The effect of the tensor force on the predicted stability of superheavy nuclei

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Abstract. - The effect of the tensor component of the Skyrme effective nucleon-nucleon interaction on the single-particle structure in superheavy elements is studied. A selection of the available Skyrme forces have been chosen and their predictions for the proton and neutron shell closures investigated. The inclusion of the tensor term with realistic coupling strength parameters leads to a small increase in the spin-orbit splitting between the proton $2f_{7/2}$ and $2f_{5/2}$ partners, opening the Z=114 shell gap over a wide range of nuclei. The Z=126 shell gap, predicted by these models in the absence of the tensor term, is found to be stongly dependent on neutron number with a $Z = 138$ gap opening for large neutron numbers, having a consequent implication for the synthesis of neutron-rich superheavy elements. The predicted neutron shell structures remain largely unchanged by inclusion of the tensor component.

The study of nuclei at the limits of stability is currently a topic of great interest in nuclear structure physics. One of the major challenges is in the regime of high mass and charge - the superheavy elements. A key question relates to the possible existence and location of the island of stability and has been a driving force behind experimental and theoretical efforts for several years [1–6].

Experimentally, superheavy elements up to Z=110-118 have been produced in heavy ion fusion reactions [7–9]. However, the data for these nuclei are scarce since the production cross-sections decrease rapidly with increasing proton number, down to ~pb for Z=112 [10]. This poses a major challenge for experimental investigations and has limited production to isotopes richer in protons than the expected most stable superheavy elements. However, more detailed spectroscopic studies are becoming possible around the transfermium region towards the island of stability [3, 11].

There are also considerable challenges from a theoretical perspective. The emergence of a region of long-lived elements beyond the actinides has been predicted since the earliest nuclear models [12, 13]. Without the shell effects and large spin-orbit splitting of single-particle levels around the magic numbers, nuclei with Z>104 should not exist, since the long-range Coulomb repulsion between protons would overcome the short-range attraction of the strong nuclear force and induce fission. The extra stability from these shell effects has been the focus of considerable theoretical efforts, with different approaches predicting different effects.

Macroscopic-microscopic models using different parameterisations of the nuclear potential predict the next proton shell gap to occur at Z=114 [14, 15], resulting from a large splitting of the $2f_{7/2}$ and $2f_{5/2}$ spin-orbit partners. A neutron gap is also predicted at N=184. These predictions are not shared by those from self-consistent mean-field models. Relativistic mean-field calculations lead to extended regions of additional shell stabilisation around Z=120, N=172,184 or Z=126, N=184 [16], whereas non-relativistic calculations favour gaps at Z=124,126 and N=184 depending on the parameterisation [5, 6, 17]. The Z=114 shell closure only appears in these models for parameterisations of the mean-field which overestimate the spin-orbit splitting in heavy nuclei by ~80%, where states of large angular momentum systematically lie too high in the single-particle spectrum. However, these are generally the forces which are better able to reproduce the bulk properties of the established superheavy elements, indicating that their features could be an essential ingredient to describe the distribution of levels within these nuclei [18].

In the region of superheavy nuclei, the single-particle level density is large. The positioning of the shell gaps is therefore sensitive to the accuracy of describing the single-particle energies and the spin-orbit interaction. Small shifts in the position of the single-particle levels will lead to gaps at different particle numbers. In self-consistent mean-field models this clearly leads to discrepancies between the different parameterisations, exposing an uncertainty in the current models, where improvements of the effective interactions beyond the existing energy functionals are needed. One current popular topic concerning the effective nucleon-nucleon interaction is the role of the tensor term in the spin-orbit splitting and shell evolution of exotic nuclei [19–24]. In this work, we study the effect of the tensor component on the predictions for superheavy nuclei using a spherical Skyrme Hartree-Fock + BCS (SHF) model.

