

## ***K*-Isomeric States in Heavy, Well-Deformed Nuclei within a Skyrme–Hartree–Fock–BCS Approach**

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**Abstract.** In this work we report on recent microscopic calculations of *K*-isomeric states of two-quasiparticle character in well-deformed rare-earth nuclei and actinide nuclei. In these calculations we employ a Skyrme energy-density functional together with a seniority residual interaction in the Hartree-Fock-BCS approximation with selfconsistent blocking (SCB). The strength of the seniority interaction is calibrated in a consistent way: as some of us showed in Ref. [1] for rare-earth nuclei, the same strength can be obtained in a fit on moments of inertia of even-even nuclei and in a fit on odd-even mass staggering. The former fitting protocol is used for the actinide nuclei studied here. Once the seniority force was adjusted we calculated properties of various *K*-isomeric states without additional parameters. Overall we have obtained a rather good agreement with available data around <sup>154</sup>Nd and in the <sup>234</sup>U–<sup>236</sup>Pu region. We also found that an octupole deformation lowers the excitation energy of the  $K^\pi = 6^-$  isomer in <sup>234</sup>U.

KEY WORDS: *K*-isomers, selfconsistent mean field, pairing, octupole deformation.

### **1 Introduction**

*K*-isomeric states of well-deformed heavy nuclei are known to yield important information about nuclear dynamics involving at the same time collective and

single-particle degrees of freedom. Studying them offers an opportunity to assess properties of nuclear mean field and residual interaction. From the point of view of collective degrees-of-freedom  $K$  isomers can provide information about the nuclear shapes that can favor appearance of such isomeric states and that determine binding energy and electromagnetic decays from these states.

Several theoretical studies have been devoted to the description of structure properties of  $K$ -isomeric states, especially the role of octupole deformation in the framework of the Deformed Shell Model [2–4] and the configuration-constrained potential-energy surface calculations [5]. More recently two-quasiparticle isomeric states have been studied also in the framework of covariant density functional theory [6]. In addition experimental efforts have increased the  $K$ -isomer database away from stability (see, e.g., Ref. [7]) providing strong challenges to our theoretical models.

In this context the description of such isomeric states appears as a relevant test of microscopic models. Here we want to assess the quality of spectroscopic results from a selfconsistent mean-field approach with pairing in deformed even-even nuclei for two-quasiparticle configurations identified as  $K$ -isomeric states. In particular we study the effects of symmetry breaking at the mean-field level on static properties of  $K$  isomers, namely time-reversal symmetry and intrinsic parity symmetry.

## 2 Theoretical Framework and Computational Details

In this work we use the Hartree–Fock–BCS approximation to the nuclear many-body problem with the Skyrme energy-density functional in the particle-hole channel, and the seniority residual interaction in the pairing channel as thoroughly described in Ref. [8]. Two important aspects of this framework are the selfconsistent symmetries and blocking.

On the one hand we impose axial symmetry as a selfconsistent symmetry, in addition to the third component of total isospin—which makes single-particle states either neutron or proton states. In the rare-earth region we also impose intrinsic parity, in contrast to the study of selected  $K$ -isomeric states in actinides in order to assess the role of octupole shapes.

On the other hand time-reversal symmetry is naturally broken by the nuclear mean field in multi-quasiparticle-like excited states of even-even nuclei. Here we describe two-quasiparticle  $K$  isomers by selfconsistently blocking two nucleons in single-particle states whose angular-momentum projections  $\Omega_1, \Omega_2$  on the intrinsic symmetry axis are such that  $\Omega_1 + \Omega_2 = K$ . By construction their occupation is set to 1 at each Hartree–Fock iteration, which induces time-odd currents and densities in the Skyrme energy-density functional and nuclear mean field which do not commute with the time-reversal operator  $\hat{T}$ . Despite this symmetry breaking it is still possible to define pairs of conjugate states

