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Study of K-Isomeric States in the Mass Region of ^{178}Hf

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Abstract. We explore the two-quasiparticle (2qp) structure of K-isomeric states in the mass region of heavy rare-earth nuclei within a self-consistent Skyrme Hartree-Fock plus BCS (SHFBCS) approach using the Skyrme-SIII parametrization. Our calculations show that the 2qp energies associated with the $K^\pi = 6^+$ and 8^- isomeric states follow the systematic behaviour of experimental data along the isotopic and isotonic chains in the vicinity of ^{178}Hf. The study outlines the frames of applicability of the approach in the region of pronounced deformation and provides a test for the relevance of alternative neutron and proton 2qp configurations and their eventual mixing in the formation of these isomeric states. The calculations provide predictions for the magnetic dipole moments in the considered K-isomeric states showing their strong sensitivity to the proton or neutron structure of the corresponding 2qp configurations.

1 Introduction

Nuclear isomers represent one of the most actively developing areas in the physics of atomic nuclei [1]. The K-isomers are of special interest, since their manifestation carries a detailed information about the intrinsic shell-structure configurations which govern the appearance of nuclear metastable states. The corresponding experimental data provide a rather precise test for the effective interactions used in the many-body theories of the nucleus. While in the regions of very heavy and superheavy nuclei the collection of data is still in progress, in the region of rare-earth nuclei an amount of data is already available for rather long continuous chains of isotopes and isotones [2]. The latter allows one to study in detail the structure and evolution of the proton or neutron configurations which

determine the K-isomeric states as well as to assess the capability of the effective interactions to reproduce it.

The aim of this work is to investigate such series of K-isomeric states in the isotopic and isotonic chains to which ^{178}Hf belongs. We consider the series of $K^\pi = 6^+$ and 8^- two-quasiparticle excitations in the isotopic chains of $^{168-184}$Hf and $^{170-186}$Hf, respectively, and the $K^\pi = 8^-$ series in the $N = 106$ isotonic chain between ^{170}Gd and ^{182}Os. (Here, K and π are the projection of the total nuclear angular momentum on the principal symmetry axis in the body-fixed frame and the parity, respectively.) We apply a Skyrme Hartree–Fock BCS (SHFBCS) approach with the SIII effective interaction [3] to calculate the $K^\pi = 6^+$ and 8^- excitation energies using the numerical algorithm as adapted for description of K-isomers in the regions of heavier actinide and transfermium nuclei [4]. For the $K^\pi = 6^+$ state we consider the two-neutron $(\frac{5}{2}^-, \frac{7}{2}^-)_{\rm n}$ and two-proton $(\frac{5}{2}^+, \frac{7}{2}^+)_{\rm p}$ q.p. configurations while for the $K^\pi = 8^-$ states we take the two-neutron $(\frac{7}{2}^-, \frac{9}{2}^+)_{\rm n}$ and two-proton $(\frac{7}{2}^+, \frac{9}{2}^-)_{\rm p}$ q.p. configurations. As it will be seen below, the obtained series of energy levels compared to experimental data allow us to assess the capability of these configurations to reproduce the systematic behaviour of the considered K-isomer excitations along the corresponding chains of nuclei.

In Section 2 we shortly present the SHFBCS approach used together with some details on the pairing and basis parameters choice and the computational algorithm, as well. The numerical results are presented and discussed in Section 3. In Section 4 we give a summary and concluding remarks.

2 Theoretical Framework

The theoretical approach applied in this work includes a Skyrme HFBCS energy-density functional with cylindrical symmetry (axial deformation) in the intrinsic frame and self-consistent blocking of the single-particle (s.p.) orbitals entering the excited 2q.p. configuration [4]. We employ the SIII Skyrme parametrization with a "minimal" scheme including the spin and current vector time-odd fields only as explained in Ref. [5]. The latter causes a time-reversal symmetry breaking at the one-body level in the excited states leading to a removal of the Kramers degeneracy in the single-particle energy spectrum via the self-consistent blocking.