The role of the tensor force was first discussed in the context of mean-field models 50 years ago [25]. A tensor component was originally included as part of Skyrme's effective zero-range nucleon-nucleon interaction. However, it has been neglected in the fitting process of most modern mean-field forces. Only recently has its significance been realised for the evolution of shell structure in nuclei [26, 27], with systematic disrepancies between theoretical calculations and experimental data being at least partly attributed to the tensor force. It induces strong correlations between single-nucleon orbitals with different isospin [27] and is understood in a transparent way within the Skyrme Hartree-Fock equations. The tensor part of the Skyrme effective interaction is written as [25]: where the momentum operators $\boldsymbol{k} = (\overrightarrow{\nabla}_1 - \overrightarrow{\nabla}_2)/2i$ and $\boldsymbol{k}' = -(\overleftarrow{\nabla}_1 - \overleftarrow{\nabla}_2)/2i$. The tensor coupling constants T and U denote the strength of the interaction and are free parameters of the SHF model. Expressing the tensor force in terms of a short-range approximation is justified, since the effect of its finite-range is to introduce a factor that is almost constant for nuclei with A>28, which is incorporated through the coupling strengths with values that are applicable to all nuclei [20] in keeping with the philosophy of the Skyrme mean-field approach.

Tensor interactions result in contributions to binding energy and spin-orbit splitting. However, in the self-consistent mean-field approach most of the effect on the binding energy is minimised through careful selection of the tensor coupling constants. The main manifestation of the tensor force within these models is therefore a correction to the magnitude of the spin-orbit splitting which arises due to the spin-orbit potential, given by [21]:

$$U_{so} = \frac{W_0}{2r}\left(2\frac{d\rho_q}{dr} + \frac{d\rho_{q'}}{dr}\right) + \left(\alpha\frac{J_q}{r} + \beta\frac{J_{q'}}{r}\right). \quad (2)$$

Interactions between like (unlike) particles are denoted by q (q'), where the first term comes from the spin-orbit interaction and the second term contains the central exchange and tensor contributions to the Skyrme interaction. The strength of these contributions, $\alpha = \alpha_c + \alpha_t$ and $\beta = \beta_c + \beta_t$, are written in terms of the Skyrme parameters as [28, 29]:

$$\alpha_c = \frac{1}{8}(t_1 - t_2) - \frac{1}{8}(t_1x_1 + t_2x_2), \quad \alpha_t = \tfrac{5}{12}U$$

$$\beta_c = -\frac{1}{8}(t_1x_1 + t_2x_2), \quad \beta_t = \tfrac{5}{24}(T + U). \quad (3)$$

Imposing spherical symmetry within the SHF equations removes all the time-odd densities from the mean-field and all but the vector component of the spin-current tensor $J_{\mu\nu}$, leading to the simplified expression for the for the spn-orbit potential, (2) [30]. The study of deformed nuclei requires the inclusion of the scalar and tensor component of $J_{\mu\nu}$ as well as the time-odd parts of the energy functional for odd-A nuclei.

There have recently been several systematic studies of the tensor component within the SHF model [19–24, 29]. The tensor strengths have been fixed through fits to experimental single-particle data and included either by making refits to the full set of Skyrme parameters [19, 22], or by adding the optimised values of the tensor strengths to existing Skyrme forces perturbatively [20, 21, 29]. Introduction of the tensor force in this way does not destroy the capabilities of the models to reproduce the binding energy and other bulk properties for reasons discussed earlier. It was found that the optimum values for the tensor coupling strengths, α_t and β_t should be located in a triangle in the 2D (α_t,β_t) plane with negative α_t, postive β_t and $-\alpha_t \approx \beta_t$. These findings were originally based on the SIII force [29]. However, all work based on different forces have led to similar conclusions. The effect of the tensor contribution to spin-orbit splitting in superheavy nuclei is studied using both approaches within the SHF plus BCS model, using a density-dependent delta interaction for the pairing channel with a cutoff prescription as in [31].