in BCS because, for a given single-particle state  $|i\rangle$  with angular-momentum projection  $\Omega > 0$ , the Hartree–Fock basis always contains a state  $|\tilde{i}\rangle$  of opposite angular-momentum projection  $-\Omega$  having an overlap with the time-reversed state  $|\tilde{i}\rangle = \hat{T}|i\rangle$  very close to 1 in absolute value. Because the blocked states and their “pairing partners”, in practice close to the Fermi level of the ground state solution, are excluded from the BCS equations, a lower state density occurs around this Fermi level, hence producing a quenching of pairing correlations. It is worth recalling that in the DSM approach used, e.g., in Ref. [2] the excitation energy of a two-quasiparticle isomeric state is given by

$$E_{2qp} = \sqrt{(e_{i_1} - \lambda)^2 + \Delta^2} + \sqrt{(e_{i_2} - \lambda)^2 + \Delta^2} \quad (1)$$

where  $i_1$  and  $i_2$  denote the two involved single-particle states (neutrons or protons) and  $\Delta$  is the pairing gap of the corresponding charge state.

In practice the Hartree–Fock–BCS (HFBCS) equations are solved in an axially-deformed harmonic-oscillator basis characterized by the number of major shells (in the spherical case) noted  $N_0 + 1$  and the oscillator frequencies  $\omega_z$  along the symmetry axis and  $\omega_\perp$  in the perpendicular direction. These parameters are optimized for a given  $N_0$  value in each nucleus. The strength of the seniority interaction is defined as

$$\langle i\tilde{i}|\hat{V}(1 - \hat{P}_{12})|j\tilde{j}\rangle = \frac{G_0^{(q)}}{11 + N_q} \quad q = \text{n or p}, \quad (2)$$

where  $\hat{P}_{12}$  is the two-nucleon exchange operator to antisymmetrize the matrix element. It was recently shown [1] that fitting the values  $G_0^{(q)}$  for neutrons and protons independently on the following two quantities essentially yield the same results in the rare-earth region,  $G_0^{(n)} = 16.20$  MeV and  $G_0^{(p)} = 15.05$  MeV (see also [9])

- moment of inertia deduced from the  $2^+$  excitation energy  $E_{\text{exp}}^*(2_1^+)$  in the ground-state rotational band

$$\frac{\hbar^2}{2\mathcal{I}_{\text{Bel}} \times \alpha} = \frac{1}{6} E_{\text{exp}}^*(2_1^+), \quad (3)$$

where  $\mathcal{I}_{\text{Bel}}$  is the Belyaev moment of inertia and  $\alpha = 1.32$  is a corrective factor for Thouless–Valatin effect. The particular value of  $\alpha$  is taken from the estimate of Ref. [10] deduced from a systematical study within Hartree–Fock–Bogolyubov calculations using the D1S interaction, whose spectroscopic properties are very close to those of the Skyrme SIII interaction used here;

- three-point odd-even binding-energy differences

$$\Delta_3^{(n)} = \frac{(-1)^N}{2} [E(N + 1, Z) + E(N - 1, Z) - 2E(N, Z)], \quad (4)$$

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where  $E(N, Z)$  represents the expectation value of the Hamiltonian of the nucleus (negative binding energy).

The pairing window considered in the seniority residual interaction is made up of all single-particle states up to 6 MeV above the chemical potential, with a smearing Fermi-like function of diffuseness 0.2 MeV (see Ref. [11] for the precise definition).

In the actinide region we have used the moment of inertia as an observable to calibrate pairing strengths  $G_0^{(q)}$ , imposing the same ratio  $G_0^{(p)}/G_0^{(n)} \approx 0.9$  in this preliminary study as in the rare-earth region. For the four considered nuclei, namely  $^{234,236}\text{U}$  and  $^{236,238}\text{Pu}$  we obtained the results collected in Table 1 with  $G_0^{(n)} = 16$  MeV.

