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Effect of tensor interaction on deformation and shell structure of medium-heavy and superheavy nuclei

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Abstract

The effect of tensor interaction is studied on deformation and shell structure of various nuclei within the deformed Skyrme Hartree–Fock+BCS model. We discuss first the effect of tensor interaction on the deformations of Kr isotopes and \textsuperscript{80}Zr. Second, the same model is applied to investigate the role of tensor correlations on the evolution of shell structure in superheavy nuclei. To this end, we adopt four different Skyrme interactions: SLy5 without tensor interaction, and SLy5+T, T24 and T44 with tensor interaction. It is shown that the SLy5+T interaction gives the shape changes of the lowest configurations of Kr isotopes similar to experimental observations. The importance of the tensor correlations is also pointed out for the single-particle spectra of protons and neutrons in \textsuperscript{249}Bk and \textsuperscript{251}Cf, respectively. The large shell gaps of superheavy nuclei are found at \( Z = 114 \) and \( Z = 120 \) for protons and \( N = 184 \) for neutrons with the spherical shape irrespective of the tensor correlations. It is also shown that \( Z = 114 \) and \( N = 164 \) shell gaps are more pronounced by the tensor correlations of SLy5+T interaction. The effect of time-odd components of Skyrme energy density functionals is examined on the deformation and the stability of superheavy elements.

(Some figures may appear in colour only in the online journal)

1. Introduction

The study of the stability of superheavy nuclei is currently a problem of great interest in nuclear physics. The major challenge is to predict the possible existence and location of the island of stability for the superheavy nuclei. In general, the most stable nuclei may have the doubly closed shell configuration for both protons and neutrons, such as in \textsuperscript{16}O (\( Z = N = 8 \)), \textsuperscript{40}Ca (\( Z = N = 20 \)), \textsuperscript{132}Sn (\( Z = 50, N = 82 \)) and \textsuperscript{208}Pb (\( Z = 82, N = 126 \)). The numbers 8, 20, 50, 82 and 126 are called ‘magic numbers’ and the physical origin was explained by Mayer and Jensen via a large spin–orbit splitting in nuclei [1]. The enhancement of nuclear binding
due to the presence of shells will be quantified in terms of the shell energy [2]. Although the doubly closed shell nuclei (so-called magic nuclei) have the largest shell energies, other nuclei can also gain extra binding energies due to the oscillation of shell energy with the number of nucleons.

In superheavy nuclei, the level density of single-particle energies is quite large, so that a small change of single-particle energy may raise a significant effect on the determination of the shell stability. That is why till now we have not really known what is the next doubly magic nucleus beyond $^{208}\text{Pb}$. The macroscopic–microscopic model [3, 4] predicts the next proton shell gap at $Z = 114$, resulting from a large splitting of the $2f_{7/2}$ and $2f_{5/2}$ spin–orbit partners. At the same time, the model predicts the neutron gap at $N = 184$. On the other hand, self-consistent mean field models predict the extended region of shell stabilities. Skyrme Hartree–Fock (SHF) calculations favor gaps at $Z = 124$, 126 and $N = 184$ depending on the parameterizations [5–7], while relativistic mean field (RMF) calculations lead to shell stabilities around $Z = 120$, $N = 172$, 184 or $Z = 126$, $N = 184$ [8–10] in addition to the ($Z = 114$, $N = 184$) shell gap. Recently, the effect of tensor terms of Skyrme interactions was studied on the shell structure of superheavy elements (SHE) within the context of the spherical HF model [11]. (See [6, 8, 12, 13] for the comparisons of the predictions of different SHF and RMF calculations.)

In the heavy mass region around SHE, the single-particle level density is high. The shell gaps are therefore sensitive to the accuracy of the predicting power of the single-particle energies and the spin–orbit interactions. It turns out that the differences in single-particle energies are responsible for the divergent predictions of magic numbers in the mass region of superheavy nuclei [14, 15] and a slight modification of the spin–orbit strength will give significant changes in the single-particle spectra and the stability of heavy and superheavy nuclei [15]. One current topic is the role of tensor terms in the effective interactions on the spin–orbit splittings and the shell evolution of exotic nuclei far from the stability line. In this work, we study the effect of the tensor terms on the shell evolution and the predictions for SHE taking into account the quadrupole deformation in the SHF model.

The role of the tensor force was first discussed in the context of the mean field model more than 50 years ago [16]. However, except for an early exploratory work in [17], the role of tensor interaction had been neglected in mean field models until very recently. Only a few years ago it was revived in Gogny [18] and also in Skyrme [19–22] models. Reference [20] pointed out the role of tensor terms of the Skyrme effective interaction on the shell evolutions in the $N = 82$ isotones and $Z = 50$ isotopes. The experimental isospin dependence of the spin–orbit splittings cannot be described by the SHF calculations with standard Skyrme interactions but is well reproduced by including the tensor interaction [20]. Similar improvements were realized in the study of single-particle energies of $f$ and $p$ orbits in nuclei around $^{48}\text{Ca}$ and $^{46}\text{Ar}$ [22, 23]. These improvements of the single-particle energies induced by tensor interactions suggest the inclusion of the tensor correlations for the study of shell gaps of nuclei in the superheavy region.