Macroscopic-microscopic models traditionally predict ^{298}114 to be a spherical doubly-magic superheavy nucleus. Modern parameterisations of self-consistent models shift the predicted shell gaps for both protons and neutrons. The question therefore arises as to whether the inclusion of the tensor force within the SHF framework will lead to significant modifications of shell structure in superheavy nuclei.

A selection of some common Skyrme parameter sets has been chosen, which differ mainly in the choice of experimental data used to constrain the parameters. The SLy4 parameterisation stems from a series of fits which not only include the ground state properties of nuclei, but also reproduce the properties of neutron matter [32]. In the case of SLy4, the exchange contributions (J^2 terms) to the spin-orbit potential are disregarded. SLy5 was fitted using the same protocol as SLy4, consequently it performs to a similar quality, but the J^2 terms are included in the force. It has also been the force of choice in several recent investigations of shell evolution with the tensor force [21, 23].

$$
\begin{aligned}
\nu_t &= \frac{T}{2}\left(\left[(\boldsymbol{\sigma}_1\cdot\boldsymbol{k}')(\boldsymbol{\sigma}_2\cdot\boldsymbol{k}') - \frac{1}{3}k'^2(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\right]\delta(\boldsymbol{r}_1-\boldsymbol{r}_2) + \delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\left[(\boldsymbol{\sigma}_1\cdot\boldsymbol{k})(\boldsymbol{\sigma}_2\cdot\boldsymbol{k}) - \frac{1}{3}(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)k^2\right]\right)\\
&+ U\left((\boldsymbol{\sigma}_1\cdot\boldsymbol{k}')\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)(\boldsymbol{\sigma}_2\cdot\boldsymbol{k}) - \frac{1}{3}(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)[\boldsymbol{k}'\cdot\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\boldsymbol{k}]\right), \qquad (1)
\end{aligned}
$$

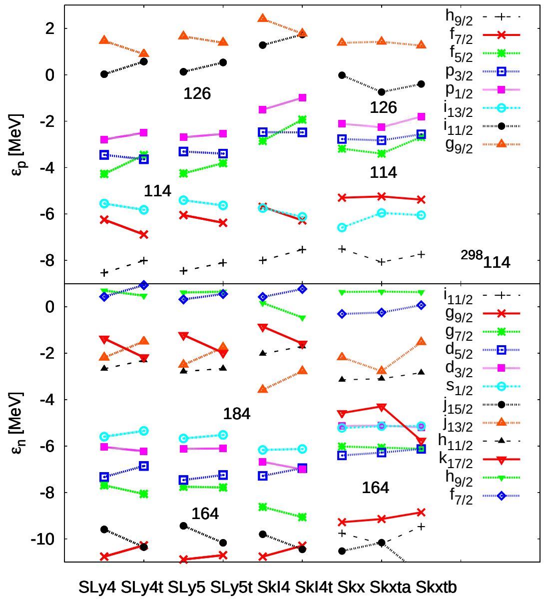

Fig. 1: Single-particle spectra of $^{298}114$ for protons (top) and neutrons (bottom) for the mean-field forces indicated with and without the tensor component.

The SkI4 fit introduced an extended spin-orbit force containing an explicit isovector component, which was found to be necessary for a description of isotope shifts across heavy nuclei [33]. Finally, the Skx set is obtained from a fit not only to binding energies and charge radii, but also to the single-particle energies of stable and exotic nuclei [34]. Skxta and Skxtb are refits, using the same protocol as Skx, which include the zero-range tensor term with strengths calibrated to finite-range G-matrix calculations [19]. The tensor coupling strengths in Skxta are calculated directly from the 1-π exchange potential, although the inclusion of the tensor force in this way was shown to produce a poorer l dependence of spin-orbit splitting. This property is restored in Skxtb by allowing α_t to be included in the variational process, but fixing β_t.