Table 1. Values of  $\frac{\hbar^2}{2\mathcal{I}_{\text{Bel}} \times \alpha}$  (in keV) calculated with the approximately optimal  $G_0^{(n)} = 16$  MeV pairing strength in four actinide nuclei compared with the experimental  $2_1^+$  excitation energy divided by 6.

| Nucleus           | $\frac{\hbar^2}{2\mathcal{I}_{\text{Bel}} \times \alpha}$ (keV) | $\frac{1}{6} E_{\text{exp}}^*(2_1^+)$ (keV) |
|-------------------|---|---|
| $^{234}\text{U}$  | 7.41  | 7.25  |
| $^{236}\text{U}$  | 8.16  | 7.53  |
| $^{236}\text{Pu}$ | 7.01  | 7.43  |
| $^{238}\text{Pu}$ | 7.48  | 7.34  |

Seemingly less success in this mass region than in the rare-earth study is encountered but prior to any definite conclusion the constraint on the proton-to-neutron strength ratio has, in a future work, to be released. Moreover the sample of nuclei has to be extended to cure for some possible minor local inaccuracies in the single-particle spectra for the limited number of considered nuclei.

Finally we are interested in some spectroscopic properties of the isomeric states, especially the static magnetic dipole moment  $\mu$ . It is calculated as in Ref. [8] for  $K = I$  bandheads (in  $\mu_N$  unit)

$$\mu = \frac{K}{K+1}(g_R + \langle \hat{\mu}_z \rangle) \quad \text{with } \hat{\mu}_z = g_\ell \hat{L}_z + g_s \hat{S}_z, \quad (5)$$

where  $\hat{L}_z$  and  $\hat{S}_z$  are the projections on the symmetry axis of orbital and spin angular momentum operators, respectively. Note in particular that no empirical attenuation factor for  $g_s$  is employed because selfconsistent blocking effectively quenches  $g_s$ , see, e.g., Ref. [8].

### 3 Numerical Results

The two mass regions considered in this two-quasiparticle  $K$ -isomers study are around  $A \sim 156$  and  $A \sim 236$ .

#### 3.1 $A \sim 156$ mass region

In the  $A \sim 156$  region we focus on the following experimentally known four  $K$ -isomeric states:  $4^-$  in  $^{154}\text{Nd}$ ,  $5^-$  in  $^{156}\text{Nd}$  and in  $^{156}\text{Sm}$ , and  $7^-$  in  $^{156}\text{Gd}$ . In the first nucleus we find a  $\Omega^\pi = 5/2^+$  level and a  $3/2^-$  level lying very close to the neutron Fermi level in the ground-state  $K^\pi = 0^+$  HFBCS solution, as shown in the left panel of Figure 1. In this figure Kramers degeneracy is indicated by the  $\pm$  signs in front of the  $\Omega$  value of the twofold degenerate states. Blocking the  $5/2^+$  and  $3/2^-$  states yields a  $K^\pi = 4^-$  configuration, for which the neutron single-particle spectrum in the HFBCS solution is displayed in the right panel of Figure 1. Kramers degeneracy is now suppressed. The blocked states are marked with full circles, and their conjugate states by open circles. Note that the blocked states lie above the Fermi level of the ground-state solution: time reversal symmetry breaking changes the sequence of states lying close to each other in the  $0^+$  solution, which increases the excitation energy of the  $K$ -isomer as compared to the value estimated in the Koopman's approximation (independent-particle picture).

