)$, due to the restoration of isobaric symmetry internally broken in SHF solutions corresponding to the $[d_{3/2}^{-1} f_{7/2}^{n+1}]_{I_{\max}}$ terminating states in $N = Z$ nuclei. The values of $\delta E_T(A)$ obtained in SkO and SLy4 models are labeled by open and filled dots, respectively.

MF present in these states do not exhibit any distinct particle number dependence.

The difference in the SHF description of $N > Z$ and $N = Z$ nuclei seen in Fig. 2 can be partly explained in terms of the spontaneous breaking of isobaric symmetry [29,30] in the $d_{3/2}^{-1} f_{7/2}^{n+1}$ terminating states in $N = Z$ nuclei. In the MF picture, those states are not uniquely defined. Indeed, by making either neutron (ν) or proton (π) $d_{3/2} \to f_{7/2}$ 1*p*-1*h* excitation, one arrives at two nearly degenerate intrinsic states $E([d_{3/2}^{-1} f_{7/2}^{n+1}]^{\nu}_{I_{\max}}) \approx E([d_{3/2}^{-1} f_{7/2}^{n+1}]^{\pi}_{I_{\max}})$, which manifestly violate isobaric symmetry. Indeed, these MF states are not eigenstates of isospin. After isospin projection, the $T = 0$ state becomes lower in energy in the laboratory system, as illustrated in the inset of Fig. 2. Due to physical symmetry-breaking caused by the Coulomb interaction, the two intrinsic states are slightly split with the proton 1*p*-1*h* excitation being always slightly lower in energy. The reason is that proton excitation from the $d_{3/2}$ orbit to a more extended $f_{7/2}$ orbit slightly increases the mean charge radius, thus reducing the Coulomb repulsion.

In order to make comparison to the data, the correlation energy δE_T due to isospin symmetry-breaking in SHF should be estimated. For the purpose of this work, we evaluate δE_T using the concept of isocranking [29,30]. That is, we compute the energy difference between the isobaric analog states at high spin, i.e., $\delta E_T \equiv E([d_{3/2}^{-1} f_{7/2}^{n+1}]_{I_{\max}}; T_z = \pm 1) - E([d_{3/2}^{-1} f_{7/2}^{n+1}]_{I_{\max}}; T_z = 0)$ using the SHF approach with Coulomb interaction switched off. The energy difference $\Delta E_{\rm HF}^{(T=0)}$ corrected in this way is marked by squares in Fig. 2.

The isospin corrections calculated self-consistently are depicted in Fig. 4. It is interesting to observe that $\delta E_T(A)$ shows a surprisingly strong decrease with increasing A. According to our analysis, see Fig. 5, this strong particle-number dependence can be attributed to the isovector time-odd fields. The preliminary calculations indicate that this effect can be reduced by decreasing the value of the isovector Landau parameter g_0'. Whether or not this can be used to further constrain the value of g_0' remains to be studied (see, however, recent work [31,32]). Coming back to Figs. 2 and 3, it is encouraging to see that after approximate isospin symmetry restoration, one obtains $\Delta E_{\rm SHF}^{(T=0)} \approx \Delta E_{\rm SM}^{(T=0)}$ also in $N = Z$ nuclei. Hence, our comparative study strongly suggests that correlations of a similar type are missing in $N = Z$ nuclei, both in the SM and the SHF approaches.

Our SM interaction strictly preserves isospin. Consequently, the Coulomb correction to ΔE, δE_C should be added afterwards. The Coulomb correction (including the associated isovector polarization) can be calculated self-consistently in SHF. Surprisingly, the many-body response against electrostatic polarization appears to be strongly sensitive to the isovector part of the EDF. This is visualized in Fig. 6 which shows a difference, δE_C, between the SHF values of ΔE calculated without ($\Delta E_{\rm HF}^{(0)}$) and with ($\Delta E_{\rm HF}$) the Coulomb term. While δE_C is very small for SLy4, the values calculated in the SkO variant are appreciable, $\delta E_C \approx 130$ keV. The difference can be traced back to the fact that these two parametrizations differ strongly in the strength of the isovector part of the spin-orbit interaction. While in SLy4 the ratio of the isovector (W_1) to the isoscalar (W_0) spin-orbit strengths equals to the standard value of $W_1/W_0 = 1/3$, SkO is a modern parametrization having $W_1/W_0 \approx -1.3$. The resulting change

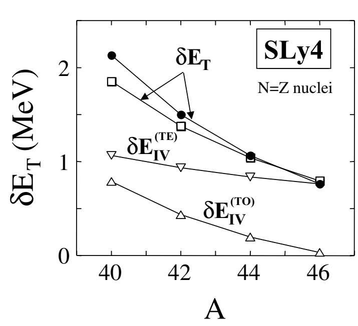

FIG. 5. The isospin energy correction calculated self-consistently (dots) and non-self-consistently (squares; from the expectation value of the isovector mean-field) within the SHF-SLy4 model. The corresponding isovector contributions associated with time-even ($\delta E_{\rm IV}^{(\rm TE)}$) and time-odd ($\delta E_{\rm IV}^{(\rm TO)}$) mean-fields are also shown. Note the strong A-dependence of $\delta E_{\rm IV}^{(\rm TO)}$ which essentially determines the A-dependence of the isospin energy correction.

