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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 Skx 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 $\epsilon(h_{11/2})$-$\epsilon(g_{7/2})$ going from ^{114}Sn to ^{132}Sn. However, the experimental ℓ dependence of the spin-orbit splittings in ^{132}Sn and ^{208}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 ℓ 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 strength 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}Sn and ^{208}Pb.

First we calculated the contribution to the single-particle proton energies 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 tensor interaction has the form

$$V^t = S_{12} \sum_{i,T} W_{i,T} \left\{ 1 + \frac{3}{x_i} + \frac{3}{x_i^2} \right\} \frac{e^{-x_i}}{x_i}, \tag{1}$$

where

$$S_{12} = 3(\vec{\sigma}_1 \cdot \hat{r})(\vec{\sigma}_2 \cdot \hat{r}) - (\vec{\sigma}_1 \cdot \vec{\sigma}_2) = Y^{(2)}(\hat{r}) \cdot \sqrt{\frac{24\pi}{5}} [\vec{\sigma}_1 \otimes \vec{\sigma}_2]^{(2)}$$

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

The contributions to the proton single-particle states for ^{132}Sn are shown in Table I. They were obtained with harmonic oscillator radial wave functions with $\hbar\omega = 7.87$ 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

$$(2j + 1)E^t_{kp} = \sum_{k',J} (2J + 1)V^t_{k,k',J,T=1}, \tag{2}$$

and from the core neutrons from

$$(2j + 1)E^t_{kn} = \sum_{k',J,T} \frac{1 + \delta_{k,k'}}{2} (2J + 1)V^t_{k,k',J,T}, \tag{3}$$

where the two-body matrix elements are $V^t_{k,k',J,T} = \langle k, k', J, T \mid V^t \mid k, k', J, T \rangle$.

In the sum over the core orbitals k' the contributions from the sum of $j'_> = \ell' + 1/2$ and $j'_< = \ell' - 1/2$ orbital pairs cancel when both are filled, as shown in Eq. (4) of Ref. [2]. Thus the E^t_{kq} are zero for LS closed cores. For non-LS closed cores with a pair of valence orbits with $j_> = \ell + 1/2$ and $j_< = \ell - 1/2$ the energy shifts are $(2j_> + 1)E^t_{k_>q} = -(2j_< + 1)E^t_{k_<q}$, which means that for a given ℓ 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 π-exchange potential by the

TABLE I. Contributions of the tensor finite-range G-matrix interaction to single-particle proton energies in ^{132}Sn. The results are given for E^t_{kp} : contribution from the $0g_{9/2}$ proton orbital, $E^t_{kn}(100)$: contribution from the $0g_{9/2}$ neutron orbital, $E^t_{kn}(114)$: $E^t_{kn}(100)$ plus the contribution from the $0g_{7/2}$ and $1d_{5/2}$ neutron orbitals, and E^t_{kn} : $E^t_{kn}(114)$ 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.

Type	$k=(n\ell_j)$	E^t_{kp} (MeV)	$E^t_{kn}(100)$ (MeV)	$E^t_{kn}(114)$ (MeV)	E^t_{kn} (MeV)	$E^t_{kp}+E^t_{kn}$ (MeV)
$\pi+s$	$0g_{7/2}$	−0.458	−1.009	−0.135	−1.032	−1.490
	$1d_{5/2}$	0.078	0.180	0.395	0.218	0.296
	$1d_{3/2}$	−0.118	−0.270	−0.593	−0.328	−0.446
	$0h_{11/2}$	0.308	0.688	0.109	0.848	1.156
s only	$0g_{7/2}$	0.251	0.408	0.072	0.465	0.716
	$1d_{5/2}$	−0.060	−0.097	−0.162	−0.100	−0.160
	$1d_{3/2}$	0.090	0.145	0.243	0.150	0.240
	$0h_{11/2}$	−0.191	−0.310	−0.050	−0.397	−0.588
$\frac{\pi+s}{s}$	$0g_{7/2}$	−1.82	−2.48	−1.88	−2.22	−2.08
	$1d_{5/2}$	−1.31	−1.86	−2.44	−2.18	−1.85
	$1d_{3/2}$	−1.31	−1.86	−2.44	−2.18	−1.88
	$0h_{11/2}$	−1.62	−2.22	−2.18	−2.14	−1.97

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}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}Sn (e.g., where only the $1d_{5/2}$ and $0g_{7/2}$ orbitals are filled) to ^{132}Sn of 1.64 MeV. ^{132}Sn is one of the best known doubly magic nuclei, and the lowest levels in ^{133}Sb are thus taken as single-particle states for adding a proton to ^{132}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}Sn are given in Table II.

