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Deformations and Magnetic Moments in High-*K* Isomeric States of Heavy and Superheavy Nuclei

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Abstract. The effect of quadrupole-octupole deformations on the energy and magnetic properties of high-K isomeric states in even-even heavy and superheavy nuclei is studied within a deformed shell model (DSM) with BCS pairing interaction. The neutron two-quasiparticle (2qp) isomeric energies and magnetic dipole moments are calculated over a wide range of quadrupole and octupole deformations. It is found that in most of the considered nuclei the magnetic moments exhibit a pronounced sensitivity to the octupole deformation. At the same time in many cases the behaviour of the 2qp energies shows minima which suggest that the presence of high-K isomeric states may be associated with the presence of octupole softness or even with octupole deformation. In the present work the influence of the BCS pairing strength on the energy of the blocked isomer configuration is examined. The analysis of the 2qp energy minima obtained in the space of quadrupole-octupole deformations for different pairing strengths shows that the formation of high-K isomeric states is a subtle effect depending on both, deformations and nuclear pairing correlations.

1 Introduction

It is well known that the basic properties of atomic nuclei are determined by the nuclear shell structure [1]. In most nuclei this structure leads to the appearance of different kinds of shape deformation. Although the quadrupole (ellipsoidal) shapes are mostly observed, many experimental data on nuclear spectra also suggest the presence of more complicated quadrupole-octupole (reflection-asymmetric) shapes [2]. The latter cause the manifestation of collective phenomena such as alternating-parity bands in even-even nuclei and quasi parity-doublet spectra in odd-mass nuclei with the observation of enhanced E1 and E3 transitions between levels with opposite parity. Also, the collective deformation modifies the intrinsic mean nucleonic field and causes strong non-linear changes in the nuclear shell structure and the attendant single-particle (s.p.) phenomena away from the zero deformation case. A phenomenon deeply originating from the shell structure is the appearance of nuclear high-K isomeric states [3].

Similarly to the origin of the reflection-asymmetric deformations, the interplay of specific s.p. orbitals near the Fermi level may lead to the formation of two- or multi- quasiparticle excites states with a large value of the angular momentum projection K on the principal symmetry axis. Due to the large amount of momentum transfer, ΔK, needed for a transition to a neighbouring lower-energy state, the decay of such a state may be strongly suppressed due to a K forbiddenness rule and thus an isomeric state is formed. In some cases the half-life of such a state can be longer than the half-life of the nucleus in the ground state. Presently a variety of high K isomeric states are known in different mass regions [4]. As far as both the phenomena, deformation and isomerism, have common shell roots it is clear that the formation of high-K isomeric states should be tightly correlated with nuclear deformation properties. Recently it was shown within a deformed shell model (DSM) with BCS-pairing interaction, that some isomer excitation energies and especially the magnetic dipole moments of heavy even-even nuclei exhibit pronounced sensitivity to the octupole deformation [5, 6]. In particular, minima in the neutron two-quasiparticle (2qp) energy surfaces were indicated at non-zero octupole deformation. The study was implemented for 2qp states in the regions of heavy actinide (U, Pu and Cm) and rare-earth (Nd, Sm and Gd) nuclei. Similar influence of the octupole deformation on the isomeric energies was found through configuration-constrained potential energy surface (PES) calculations applied in the same region of actinide nuclei [7]. A recent more systematic study involving heavier Fm and No isotopes and the superheavy nucleus ^{270}Ds showed that three different groups of nuclei can be outlined: with pronounced, shallow and missing minima in the 2qp energy surfaces with respect to the octupole deformation [8]. As a result, regions of nuclei with possible octupole softness as well as possible octupole deformation in the high-K isomeric states were indicated. This finding shows the need of further more detailed analysis of the mechanism which causes the appearance of 2qp energy minima as well as the factors which determine their evolution in deformation space.

In this article first we illustrate the evolution of the 2qp energy minima for high K-isomeric states of heavy even-even nuclei calculated within the DSM+BCS approach without blocking the excited 2qp configuration in the BCS procedure. Further we show the result of calculations performed in ^{254}No and ^{270}Ds by blocking the two excited orbitals and by varying the BCS pairing strength. As will be seen below, this allows us to assess the roles of the blocking effect and the pairing strength in the appearance of 2qp energy minima in the quadrupole-octupole deformation space. Consequently we are able to estimate the predictive value of the theoretical results which suggest different regions of deformation with possible formation of high K-isomeric states.