Recently, the stability of SHE has been studied including the tensor interactions in the SHF model with spherical symmetry. It is known however that the breaking of spherical symmetry in deformed nuclei leads to a strong modification of the single-particle spectra in the Nilsson diagram and may change the shell evolution of heavy and superheavy nuclei. At the same time, the deformation potential itself will be modified in the mean field by inclusion of the tensor effect. Thus, we need mean field calculations including both the tensor interactions and the deformation to make more reliable predictions for the stability of superheavy nuclei.

The spin–orbit potential is in general expressed by a derivative of density with the coupling strength. The mass number dependence of this potential is modest and smooth as a function
of mass number. On the other hand, the spin–orbit potential of the Skyrme tensor interaction depends on the spin–orbit density and is very sensitive to the shell occupancy. Namely, the effect of tensor correlations becomes active only when the spin–orbit partners are partially occupied. In deformed nuclei, the ordering of single-particle states is changed drastically so that the tensor correlations might be very different compared with spherical nuclei. The effect of tensor interactions on deformed nuclei was studied in [24] for magic or semi-magic nuclei with \( N \) or \( Z = 20, 28, 40, 50, 82 \). We extend the work in [24] to study the shell stability in the SHE region.

The time-odd components of Skyrme energy density can be neglected in even–even nuclei. It was pointed, however, that the time-odd components have a substantial effect on the moment of inertia and thus on the rotational spectra of deformed nuclei. We take into account the time-odd components of the central part of Skyrme energy density to study single-particle energies of odd superheavy nuclei.

In this paper, we study the effect of tensor interaction on the shapes of ground states and the shell evolution of nuclei. We discuss first how the tensor correlations change the shape of medium-heavy nuclei. Then the shell evolution of heavy and superheavy nuclei will be studied, especially focusing on the shell evolution around the proton number \( Z = 114 \). This paper is organized as follows. A brief summary of the HF-BCS model with tensor interactions is given in section 2. The effect of tensor correlations on the shape is discussed in section 3. Section 4 is devoted to the study of shell evolution of superheavy nuclei. A summary is given in section 5.

2. Formalism

We perform axially symmetric deformed SHF calculations [25–27], taking into account the triplet-even and triplet-odd zero-range tensor interactions,

\[
V_T = \frac{T}{2} \left\{ (\sigma_1 \cdot k')(\sigma_2 \cdot k') - \frac{1}{3} k'^2 (\sigma_1 \cdot \sigma_2) \right\}
+ \left\{ (\sigma_1 \cdot k)(\sigma_2 \cdot k) - \frac{1}{3} (\sigma_1 \cdot \sigma_2) k^2 \right\} \delta(r_1 - r_2)
+ U \left\{ (\sigma_1 \cdot k') \delta(r_1 - r_2)(\sigma_2 \cdot k) - \frac{1}{3} (\sigma_1 \cdot \sigma_2) [k' \cdot \delta(r_1 - r_2) k] \right\},
\]

where \( k \) and \( k' \) are the momentum operators acting on the right- and left-hand side, respectively. The time-even and time-odd tensor coupling constants \( T \) and \( U \) are free parameters in the SHF model. The tensor interaction (1) gives rise to, so-called, time-even and time-odd components in the Skyrme energy density functionals. The time-even part has the pseudo-scalar, the vector and the pseudo-tensor spin–orbit densities. Because of the symmetry restriction for the deformation, the pseudo-scalar part is dropped out. In [24], the effect of the pseudo-tensor part on deformations was studied systematically in medium and heavy nuclei and it was found that the contribution of the pseudo-tensor spin–orbit density is two orders of magnitude smaller than the vector one. For these reasons, we will not consider the pseudo-scalar and pseudo-tensor spin–orbit densities in the following calculations, but only take into account the vector part in the Skyrme energy density functionals. For even–even nuclei, the time-odd components of the density functionals have no contributions in the mean field calculations. For odd-\( A \) nuclei, however the time-odd components may have finite contributions. In this study, we take into account the time-odd contributions of the central part of Skyrme energy density functionals and study the effect of deformations and single-particle energies. Formulas are given in the appendix.
The vector part of the spin–orbit density is expressed as

$$J_q = \frac{1}{4\pi R^3} \sum_{i \in q} (2j_i + 1)v_i^2 \left[ j_i(j_i + 1) - l_i(l_i + 1) - \frac{3}{4} R_i^2(r) \right], \quad (2)$$

where $q = n(p)$ labels neutron (proton), and $R_i(r)$ and $v_i^2$ are the HF wavefunction and its occupation probability, respectively. The associated part of the SHF energy density is given by

$$\Delta H = \frac{1}{2\alpha}(J_n^2 + J_p^2) + \frac{1}{2}\beta J_n J_p, \quad (3)$$

where the $\alpha$ and $\beta$ have the contributions of central exchange and tensor term,

$$\alpha = \alpha_C + \alpha_T, \quad (4)$$
$$\beta = \beta_C + \beta_T, \quad (5)$$

$$\alpha_C = \frac{1}{2}(t_1 - t_2) - \frac{1}{2}(t_1x_1 + t_2x_2), \quad (6)$$
$$\beta_C = -\frac{1}{8}(t_1x_1 + t_2x_2), \quad (7)$$
$$\alpha_T = \frac{5}{12}U, \quad (8)$$
$$\beta_T = \frac{5}{24}(T + U). \quad (9)$$

Here, $\alpha_C$ and $\beta_C$ are written in terms of standard Skyrme parameters, while $\alpha_T$ and $\beta_T$ are related to the tensor interactions. With the contributions of tensor correlations, the spin–orbit potential is given by

$$W_q = \frac{W_0}{2r} \left( 2 \frac{d\rho_q}{dr} + \frac{d\rho_q'}{dr} \right) + \left( \alpha J_q + \beta J_q' \right), \quad (10)$$

where the first term comes from the Skyrme spin–orbit interaction, whereas the second one includes both the central exchange and tensor contributions. The interactions between like (unlike) particles are denoted as $q(q')$ in equation (10).

