Tensor interaction contributions to single-particle energies

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We calculate the contribution of the nucleon-nucleon tensor interaction to single-particle energies with finite-range G-matrix potentials and with zero-range Skyrme potentials. The Skyrme parameters including the zero-range tensor terms with strengths calibrated to the finite-range results are refitted to nuclear properties. The fit allows the zero-range proton-neutron tensor interaction as calibrated to the finite-range potential results which gives the observed change in the single-particle gap \( \epsilon(h\ell_{1/2}) - \epsilon(g\ell_{1/2}) \) going from \( ^{114}\text{Sn} \) to \( ^{132}\text{Sn} \). However, the experimental \( \ell \) dependence of the spin-orbit splittings in \( ^{132}\text{Sn} \) and \( ^{208}\text{Pb} \) is not well described when the tensor is added, owing to a change in the radial dependence of the total spin-orbit potential. The gap shift and a good fit to the \( \ell \) dependence can be recovered when the like-particle tensor interaction is opposite in sign to that required for the G matrix.

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The tensor force between nucleons is important for single-particle energy spacing and the shell structure of nuclei obtained from shell-model configuration interaction models of nuclei [1, 2]. But, except for an early exploratory work [3], its role in Hartree-Fock models has been neglected. Results for relative energy shifts have recently been obtained with a finite-range tensor in the Gogny model [4]. In this Rapid Communication we present the first systematic results for a Skyrme-type interaction with a zero-range tensor interaction from a global fit to nuclear data including data for single-particle energies. We start by calibrating the strength of the zero-range tensor with results obtained from a G-matrix interaction. Then the Skyrme parameters plus the tensor parameters are varied to obtain a best fit to data. We find that the fit will allow an isovector tensor similar to that expected from the G matrix. But the data set prefers an isoscalar tensor that is much smaller than expected from the G matrix. The reason is traced to a difference between the Skyrme spin-orbit and tensor radial shapes in the doubly closed-shell nuclei \( ^{132}\text{Sn} \) and \( ^{208}\text{Pb} \).

First we calculated the contribution to the single-particle proton energy for single-particle states above the \( Z = 50 \) closed shell from the tensor part of the Hosaka-Kubo-Toki (HKT) G matrix [5]. HKT is a one-boson exchange potential that reproduces the G-matrix elements obtained from the Paris potential. This interaction has the form

\[
V' = S_{12} \sum_{i,T} W_i, T \left\{ \frac{1 + 3 \kappa}{2 x_i^2} - \frac{3}{x_i^2} \right\} \frac{e^{-x_i}}{x_i},
\]

where

\[
S_{12} = \frac{5}{3} \left( \Delta \cdot \hat{r} \right) \Delta \cdot \hat{r} - \left( \Delta \cdot \hat{r} \right)^2 = Y^{(2)}(\hat{r}) \cdot \sqrt{\frac{24 \pi}{5}} [\Delta \otimes \Delta]^2,
\]

and \( x_i = r_i / r_i \), where \( r_i \) are the range parameters. This interaction consists of the one-pion exchange potential with \( r_\pi = 1.414 \text{ fm} \), \( W_{i,T=0}/W_{i,T=1} = -3 \), and \( W_{i,T=1} = 3.49 \text{ MeV} \) plus a short-range potential with \( r_s = 0.25 \text{ fm} \) and with the strengths \( W \) determined from the G-matrix elements: \( W_{i,T=0} = 3105 \text{ MeV} \) and \( W_{i,T=1} = -1382 \text{ MeV} \).