The paper is organized as follows. In Section 2 the DSM+BCS calculation is briefly explained. In Section 3 numerical results for 2qp energies with and without blocking are given. In Section 4 the results are summarized.

2 Deformed Shell Model with Pairing Interaction

We apply a deformed shell model (DSM) with a Woods-Saxon potential allowing axial quadrupole and octupole deformations [9]. The DSM Hamiltonian is

$$H_{\text{sp}} = T + V_{\text{ws}} + V_{\text{s.o.}} + V_{\text{c}}, \tag{1}$$

where

$$V_{\text{ws}}(\mathbf{r}, \hat{\beta}) = V_0 \left[1 + \exp\left(\frac{\text{dist}_\Sigma(\mathbf{r}, \hat{\beta})}{a} \right) \right]^{-1} \tag{2}$$

is the Woods-Saxon potential with $\hat{\beta} \equiv (\beta_2, \beta_3, \beta_4, \beta_5, \beta_6)$. The quantity $\text{dist}_\Sigma(\mathbf{r}, \hat{\beta})$ is the distance between the point $\mathbf{r}$ and the nuclear surface represented by

$$R(\theta, \hat{\beta}) = c(\hat{\beta}) R_0 \left[1 + \sum_{\lambda=2,3,\ldots} \beta_\lambda Y_{\lambda 0}(\cos\theta) \right], \tag{3}$$

where $c(\hat{\beta})$ is a scaling factor to keep the volume fixed. $V_{\text{s.o.}}$ and V_{c} are the spin-orbit and Coulomb terms whose analytic form is given in [9].

The Hamiltonian (1) is diagonalized in the axially symmetric deformed harmonic oscillator basis $|N n_z \Lambda \Omega\rangle$, and the s.p. wave function is obtained in the form

$$\mathcal{F}_\Omega = \sum_{N n_z \Lambda} C^\Omega_{N n_z \Lambda} |N n_z \Lambda \Omega\rangle. \tag{4}$$

In the case of non-zero octupole deformation the wave function (4) appears with mixed s.p. parity given by

$$\begin{aligned} \langle \hat{\pi}_{\text{sp}} \rangle &= \langle \mathcal{F}_\Omega | \hat{\pi}_{\text{sp}} | \mathcal{F}_\Omega \rangle \\ &= \sum_{N n_z \Lambda} (-1)^N |C^\Omega_{N n_z \Lambda}|^2. \end{aligned} \tag{5}$$

Hereafter we imply that in the physically meaningful cases the average parity remains close to one of the good values $+1$ or -1.

The pairing effect is taken into account through a BCS procedure with constant pairing interaction applied to the DSM s.p. levels. The pairing constants $G_{n/p}$ for neutrons(n)/protons(p) are taken as [10] (see page 311):

$$G_{n/p} = \left(g_0 \mp g_1 \frac{N-Z}{A} \right) / A. \tag{6}$$

The parameters g_0 and g_1 are originally taken in [10] as $g_0 = 19.2$ MeV and $g_1 = 7.4$ MeV. The BCS equation for the pairing gap Δ and the chemical potential λ is solved within energy windows including $(15\,N)^{1/2}$ orbitals for neutrons and $(15\,Z)^{1/2}$ orbitals for protons below and above the Fermi surface. As a starting point in the numerical solution of the gap equation, the phenomenological value $\Delta = 12 \cdot A^{-1/2}$ is used for the pairing gap, and the average value between the energies of the last occupied orbital and the first unoccupied orbital is used for the chemical potential λ.

In the DSM+BCS calculations performed in [5, 6, 8] without blocking the excited orbitals the parameter g_0 was slightly decreased to $g_0 = 17.8$ MeV, to provide for the different deformations overall gap values comparable with the experimentally estimated gaps in the considered nuclei. For tuning the pairing constants one should also mind the above mentioned empirical behaviour of the pairing gap $\Delta = 12 \cdot A^{-1/2}$. In sec. 3 we shall see that if in the same calculations the blocking is taken into account, in contrast, one may need to consider larger g_0-values, even larger than 20 MeV.