There have been several systematic studies of the tensor interactions in the SHF model [20, 28, 19, 21, 23]. The tensor strengths have been fixed by adding the optimized values to the existing Skyrme parameters through fits to isotope and/or isotone dependence of experimental single-particle energies in [20, 21]. The tensor parameters are obtained by making refits of the full Skyrme parameters to reproduce the binding energies of reference nuclei and other bulk properties in [19, 28]. We choose four parameter sets in the following study: SLy5 force without tensor interactions and three parameter sets SLy5+T [20], T24 and T44 [28] with tensor interactions. For SLy5+T, the tensor interactions are added on top of the existing parameter set SLy5 to describe the spin–orbit splittings of $N = 82$ isotones and $Z = 50$ isotopes [20]. On the other hand, the interactions T24 and T44 are determined by the fitting procedure of all the parameters including tensor terms to reproduce various empirical data. These four parameter sets can be considered as representatives of the parameter sets classified in the neutron and proton spin–orbit density 2D $(C_0^t, C_1^t)$ parameter plane [28]. The parameters $C_0^t$ and $C_1^t$ are expressed by $\alpha$ and $\beta$ through the relations $C_0^t = \frac{1}{2}(\alpha + \beta)$ and $C_1^t = \frac{1}{2}(\alpha - \beta)$, respectively. SLy5 has positive $C_1^t$ and zero value for $C_0^t$, while SLy5+T has negative values for both $C_0^t$ and $C_1^t$. The parameter sets T24 and T44 are two members among 36 members of the TJ family. The parameter set T24 has positive values for both $C_0^t$ parameters, while T44 has a larger positive value for $C_0^t$ and a small positive value for $C_1^t$. These four sets of parameters spread over the $(C_0^t, C_1^t)$ plane and can be considered to simulate the major effect of the tensor correlations in Skyrme interactions.
Figure 1. The odd–even mass difference for Nι isotopes. The three-point formula is used to calculate the odd–even mass difference [29, 30]. Experimental data are indicated by filled circles. The results for the pairing strength $V_0' = -1250$ and $-625$ MeV fm$^{-3}$ are indicated by open circles and open diamonds, respectively, while the corresponding results with odd-term fields are indicated by open squares and open triangles, respectively.

Table 1. Parameters of tensor interactions $T$, $U$ and also $\alpha$, $\beta$ for Skyrme interactions SLy5, SLy5+T, T24 and T44. All the parameters are given in units of MeV fm$^{-5}$. See the text for details.

<table>
<thead>
<tr>
<th>Skyrme parameters</th>
<th>$T$</th>
<th>$U$</th>
<th>$\alpha_\xi$</th>
<th>$\beta_\xi$</th>
<th>$\alpha_T$</th>
<th>$\beta_T$</th>
<th>$\alpha$</th>
<th>$\beta$</th>
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<td>0.0</td>
<td>0.0</td>
<td>80.20</td>
<td>-48.87</td>
</tr>
<tr>
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<td>-408.0</td>
<td>80.20</td>
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<td>-170</td>
<td>100</td>
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<tr>
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<td>59.22</td>
<td>95.33</td>
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<td>24.67</td>
<td>19.37</td>
<td>120</td>
<td>0</td>
</tr>
<tr>
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<td>21.52</td>
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<td>6.98</td>
<td>8.97</td>
<td>113.02</td>
<td>120</td>
<td>120</td>
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</tbody>
</table>

3. Results of medium-heavy nuclei: Kr isotopes and $^{90}$Zr

We discuss how the deformations of medium-heavy and heavy nuclei are affected by the tensor correlations in SHF+BCS calculations. The parameters for tensor interactions employed are taken from [20, 24]. The adopted parameters of tensor interactions $T$, $U$ and also $\alpha$, $\beta$ are summarized in table 1. The sign of $\alpha_T$ is negative for SLy5+T, while T24 and T44 have positive values. On the other hand, the sign of $\beta_T$ is always positive for these three parameter sets. The bare meson exchange as well as G-matrix interactions suggests a positive sign for both $\alpha_T$ and $\beta_T$. Such tensor forces applied to study the shell evolutions of medium-heavy nuclei in [18, 19]. In contrast, in [20, 21], better descriptions of single-particle energies in various isotopes have been obtained by the negative $\alpha$ and positive $\beta$ values of the tensor interactions. In this respect, the Skyrme-type tensor interaction is not fully understood in the context of the bare and G-matrix ones. We may need to examine the role of correlations beyond mean fields such as the particle-vibration couplings to obtain better understanding of the effective tensor interactions.
Figure 2. Calculated energies and shapes of the ground states and the first excited $0^+$ states in Kr isotopes with SLy5, SLy5+T, T24 and T44 interactions. The prolate and oblate deformations are shown by open circles and open triangles, respectively. Experimental data are indicated by filled circles and filled triangles for prolate and oblate deformations, respectively. Results of the macroscopic–microscopic model [32] are indicated by open and filled stars for prolate and oblate deformations, respectively, in the upper-right panel. Experimental data are taken from [33–35]. See the text for detailed discussions.