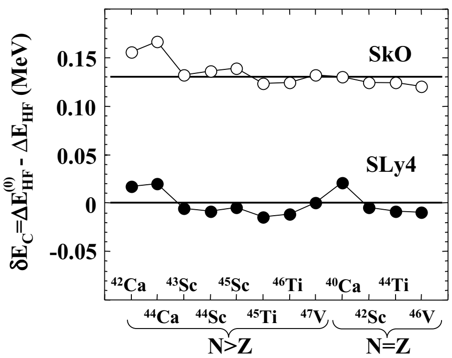

FIG. 6. Coulomb correction, δE_C, to ΔE calculated in the SkO and SLy4 models by performing SHF calculations without ($\Delta E_{\rm HF}^{(0)}$) and with ($\Delta E_{\rm HF}$) Coulomb interaction.

in the radial form factor leads to a large Coulomb effect at high spin, an effect that is of the same order as the measured Coulomb energy differences in *fp*-shell nuclei [12]. Based on our study, the Coulomb interaction can give rise to an overall displacement of the order of 100 keV that very weakly depends on Z and N.

In summary, the self-consistent SHF analysis of terminating states in the $A \sim 44$ nuclei agrees nicely with SM studies, after correcting the former for the isospin-breaking effects in $N = Z$ nuclei. For $N > Z$ nuclei, both theories provide a good reproduction of experimental data. This validates the assumption of previous studies [17,18] regarding the single-particle character of the maximally-aligned states. We believe that the origin of the remaining deviation from the data seen in the $N = Z$ systems has its source in the $T = 0$ pairing channel. The SM provides an excellent description of spectroscopic properties in the whole *fp* shell. Most likely, any discrepancy involving intruder configurations has its source in the assumed truncation to $1p$-$1h$ cross-shell excitations. This configuration-space restriction is expected to impact the isoscalar channel associated with the $sd \rightarrow fp$ pair scattering. The single main obstacle that prevents us from carrying out calculations in an extended space involving $2p$-$2h$, $3p$-$3h, \ldots,$ cross-shell transitions is the lack of an appropriate effective interaction. A possibility of an onset of isoscalar proton-neutron pairing nearby band-termination was already discussed in Ref. [33] within the mean-field formalism. At this level of approximation, however, while the extended proton-neutron local EDF formalism has been developed [4], its practical implementation is still in an early stage.

The discrepancy between the SM description of $N > Z$ and $N = Z$ nuclei and the characteristic seesaw pattern of $\Delta E_{\rm th} - \Delta E_{\rm exp}$ (see Fig. 2) may be caused also (or partly) by incorrect isospin dependence of the SM matrix elements. According to the BFZ mechanism, the isospin-dependent contribution to the excitation energy of a $1p$-$1h$ state is

$$\Delta E^T = \tfrac{1}{2} b[T(T+1) - T_p(T_p+1) - T_h(T_h+1)], \qquad (2)$$

where T is the total isospin of the intruder state, $T_h = 1/2$, $T_p = T \pm 1/2$, and b denotes the average difference between $T = 0$ and $T = 1$ two-body SM matrix elements. Since for the spin-aligned states $T_p = T - 1/2$ in $N > Z$ nuclei and $T_p = 1/2$ in $N = Z$ nuclei, the isospin-dependent term is $\Delta E^T_{N>Z} = b(T - 1/2)/2$ and $\Delta E^T_{N=Z} = -3b/4$. Hence, the reduction of b by $\delta b \sim 700$ keV would lead to an almost perfect agreement with the data. Unfortunately, our attempt to modify b in Eq. (2) through a simple renormalization of $T = 0$ and $T = 1$ SM matrix elements was not successful as it spoiled the previously obtained nice agreement between SM and experimental binding energies. An open question, which is a subject of our ongoing work [34], is whether the simultaneous improvement in ΔE *and* binding energies can be obtained by a systematic refinement of SM interaction.

Finally, we have demonstrated that the state-dependent Coulomb polarization at high spins noticeably depends on the choice of the EDF. The resulting uncertainty in the Coulomb energy shift can be as large as the measured Coulomb energy displacement. This is likely to result in ambiguities when estimating Coulomb effects at high spins.

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