The energy of a 2qp configuration with a broken pair is taken as $E_{2qp}^{K\pi} = E_{1qp}^{\Omega_1\pi_1} + E_{1qp}^{\Omega_2\pi_2}$, with

$$E_{1qp}^{\Omega\pi} = \sqrt{(E_{sp}^{\Omega\pi} - \lambda)^2 + \Delta^2} \tag{7}$$

being the one-quasiparticle energy. The K-value is determined as $K = \Omega_1 + \Omega_2$, while the parity of the configuration is $\pi = \pi_1 \cdot \pi_2$. More precisely, in the case of non-zero octupole deformation one has $\pi = \mathrm{sign}\langle\pi_1\rangle \cdot \mathrm{sign}\langle\pi_2\rangle$.

The magnetic moment of the 2qp configuration is determined as [11]

$$\mu = \mu_N \left[g_R \frac{I(I+1) - K^2}{I+1} + g_K \frac{K^2}{I+1} \right], \tag{8}$$

with $\mu_N = e\hbar/(2mc)$, $g_R = Z/A$ and

$$g_K = \frac{1}{K} \sum_{n=1,2} \langle \mathcal{F}_{\Omega_n} | g_s \cdot \Sigma + g_l \cdot \Lambda | \mathcal{F}_{\Omega_n} \rangle, \tag{9}$$

where $\Sigma = \Omega \mp \Lambda$ is the intrinsic spin projection, and g_l and g_s are the standard gyromagnetic ratios. The proton and neutron g_s values are attenuated by a commonly used factor of 0.6 compared to the free values.

3 Numerical Results and Discussion

By using the DSM+BCS approach of the previous section, the energies and magnetic moments of 2qp high-K isomeric states in several groups of heavy even-even nuclei were calculated over a net of quadrupole (β_2) and octupole (β_3) deformation parameters. For each isomeric state/nucleus the calculation provides a 2qp-energy surface in the (β_2, β_3) deformation space and a two-dimensional pattern for the magnetic dipole moment in the isomeric state as a function of β_2 and β_3.

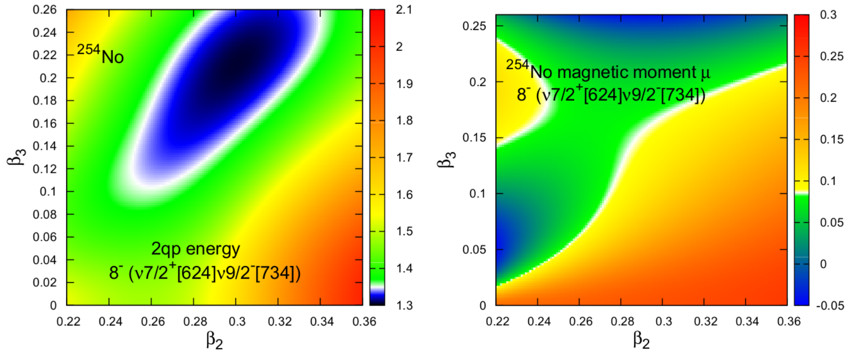

Figure 1. Two-quasiparticle energy and magnetic moment of the $K^{\pi} = 8^{-}\{\nu 7/2[624] \otimes \nu 9/2[734]\}$ configuration in ^{254}No calculated within DSM+BCS without blocking as a functions of β_2 and β_3.