The contributions to the proton single-particle states for \( ^{132}\text{Sn} \) are shown in Table I. They were obtained with harmonic oscillator radial wave functions with \( h\omega = 7.87 \text{ MeV} \). (The results with the tensor part of the M3Y potential [6] are the same as HKT within about 3%). The contribution to the single-particle energy of the valence proton in orbital \( k = (n, \ell, j) \) from the core protons is obtained from

\[
(2j + 1)E_{kp}^t = \sum_{k',T}(2j + 1)V_{k,k',J,T=1}^t,
\]

and from the core neutrons from

\[
(2j + 1)E_{kn}^t = \sum_{k,T}(1 + \delta_{k,k'}) \frac{1}{2}(2j + 1)V_{k,k',J,T}^t,
\]

where the two-body matrix elements are

\[
V_{k,k',J,T}^t = \langle k, k', J, T | V' | k, k', J, T \rangle.
\]

In the sum over the core orbitals \( k' \) the contributions from the sum of \( j_{k'} = \ell + 1/2 \) and \( j_{k'} = \ell - 1/2 \) orbitals pairs cancel when both are filled, as shown in Eq. (4) of Ref. [2]. Thus the \( E_{kp}^t \) are zero for LS closed cores. For non-LS closed cores with a pair of valence orbits with \( j_\nu = \ell + 1/2 \) and \( j_\nu = \ell - 1/2 \) the energy shifts are \( (2j_\nu + 1)E_{k,q}^t = -(2J_\nu + 1)E_{k,q}^t \), which means that for a given \( \ell \) value the tensor interaction with the core contributes to the effective spin-orbit splitting (see Eq. (4) of Ref. [2]). The short-range contribution \( s \) to the energy shifts are given in the middle part of Table I. One observes the change in sign, which is related to the partial cancellation of the \( \pi \)-exchange potential by the
TABLE I. Contributions of the tensor finite-range $G$-matrix interaction to single-particle proton energies in $^{132}\text{Sn}$. The results are given for $E_1^{kn}$: contribution from the $0g_{7/2}$ proton orbital, $E_2^{kn}(100)$: contribution from the $0g_{7/2}$ neutron orbital, $E_4^{kn}(114)$: $E_1^{kn}(100)$ plus the contribution from the $0g_{7/2}$ and $1d_{5/2}$ neutron orbitals, and $E_4^{k}$: $E_4^{kn}(114)$ plus the contribution from the $1d_{3/2}$ and $0h_{11/2}$ neutron orbitals. The short-range tensor contribution is given by the “$s$-only” results.

<table>
<thead>
<tr>
<th>Type</th>
<th>$k = (n\ell_j)$</th>
<th>$E_1^{kn}$ (MeV)</th>
<th>$E_2^{kn}(100)$ (MeV)</th>
<th>$E_4^{kn}(114)$ (MeV)</th>
<th>$E_1^{kn}(100)$ (MeV)</th>
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<tbody>
<tr>
<td>$\pi + s$</td>
<td>$0g_{7/2}$</td>
<td>-0.458</td>
<td>-1.009</td>
<td>-0.135</td>
<td>-1.032</td>
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<td></td>
<td>$1d_{5/2}$</td>
<td>0.078</td>
<td>0.180</td>
<td>0.395</td>
<td>0.218</td>
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<tr>
<td></td>
<td>$1d_{3/2}$</td>
<td>-0.118</td>
<td>-0.270</td>
<td>-0.593</td>
<td>-0.328</td>
</tr>
<tr>
<td></td>
<td>$0h_{11/2}$</td>
<td>0.308</td>
<td>0.688</td>
<td>0.109</td>
<td>0.848</td>
</tr>
<tr>
<td>$s$ only</td>
<td>$0g_{7/2}$</td>
<td>0.251</td>
<td>0.408</td>
<td>0.072</td>
<td>0.465</td>
</tr>
<tr>
<td></td>
<td>$1d_{5/2}$</td>
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<td>-0.097</td>
<td>-0.162</td>
<td>-0.100</td>
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<tr>
<td></td>
<td>$1d_{3/2}$</td>
<td>0.090</td>
<td>0.145</td>
<td>0.243</td>
<td>0.150</td>
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<td>$0h_{11/2}$</td>
<td>-0.191</td>
<td>-0.310</td>
<td>-0.050</td>
<td>-0.397</td>
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<tr>
<td>$s + \pi$</td>
<td>$0g_{7/2}$</td>
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<td>-2.48</td>
<td>-1.88</td>
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<td></td>
<td>$1d_{5/2}$</td>
<td>-1.31</td>
<td>-1.86</td>
<td>-2.44</td>
<td>-2.18</td>
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<td>$1d_{3/2}$</td>
<td>-1.31</td>
<td>-1.86</td>
<td>-2.44</td>
<td>-2.18</td>
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<tr>
<td></td>
<td>$0h_{11/2}$</td>
<td>-1.62</td>
<td>-2.22</td>
<td>-2.18</td>
<td>-2.14</td>
</tr>
</tbody>
</table>