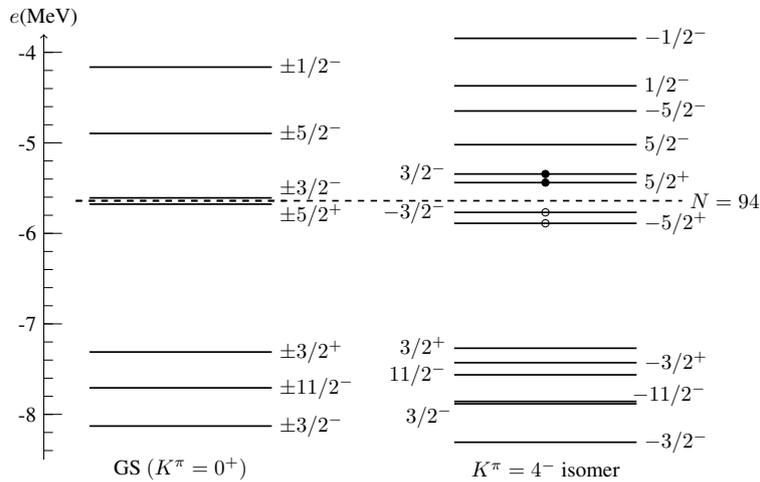


Figure 1. Neutron single-particle level scheme of  $^{154}\text{Nd}$  in the ground state (left panel) and in the  $K^\pi = 4^-$  two-quasiparticle configuration (right panel) of  $^{154}\text{Nd}$ . The solid circles show the blocked states, whereas the open circles correspond to the conjugate states.

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However if one takes pairing into account and calculates the excitation energy  $E^*$  of this isomeric state as the sum of two quasiparticle energies from the ground-state  $K^\pi = 0^+$  solution as in the Deformed Shell Model [3], one obtains a larger value than in the independent-particle picture. In contrast in the above-described HFBCS approach the excitation energy of the isomeric state is calculated directly by subtracting the expectation value of the nuclear Hamiltonian in the  $0^+$  solution from that in the  $4^-$  solution. In this way we account selfconsistently for the pairing quenching and core polarization effects. It is worth noting that the two Hartree–Fock states blocked in the  $4^-$  solution are found to have the same dominant Nilsson numbers ( $5/2^+[642], 3/2^-[521]$ ) as in Ref. [3].

Similarly to  $^{154}\text{Nd}$ , a non-ambiguous two-quasiparticle neutron configuration is found in two other nuclei:  $(\frac{5}{2}^+, \frac{5}{2}^-)$  configuration for the  $K^\pi = 5^-$  isomeric state in  $^{156}\text{Nd}$ , and  $(\frac{11}{2}^-, \frac{3}{2}^+)$  for the  $K^\pi = 7^-$  isomeric state in  $^{156}\text{Gd}$ . In contrast two low-lying candidate configurations are found for the  $K^\pi = 5^-$  isomeric state in  $^{156}\text{Sm}$ : a two-neutron  $(\frac{5}{2}^+, \frac{5}{2}^-)$  configuration and a two-proton  $(\frac{5}{2}^+, \frac{5}{2}^-)$  configuration.

In Table 2 calculated quadrupole deformation parameter  $\beta_2$  and excitation energies of  $K$ -isomeric states in the four studied rare-earth nuclei are displayed together with experimental excitation energies taken from Ref. [7].

A good agreement is obtained for the HFBCS solution with SCB in the Nd and Sm isotopes, with less than 150 keV difference with the experimental value.

Table 2. Calculated quadrupole deformation parameter  $\beta_2$  and excitation energies (in MeV) in the four studied  $K$ -isomeric states in the rare-earth region. The values of  $E_{2qp}$  are obtained using Eq. (1) from the HFBCS solution of the  $K^\pi = 0^+$  ground state, whereas  $E_{SCB}^*$  is obtained from the HFBCS solution for the actual  $K^\pi$  configuration with selfconsistent blocking. The total angular momentum projection quantum number on the symmetry axis,  $\Omega$ , and intrinsic parity  $\pi$  of each blocked single-particle state is indicated in parenthesis, together with the charge state  $q = n$  for neutron or  $p$  for proton.

