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

G. Stoitcheva,$^1,2$ W. Satula,$^{3,4}$ W. Nazarewicz,$^{2,1,3}$ D.J. Dean,$^1$ M. Zalewski,$^3$ and H. Zduńczuk$^3$

$^1$ Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831
$^2$ Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996
$^3$ Institute of Theoretical Physics, University of Warsaw, ul. Hoża 69, 00-681 Warsaw, Poland
$^4$Joint Institute for Heavy Ion Research, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, Tennessee 37831

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We perform a systematic shell-model and mean-field study of fully-aligned, high-spin $f^n_p I_{max}$ intruder states in the $A\sim 44$ nuclei from the lower-$fp$ shell. The shell-model calculations are performed in the full sdfp configuration space allowing 1p-1h cross-shell excitations. The self-consistent mean-field calculations are based on the Hartree-Fock approach with the Skyrme energy density 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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The triumph of the nuclear shell model (SM) in the sd-p-shell region$^1$ proves that many spectroscopic properties of those fairly heavy nuclei can be well accounted for by an effective two-body $G$-matrix augmented by the monopole corrections. 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 shift light on isospin breaking effects$^2,3$. 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$^4,5$. 

From a theoretical standpoint, the $fp$-shell nuclei are particularly good candidates to study the competition between collective and single-particle excitations. 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 the mean-field (MF) theory$^6$. The diversity of nuclear structure phenomena, rich amount of spectroscopic data collected, and a possibility of direct SM verification of MF calculations in the $fp$ region, offer a unique opportunity for fine tuning of the underlying nuclear energy density functional (EDF).

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$^7,8$ for the $[f^n_p I_{max}]$ and $[d^{−1}_3 f^n_{7/2} I_{max}]$ configurations ($n$ denotes the number of valence particles outside the $^40$Ca core). Those fully-aligned states, experimentally known in a number of $20 \leq Z < N \leq 24$ nuclei, have fairly simple SM configurations, and they provide an excellent testing ground for 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,

$$\Delta E = E([d^{−1}_3 f^n_{7/2} I_{max}]) - E([f^n_p I_{max}]),$$

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$^9$ 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$^{10,11}$ based on different theoretical methodology and experimental input (such as giant resonances, beta decays, and moments of inertia).

The MF studies of Refs.$^{12,17}$ rely on the assumption that the terminating states are almost ideal examples of unperturbed single-particle motion, which further implies that $\Delta E$, unlike the absolute excitation energies $E([d^{−1}_3 f^n_{7/2} I_{max}])$ and $E([f^n_p I_{max}])$, mainly depends on properties of the underlying MF. In particular, $\Delta E$ depends on the energy of the cross-shell excitation and symmetry-breaking effects. The main objective of the present work is to (i) study the role of dynamical correlations on $\Delta E$, and (ii) investigate the origin of large deviations between MF results and experimental data for $N=\!Z$ nuclei. For this purpose, we carry SM calculations. Preliminary results of this analysis were published in Refs.$^{18,19}$.

Our SM calculations were carried out using the code ANTOINE$^{10}$ in the sdfp configuration space limited
to 1p-1h cross-shell excitation from the sd shell to the fp shell. In the fp-shell SM space we took the FPD6 interaction [20]. The remaining matrix elements are those of Ref. [21]. As compared to the earlier work [11], the mass scaling of the SM matrix elements was done here consistently, thus reducing the sd interaction channel by \(\sim 4\%\).

As seen in Fig. 1 excellent agreement was obtained between the SM and experiment for the absolute excitation energies of terminating states for both \(E(\{f_{7/2}\}_{n=0}^{\text{max}} + t_{1/2}^{\text{max}}\})\) and \(E(d_{5/2}^{\text{max}} + f_{7/2}^{\text{max}})\).

The calculated SM and SHF energy differences \(\Delta E\) are shown in Fig. 2 relative to experimental values. We note that while Fig. 1 suggests a similar level of agreement between 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 \(\sim 280\text{ keV}\). On the contrary, in \(N=Z\) nuclei the SM systematically underestimates the data by \(\sim 410\text{ keV}\). 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 [22] parameterization slightly modified along the prescription given in Refs. [12, 17]. Without entering into details, we recall that the modifications concern coupling constants related to the time-odd spin fields \(C_t s^2\) and \(C_\Delta s \Delta s\) 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 \(\Delta E\) in \(N>Z\) nuclei by \(\sim 200\text{ keV}\) giving rise to an average offset of \(\sim 480\text{ keV}\) 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 \(\Delta E\) can easily be accounted for by varying the size of the \(N=Z=20\) gap in SM or by a 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 parameterization [23], modified according to Ref. [12].