short-range potential. The variation of the ratio over several valence orbitals shown at the bottom of Table I is a measure of how well the finite-range tensor can be approximated by a zero-range form. This is important since the zero-range approximation leads to an analytic form for the tensor density functional and an efficient implementation in the Skyrme Hartree-Fock method [3]. The ratio varies, by up to a factor of 2, depending on which orbits are filled in the core. But in the case of the total energy for protons in $^{132}\text{Sn}$ the orbit dependence in the ratio is small.

One observes from Table I that the tensor interaction results in a change in the $0g_{7/2}$-$0h_{11/2}$ gap going from $^{114}\text{Sn}$ (e.g., where only the $1d_{5/2}$ and $0g_{7/2}$ orbitals are filled) to $^{132}\text{Sn}$ of 1.64 MeV. $^{132}\text{Sn}$ is one of the best known doubly magic nuclei, and the lowest levels in $^{133}\text{Sn}$ are thus taken as single-particle states for adding a proton to $^{132}\text{Sn}$, although the experimental measurement of spectroscopic strength from one-proton transfer reactions has not yet been carried out. The single-particle proton energies for $^{132}\text{Sn}$ are given in Table II.

Proton transfer experiments have been carried out for $^{114}\text{Sn}$ to $^{115}\text{Sb}$. But the interpretation of the experimental results in terms of single-particle energies is not so simple since the neutron configuration in $^{114}\text{Sn}$ is not magic with significant configuration mixing between the lowest neutron orbits of $0g_{7/2}$ and $1d_{5/2}$ and the upper orbits of $1d_{3/2}$, $2s_{1/2}$, and $0h_{11/2}$. To estimate the effect of splitting of single-particle strength we carry out a large-basis shell-model calculation that includes up to three neutrons being excited from the lower to the upper orbits with the renormalized $G$-matrix interaction from Ref. [7]. The spectroscopic strength obtained is shown

TABLE II. Proton single-particle energies in $^{114}\text{Sn}$ and $^{132}\text{Sn}$. The gap is the energy difference between $0g_{7/2}$ and $0h_{11/2}$.

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>$n\ell_j$</th>
<th>Exp. lowest $J$ (MeV)</th>
<th>Exp. centroid (MeV)</th>
<th>Skx (MeV)</th>
<th>Skxta (MeV)</th>
<th>Skxtb (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{132}\text{Sn}$</td>
<td>0$g_{7/2}$</td>
<td>-9.68</td>
<td>-9.68</td>
<td>-9.87</td>
<td>-10.82</td>
<td>-9.86</td>
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<tr>
<td></td>
<td>1$d_{5/2}$</td>
<td>-8.72</td>
<td>-8.72</td>
<td>-9.20</td>
<td>-9.22</td>
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</tr>
<tr>
<td></td>
<td>1$d_{3/2}$</td>
<td>-6.97</td>
<td>-6.97</td>
<td>-7.38</td>
<td>-7.50</td>
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<tr>
<td></td>
<td>2$s_{1/2}$</td>
<td>-6.89</td>
<td>-6.89</td>
<td>-6.82</td>
<td>-6.93</td>
<td>-6.78</td>
</tr>
<tr>
<td></td>
<td>$0h_{11/2}$ gap</td>
<td>2.79</td>
<td>2.79</td>
<td>2.84</td>
<td>4.52</td>
<td>3.20</td>
</tr>
<tr>
<td>$^{114}\text{Sn}$</td>
<td>0$g_{7/2}$</td>
<td>-3.01</td>
<td>-2.48</td>
<td>-2.78</td>
<td>-2.70</td>
<td>-1.59</td>
</tr>
<tr>
<td></td>
<td>1$d_{5/2}$</td>
<td>-3.73</td>
<td>-3.02</td>
<td>-2.91</td>
<td>-2.81</td>
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</tr>
<tr>
<td></td>
<td>1$d_{3/2}$</td>
<td>-2.66</td>
<td>-1.63</td>
<td>-0.88</td>
<td>-1.06</td>
<td>-1.16</td>
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<td></td>
<td>2$s_{1/2}$</td>
<td>-2.96</td>
<td>-1.32</td>
<td>-0.81</td>
<td>-0.87</td>
<td>-0.85</td>
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<tr>
<td></td>
<td>$0h_{11/2}$ gap</td>
<td>0.58</td>
<td>1.03</td>
<td>2.97</td>
<td>2.81</td>
<td>0.83</td>
</tr>
</tbody>
</table>