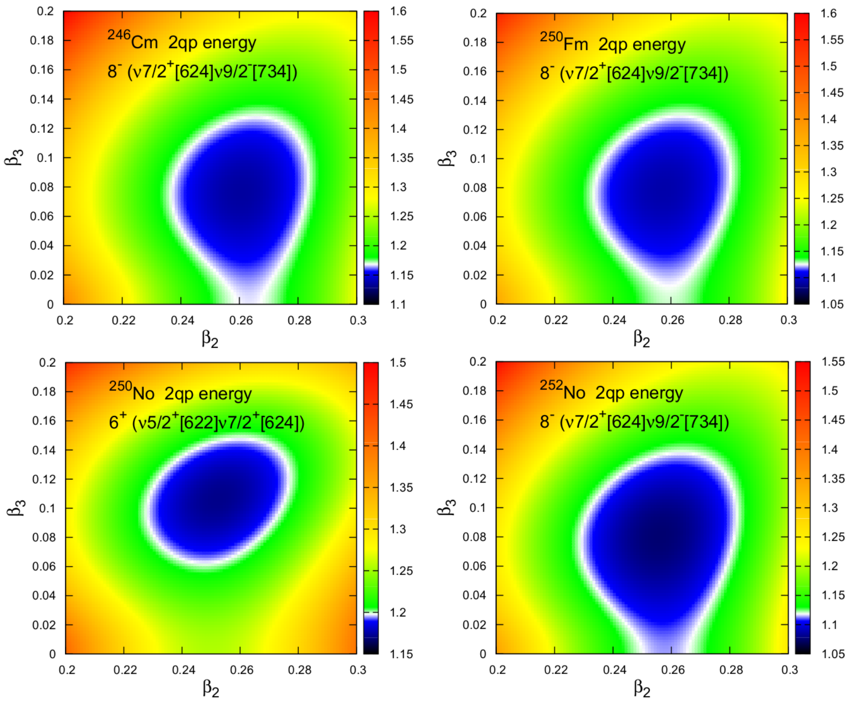

Figure 2. Two-quasiparticle energies for $K^{\pi} = 8^{-}$ isomeric states in ^{246}Cm, ^{250}Fm and ^{252}No and the $K^{\pi} = 6^{+}$ isomer in ^{250}No calculated within DSM+BCS without blocking as functions of β_2 and β_3.

Here, first we illustrate results of calculations in which the orbitals from which the isomeric state is formed are not blocked in the BCS procedure. In Figure 1 the result for the $K^\pi = 8^-$ isomeric state based on the neutron (ν) $\{\nu 7/2[624] \otimes \nu 9/2[734]\}$ configuration in ^{254}No is given as one of the best examples for the influence of the octupole deformation. The 2qp energy surface in Figure 1 (left) shows the presence of a considerably deep minimum, about 0.32 MeV, at non-zero octupole deformation ($\beta_2 = 0.302, \beta_3 = 0.212$). The obtaining of such a minimum suggests the possibility for stable octupole deformation in this state. In a similar way the presence of a 0.42 MeV minimum was obtained for the $K^\pi = 6^-\{\nu 5/2[633] \otimes \nu 7/2[743]\}$ isomer in ^{234}U [8]. We remark that the configuration-constrained potential energy surface (PES) calculations reported for the same isomeric state in Ref. [7] show the presence of a minimum at non-zero octupole deformation, $(\beta_2, \beta_3) \approx (0.22, 0.03)$. These results emphasize the need of a detailed comparative examination of the quadrupole-octupole deformation effects in the high-K isomeric states through different model approaches.

The plot in Figure 1 (right) shows that the magnetic moment in the $K^\pi = 8^-$ isomer of ^{254}No essentially changes in the direction of non-zero octupole deformation, whereas its value at $\beta_3 = 0$ shows a very weak dependence on the quadrupole deformation. The appearance of the 2qp energy minimum in Figure 1 (left) as well as the behaviour of the magnetic moment in Figure 1 (right) can be explained in relation to the crossing of the neutron $7/2[624]$ and $9/2[734]$ orbitals at some non-zero octupole deformation similarly to the case of $K^\pi = 8^-$ isomer in ^{244}Pu (see Figure 1 in [5]).

In Figure 2 we illustrate the calculated 2qp energy surfaces in the (β_2, β_3) space for the $K^\pi = 8^-$ isomeric states in ^{246}Cm, ^{250}Fm and ^{252}No based on the same $\{\nu 7/2[624] \otimes \nu 9/2[734]\}$ configuration as in ^{254}No, and the $K^\pi = 6^+$ isomer in ^{250}No based on the $\{\nu 5/2[622] \otimes \nu 7/2[624]\}$ configuration. The 2qp energy surfaces in Figure 2 correspond to the presence of shallow minima at non-zero octupole deformations, with the depth of the minima being between 40 and 80 keV (see Table 1 in [8]). The obtained result gives an indication of possible softness of the nucleus against octupole deformation in these states.