The HF Hamiltonian is diagonalized and the s.p. spectrum is obtained as an expansion in the axially-symmetric deformed harmonic oscillator (ASDHO) basis [6] truncated at the $N_0+1 = 15$ major oscillator shell. The matrix elements are calculated through quadratures using 30 Gauss–Hermite mesh points in the z and 15 Gauss–Laguerre mesh points in the perpendicular direction. The basis parameters b and q (defined in [6]) are optimized for the considered nuclei. The values obtained for the Hf isotopes and the $N = 106$ isotones are given in Tables 1 and 2, respectively.

Table 1. Optimized ASDHO basis parameters b (fm^{-1}) and q (dimensionless) (see text and Ref. [6] for definitions), experimental R_4-values [7] and longitudinal quadrupole deformation β [8] for several Hf ($Z = 72$) isotopes. See the text for explanations.

A	N	R_4	β	b (fm^{-1})	q
168	96	3.1098(13)	0.2781(11)	0.4820	1.1890
170	98	3.1938(14)	0.2976(52)	0.4820	1.1890
172	100	3.2476(15)	0.314(3)	0.4805	1.1890
174	102	3.268	0.301(6)	0.4789	1.1890
176	104	3.284	0.299(5)	0.4770	1.1890
178	106	3.291	0.2779(18)	0.4755	1.1890
180	108	3.307	0.273190(88)	0.4740	1.1840
182	110	3.295(3)	—	0.4714	1.1890
184	112	3.264(4)	—	0.4690	1.1891
186	114	—	—	0.4690	1.1891

Table 2. The same as in Table 1, but for several $N = 106$ isotones.

Nucl.	Z	R_4	β	b (fm^{-1})	q
170Gd	64	—	—	0.4803	1.1891
172Dy	66	—	—	0.4803	1.1891
174Er	68	—	—	0.4790	1.1891
176Yb	70	3.31	0.3014(26)	0.4772	1.1891
178Hf	72	3.291	0.2779(18)	0.4755	1.1890
180W	74	3.26	0.251(5)	0.4755	1.1401
182Os	76	3.1546(21)	0.2352(26)	0.4755	1.1401

The pairing correlations are taken into account through the expectation values of a seniority residual interaction in the BCS states with a subsequent blocking at each iteration of the s.p. states entering the excited state configuration. The nucleon-number dependence of the corresponding matrix elements is parameterized as in Ref. [5]. The BCS equations are solved for all s.p. states with a smearing factor $f(e_i) = \left[1+\exp\left((e_i-X-\lambda_\tau)/\mu\right)\right]^{-1}$ where e_i is the energy of the s.p. state $|i\rangle$, X is a limiting factor with $X = 6$ MeV, λ_τ is the chemical potential for $\tau = n, p$ (neutrons and protons) and $\mu = 0.2$ MeV is a diffuseness parameter. The neutron and proton pairing constants are taken for all considered nuclei as $G_\mathrm{n} = 16$ MeV and $G_\mathrm{p} = 15$ MeV based on earlier proposed concept of overall adjustment with respect to experimental estimations for the moment of inertia [9] (see also Section IV in Ref. [4]).

The theoretical two-quasiparticle excitation energy is determined as

$$E^*_\mathrm{th}(K^\pi) = E^{2qp}_\mathrm{tot}(K^\pi) - E^\mathrm{GS}_\mathrm{tot}\,, \tag{1}$$

where $E^{2qp}_{\rm tot}(K^\pi)$ is the total HFBCS energy energy of the nucleus, obtained in the solution with blocked isomer configuration orbitals and $E^{\rm GS}_{\rm tot}$ is the total energy in the ground-state solution.

The magnetic dipole moments in the 2q.p. configurations are calculated by taking into account polarization effects according to the approach proposed in Ref. [5].