| Nucleus           | $K^\pi$ | Configuration<br>$q(\Omega_1^{\pi_1}, \Omega_2^{\pi_2})$ | $\beta_2$ | $E_{2qp}$ | $E_{SCB}^*$ | $E_{\text{exp}}^*$ [7] |
|-------------------|---------|--|-----------|-----------|-------------|------------------------|
| $^{154}\text{Nd}$ | $4^-$   | $n(\frac{5}{2}^+, \frac{3}{2}^-)$                        | 0.32      | 1.681     | 1.165       | 1.298                  |
| $^{156}\text{Nd}$ | $5^-$   | $n(\frac{5}{2}^+, \frac{5}{2}^-)$                        | 0.32      | 1.955     | 1.447       | 1.431                  |
| $^{156}\text{Sm}$ | $5^-$   | $n(\frac{5}{2}^+, \frac{5}{2}^-)$                        | 0.31      | 1.929     | 1.659       | 1.398                  |
|                   |         | $p(\frac{5}{2}^+, \frac{5}{2}^-)$                        | 0.32      | 1.988     | 1.233       |                        |
| $^{156}\text{Gd}$ | $7^-$   | $n(\frac{11}{2}^-, \frac{3}{2}^+)$                       | 0.31      | 2.642     | 3.115       | 2.138                  |

In these cases the two-quasiparticle energy expression (1) overestimates the excitation energy. Similarly good results for  $^{154,156}\text{Nd}$  and  $^{156}\text{Sm}$  isotopes were obtained by Gautherin and collaborators [12] within the Hartree–Fock–Bogolyubov approach with the D1S Gogny effective interaction. Interestingly they report a proton  $5^-$  configuration close to the experimental isomeric state in  $^{156}\text{Sm}$  but no neutron  $5^-$  configuration, whereas a neutron  $5^-$  configuration and a proton  $5^-$  configuration are reported in  $^{158}\text{Sm}$  (both close to the experimental isomeric state, at about 1.5 MeV). In this nucleus our proton configuration lies closer to the experimental state than our neutron configuration. Of course the validity of such a bold conclusion is contingent upon the assumption of the absence of any significant coupling between those two states, which is to be confirmed or not.

In contrast a large discrepancy between our calculated excitation energy and experiment (of the order of 1 MeV) is found for the  $K^\pi = 7^-$  state in  $^{156}\text{Gd}$ . To understand the origin of this discrepancy it is useful to consider the corresponding neutron single-particle spectrum in Figure 2.

One observes that both the  $11/2^-$  and  $3/2^+$  states lie below the Fermi level of the ground state (left panel of Figure 2), and are rather far from it (approximately 1.5 and 0.6 MeV, respectively). This yields this  $7^-$  configuration at a particularly high excitation energy comparable to that of a four-quasiparticle configuration with respect to the  $K^\pi = 0^+$  configuration. This argument is consistent with the fact that in the other three studied isomeric states, for which good agreement is found with comparatively much smaller calculated excitation energies, the two blocked states are of hole and particle characters (providing the isomeric state with a two-quasiparticle nature with respect to the  $0^+$  configuration). This is exemplified in Figure 1 for the  $4^-$  isomer in  $^{154}\text{Nd}$ .

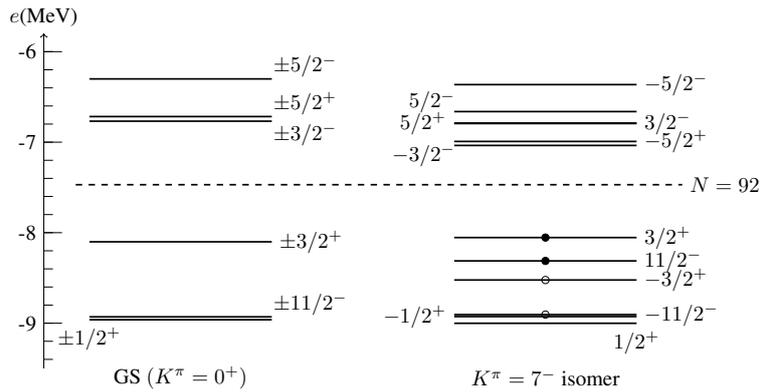


Figure 2. Neutron single-particle level scheme of  $^{156}\text{Gd}$  in the ground state (left panel) and in the  $K^\pi = 7^-$  two-quasiparticle configuration (right panel) of  $^{156}\text{Gd}$ . The solid circles show the blocked states, whereas the open circles correspond to the conjugate states.