An appropriate example for the effect of the octupole deformation in the forming of high-K isomeric states in superheavy nuclei is the case of the nucleus ^{270}Ds. For this nucleus two possible isomeric configurations, $K^\pi = 9^-\{\nu 7/2[613] \otimes \nu 11/2[725]\}$ and $K^\pi = 10^-\{\nu 9/2[615] \otimes \nu 11/2[725]\}$, are proposed [13]. We have examined both of them and the result for the 2qp energy surfaces in the quadrupole-octupole space is given in Figure 3. We see that in both cases, $K^\pi = 9^-$ and $K^\pi = 10^-$, the DSM+BCS calculations predict non-zero octupole deformation in the 2qp energy minimum. Especially for the $K^\pi = 9^-$ configuration the depth of the minimum (~ 0.14 MeV) is considerable. This example shows that the quadrupole-octupole shape effects may also be of essential importance in determining the isomeric properties of the superheavy nuclei.

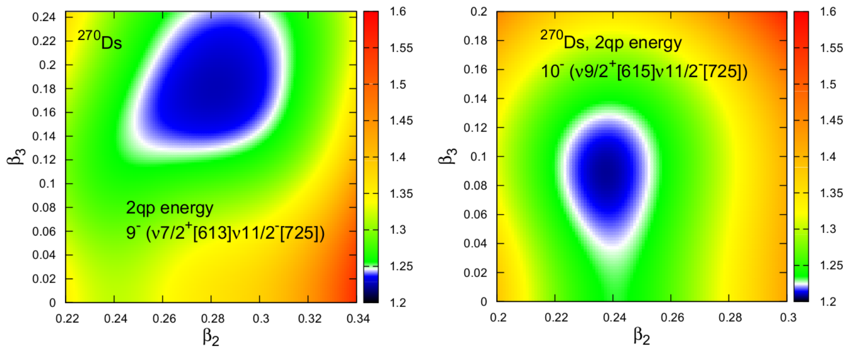

Figure 3. Two-quasiparticle energies for possible $K^\pi = 9^-$ and $K^\pi = 10^-$ isomeric states in ^{270}Ds calculated within DSM+BCS without blocking as functions of β_2 and β_3.

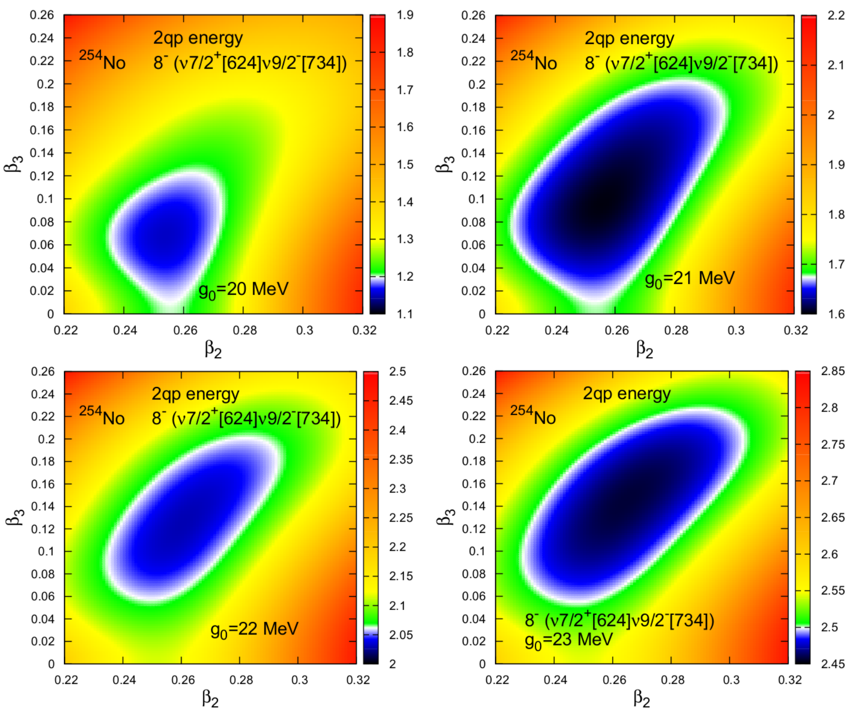

Figure 4. Two-quasiparticle energy of the $K^\pi = 8^-\{\nu 7/2[624] \otimes \nu 9/2[734]\}$ configuration in ^{254}No as a function of β_2 and β_3 calculated by DSM+BCS with blocking for different values of the pairing parameter g_0.