3 Numerical Results and Discussion

The numerical SHFBCS calculations for the $K^\pi = 6^+$ and 8^- 2q.p. configurations in the isotopic and isotonic chains around ^{178}Hf were performed as explained above. The results are given in Tables 3 and 4. For each nucleus the ob-

Table 3. Theoretical (HFBCS) excitation energies $E^{*n}_{\rm th}$ and $E^{*p}_{\rm th}$ [in MeV] for neutron $K^\pi = 6^+(\frac{5}{2}^-, \frac{7}{2}^-)_{\rm n}$ and proton $6^+(\frac{5}{2}^+, \frac{7}{2}^+)_{\rm p}$ 2-qp configurations, respectively, as well as $8^-(\frac{7}{2}^-, \frac{9}{2}^+)_{\rm n}$ and $8^-(\frac{7}{2}^+, \frac{9}{2}^-)_{\rm p}$ configurations, respectively, compared with the experimental $K^\pi = 6^+$ [2] and 8^- [10] isomeric energies in several Hf ($Z = 72$) isotopes. The magnetic dipole moments $\mu^n_{\rm th}$ and $\mu^p_{\rm th}$ [in the units of nuclear magneton μ_N], calculated in the neutron and proton configurations, respectively, are also given.

A	N	K^π	$E^{*n}_{\rm th}$	$E^{*p}_{\rm th}$	$E^{*}_{\rm exp}$	$\mu^n_{\rm th}$	$\mu^p_{\rm th}$
168	96	6^+	3.409	2.236	—	1.832	5.740
		8^-					
170	98	6^+	3.824	2.306	1.773	0.136	5.652
		8^-	4.667	2.266	—	0.148	7.348
172	100	6^+	2.941	2.341	1.685	0.036	5.670
		8^-	3.723	2.130	2.006	0.062	7.338
174	102	6^+	2.073	2.282	1.549	0.074	5.676
		8^-	2.778	1.914	1.798	0.150	7.335
176	104	6^+	1.064	2.159	1.333	−0.029	5.697
		8^-	1.740	1.600	1.559	0.267	7.343
178	106	6^+	1.919	2.143	1.554	0.108	5.704
		8^-	1.141	1.352	1.147	0.311	7.349
180	108	6^+	3.739	2.190	1.703	0.167	5.697
		8^-	3.017	1.179	1.142	0.378	7.343
182	110	6^+	4.002	2.219	—	−2.051	5.757
		8^-	3.193	1.085	1.173	−1.880	7.378
184	112	6^+	4.042	2.258	—	−2.045	5.825
		8^-	3.214	1.031	1.272	−1.931	7.414
186	114	6^+					
		8^-	3.204	1.071	—	−2.028	7.455

Table 4. Theoretical (HFBCS) excitation energies $E^{*n}_{\rm th}$ and $E^{*p}_{\rm th}$ [in MeV] for neutron $K^\pi = 8^-(\frac{7}{2}^-, \frac{9}{2}^+)_{\rm n}$ and proton $8^-(\frac{7}{2}^+, \frac{9}{2}^-)_{\rm p}$ 2-qp configurations, respectively, compared with the experimental 8^- [2] isomeric energies in several $N = 106$ isotones. The magnetic dipole moments $\mu^n_{\rm th}$ and $\mu^p_{\rm th}$ [in the units of nuclear magneton μ_N], calculated in the neutron and proton configurations, respectively, are also given.

A	N	$E^{*n}_{\rm th}$	$E^{*p}_{\rm th}$	$E^{*}_{\rm exp}$	$\mu^n_{\rm th}$	$\mu^p_{\rm th}$
^{170}Gd	64	1.117	6.748	—	0.331	7.491
^{172}Dy	66	1.060	5.631	1.278	0.356	7.521
^{174}Er	68	1.020	4.331	1.112	0.334	7.571
^{176}Yb	70	1.031	3.015	1.050	0.359	7.422
^{178}Hf	72	1.141	1.352	1.147	0.311	7.349
^{180}W	74	1.308	2.532	1.529	0.256	7.354
^{182}Os	76	1.412	3.434	1.831	0.253	7.391

tained neutron and proton 2q.p. excitation energy $E^{*\tau}_{\rm th}(K^\pi)$ ($\tau = n, p$) is compared with the experimental value for the corresponding K-isomeric state [2,10]. In few cases towards the ends of the considered isotopic and isotonic chains, where no data are available, the theoretical predictions are still given for better understanding the model performance along the corresponding series of states. In the tables we also give theoretical predictions for the magnetic dipole moments calculated for each 2q.p. configuration as explained in Ref. [4] following the prescription in Ref. [5].