Figure 1 shows the proton and neutron single-particle levels in $^{298}114$ for each of the chosen Skyrme parameter sets both with and without the tensor component. The tensor term has been added to the SLy4, SLy5 and SkI4 Skyrme forces with coupling strengths of $\alpha_t = -170$MeV fm^5 and $\beta_t = 100$MeV fm^5 as in [21]. The Skxta and Skxtb sets are also shown, along with Skx for comparison. For nuclei around Z=114 the important proton shells are $1i_{13/2}$ and $2f_{7/2}$, which are filled at Z=114, and the $2f_{5/2}$ and $3p_{3/2}$ levels, which lie above Z=114. The difference between the $3p_{1/2}$ and $1i_{11/2}$ proton orbitals determines the size of the Z=126 gap. In the absence of the tensor component the level ordering of single-proton states is identical for all forces, except for Skx, which places the $2f_{7/2}$ orbital above $1i_{13/2}$. The possible shell closure at Z=114 is therefore determined by the amplitude of the spin-orbit splitting between the two $2f$ coupled states and the location of the $1i_{13/2}$ state. A strong shell gap at Z=114 appears only for SkI4, with a smaller, but still pronounced Z=114 gap in Skx. In most cases, a more convincing closure appears at Z=126. However it has been shown that this gap is closed as the number of protons in the nucleus is increased from Z=114 to Z=126 for most parameterisations of self-consistent methods [4].

Inclusion of the tensor term generally leads to an increase in spin-orbit splitting between the $2f_{7/2}$ and $2f_{5/2}$ partners, opening the Z=114 shell gap. For SLy4t, SLy5t and SkI4t the $1i_{13/2}$ state is also lowered in energy, increasing this gap by ~1MeV in total. The only exception is Skxta, which predicts a decrease in the splitting between the two $2f$ levels compared to Skx. However, in this case the Z=126 shell gap is also decreased due to a lowering in energy of the $1i_{11/2}$ state. This is also the case for Skxtb, where the magnitude of the shell gap at Z=126 is smaller than that of Z=114 for both forces. The Z=126 closure remains more or less unchanged by the tensor component for all other Skyrme parameterisations, with the Z=114 and Z=126 shell gaps having a similar magnitude, for all but SkI4t. The main difference between the SLy4 and SLy5 forces is the magnitude of the change in splitting between the $2f$ spin-orbit partners once the tensor term is added. SLy5t, which is the force that the tensor coupling strengths used in this work are specifically tuned to, predicts a smaller increase than SLy4t, although the qualitative features remain identical.

In the case of neutrons, the SLy4, SLy5 and SkI4 variants all produce a spherical shell gap at N=184 whose size is determined by the splitting between the $4s_{1/2}$ orbital below the gap and either the $1h_{11/2}$ or the $1j_{13/2}$ orbitals above the gap. In all these cases, the inclusion of the tensor term keeps the size of the gap either constant or increases it, maintaining N=184 as a robust neutron shell gap. Skx does not give a clear gap at N=184 due to the intrusion of the $1k_{17/2}$ state from above. Skxta gives a similar result, but Skxtb pushes the $1k_{17/2}$ level even lower, giving a gap of around 2 MeV at N=184. On the other hand, the N=164 gap is evident in the Skx forces, a conclusion which is unchanged with the addition of the

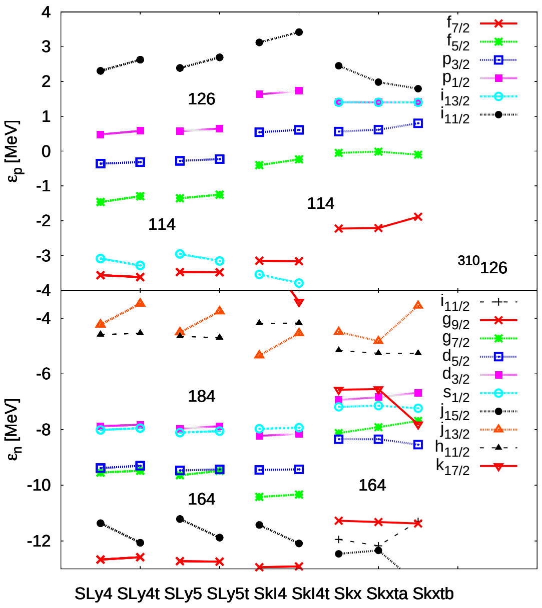

Fig. 2: Single-particle spectra of $^{310}126$ for protons (top) and neutrons (bottom) for the mean-field forces indicated with and without the tensor component.