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 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 in the \(d_{3/2}^{\text{max}} f_{7/2}^{\text{max}}\) terminating states in \(N=Z\) nuclei. In the MF picture, those states are not uniquely defined. Indeed, by making either neutron (\(\nu\)) or proton (\(\pi\)) \(d_{3/2} \rightarrow f_{7/2}\) 1p-1h excitation, one arrives at two nearly degenerate intrinsic states \(E(\text{SHF}) = E(d_{3/2}^{\text{max}} f_{7/2}^{\text{max}}) \approx E(d_{3/2}^{\text{max}} f_{7/2}^{\text{max}})\), which manifestly violate isobaric
extended is that proton excitation from the intrinsic states are slightly split with the proton 1p-1h excitation caused by the Coulomb interaction, the two in-orbit of isospin. After isospin projection, the 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 1p-1h 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 $\delta E_T$ due to isospin symmetry-breaking in SHF should be estimated. For the purpose of this work, we evaluate $\delta E_T$ using the self-consistent isoranking. That is, we compute the energy difference between the isobaric analogue states at high spin, i.e., $\delta E_T \equiv E(\{d_{3/2}^{-1}f_{7/2}^{n+1}\}_{\text{max}}; T_z = \pm 1) - E(\{d_{3/2}^{-1}f_{7/2}^{n+1}\}_{\text{max}}; T_z = 0)$ using the SHF approach with Coulomb interaction switched off. The energy difference $\Delta E_{HF}^{(T=0)}$ corrected in this way is marked by squares in Fig. 2.

The calculated isospin corrections 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, this strong particle-number dependence can be attributed to the time-odd fields, and the 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 [23, 24]). Coming back to Figs. 2 and 3, it is encouraging to see that after approximate isospin symmetry restoration, one obtains $\Delta E_{HF}^{(T=0)} \approx \Delta E_{HF}^{(T=0)}$ 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 conserves isospin. Consequently, the Coulomb correction to $\Delta E$, $\delta EC_c$ 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. 4, which shows a difference, $\delta EC$, between the SM values of $\Delta E$ calculated without ($\Delta E_{HF}^{(0)}$) and with ($\Delta E_{HF}$) the Coulomb term. While $\delta EC$ is very small for SLy4, the values calculated in the SkO variant are appreciable, $\delta EC \approx 130$ keV. The difference can be traced back to the fact that these two parameterizations differ strongly in the shape of the isovector part of the spin-orbit interaction. While in SLy4 the ratio of the isovector ($W_J$) to the isoscalar ($W_0$) spin-orbit strengths equals to the standard value of $W_J/W_0 = 1/3$, SkO is a modern parameterization having $W_J/W_0 \approx -1.3$. The resulting change 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 [3]. 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 [12, 13] regarding the single-particle character of the maximally-aligned states. We believe that the origin

![Figure 3](image3.png)

**Fig. 3:** Difference between SM and SHF values of $\Delta E$. Two Skyrme parametrizations are used: SkO (dots) and SLy4 (circles), modified according to Ref. [12]. As in Fig. 2 the SHF results were shifted by 480 keV.

![Figure 4](image4.png)

**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 $\{d_{3/2}^{-1}f_{7/2}^{n+1}\}_{\text{max}}$ 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.
FIG. 5: Coulomb correction, $\delta E_C$, to $\Delta E$ calculated in the SkO and SLy4 models by performing SHF calculations without $(\Delta E_{HF}^{(0)})$ and with $(\Delta E_{HF})$ Coulomb interaction.

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 the whole $fp$ shell. Therefore, any discrepancy involving intruder configurations must have 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,..., cross-shell transitions is the lack of an appropriate effective interaction. On the SHF level, while the extended proton-neutron self-consistent SHF formalism has been developed, its practical implementation is still in an early stage; see, e.g., Refs. [27], [28] and references quoted therein.

Finally, we have demonstrated that the state-dependent Coulomb polarization at high spins noticeably depends on the choice of the energy density functional, in particular its spin-dependent terms. 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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