The energy levels obtained for the $K^\pi = 6^+$ excitations in the $^{168-184}$Hf isotopic chain are given in Figure 1 in dependence on the neutron number. It should be noted that the considered series of nuclei comprises the overall rotation region in the Hf isotopic chain with the experimental $R_4 = E(4^+_1)/E(2^+_1)$ ratio in the ground-state bands varying between $3.11 - 3.19$ in $^{168-170}$Hf and 3.31 in ^{180}Hf [7] (see Table 1). The corresponding quadrupole deformation parameter β takes values $\beta \approx 0.27 - 0.28$ in ^{168}Hf and ^{180}Hf and $\beta \approx 0.3 - 0.31$ in $^{170-176}$Hf [8] (Table 1). We see in Figure 1 that the energies corresponding to the two-proton $(\frac{5}{2}^+, \frac{7}{2}^+)_{\rm p}$ q.p. configuration (red level-bars) follow the overall behaviour of experimental data for the $K^\pi = 6^+$ isomers overestimating them by between 0.5 and 0.8 MeV (see also Table 3). On the other hand the energy levels from the two-neutron $(\frac{5}{2}^-, \frac{7}{2}^-)_{\rm n}$ q.p. configuration (blue level-bars) only approach the experiment at $^{174-178}$Hf while aside (left and right) of that region they sharply raise above by more that 1–2 MeV. In ^{176}Hf the theoretical value of $E^{*n}_{\rm th}(6^+) = 1.064$ MeV underestimates the experimental value of 1.333 MeV by 269 keV while in ^{174}Hf and ^{178}Hf the theory overestimates the experiment by 524 keV and 365 keV, respectively (see Table 3). Thus, one may consider that the overall systematic behavior of the theoretical 6^+ excitations compared with the experimental data points on the relevance of the proton structure of the 2qp configurations. In the narrow region of ^{174,176,178}Hf the energy proxim-

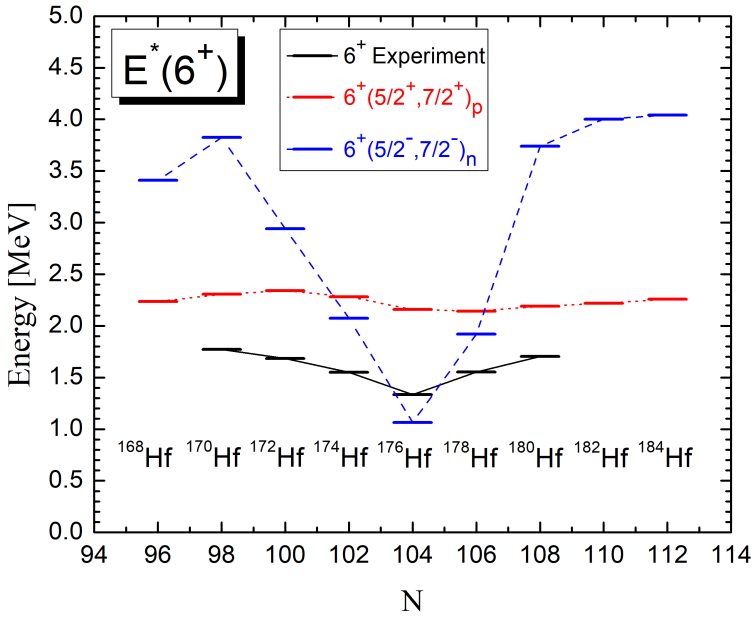

Figure 1. Theoretical $K^\pi = 6^+$ excitation energies from neutron (blue level-bars) and proton (red bars) 2q.p. configurations obtained for the $^{168-184}$Hf isotopic chain compared with experimental data [2]. See the text for details.