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in Fig. 1. One observes that the lowest $J = j$ states contain the largest fraction of single-particle strength but that there is significant spreading to higher energy. The isolation of one large part of the spectroscopic strength into the lowest state is consistent with experimental observation [8]. This spreading is due to coupling with the neutron vibrations within the $0g_{7/2}, 1d_{5/2}, 1d_{3/2}, 1s_{1/2}, h_{11/2}$ model space as well as isospin splitting of the strength to the $T_2 = 15/2$ states. The centroid energies obtained from the results of Fig. 1 are within about 10 keV of the single-particle energies obtained with the simplest \([\nu, 0g_{7/2}, 1d_{5/2}] [\pi_{n,\ell,j}]\) configuration. This simple configuration is the one assumed for the finite-range tensor contribution already discussed as well as for the Skyrme Hartree-Fock calculations to be discussed in the following. (This configuration does not necessarily have good isospin, but configuration mixing restores isospin.) To estimate the proton single-particle energies in $^{115}$Sb we add a correction to the separation energy of the lowest states of a given $J = j$ in the experimental spectrum based on the configuration mixing results of Fig. 1, giving the experimental centroid energies in column 3 of Table II.

In addition to configuration mixing within the $0g_{7/2}, 1d_{5/2}, 1d_{3/2}, 1s_{1/2}, h_{11/2}$ model space, one could consider the effects of protons excited across the $Z = 50$ shell gap and neutrons excited across the $N = 50$ and $N = 82$ shell gaps. The proton excitations have a direct effect on enhancing the $B(E2)$ values for low-lying $2^+$ states of Sn [9]. This type of configuration mixing affects single-particle energies for all of the Sn isotopes, including those for $^{131}$Sb. However, this is already partly accounted for in Skx with its empirical effective mass of near unity [10]. The enhancement of the bare $G$-matrix effective mass of $m^*/m = 0.6–0.7$ toward its empirical value of near unity in Skx can be attributed to coupling with the multipole vibrations of the core [11,12].

The experimental centroid energies are compared with the results of Skyrme Hartree-Fock calculations in Table II. The Skx interaction [10] was obtained from a fit to binding energies, rms charge radii, and single-particle energies, including those for the $^{132}$Sn core [10]. Thus the rather good agreement between the experimental and Skx proton single-particle energies for $^{132}$Sn is not an accident. The $^{114}$Sn data were not included in the original Skx fit since, as discussed, this does not have a magic neutron number. However, the agreement with the centroid energies is not bad except for the $0h_{11/2}$.

The gap between the $0h_{11/2}$ and $0g_{7/2}$ single-particle energies is particularly sensitive to the tensor interaction. Experimentally the gap changes by 1.76 MeV: from 2.79 MeV in $^{132}$Sn to 1.03 MeV in $^{114}$Sn. The gap for Skx is about the same for $^{114}$Sn and $^{132}$Sn and this is similar to what we find for other Skyrme interactions. But the finite-range tensor interaction discussed here leads to a gap shift of 1.64 MeV—close to the observed shift of 1.76 MeV and to the values shown in Fig. 4 (d) of Ref. [2] and Fig. 4 of Ref. [4]. Thus we are motivated to add a tensor interaction to the Skyrme functional.