Proton transfer experiments have been carried out for ^{114}Sn to ^{115}Sb. But the interpretation of the experimental results in terms of single-particle energies is not so simple since the neutron configuration in ^{114}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}Sn and ^{132}Sn. The gap is the energy difference between $0g_{7/2}$ and $0h_{11/2}$.

Nucleus	$n\ell_j$	Exp. lowest J (MeV)	Exp centroid (MeV)	Skx (MeV)	Skxta (MeV)	Skxtb (MeV)
^{132}Sn	$0g_{7/2}$	−9.68	−9.68	−9.87	−10.82	−9.86
	$1d_{5/2}$	−8.72	−8.72	−9.20	−9.22	−9.30
	$1d_{3/2}$	−6.97	−6.97	−7.38	−7.50	−7.14
	$2s_{1/2}$			−6.82	−6.93	−6.78
	$0h_{11/2}$	−6.89	−6.89	−6.92	−6.08	−6.66
	gap	2.79	2.79	2.84	4.52	3.20
^{114}Sn	$0g_{7/2}$	−3.01	−2.48	−2.78	−2.70	−1.59
	$1d_{5/2}$	−3.73	−3.02	−2.91	−2.81	−2.66
	$1d_{3/2}$	−2.66	−1.63	−0.88	−1.06	−1.16
	$2s_{1/2}$	−2.96	−1.32	−0.81	−0.87	−0.85
	$0h_{11/2}$	−2.43	−1.45	0.19	0.11	−0.76
	gap	0.58	1.03	2.97	2.81	0.83

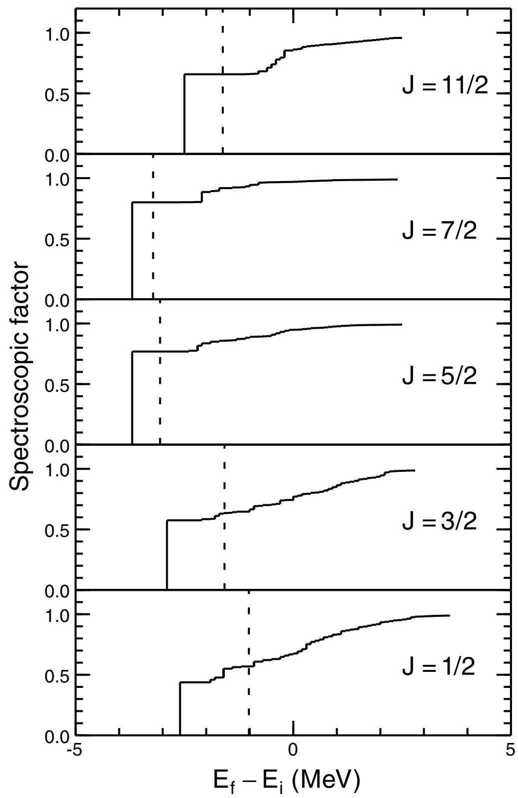

FIG. 1. Single-particle proton spectroscopic factors for ^{114}Sn to ^{115}Sb from the shell-model calculations. The lines for each n, ℓ, j value correspond to the cumulative sum of spectroscopic strength as a function of the energy difference $E_f - E_i$. The centroid energies are indicated by the dashed lines.