Now, let us consider the case of DSM+BCS calculations in which the two orbitals providing the high-K isomeric state are blocked in the solution of the BCS gap equation. Hereafter some preliminary results are discussed. Initially the calculation was applied to the $K^\pi = 8^-$ isomer in ^{254}No with Nilsson's original parameter values $g_0 = 19.2$ MeV and $g_1 = 7.4$ MeV [10] used in the paring constants in Eq (6). The analysis of the results showed that in most of parts of the (β_2, β_3) deformation space the gap equation does not possess a solution and the 2qp energy surface can not be obtained with a relevant shape allowing us to make any conclusion. For the previously used value of the parameter $g_0 = 17.8$ MeV [5, 6, 8] the problem with the BCS solution becomes even stronger. The collapse of the BCS pairing with the appearance of broken pairs is a known effect which can be prevented by increasing the pairing constants. Though the reduction of the gap due to the blocking effect has reasonable physical grounds the arbitrary increase of the pairing strength to take it into account may lead to inconsistencies in the description of different nuclear characteristics [12]. Therefore any change in the pairing strength has to be performed with caution. Thus we performed calculations with slightly larger values of the parameter $g_0 > 19$ MeV by keeping $g_1 = 7.4$ MeV. The results of calculations with several g_0 values, $g_0 = 20, 21, 22$ and 23 MeV, are given in Table 1, and the respective patterns for the 2qp energy in the deformation space are illustrated in Figure 4. It is seen that both the positions and the depths of the obtained energy minima strongly depend on the value of the pairing parameter g_0. Thus for the lowest considered $g_0 = 20$ MeV the minimum is positioned at $(\beta_2 = 0.254, \beta_3 = 0.07)$ with a relative depth of 0.05 MeV. For the largest $g_0 = 23$ MeV the minimum is shifted at $(\beta_2 = 0.268, \beta_3 = 0.150)$ with a depth of 0.11 MeV. At the same time the neutron pairing gap Δ_n raises from 0.45 MeV to 1.22 MeV together with the raising octupole deformation in the minimum. For ^{254}No the empirical ground-state gap is $\Delta = 12 \cdot A^{-1/2} = 0.75$ MeV and we may assume that in the case of blocking the neutron gap Δ_n can not exceed it. Then a reasonable estimation for the 2qp energy minimum could be associated to $(\beta_2 = 0.25, \beta_3 = 0.1)$ with a depth of about 0.08 MeV. Thus we see that the 2qp minimum may appear to be shallower when the blocking effect is taken into account.

Table 1. Location and depth (in MeV) of the energy minima obtained for the $8^-\{\nu 7/2[624] \otimes \nu 9/2[734]\}$ configuration in ^{254}No and the $9^-\{\nu 7/2[613] \otimes \nu 11/2[725]\}$ configuration in ^{270}Ds in dependence on the pairing parameter g_0 (in MeV). The corresponding neutron pairing gaps Δ_n (in MeV) are also given

^{254}No				^{270}Ds			
g_0	(β_2, β_3)	depth	Δ_n	g_0	(β_2, β_3)	depth	Δ_n
20	0.254, 0.070	0.050	0.454	19	0.255, 0.208	0.315	0.258
21	0.256, 0.096	0.075	0.743	20	0.258, 0.158	0.097	0.575
22	0.261, 0.126	0.094	0.989	21	0.260, 0.100	0.021	0.791
23	0.268, 0.150	0.110	1.217	22	0.251, 0.038	0.001	0.954