In the calculation, a density-dependent surface delta interaction (DDDI)

$$V(r_1, r_2) = V_0' \left(1 - \frac{\rho(r)}{\rho_0}\right) \delta(r_1 - r_2)$$

(11)

is used for the pairing (particle–particle) channel, where $\rho(r)$ is the HF density at $r = (r_1 + r_2)/2$ and $\rho_0 = 0.16$ fm$^{-3}$. We employ the BCS model with Lipkin–Nogami (LN) number projection for the calculations of pairing correlations. We use the same pairing strength for medium and heavy nuclei with the cutoff prescription as was adopted in [24], namely $V_0' = -1000$ MeV fm$^{-3}$ for medium and heavy nuclei. In order to obtain a proper estimate of the pairing correlations in superheavy nuclei, we checked the odd–even mass difference by the three-point formula $\Delta^{(3)}$ [30] for No isotopes as shown in figure 1. We find that the pairing strength $V_0' = -1250$ MeV fm$^{-3}$ adopted in [24] is too large for superheavy nuclei and the paring strength $V_0' = -625$ MeV fm$^{-3}$ can well reproduce the odd–even difference compared with the experimental data. Therefore, in the following calculations, we use the pairing strength $V_0' = -625$ MeV fm$^{-3}$ for superheavy nuclei. In the case of a nucleus with an odd number of nucleons, the orbit occupied by the last odd nucleon is blocked, as described in [31]. The time-odd components of energy density functionals are included in the study of odd and odd–odd nuclei.
We calculate the binding energies of Kr isotopes using four different Skyrme parameters SLy5, SLy5+T, T24 and T44. We plot in figure 2 the energies of the ground states and the first excited local minima of Kr isotopes. The experimental data are shown by the filled circles and filled triangles for prolate and oblate shapes, respectively. The calculated results of the macroscopic–microscopic model [32] are also shown by open and filled stars for prolate and oblate deformations, respectively, in the upper-right panel in figure 2. Experimental data show that the prolate and oblate deformation minima coexist near the ground states of Kr isotopes and the inversion of the prolate and the oblate minima occurs at $^{74}$Kr, the dominant configuration of the ground state of $^{72}$Kr is identified experimentally to be prolately deformed [33], while those of $^{74,76,78}$Kr are suggested to be oblate deformations [33–35]. SLy5 (without the tensor interactions) in the upper-left panel gives the lowest configurations for all Kr isotopes to be oblate, except the spherical shape for $^{76}$Kr. The prolate minima compete with the oblate minima in $^{76,78}$Kr. The calculated lowest configurations of SLy5+T (the upper-right panel) become prolate in $^{76,78}$Kr being consistent with the empirical findings. In $^{74}$Kr, the result of SLy5+T interaction gives almost degenerate prolate and oblate minima near the ground state, while SLy5 without tensor gives a clear oblate minimum. The T24 and T44 interactions give oblate or spherical minima for all the ground states except in $^{78}$Kr where the prolate minimum appears in the case of T24 interaction. Thus, the two interactions in the lower panels do not show any sign of the proper inversion of prolate and oblate shapes at $^{74}$Kr. The macroscopic–microscopic model gives a reasonable description of the shapes of the ground states of Kr isotopes up to $A = 76$, but the model has a problem to predict the proper shapes of $^{78}$Kr. It is pointed out that the configuration mixing between the prolate and oblate minima is important for the quantitative description of the shape isomers of Kr isotopes [36]. In [36], the generator coordinate method (GCM) was performed with HF+BCS wavefunctions. Although the GCM calculations produce many global features of Kr isotopes, the ordering of low-lying states is at variance with the experimental data. The HFB+GCM calculations with the Gogny D1S interaction have been performed for $^{74}$Kr and $^{76}$Kr in [37]. The results give a proper ordering of the prolate and the oblate states in these two nuclei. All Kr isotopes with the Gogny interaction together with the tensor correlations is an interesting problem to study.

Let us discuss next the shape of $^{80}$Zr. It might be reasonable to consider $^{80}$Zr as a double closed subshell nucleus because of $N = Z = 40$, but experimental data suggest a large quadrupole deformation with $\beta_2 \sim 0.4$ for the ground state [38–40]. In figure 3, we plot the binding energy of $^{80}$Zr as a function of quadrupole deformation for different Skyrme interactions SLy5, SLy5+T, T24 and T44. We find that the addition of the tensor interaction to SLy5 leads to a drastic change of the potential energy surface of $^{80}$Zr. According to the result of SLy5+T, the ground state is prolate with $\beta_2 = 0.51$ and a spherical local minimum becomes 0.6 MeV above the deformed ground state, while the ground state is spherical for the other three interactions SLy5, T22 and T24. In $^{80}$Zr, it is shown that a parameter set SLy5+T improves clearly the deformation property in comparison with experimental data.

4. Shell structure of superheavy nuclei

4.1. Single-particle energies of $^{249}$Bk ($Z = 97$) and $^{251}$Cf ($Z = 98$)

Before applying our method to superheavy nuclei, let us first focus on the proton and neutron single-particle spectra of $^{249}$Bk ($Z = 97$) and $^{251}$Cf ($Z = 98$) which are known experimentally [41, 43]. Figures 4 and 5 show the calculated single-particle energies of $^{249}$Bk and $^{251}$Cf, respectively, by the deformed SHF+BCS model with the four different Skyrme interactions. The time-odd terms in the HF Hamiltonian are examined in the figures. Detailed discussions
Figure 3. The calculated binding energy for $^{80}$Zr as a function of quadrupole deformation $\beta_2$ with the parameter sets SLy5, SLy5+T, T24 and T44.