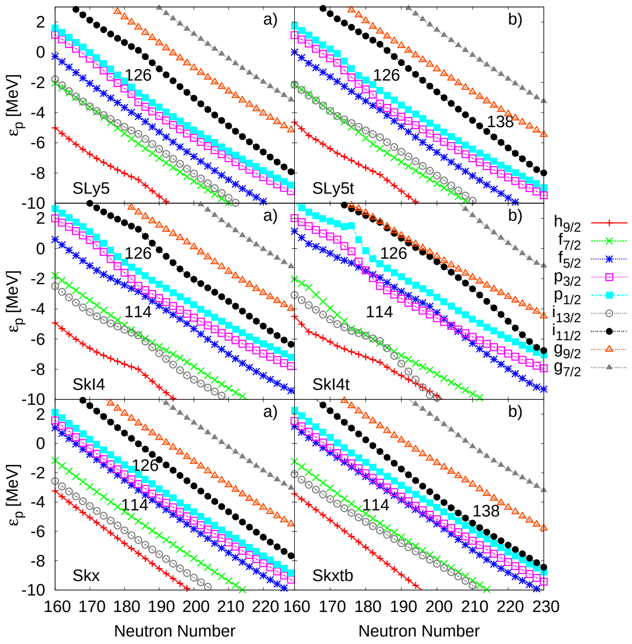

Fig. 3: Proton shell structures across the Z=114 isotopes using SLy6 a) without tensor and b) with the tensor term.

tensor term. Though the additon of this term does serve to decrease the splitting between the $2g_{9/2}$ and $2g_{7/2}$ spin-orbit parters in all cases, this decrease is not enough to affect the presence or absence of a gap at N=164 in any parameter set.

Figure 2 shows the calculated single-particle structure for $^{310}126$. As mentioned previously, the proton shell gap at Z=126 is closed as the number of protons in the nucleus is increased from 114 to 126, and is completely absent in the Skx predictions. In contrast, the shell gap at Z=114 remains of a similar order of magnitude as for $^{298}114$. The tensor component again leads to an opening of the Z=114 gap, which is now of a similar magnitude to the Z=126 gap for most forces. Only for the Skxtb force does the splitting between the $2f_{7/2}$ and $2f_{5/2}$ levels decrease, with Skxta now predicting no change for the Z=114 shell gap compared with Skx. The proton states below the Z=126 gap have a slightly positive energy suggesting the nuclei to be unstable against proton emission, although the high Coulomb barrier would make other decay channels more probable [4]. The single-neutron structure is similar to that of $^{298}114$, with shell closures appearing at N=184 for the SLy4, SLy5 and SkI4 sets and N=164 for Skx. The tensor term produces small changes in the spin-orbit splitting around these gaps. However, its effect is not large enough to modify the shell and subshell closures.

The effect of the tensor term on the behaviour of the single-proton shell structures has been calculated across the Z=114 isotopes for a selection of forces (figure 3). In the absence of the tensor term (a) the Z=126 shell gap is the more convincing closure over the full range of isotopes for SLy5, which has an enhanced magnitude around the N=184 shell gap. For SkI4 and Skx it is less clear. Although SkI4 is the only force used within this study that shows a clear agreement with the predictions of macroscopic-microscopic calculations for a Z=114 shell closure, it is known to overestimate the spin-orbit splitting in heavy nuclei such as ^{208}Pb, questioning the reliability of the force when extrapolating into the superheavy region. However, it has been demonstrated that SkI4 is among one of the best forces for describing the properties of superheavy nuclei for which experimental data is available. Skx is one of the few widely used forces in which single-particle data was used to constrain the parameters, rather than simply bulk properties such as binding eneries, radii and masses. The fact that Skx alreday predicts different single-particle structures to most other forces indicates the need for further fits whose motivation is based on an accurate reproduction of single-particle spectra.