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 $T_> = 15/2$ 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 $[\nu, 0g^8_{7/2}, 1d^6_{5/2}][\pi_{n,\ell,j}]$ 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 ^{133}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

$$\Delta W_n = \alpha J_n + \beta J_p, \quad \Delta W_p = \alpha J_p + \beta J_n, \tag{4}$$

where the coefficients α and β (given in units of MeV fm^5) come from the zero-range form of the tensor interaction (α_t and β_t) as well as from the exchange part of the central interaction:

$$\alpha_c = \tfrac{1}{8}(t_1 - t_2) - \tfrac{1}{8}(t_1 x_1 + t_2 x_2) \tag{5}$$

and

$$\beta_c = -\tfrac{1}{8}(t_1 x_1 + t_2 x_2). \tag{6}$$

The J_q are the spin densities defined by

$$J_q(r) = \frac{1}{4\pi r^3} \sum_\alpha (2j_\alpha + 1) \times \left[j_\alpha(j_\alpha + 1) - \ell_\alpha(\ell_\alpha + 1) - \frac{3}{4} \right] R^2_\alpha(r),$$

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 χ^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

TABLE III. Contributions to proton single-particle energies in ^{132}Sn for the Skxta and Skx Hartree-Fock calculations. E^t is the total tensor contribution with $\alpha = 93$ and $\beta = 94$, with the zero-range tensor interaction contribution for $\alpha_t = 60$ and $\beta_t = 110$ shown in brackets. E^{so} is the spin-orbit potential contribution to the energy. The total for Skxta $E^t_{kp} + E^t_{kn} + E^{so}$ is compared with the spin-orbit for Skx.

$n\ell_j$	E^t_{kp} Skxta (MeV)	E^t_{kn} Skxta (MeV)	E^{so} Skxta (MeV)	Total Skxta (MeV)	E^{so} Skx (MeV)
$0g_{7/2}$	−0.723 (−0.476)	−0.828 (−0.984)	3.20	1.65	2.64
$1d_{5/2}$	0.117 (−0.079)	0.089 (0.094)	−0.83	−0.62	−0.68
$1d_{3/2}$	−0.181 (−0.121)	−0.158 (−0.171)	1.34	1.00	1.11
$0h_{11/2}$	0.640 (−0.421)	0.864 (1.034)	−3.84	−2.34	−3.19

to the data set of [10]. For this original Skx the α_c and β_c terms were not included. If they are included, the χ^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 α_t and β_t parameters were chosen to reproduce the calculated E^t_{pk} and E^t_{nk} 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 α_c and β_c. For comparison with Stancu *et al.* [3], our values of α_t and β_t are close to those they estimate from the interaction of Sprung and Banerjee [13] with $q = 1.0$ fm^{-1} (Table 1 of Ref. [3]).

The Skyrme parameters $t_0, t_1, t_2, t_3, x_0, x_1, x_2, x_3$, and W_{so} were then refit for these fixed values of α_t and β_t and the resulting set of parameters were called Skxta. The χ^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 χ^2 increase is due to a poorer ℓ 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 contribution, 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 ℓ dependence of the

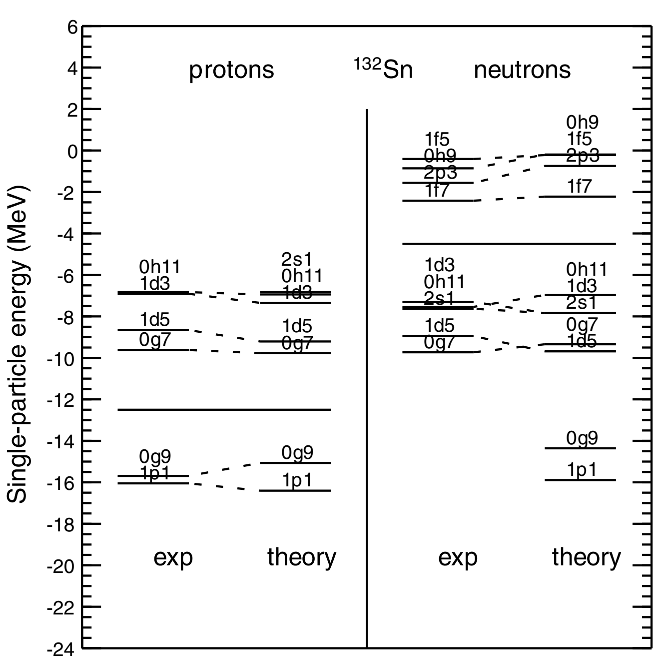

FIG. 2. Comparison of experimental and theoretical single-particle energies in ^{132}Sn for the Skx interaction.