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Table 3. Calculated magnetic dipole moments  $\mu$  together with their single-particle contribution  $\langle \hat{\mu}_z \rangle$  and the calculated collective gyromagnetic ratio  $g_R$

| Nucleus           | $K^\pi$ | Configuration<br>$q(\Omega_1^{\pi_1}, \Omega_2^{\pi_2})$ | $\langle \hat{\mu}_z \rangle$ | $g_R$ | $\mu$  |
|-------------------|---------|--|-------------------------------|-------|--------|
| $^{154}\text{Nd}$ | $4^-$   | $n(\frac{5}{2}^+, \frac{3}{2}^-)$                        | −1.962                        | 0.476 | −1.189 |
| $^{156}\text{Nd}$ | $5^-$   | $n(\frac{5}{2}^+, \frac{5}{2}^-)$                        | −0.117                        | 0.475 | 0.298  |
| $^{156}\text{Sm}$ | $5^-$   | $n(\frac{5}{2}^+, \frac{5}{2}^-)$                        | −0.097                        | 0.358 | 0.217  |
|                   |         | $p(\frac{5}{2}^+, \frac{5}{2}^-)$                        | 4.925                         |       | 4.402  |
| $^{156}\text{Gd}$ | $7^-$   | $n(\frac{11}{2}^-, \frac{3}{2}^+)$                       | −2.189                        | 0.269 | −1.680 |

Finally we show in Table 3 the calculated magnetic dipole moments  $\mu$  together with their single-particle contribution  $\langle \hat{\mu}_z \rangle$  and the collective gyromagnetic ratio  $g_R$  calculated as in Ref. [13].

The latter are found to significantly differ from the  $Z/A \approx 0.39$  estimate. It is worth mentioning that in Ref. [14] a value of  $\mu$  of  $-1.6 \mu_N$  in the  $4^-$  isomer of  $^{154}\text{Nd}$  was obtained within the quasiparticle-rotor model. This is of the same order of magnitude as our calculated value  $-1.2 \mu_N$ . Moreover the two candidate  $K^\pi = 5^-$  configurations that we find in  $^{156}\text{Sm}$  could be discriminated, or their mixing assessed, if their magnetic dipole moment could be measured as we predict a quite small value for the neutron configuration in contrast with the large value found for the proton configuration.

### 3.2 $A \sim 236$ mass region

In the actinide region we focus on four isomeric states whose considered configurations are given in Table 4.

Using the seniority strengths calibrated as explained in section 2 and assuming first intrinsic parity selfconsistent symmetry, we obtain the results displayed in Table 5.

Table 4. *K*-isomeric states studied in the actinide region and their considered configurations.

| Nucleus          | $K^\pi$ | Configuration<br>$q(\Omega_1^{\pi_1}, \Omega_2^{\pi_2})$ | Nucleus           | $K^\pi$ | Configuration<br>$q(\Omega_1^{\pi_1}, \Omega_2^{\pi_2})$ |
|------------------|---------|--|-------------------|---------|--|
| $^{234}\text{U}$ | $6^-$   | $n(\frac{7}{2}^-, \frac{5}{2}^+)$                        | $^{236}\text{Pu}$ | $5^-$   | $p(\frac{5}{2}^-, \frac{5}{2}^+)$                        |
| $^{236}\text{U}$ | $4^-$   | $n(\frac{7}{2}^-, \frac{1}{2}^+)$                        | $^{238}\text{Pu}$ | $4^-$   | $n(\frac{7}{2}^-, \frac{1}{2}^+)$                        |
|                  |         | $\pi(\frac{5}{2}^-, \frac{3}{2}^+)$                      |                   |         |  |