We use the zero-range form of the tensor potential given by Stancu et al. [3] [Eq. (1) of their paper]. The zero-range tensor gives an additional contribution to the one-body spin-orbital potential of the form

$$\Delta W_n = \alpha J_n + \beta J_p, \quad \Delta W_p = \alpha J_p + \beta J_n,$$

where the coefficients $\alpha$ and $\beta$ (given in units of MeV fm$^5$) come from the zero-range form of the tensor interaction ($\alpha_t$ and $\beta_t$) as well as from the exchange part of the central interaction:

$$\alpha_t = \frac{1}{8}(t_1 - t_2) - \frac{1}{8}(t_1 x_1 + t_2 x_2)$$

and

$$\beta_t = -\frac{1}{8}(t_1 x_1 + t_2 x_2).$$

The $J_q$ are the spin densities defined by

$$J_q(r) = \frac{1}{4\pi r^2} \sum_a (2j_a + 1) \times [j_a(j_a + 1) - \ell_a(\ell_a + 1) - \frac{3}{4}] R_a^2(r),$$

where the sum is over the occupied orbits with protons ($q = p$) or neutrons ($q = n$).

We start with the Skx interaction [10] and the data base that was used to determine its parameters. Skx is the only interaction for which a large number of experimental single-particle energies were used to constrain the parameters. As a baseline for our new fits, Skx gives a $\chi^2$ value of 0.60 when the parameters $t_0, t_1, t_2, t_3, x_0, x_1, x_2, x_3$, and $W_{so}$ are fitted
to the data set of [10]. For this original Skx the $\alpha_c$ and $\beta_c$ terms were not included. If they are included, the $\chi^2$ increases slightly to 0.62 and the central-exchange values are $\alpha_c = 24$ and $\beta_c = -23$.

For the tensor contribution, the initial set of $\alpha_t$ and $\beta_t$ parameters were chosen to reproduce the calculated $E^t_{sk}$ and $E^t_{xt}$ values for the $0g_{7/2}$ proton orbit from the finite-range $G$ matrix given in Table I. The results are $\alpha_t = 60$ and $\beta_t = 110$. These are larger than the Skx central-exchange values of $\alpha_c = 24$ and $\beta_c = -23$, but both should be considered for the total and the refits we carry out include the effects of $\alpha_t$ and $\beta_t$. For comparison with Stancu et al. [3], our values of $\alpha_t$ and $\beta_t$ are close to those they estimate from the interaction of Sprung and Banerjee [13] with $q = 1.0$ fm$^{-1}$ (Table I of Ref. [3]).

The Skyrme parameters $t_0$, $t_1$, $t_2$, $x_0$, $x_1$, $x_2$, $x_3$, and $W_{so}$ were then refit for these fixed values of $\alpha_t$ and $\beta_t$ and the resulting set of parameters were called Skxta. The $\chi^2$ value increased significantly to 1.50. The contributions from the zero-range tensor and central-exchange and spin-orbit interactions to the proton single-particle energies in $^{132}$Sn are shown in Table III. The central exchange values from the fit are $\alpha_c = 33$ and $\beta_c = -16$.

The single-particle energies for orbitals around $^{132}$Sn obtained with Skx and Skxta are shown in Figs. 2 and 3, respectively. Comparison of these figures shows that the $\chi^2$ increase is due to a poorer $\ell$ dependence of the spin-orbit splitting for Skxta compared to Skx. This can be traced to a difference in the radial functional form of the spin-orbit contributions that are shown in Fig. 4. The tensor contribution peaks at a 0.5-fm smaller radius compared to the Skyrme spin-orbit potential. Since the tensor contribution with $\alpha_t = 60$ and $\beta_t = 110$ is opposite in sign to the normal spin-orbit potential, the strength of the Skyrme spin-orbit parameter $W_{so}$ has to increase by about 20% to recover an overall fit to the single-particle energy data. But the $\ell$ dependence of the single-particle energy data. But the $\ell$ dependence of the