Regardless of the predicted shell structures for the different forces in the absence of the tensor term, its inclusion consistently leads to an increase in the spin-orbit splitting of the $2f$ partners, opening the shell gap at Z=114 over the range N=160-200. There is a decrease in splitting at Z=114 beyond N=200 for all three forces due to a lowering of the $f_{5/2}$ level, in agreement with the findings of [35], which uses a Woods-Saxon plus $\pi+\rho$ tensor exchange potential. This work showed a decrease in splitting between the $2f$ partners in nuclei up to N=240, and an increase in spin-orbit splitting at Z=92. This opening at Z=92 is also predicted by Skxtb in figure 3. A decrease in splitting between $1i_{11/2}$ and $3p_{1/2}$ also opens a possible shell gap at Z=138 beyond N=200 in the neutron-rich isotopes.

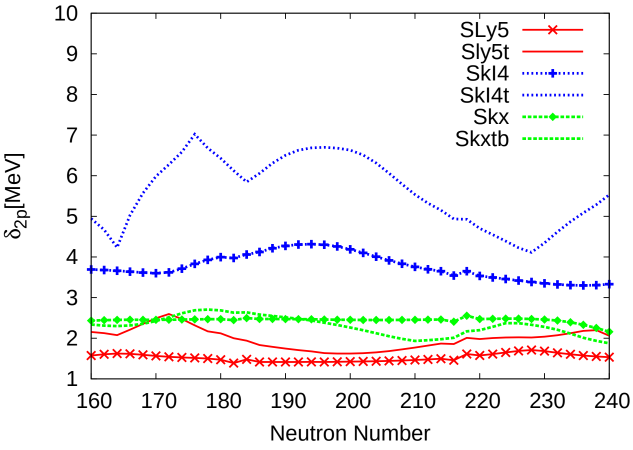

Fig. 4: Two-proton shell gap across the Z=114 isotopes.

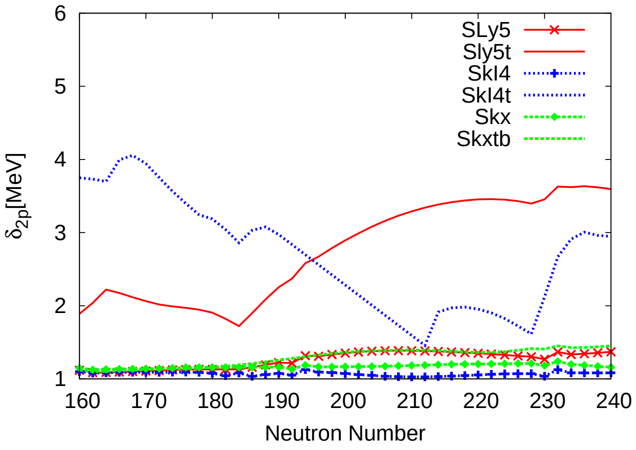

Fig. 5: Two-proton shell gap across the Z=138 isotopes.

This was also reflected in the single-proton spectra across the Z=126 isotopes, although the Z=126 shell gap was significantly decreased in comparison to the Z=114 gap, indicating a clear dependence on proton number.