Figure 4. Proton single-particle energies of $^{249}$Bk calculated by the deformed SHF+BCS model with LN number projection. The parameter sets SLy5, SLy5+T, T24 and T44 are used. The deformation parameter is set to the calculated energy minimum at $\beta_2 = 0.3$. The long and short lines show the calculated results of single-particle energies without and with the time-odd terms in the HF Hamiltonian, respectively. Experimental data are taken from [41].

The calculated results of the time-odd terms in the HF Hamiltonian are given in the appendix. Experimental data are also given in the figures. The energy minima are found at the prolate deformation $\beta_2 \sim 0.3$ both in $^{249}$Bk and $^{251}$Cf for all the interactions. For $^{249}$Bk, the SLy5+T interaction can reproduce the correct ordering of the experimental proton single-particle energies, while the other interactions show the different level schemes for several single-particle states compared with the empirical spectra. The energy gaps around the Fermi surface appear at $Z = 96$ for SLy5 and at $Z = 96, 98$ and 100 for SLy5+T, respectively. Both the T24 and T44 interactions do not show the energy gap at $Z = 98$ since the $[633]7/2^+$ level is much higher in energy compared with the empirical value.

Let us explain how the tensor force in SLy5+T interaction produces the $Z = 98$ shell gap of $^{249}$Bk in comparison with the SLy5 interaction. The relative positions of three states
Figure 5. Neutron single-particle energies of $^{251}$Cf calculated by the deformed SHF+BCS model with LN number projection. The parameter sets SLy5, SLy5+T, T24 and T44 are used. The deformation parameter is set to the calculated energy minimum at $\beta_2 = 0.3$. The long and short lines show the calculated results of single-particle energies without and with the time-odd terms in the HF Hamiltonian, respectively. Experimental data are taken from [42].

$^{[521]}3/2^-$ (from $2f_7/2$ in the spherical limit), $^{[633]}7/2^+$ (from $1i_{13/2}$ in the spherical limit) and $^{[521]}1/2^-$ (from $2f_5/2$ in the spherical limit) determine the appearance of $Z = 98$ and $Z = 96$ shell gaps. The tensor interactions have significant contributions to the spin–orbit splittings when one of the spin–orbit partners is unoccupied. For the SLy5+T interaction, we take $(\alpha_T, \beta_T) = (-170, 100) \text{ MeV fm}^2$ and $(\alpha = \alpha_C + \alpha_T, \beta = \beta_C + \beta_T) = (-88.8, 51.1) \text{ MeV fm}^2$. As is expected from equation (10), when a $j_c > l + 1/2$ proton orbit is occupied and the spin–orbit partner $j_c < l - 1/2$ proton orbit is unoccupied, the negative $\alpha$ value increases the spin–orbit splitting of protons, while the positive $\beta$ value decreases the spin–orbit splitting of neutrons. The same effect is induced by the neutron configurations when one of the spin–orbit partners is unoccupied. The net effect of tensor correlations in the SLy5+T interaction makes a larger spin–orbit splitting for both neutrons and protons since the absolute value of $\alpha_T$ is larger than that of $\beta_T$. Because the proton orbits $2f_7/2$ and $1i_{13/2}$ in $^{249}$Bk are partially occupied in the spherical limit, the proton spin–orbit splittings of $2f_7/2-2f_5/2$ and $1i_{13/2}-1i_{11/2}$ partners are enlarged by the tensor correlations. These energy changes of orbits $2f_7/2$, $2f_5/2$ and $1i_{13/2}$ in the spherical limit turn out to create the upward shift of $^{[521]}1/2^-$ orbit and the downward shifts of $^{[725]}11/2^-$ and $^{[622]}3/2^+$ states compared with the empirical energy spectra. In the case of SLy5+T interaction, there is no inversion of the two states. The different results between SLy5 and SLy5+T interactions originate from the tensor forces which enlarge the neutron spin–orbit splitting of $1j_{15/2}-1j_{13/2}$ partner due to the partial occupation of $1j_{15/2}$ orbit. The Skyrme parameters T24 and T44 have large gaps at $N = 160$ and 164, while the positions of $^{[750]}1/2^-$ and $^{[622]}3/2^+$ states are inverted in the level diagram compared with the experimental data.
The single-particle energies for neutrons (upper panels) and protons (lower panels) calculated for $^{254}$No ($Z = 102, N = 152$) with SLy5 (left panels) and SLy5+T (right panels), respectively. The Fermi energy is indicated by the long-dashed line and the ground state deformation is indicated by the vertical dashed line.