<table>
<thead>
<tr>
<th>$n\ell_j$</th>
<th>$E_{ip}^{sk}$ (MeV)</th>
<th>$E_{ix}^{sk}$ (MeV)</th>
<th>$E^{so}$ (MeV)</th>
<th>Total (MeV)</th>
<th>$E^{so}$ (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0g_{7/2}$</td>
<td>$-0.723$ ($-0.476$)</td>
<td>$-0.828$ ($-0.984$)</td>
<td>$3.20$</td>
<td>$1.65$</td>
<td>$2.64$</td>
</tr>
<tr>
<td>$1d_{5/2}$</td>
<td>$0.117$ ($-0.079$)</td>
<td>$0.089$ ($0.094$)</td>
<td>$-0.83$</td>
<td>$-0.62$</td>
<td>$-0.68$</td>
</tr>
<tr>
<td>$1d_{3/2}$</td>
<td>$-0.181$ ($-0.121$)</td>
<td>$-0.158$ ($-0.171$)</td>
<td>$1.34$</td>
<td>$1.00$</td>
<td>$1.11$</td>
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<tr>
<td>$0h_{11/2}$</td>
<td>$0.640$ ($-0.421$)</td>
<td>$0.864$ ($1.034$)</td>
<td>$-3.84$</td>
<td>$-2.34$</td>
<td>$-3.19$</td>
</tr>
</tbody>
</table>

FIG. 2. Comparison of experimental and theoretical single-particle energies in $^{132}$Sn for the Skx interaction.

FIG. 3. Comparison of experimental and theoretical single-particle energies in $^{132}$Sn for the Skxta interaction.
Experimental single-particle energies is better reproduced with the Skyrme spin-orbit shape. The quality of the Skx and Skxta fit results for single-particle energies around $^{208}$Pb are similar to those we show for $^{132}$Sn.

Given that $\beta_t = 110$ is needed to reproduce the shift of the $0_{7/2}^+ - 0_{5/2}^+$ gap going from $^{114}$Sn to $^{132}$Sn, we next fix $\beta_t = 110$ and include $\alpha_c$ in the Skyrme fit to the data. We recover a good fit of $\chi^2 = 0.63$ with $\alpha_c = -118$ for a parameter set we call Skxtb. In general we find a good fit with values of $\beta_t$ in the range of 0 to 110 as long as $\alpha_c \approx -\beta_t$. This happens because the proton and neutron contributions then cancel in the $jj$ closed shell nuclei $^{132}$Sn and $^{208}$Pb, giving the good reproduction of the single-particle energies from the Skyrme spin-orbit shape. The Skxtb single-particle energies are compared with experiment in Table II. Skxtb gives a best account of the $^{132}$Sn single-particle energies and the $0_{7/2}^+ - 0_{5/2}^+$ gap shift. However, the absolute single-particles energies in $^{114}$Sn still differ from experiment by as much as one MeV.

In conclusion, we find that the finite-range tensor interaction is important for the $0_{7/2}^+ - 0_{5/2}^+$ gap shift. However, a zero-range implementation of the tensor interaction in the Skyrme interaction is problematic. The radial form of the tensor contribution to the spin-orbit potential does not give a good reproduction of the $\ell$ dependence of the spin-orbit splittings in $^{132}$Sn and $^{208}$Pb. Reproduction of the observed $0_{7/2}^+ - 0_{5/2}^+$ gap shift plus a good fit to absolute single-particle energies in $^{132}$Sn and $^{208}$Pb requires $\beta_t \approx 110$ for the proton-neutron tensor interaction (consistent with the $G$-matrix value) and $\alpha_c \approx -\beta_t$ for the $T = 1$ tensor interaction between like particles, which is opposite in sign to the $G$ matrix value of $\alpha_c \approx 60$. Although our finite-range calculations indicate that the zero-range approximation may be adequate, further investigation is required. Also we need to understand the role of correlations (coupling to vibrations) and three-body forces on the effective tensor interactions in nuclei. The central part of the Skyrme functional also needs to be constrained and extended to reproduce realistic properties of nuclear matter [14]. These changes may lead to different values for $\alpha_c$ and $\beta_t$ than those obtained with Skx that also need to be taken into account when the tensor interaction is included.

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