ity of the two-neutron $(\frac{5}{2}^-, \frac{7}{2}^-)_{\rm n}$ and two-proton $(\frac{5}{2}^+, \frac{7}{2}^+)_{\rm p}$ q.p. configurations may be interpreted as the result of a possible mixture between them. Aside from that region (of large quadrupole deformations, see Table 1) the two-neutron configuration is definitely off, while the two-proton configuration still follows the experiment from above. The so-obtained descriptions of the $K^\pi = 6^+$ isomer determine a corresponding area of applicability of the axially-symmetric SHF-BCS approximation in the Hf isotopes and allow one to assess the relevance of the above considered neutron and proton 2q.p. configurations.

Further test for the SIII interaction used and the applicability of the model in the Hf isotopic chain is provided by the calculations for the $K^\pi = 8^-$ two-neutron $(\frac{7}{2}^-, \frac{9}{2}^+)_{\rm n}$ and two-proton $(\frac{7}{2}^+, \frac{9}{2}^-)_{\rm p}$ q.p. configurations. The obtained energy levels are given in Figure 2 in dependence on N. Here, similarly to the 6^+ isomer we observe that the energy of the two-proton configuration closely follows the overall behaviour of the experimental $K^\pi = 8^-$ isomer energy, well approaching it at ^{176}Hf and ^{180}Hf with an overestimation of 41 keV and 37 keV, respectively (see also Table 4). At the same time the energy of the two-neutron configuration $(\frac{7}{2}^-, \frac{9}{2}^+)_{\rm n}$ only approaches the experiment at ^{176}Hf and ^{178}Hf. In ^{176}Hf the experiment is overestimated by 181 keV while in ^{178}Hf it is rather well reproduced by 6 keV underestimation. In the other isotopes the theoretical

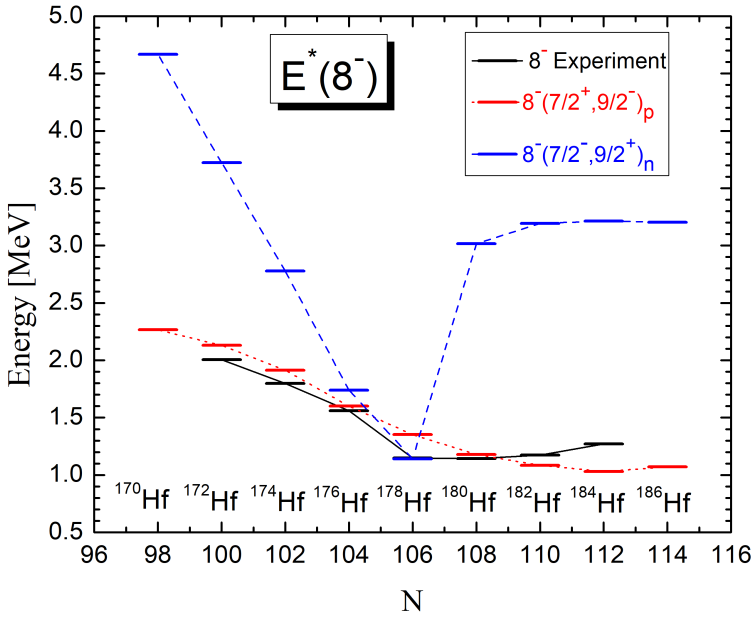

Figure 2. Theoretical $K^\pi = 8^-$ 2q.p. excitation energies from neutron (blue level-bars) and proton (red bars) 2q.p. configurations obtained for the $^{170-186}$Hf isotopic chain compared with experimental data [10].