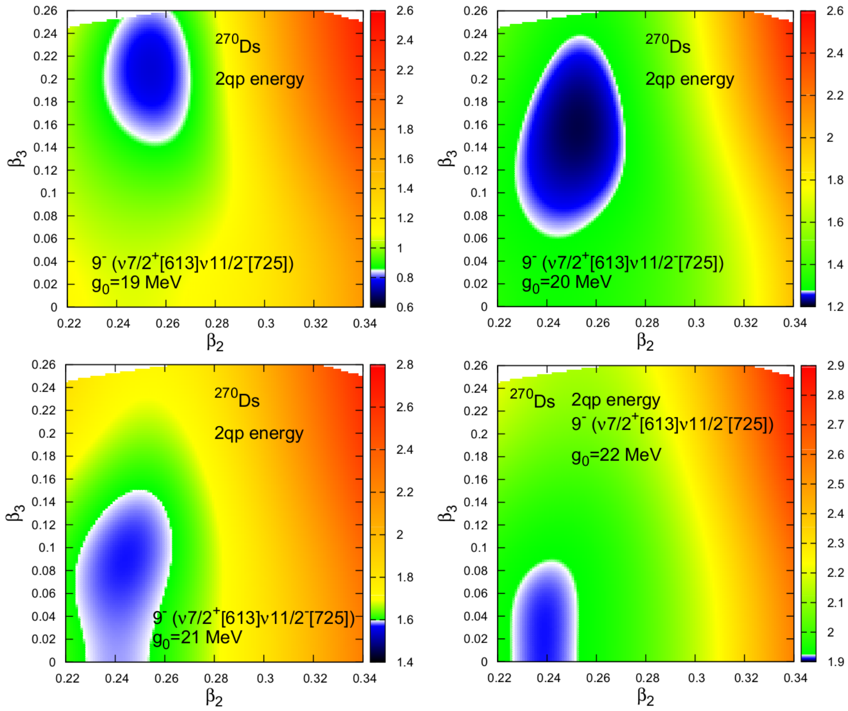

Figure 5. The same as Figure 4, but for the $K^{\pi} = 9^{-}\{\nu 7/2[613] \otimes \nu 11/2[725]\}$ configuration in ^{270}Ds.

Similar calculations (DSM+BCS+blocking) were performed for the $K^{\pi} = 9^{-}\{\nu 7/2[613] \otimes \nu 11/2[725]\}$ configuration in ^{270}Ds. The obtained result is shown in Table 1 and in Figure 5. Again, we see a pronounced dependence of the 2qp energy minima on the pairing strength. We notice a slightly stronger variation of the positions of the minima in octupole direction with the change of g_0 compared to ^{254}No. Moreover, in contrast to ^{254}No we find that here the octupole deformation and the depth of 2qp energy minima decrease with the increase of g_0. For $g_0 = 19$ MeV the minimum is at $(\beta_2 = 0.255, \beta_3 = 0.208)$ with a depth of 0.315 MeV. For $g_0 = 22$ MeV the pattern moves to essentially lower octupole deformation $\beta_3 = 0.04$ while the 2qp minimum practically vanishes. Considering that for ^{270}Ds the empirical pairing gap in the ground state is 0.73 MeV one may assume that the physically reasonable Δ_n is much lower. According to the correlation in Table 1 this can lead to the estimation that a minimum in the energy of the considered 9^{-} state may be located at relatively large octupole deformation $\beta_3 \geq 0.15$ with a depth larger than 0.1 MeV.

We remark that for both considered configurations in ^{254}No and ^{270}Ds the obtained dependencies of the octupole deformations and the depths of the 2qp energy minima on the increasing pairing strength are different. However, in order to make any conclusion one has to estimate the pairing strength corresponding to the broken neutron pairs in a more unambiguous way. For the moment we can only say that the present preliminary results emphasize the need for further detailed study of the effects of the deformation and pairing on the formation of high-K isomeric states in heavy and superheavy nuclei.

4 Summary

The implemented DSM+BCS calculations suggest that octupole deformation may play a considerable role in the formation of two-quasiparticle high-K isomeric states in even-even heavy and superheavy nuclei. The cases of shallow octupole minima obtained for the 2qp energies indicate an octupole softness of the nuclei in their respective isomeric states. The pronounced octupole minima observed in several nuclei give an indication for the possible presence of octupole deformation in some isomeric states. The pronounced sensitivity of the magnetic dipole moments to the octupole deformation suggests that future magnetic-moment measurements would provide useful constraints on the degree of octupole deformation. The physically more relevant DSM+BCS calculations taking the blocking effect into account indicate strong dependence of the eventual octupole softness/deformation in the high-K isomeric states of heavy and superheavy nuclei on the pairing interaction strength. It is shown that in the case of blocking the role of the deformation may be a bit more subtle. Further detailed study will be needed to unambiguously clarify this role and to improve the predictive value of the approach used with respect to the appearance of complex deformed shapes in nuclear isomeric states.

5 Acknowledgments

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