Table 5. Calculated quadrupole deformation, excitation energy (in MeV) and magnetic dipole moment of the isomeric states listed in Table 4. Experimental excitation energies  $E_{\text{exp}}^*$  (in MeV) are taken from Ref. [7].

| Nucleus           | $K^\pi$ | $\beta_2$ | $E_{\text{SCB}}^*$ | $E_{\text{exp}}^*$ | $\langle \hat{\mu}_z \rangle$ | $g_R$ | $\mu$ |
|-------------------|---------|-----------|--------------------|--------------------|-------------------------------|-------|-------|
| $^{234}\text{U}$  | $6^-$   | 0.25      | 1.595              | 1.421              | -0.190                        | 0.303 | 0.097 |
| $^{236}\text{U}$  | $4_n^-$ | 0.25      | 1.067              | 1.052              | -0.239                        | 0.322 | 0.066 |
|                   | $4_p^-$ | 0.25      | 1.457              |                    | 3.528                         |       |       |
| $^{236}\text{Pu}$ | $5^-$   | 0.26      | 1.236              | 1.185              | 4.899                         | 0.365 | 4.387 |
| $^{238}\text{Pu}$ | $4^-$   | 0.26      | 1.071              | -                  | -0.216                        | 0.379 | 0.130 |

As a typical example Figure 3 shows the neutron single-particle spectrum near the Fermi level in the ground state  $K^\pi = 0^+$  and isomeric state  $K^\pi = 6^-$  HFBCS solutions.

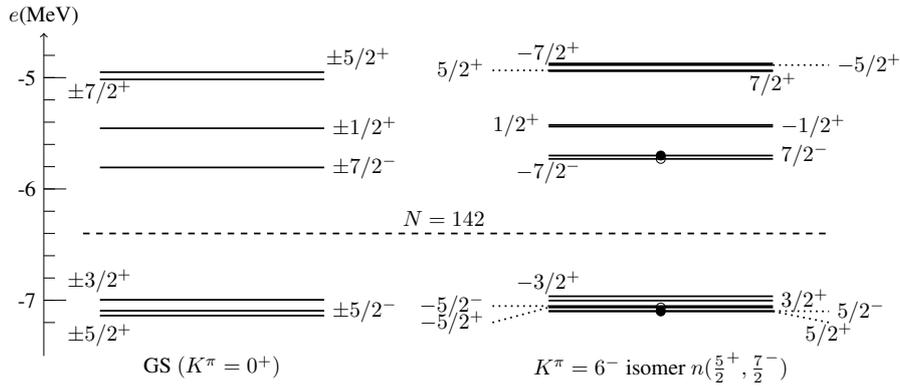


Figure 3. Neutron single-particle level in the ground-state  $K^\pi = 0^+$  and isomeric-state  $K^\pi = 6^-$  HFBCS solutions for  $^{234}\text{U}$  with imposed intrinsic parity symmetry.

Finally we study the role of octupole deformation in  $K$ -isomerism states by performing an unconstrained parity-breaking HFBCS calculation with selfconsistent blocking starting from an octupole-deformed Woods–Saxon potential. In this case the blocked states are only characterized by their total angular-momentum projection on the symmetry axis,  $\Omega$ . In this preliminary study we focus on the  $K^\pi = 6^-$  isomeric state of  $^{234}\text{U}$  in which the Deformed Shell Model predicts the parity-breaking effect to be the largest among many considered actinide nuclei [4]. At the end of the Hartree–Fock iterative process our converged solution is indeed found to have a finite expectation value of the (axial) octupole moment, corresponding to  $\beta_3 = 0.05$  calculated as  $\beta_\ell = \frac{4\pi}{3} \frac{\langle r^\ell Y_\ell^0 \rangle}{r_0^\ell A^{1+\ell/3}}$ , where  $\langle r^\ell Y_\ell^0 \rangle$  is the expectation value of  $r^\ell$  times the spherical hamonics  $Y_\ell^0$  in the