two-neutron configuration energy is obtained highly above the experiment. The overall good reproduction of the 8^- isomer energy in ^{176}Hf and ^{178}Hf by the two-neutron configuration together with its good description provided by the two-proton configuration suggests a mixture between the two configurations, an effect long known in these nuclei [11]. Totally for both configurations, the best reproduction of the 8^- isomer energy is achieved in ^{176,178,180}Hf which also represent the best rotators in the isotopic chain with $R_4 = 3.28 - 3.31$ (see Table 1). This result outlines a region of the most relevant applicability of the SHFBCS approximation with SIII interaction in the Hf isotopic chain.

In Figure 3 the excitation energies corresponding to the $K^\pi = 8^-$ isomer in the $N = 106$ isotones are given in dependence on the proton number Z. Here we see that the theoretical $E^{*n}_{\rm th}(8^-)$ energy of the two-neutron $(\frac{7}{2}^-, \frac{9}{2}^+)_{\rm n}$ configuration closer follows the experimental 8^- energies compared to the two-proton configuration $(\frac{7}{2}^+, \frac{9}{2}^-)_{\rm p}$ which only in ^{178}Hf approaches the experiment by 204 keV overestimation while otherwise sharply jumps to irrelevantly high values (see also Table 4). The two-neutron configuration provides a rather good agreement with data for ^{176}Yb with 19 keV underestimation and for the above mentioned case of ^{178}Hf with 6 keV underestimation. Aside of these two isotones the disagreement between the theory and experiment varies between 90

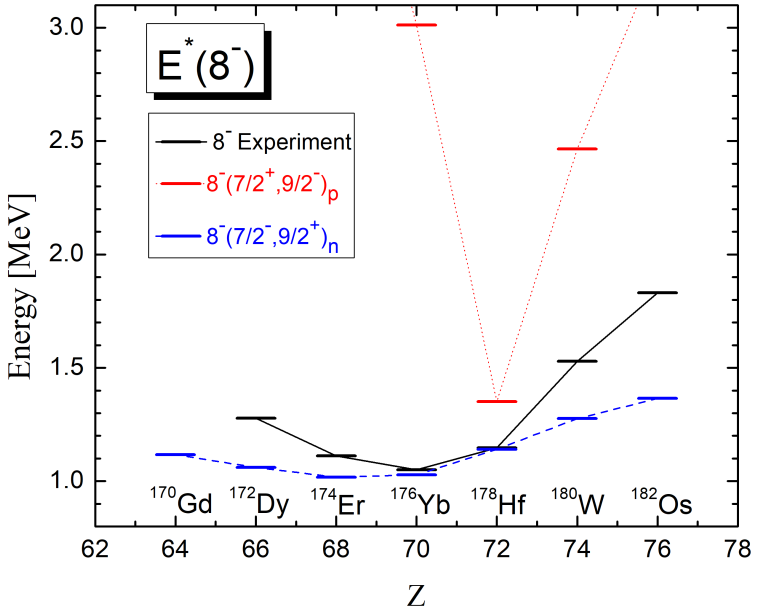

Figure 3. Theoretical $K^\pi = 8^-$ 2q.p. excitation energies from neutron (blue level-bars) and proton (red bars) 2q.p. configurations obtained for the $N = 106$ isotonic chain between ^{170}Gd and ^{182}Os compared with experimental data [10].

and 420 keV underestimation, between ^{172}Dy and ^{182}Os (see Table 4). Now we remark that between ^{176}Yb and ^{182}Os the R_4 ratio takes values between 3.31 and 3.15 (see Table 2), which indicates their presence in the rotation part of the rare earth region. No experimental information on R_4 is available for ^{172}Dy and ^{174}Er, but one may guess that it is close to the rotation values. We may conclude that the present calculations provide reasonably motivated model predictions for the $K^\pi = 8^-$ isomer from ^{172}Dy to ^{180}W which outline the corresponding region of applicability of the present SHFBCS approach with SIII parametrization.