Perhaps a clearer indicator to quantify the magicity of a given nucleus is given by the two-nucleon shell gap, derived from the total binding energies, $E(N_q)$ [36]

$$\delta_{2q}(N_q) = E(N_q + 2) - 2E(N_q) + E(N_q - 2). \qquad (4)$$

Figure 4 shows the two-proton shell gap calculated for the same forces across the Z=114 isotopes. Once again only SkI4 predicts a clear shell closure for Z=114. However, inclusion of the tensor component generally leads to an increase in δ_{2p} over the full range of isotopes for both SkI4t and SLy5t.

Figure 5 shows a similar calculation across the Z=138 isotopes. In this case the tensor term leads to significant increases (>1MeV) in δ_{2p} for both SLy5t abd SkI4t, although a clear shell closure is only predicted by SLy5t in the range N=200-240 and SkI4t in the range N=160-200. Note that this is not evident from figure 1 since the Z=138 gap is strongly dependent on proton number. Skxtb also shows a small increase δ_{2p} in the more neutron-rich isotopes compared to Skx. However, only for SLy5t is the calculated two proton shell gap larger for the Z=138 isotopes than across the Z=114 nuclei.

In all cases as a consequence of including the tensor component within the calculations, a changed dependence of the shell structure on nucleon number is introduced. This feature is also known to occur in light nuclei, although only at the very limits of stability.

We have investigated the influence of the tensor component of the effective nucleon-nucleon interaction on the single-particle structure of nuclei in the superheavy region within the spherical SHF model. There is evidence for an opening of the Z=114 shell gap over a range of nuclei as a result of the tensor interaction, with δ_{2p} remaining a stable function over the full range of Z=114 isotopes studied. However, the increase in splitting between the $2f$ spin-orbit partners and δ_{2p} function are not conclusive to predict a Z=114 shell closure. This is in agreement with the current experimental status [37], which suggests that a shell closure is more probable around Z=120-126, particularly in neutron-deficient nuclei. The Z=126 shell gap is shown to be strongly dependent on nucleon number, with the tensor term serving to open a possible Z=138 shell closure in neutron-rich isotopes of superheavy elements, although this is again shown to be dependent on neutron number. The predictions for the single-neutron structures remain robust after the inclusion of the tensor term, with either N=184 or N=164 suggested to be possible magic numbers over a range of nuclei.

The strong nucleon number dependence of shell structure in this region is a consequence of the high level density in the superheavy nuclei. The theoretical predictions are therefore sensitive to the details of the individual forces employed. Due to the high ratio of neutrons in these systems, it may also become important to consider the performance of a particular force for describing the density dependence in asymmetric matter, which becomes relevant at the very extremes of nuclear existence. We note that the SLy and SkI4 forces exhibit similar density dependence of both symmetric nuclear matter (SNM) and pure neutron matter (PNM), with SNM remaining energetically favourable at all densities, whereas SkX favours pure neutron matter at high particle densities [38]. Such distinctions as given in [38] may be relavent for the properties of very neutron-rich superheavy nuclei, though further systematic study beyond our present work will be necessary to draw further conclusions. Each of the Skyrme parameter sets in this study was chosen for their particular strengths. SkI4 was chosen for its ability to reproduce the bulk properties of superheavy nuclei for which experimental data is available. However, its overestimation of the spin-orbit splitting in heavy nuclei limits its reliability for studying single-particle properties when extrapolating beyond this region. Both SLy5 and Skx have been forces of choice for investigations into nuclear structure properties with the addition of the tensor force. In the case of SLy5 the tensor coupling strength parameters have been added perturbatively (without refitting the remaining parameters). The conclusions of [22] point out that a complete refit of the entire parameter set is imperative when adding the tensor terms, which is the case for Skxta and Skxtb. However, these forces, including Skx, tend to predict a different ordering of single-particle levels for the superheavy nuclei compared to other common parameter sets.

In order to make more reliable predictions about the single-particle properties of superheavy nuclei, it is therefore essential that further investigations and new fits are made, incorporating missing ingredients such as the tensor term, with an emphasis on reproducing single-particle properties of a wide range of nuclei including the properties of superheavy nuclei for which experimental data is available.

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