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Table 6. Calculated properties of the  $K = 6$  isomeric state in  $^{234}\text{U}$  with intrinsic-parity breaking compared to those with selfconsistent parity symmetry: axial quadrupole and octupole deformation parameters  $\beta_2$  and  $\beta_3$ , expectation value of the parity operator in the blocked single-particle states  $\langle \hat{\pi} \rangle$ , excitation energy  $E_{\text{SCB}}^*$  (in MeV) and magnetic dipole moment (in nuclear magneton unit). The experimental excitation energy  $E_{\text{exp}}^*$  (in MeV) is taken from Ref. [7].

| $K^\pi$ | $\beta_2$ | $\beta_3$ | Single-particle $\langle \hat{\pi} \rangle$  | $E_{\text{SCB}}^*$ | $E_{\text{exp}}^*$ | $\mu$  |
|---------|-----------|-----------|--|--------------------|--------------------|--------|
| $0^+$   | 0.25      | 0.00      | —  | 0                  | 0                  | 0      |
| $6^-$   | 0.25      | 0.05      | $\langle \hat{\pi} \rangle(\frac{5}{2}) = +0.086$<br>$\langle \hat{\pi} \rangle(\frac{7}{2}) = -0.775$ | 1.481              | 1.421              | -0.081 |
|         | 0.25      | set to 0  | —  | 1.595              |                    | 0.097  |

HFBCS solution, with  $\ell = 3$ , using  $r_0 = 1.2$  fm.

In Table 6 we report several calculated properties of the isomeric  $K = 6$  HFBCS solution with selfconsistent blocking: axial quadrupole and octupole deformation parameters  $\beta_2$  and  $\beta_3$ , expectation value of the parity operator in the blocked single-particle states  $\langle \hat{\pi} \rangle$ , excitation energy  $E_{\text{SCB}}^*$  and magnetic dipole moment. They are compared to the same properties obtained with selfconsistent parity symmetry, and to experimental excitation energy. The effect of octupole degrees of freedom is to lower the isomeric state by 100 keV, bring it in very good agreement with experiment, and to flip the sign of magnetic moment. The latter effect might be tested in an experimental measurement of magnetic moment sensitive to its sign despite a rather small absolute value.

## 4 Conclusions and Perspectives

Overall the Hartree–Fock–BCS calculations with selfconsistent blocking of two nucleon single-particle states, performed with the Skyrme energy-density functional in the particle-hole channel and the seniority residual interaction in the particle-particle channel, allow for a rather good reproduction of excitation energies of  $K$ -isomers around  $A \sim 156$  and  $A \sim 236$ . This success confirms the good spectroscopic properties of the employed Skyrme parametrization SIII and the relevance of our pairing strength adjusted to ground-state properties. Moreover selfconsistent blocking yields a sizable effect on isomer excitation energies, as compared to the Koopmans approximation or the independent quasi-particle picture. Finally a static octupole deformation is found from intrinsic-parity breaking calculations in the  $K = 6$  isomer in  $^{234}\text{U}$  as predicted from the Deformed Shell Model in Ref. [4].

Despite this fair success at the Hartree–Fock–BCS level, it remains to investigate the role of particle-number symmetry restoration. Indeed the BCS approximation is expected to overestimate pairing quenching in low-pairing regimes, such

as multi-quasiparticle  $K$ -isomeric states. This can be done for example in the particle-number conserving Highly-Truncated Diagonalization approach which amounts to a shell-model like calculation in the  $m$  scheme in which the many-body basis is built from multi-particle–multi-hole excitations on a selfconsistent mean-field solution (see, e.g., Refs. [11, 15, 16]). Moreover, at the HFBCS level, we have to extend the search for possible static octupole deformation in two-quasiparticle  $K$ -isomers around  $^{154}\text{Nd}$ ,  $^{254}\text{No}$  and  $^{270}\text{Ds}$  where the Deformed Shell Model predicts some effects. Finally the present approach can be in principle straightforwardly applied to  $K$ -isomers in odd-mass and odd-odd nuclei, planned to be addressed in a near future.

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