Regarding the magnetic dipole moments given in Tables 3 and 4 we observe a rather stable behavior of the values calculated for the proton 2q.p. configurations with $\mu^p_{\rm th} = 5.7 - 5.8\ \mu_N$ for the $K^\pi = 6^+$ states and $\mu^p_{\rm th} = 7.3 - 7.5\ \mu_N$ for the $K^\pi = 8^-$ states. For the magnetic moment values in the neutron 2q.p. configurations we observe rather small positive values in the $K^\pi = 6^+$ states in $^{170-174,178,180}$Hf with $\mu^n_{\rm th}$ between $0.04\mu_N$ and $0.17\mu_N$ and a small negative value of $\mu^n_{\rm th} = -0.029\mu_N$ in ^{176}Hf. These small absolute values can be ascribed to a strong cancelation of the spin contribution to the magnetic moment content coming from the blocked neutron orbitals, as explained in [4]. This cancellation is less pronounced in the neutron $K^\pi = 8^-$ states of $^{176-180}$Hf and in the considered $N = 106$ isotones (see Table 4) with $\mu^n_{\rm th} = 0.27 - 0.38\ \mu_N$, while a large $\mu^n_{\rm th} = 1.83$ value is obtained for the $K^\pi = 6^+$ state in ^{168}Hf. On the other hand

large negative $\mu^n_{\rm th} = (-1.9) - (-2.1)\ \mu_N$ values are obtained for $K^\pi = 6^+$ and 8^- states in $^{182-186}$Hf. This may be an indication for a change in the contents of the HF s.p. wave function and could be a subject of further detailed examination. In all cases it is clear that the calculated values for the magnetic dipole moments in the considered 2q.p. configurations would strongly constrain the choice of the corresponding neutron or proton configuration whenever relevant experimental information is obtained.

4 Summary and Concluding Remarks

We explored series of $K^\pi = 6^+$ and $K^\pi = 8^-$ isomeric states in the isotopic and isotonic chains of even-even nuclei around ^{178}Hf within the Skyrme (SIII) Hartree–Fock–BCS approach. The calculations made for the corresponding neutron and proton 2q.p. configurations outline the systematic behaviour of the theoretical 6^+ and 8^- excitation energies in the Hf isotopes and 8^- energies in the $N = 106$ isotones and provide a comparison to available experimental data. This result allows us to determine the limits of relevance of the SIII parametrization used as well as of the neutron and proton configurations considered. Thus, we find that in Hf isotopes the two-proton $6^+(\frac{5}{2}^+, \frac{7}{2}^+)_{\rm p}$ configuration closer follows the experiment compared to the two-neutron $6^+(\frac{5}{2}^-, \frac{7}{2}^-)_{\rm n}$ configuration, while the latter approaches it in $^{174-178}$Hf where a mixing between the two configurations seems to be possible. Similarly for the $K^\pi = 8^-$ isomer the two-proton $8^-(\frac{7}{2}^+, \frac{9}{2}^-)_{\rm p}$ energy stays close to the experiment along the considered isotopic chain while the two-neutron $(\frac{7}{2}^-, \frac{9}{2}^+)_{\rm n}$ one only in ^{176}Hf and ^{178}Hf approaches it, confirming the known mixture between the two configurations. In the $N = 106$ isotones the study outlines the region from ^{172}Dy to ^{180}W where the two-neutron $8^-(\frac{7}{2}^-, \frac{9}{2}^+)_{\rm n}$ configuration reasonably well describes the $K^\pi = 8^-$ isomer energy, whereas the two-proton $8^-(\frac{7}{2}^+, \frac{9}{2}^-)_{\rm p}$ configuration remains essentially off. Our predictions for the magnetic dipole moment suggest its stable behaviour in the two-proton configurations and certain sensitivity in the two-neutron excitations to the spin contents of the corresponding s.p. states. The comparison with experimental data where available would provide a clear test for the configurations used. This is a subject of forthcoming work.

Acknowledgments

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