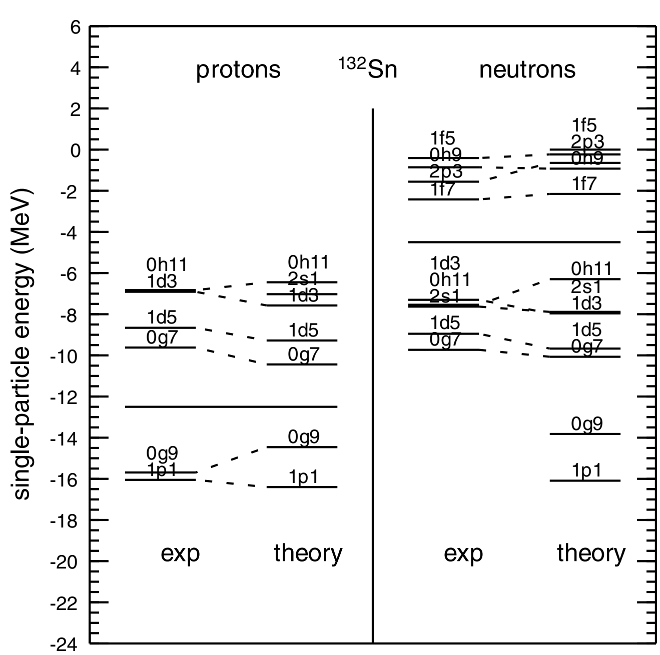

FIG. 3. Comparison of experimental and theoretical single-particle energies in ^{132}Sn for the Skxta interaction.

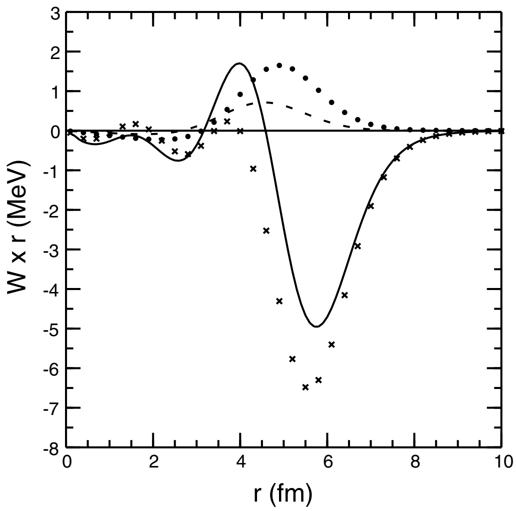

FIG. 4. Spin-orbit potentials for protons in ^{132}Sn for the Skxta interaction: the Skyrme spin-orbit potential (crosses); the zero-range tensor contributions from the core protons (dashed line) and core neutrons (dotted line); and the total (solid line). The total also includes the smaller α_c and β_c terms from the exchange part of the central 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 $0g_{7/2}$-$0h_{11/2}$ gap going from ^{114}Sn to ^{132}Sn, we next fix $\beta_t = 110$ and include α_t in the Skyrme fit to the data. We recover a good fit of $\chi^2 = 0.63$ with $\alpha_t = -118$ for a parameter set we call Skxtb. In general we find a good fit with values of β_t in the range of 0 to 110 as long as $\alpha_t \approx -\beta_t$. 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 $0g_{7/2}$-$0h_{11/2}$ 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 $0g_{7/2}$-$0h_{11/2}$ gap shift. However, a zero-range implementation of the tensor interaction in the Skryme interaction is problematic. The radial form of the tensor contribution to the spin-orbit potential does not give a good reproduction of the ℓ dependence of the spin-orbit splittings in ^{132}Sn and ^{208}Pb. Reproduction of the observed $0g_{7/2}$-$0h_{11/2}$ 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 $\alpha_t \approx -\beta_t$ for the $T = 1$ tensor interaction between like particles, which is opposite in sign to the G matrix value of $\alpha_t \approx 60$. 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 α_c and β_c than those obtained with Skx that also need to be taken into account when the tensor interaction is included.

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