4.2. $^{254}$No ($Z = 102$)

Next, we perform DSHF+BCS calculations with SLy5 and SLy5+T interactions for $^{254}$No ($Z = 102$), which is one of the heaviest even–even nuclei experimentally observed. The single-particle energies of neutrons (upper panels) and protons (lower panels) for $^{254}$No are plotted in figure 6 as a function of deformation parameter $\beta_2$. For the SLy5 interaction (lower-left panel), around the energy minimum at $\beta_2 = 0.30$, there are several deformed proton shells, namely $Z = 98, 102, 104$ and 108. When including the tensor interaction, the deformed closed shells become $Z = 98$ and 104 (see the lower-right panel). In the spherical case, the proton gaps are $Z = 92, 100$ and 120 for the SLy5 interaction, while the gap at $Z = 114$ is increased with the SLy5+T interaction. Here, we see again the effect of tensor correlations on the shell structure of single-particle states as were seen in $^{249}$Bk and $^{251}$Cf.
Because the $1i_{13/2}$ proton orbit is partially occupied in $^{254}_{114}$No in the spherical limit, the spin–orbit splittings of $(2f_{7/2}-2f_{5/2})$, $(1i_{13/2}-1i_{11/2})$ and $(1h_{11/2}-1h_{9/2})$ proton orbits are enlarged, respectively, by the effect of $\alpha$ in equation (10). The net effect makes a large shell gap at $Z = 114$, but a smaller gap at $Z = 92$ compared with those of SLy5 without tensor. Similarly, the occupations of $2g_{9/2}$ and $1j_{15/2}$ neutron orbits (the upper panels) make the neutron spin–orbit splittings between $(2g_{9/2}-2g_{7/2})$ and $(1j_{15/2}-1j_{13/2})$ larger. This is the reason why a large shell gap at $N = 164$ appears in the spherical limit in the case of SLy5+T (the upper-right panel). In the Nilsson diagram of figure 6, we see $N = 152$ and 162 deformed gaps for neutrons at $\beta^2 \sim 0.3$ with SLy5, while $N = 150$, 152 and 160 shell gaps appear for SLy5+T.

In recent experimental observations of synthesis of heavy nuclei by cold fusion, the deformed shell gaps are pointed out at $N = 152$ with $Z \sim 100$ and $N = 162$ with $Z = 108$ [48]. These experimental findings give a crucial test of the theoretical predictions of shell gaps. In figure 6 with SLy5 interaction, we can see magnified shell gaps at $N = 152$ and 162 for neutrons and at $Z = 98$, 102 and 108 for protons at the deformation $\beta^2 \sim 0.3$. These calculations can be identified to the empirical observations in the nuclear synthesis of heavy nuclei. On the other hand, the interaction SLy5+T gives the deformed shell gaps at $N = 150$ and 160 for neutrons and $Z = 98$ and 104 for protons. The shell gap at $Z = 108$ is also somewhat quenched compared with that of SLy5.

4.3. $^{298}_{114}$I$_{184}$

The total energies of a nucleus $^{298}_{114}$I$_{184}$ are shown in figure 7 as a function of quadrupole deformation $\beta^2$ with SLy5, SLy5+T, T24 and T44 interactions, respectively. As can be seen from figure 7, the presence of tensor terms in the energy functional has an obvious effect on the energy surface. The SLy5+T interaction gives the spherical minimum lower by about 5 MeV than the local minimum at $\beta^2 \sim 0.65$. The three interactions, SLy5, T24 and T44, give
Figure 8. The single-particle energies of protons in $^{298}$114 as a function of deformation parameter $\beta_2$ with SLy5, SLy5+T, T24 and T44. The Fermi energy is indicated by a long-dashed line. The position of the local minimum is shown by a vertical dashed line.

Table 2. The $Z = 114$ and $Z = 120$ gaps (in units of MeV) at $\beta_2 = 0$ in $^{298}$114 for different Skyrme parameters SLy5, SLy5+T, T24 and T44. See the text for details.

<table>
<thead>
<tr>
<th>Skyrme parameters</th>
<th>$Z = 114$</th>
<th>$Z = 120$</th>
<th>$Z = 126$</th>
</tr>
</thead>
<tbody>
<tr>
<td>SLy5</td>
<td>0.93</td>
<td>1.0</td>
<td>2.89</td>
</tr>
<tr>
<td>SLy5+T</td>
<td>1.89</td>
<td>0.36</td>
<td>3.18</td>
</tr>
<tr>
<td>T24</td>
<td>0.65</td>
<td>0.94</td>
<td>2.67</td>
</tr>
<tr>
<td>T44</td>
<td>0.54</td>
<td>0.75</td>
<td>2.41</td>
</tr>
</tbody>
</table>

the competing ground and excited states at $\beta_2 \sim 0.55$ with smaller energy differences of 2.5, 1.4 and 0.2 MeV, respectively. Furthermore, the barrier height in the case of SLy5+T is higher by about 2 MeV than the other three interactions.

The single-particle energies of protons in $^{298}$114 are shown in figure 8 as a function of deformation parameter $\beta_2$ for the four Skyrme interactions. In all cases, we find that $Z = 126$ is the major shell gap in the spherical limit. For subshells, as discussed in [49], the $Z = 114$ and 120 shell gaps appear depending on the relative positions of $2f_5/2$, $2f_7/2$ and $1i_{13/2}$ orbits. All the Skyrme calculations show the results in which the $1i_{13/2}$ orbit lies between the $2f_5/2$ and $2f_7/2$ orbits. The shell gap energies at $Z = 114$, $Z = 120$ and $Z = 126$ at the spherical minimum $\beta_2 = 0$ are listed in table 2. We recognize in the table that for the SLy5, T24 and T44 interactions, $Z = 114$ and 120 gaps are competing, while the energy gap at $Z = 114$
Figure 9. Same as figure 8, but for the single-particle energies of neutrons in $^{298}\text{114}$. 

is more pronounced and the $Z = 120$ gap has almost disappeared in the case of the SLy5+T interaction. It should also be noted that the $Z = 126$ gap is always much larger than those of $Z = 114$ and 120.

As was mentioned in section 4.1, the occupations of the $1i_{13/2}$ and $2f_{7/2}$ orbits enhance the spin–orbit splittings and make the $Z = 114$ shell gap for the SLy5+T interaction larger than that for SLy5. On the other hand, for T24 and T44, the tensor effect is not clearly seen in the Nilsson diagram of figure 8 as far as the gaps $Z = 114$ and 120 are concerned. This is because of large spin–orbit strengths $W_0$ for T24 and T44 interactions, i.e. $W_0 = 139.272$ and 161.367 MeV fm$^{-5}$, respectively, compared to $W_0 = 126$ MeV fm$^{-5}$ for SLy5 and SLy5+T. Then the values $\alpha$ are taken to be positive for T24 and T44 as given in table 1. These positive values for $\alpha$ quench the spin–orbit splittings. Thus, in figure 8, the tensor effects of T24 and T44 interactions compensate with the larger $W_0$ strength and the net results give similar level schemes to that of SLy5. In the large prolate deformation side, it is interesting to note that the SLy5 and SLy5+T interactions give clear energy gaps at $Z = 114$ and 120, while the T24 and T44 interactions show a shell gap at $Z = 122$.

The single-particle energies of neutrons in $^{298}\text{114}$ with the four interactions are shown in figure 9. We obtain a large energy gap at $N = 184$ for the SLy5 and SLy5+T interactions in the spherical limit. We can also see that the $N = 164$ gap becomes much larger for SLy5+T because of the occupation of $1j_{15/2}$ orbit and the negative $\alpha$ value. In the large prolate deformation region, the $N = 184$ gap and somewhat smaller $N = 172$ gap appear at the deformation $\beta_2 \sim 0.6$ in the cases of T24, T44 and SLy5. However, the deformed $N = 184$ and $N = 172$ gaps disappear for SLy5+T because the $1i_{11/2}$ orbit
becomes close to the $2g_{9/2}$ and $1j_{15/2}$ orbits due to the tensor interactions and kills the energy gaps at $\beta_2 \sim 0.6$.

In contrast to the deformed shell gaps at $N = 152$ and $N = 162$, the gap at $N = 184$ is predicted to be a spherical shape and may influence the decay properties of a much wider charge and mass region of heavy nuclei. In order to synthesize nuclei with $Z \geqslant 112$ and $N \geqslant 172$, hot fusion reactions with massive nuclei are a promising reaction mechanism rather than the well-studied cold fusion reactions. It would be extremely interesting to study the decay properties of these synthesized heavy nuclei to establish a possible spherical shell gap at $N = 184$.

5. Summary

In order to study the effect of the tensor interaction on the deformation and shell evolution of medium-heavy and superheavy nuclei, we performed the deformed SHF+BCS calculations with four different Skyrme interactions SLy5, SLy5+T, T24 and T44. There is no tensor interaction in SLy5, while the tensor interactions are included perturbatively in SLy5+T and by the variational procedure in the T24 and T44 parameter sets. We discussed first the effect of tensor force on the shape isomers in Kr isotopes and the ground state of $^{80}$Zr. The single-particle energies and the shell evolution of superheavy nuclei $^{249}$Bk, $^{251}$Cf, $^{254}$No and $^{280}$114 are then examined by the same model.

Our calculations indicate that the SLy5+T interaction gives a proper description of shape changes near the ground states of Kr isotopes and also the deformation of the ground state of $^{80}$Zr. Furthermore, it is shown that the single-particle spectra of $^{249}$Bk and $^{251}$Cf are largely influenced by the tensor correlations. The energies of proton and neutron single-particle states are better described by the SLy5+T interaction than by the other three interactions in comparison with the experimental data. For superheavy nuclei, we find the pronounced energy gaps at $Z = 114$ and $Z = 120$ at the spherical minimum in general. However, the tensor correlations of the SLy5+T interaction make a larger shell gap at $Z = 114$ and that at $Z = 120$ has almost disappeared. Near the deformed local minimum at $\beta_2 \sim 0.6$, the $Z = 114$ and 120 shell gaps appear for the SLy5 and SLy5+T interactions. For neutron shells, we point out that the $N = 184$ closure is robust for all the interactions. It is noted that the tensor terms of the SLy5+T interaction enhance the subshell closure at $N = 164$ in the spherical limit. The large shell gap at $N = 184$ appears both at the spherical minimum and the deformed local minimum of $\beta_2 \sim 0.6$. The $N = 172$ gap also appears at the deformed local minimum in the cases of SLy5, T24 and T44. However, the two deformed gaps disappear by the tensor correlations of the SLy5+T interaction. The time-odd components of the HF potential are examined in odd nuclei $^{249}$Bk and $^{251}$Cf. It is found that the effect is rather small on the single-particle energies and does not change the ordering of single-particle levels of both nuclei.

While the parameter set SLy5+T has several good properties to describe the single-particle energies and the shell structure, the fine agreement of mass systematics of the original SLy5 interaction is missing because of the perturbative adjustment of the tensor interactions. It is desperately desired to establish a new fitting protocol of the Skyrme parameter set with the tensor terms to obtain both the fine mass systematics and the proper shell structure of heavy nuclei. Furthermore, the dynamical effect beyond the mean field approximation [43] may play a role in predicting the shell structure of superheavy nuclei although it is expected to be smaller than the other mass region due to the less collectivity of low-lying excitations. This is an interesting issue to pursue in a future project.
Acknowledgments

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Appendix. Time-odd components in the mean field of the Skyrme interaction

In odd nuclei, the energy density $\mathcal{H}$ acquires a dependence on the spin density $\rho_{s} = \rho_{m} + \rho_{sp}$ [44–47]. Respecting the decomposition of the Skyrme energy functional proposed in [44, 46], the components of $\mathcal{H}$ are

$$\mathcal{H}_{0}^{\text{odd}} = \frac{1}{2} t_0 (x_0 \rho_{s}^2 - \rho_{m}^2 - \rho_{sp}^2),$$  \hspace{1cm} (A.1)

$$\mathcal{H}_{3}^{\text{odd}} = \frac{1}{24} t_3 \rho^{\gamma} \left[ (x_3 \rho_{s}^2 - \rho_{m}^2 - \rho_{sp}^2) \right], \hspace{1cm} (A.2)

$$\mathcal{H}_{\text{fin}}^{\text{odd}} = \frac{1}{32} [3 t_1 (1-x_1) + t_2 (1+x_2)] (\rho_{m} \cdot \nabla^2 \rho_{m} + \rho_{sp} \cdot \nabla^2 \rho_{sp}) + \frac{1}{28} [t_2 x_2 - 3 t_1 x_1] (\rho_{m} \cdot \nabla^2 \rho_{sp} + \rho_{sp} \cdot \nabla^2 \rho_{m}), \hspace{1cm} (A.3)

$$\mathcal{H}_{\text{current}}^{\text{odd}} = \frac{1}{8} [-t_1 (1-x_1) - t_2 (1+x_2)] \hat{J}^2 + \frac{1}{8} [t_1 (1+2 x_1) - t_2 (1+2 x_2)] [\hat{j}_{x}^2 + \hat{j}_{y}^2], \hspace{1cm} (A.5)

where $\rho_{s}$ is the spin kinetic energy density and $\hat{J}$ is the current. The variation of time-odd Hamiltonian (A.1)–(A.5) reads

$$\delta \mathcal{H}^{\text{odd}} = \Sigma_{q}(r) \cdot \delta \rho_{aq}(r) + C_{q}(r) \cdot \delta \tau_{aq}(r) + I_{q}(r) \cdot \delta \hat{j}_{q}(r), \hspace{1cm} (A.6)

where

$$\Sigma_{q}(r) = \frac{1}{2} t_0 (x_0 \rho_{s} - \rho_{aq}) + \frac{1}{24} t_3 \rho^{\gamma} (x_3 \rho_{s} - \rho_{aq}) + \frac{1}{8} [t_1 x_1 + t_2 x_2] \rho_{s} + \frac{1}{15} [3 t_1 (1-x_1) + t_2 (1+x_2)] \nabla^2 \rho_{aq} + \frac{1}{28} [t_2 x_2 - 3 t_1 x_1] \nabla^2 \rho_{aq}

+ \frac{1}{8} [t_2 - t_1] \tau_{aq} + \frac{1}{24} W_{0} \nabla \times (\hat{j} + \hat{j}_{q}), \hspace{1cm} (A.7)

$$C_{q}(r) = \frac{1}{8} [t_1 x_1 + t_2 x_2] \rho_{s} + \frac{1}{8} [t_2 - t_1] \rho_{aq}, \hspace{1cm} (A.8)

$$I_{q}(r) = \frac{1}{8} [-t_1 (2+x_1) - t_2 (1+2 x_2)] \hat{J} + \frac{1}{8} [t_1 (1+2 x_1) - t_2 (1+2 x_2)] \hat{j}_{y}

- \frac{1}{8} W_{0} \nabla \times (\rho_{s} + \rho_{aq}), \hspace{1cm} (A.9)

with the isospin index $q$. Then, the time-odd components for the HF equation read

$$U_{\text{odd}}^{q} = - \nabla \cdot (\sigma \cdot C_{q}) \nabla + \sigma \cdot \Sigma_{q} + \frac{1}{24} (\nabla \cdot \hat{J}_{q} + \hat{I}_{q} \cdot \nabla), \hspace{1cm} (A.10)

There is also an extra term to $U_{\text{even}}^{q}$ from the spin density,

$$\delta U_{\text{even}}^{q} = \frac{1}{24} t_3 \rho^{\gamma-1} (x_3 \rho_{s}^2 - \rho_{m}^2 - \rho_{sp}^2). \hspace{1cm} (A.11)

For the odd nucleus (one nucleon is unpaired), the spin densities are written as $\rho_{s} = \rho_{aq}$ and

$$\sigma \cdot C_{q} = \frac{1}{8} [t_1 x_1 + t_2 x_2] \sigma \cdot \rho_{s} + \frac{1}{8} [t_2 - t_1] \sigma \cdot \rho_{s}, \hspace{1cm} (A.12)$$
and
\[ \sigma \cdot \rho_i = \rho_i(r), \]  
(A.13)
where \( \rho_i(r) = |\phi_i(r)|^2/4/\pi \) is a radial density of the last unpaired particle. In \( \Sigma_q(r) \), the scalar products become
\[ \sigma \cdot \tau_i = \tau_i(r), \]  
(A.14)
\[ \sigma \cdot \nabla^2 \rho_i = \nabla^2 \rho_i(r), \]  
(A.15)
where \( \tau_i(r) \) is the kinetic energy density of the last unpaired particle.

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