Evolution of nuclear shells with the Skyrme density dependent interaction

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Abstract

We present the evolution of the shell structure of nuclei in Hartree-Fock calculations using Skyrme’s density-dependent effective nucleon-nucleon interaction. The contribution of the tensor part of the Skyrme interaction to the Hartree-Fock spin-orbit splitting in spherical spin unsaturated nuclei is reanalyzed.

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I. INTRODUCTION

The shell structure is a distinctive feature of nuclei and is characterized by the existence of magic numbers which are a consequence of the spin-orbit interaction [1, 2]. The spin-orbit interaction can be understood in a mean field approach which leads to a one-body potential containing a central part and a spin-orbit part. In spin-saturated nuclei the spin-orbit part stems from the spin-orbit nucleon-nucleon interaction. In spin unsaturated nuclei there are additional contributions coming either from the exchange part of the central two-body force or from the tensor force. In view of the recent progress related to the discovery of exotic nuclei (neutron or proton rich) a major problem is to understand how the shell structure evolves from stable to unstable nuclei. Presently there is much concern about the role of the tensor force in the shell evolution and the structure of exotic nuclei [6–11].

In a previous work [3] we estimated the contribution of the tensor part of the Skyrme interaction to the Hartree-Fock spin-orbit splitting in several magic nuclei and adjusted the strength of the tensor force such as to obtain a good global fit. In the present paper we extend the previous study to exotic nuclei, most of which were unknown at that time. This extension sheds a new light on the previous results.

The tensor term in the Skyrme interaction is written as a $\delta$-function in the internucleon separation multiplied by momentum dependent terms. The momentum dependence takes the finite range of the interaction into account. Contrary to the view that it plays a minor role because of its $\delta$-type structure [6], this interaction has the same effect as a finite size interaction due to its momentum dependence. We will show that the Skyrme interaction provides a good mechanism for describing the evolution of the shell structure in exotic nuclei.

Otsuka et al. [6] have pointed out that the nuclear tensor force has a rather long range and that the use of the energy density (1) may not be justified. The goal of the present paper is to show that expressions (1) of section 1 together with (16) and (17) given in section 2 of this paper can still be used to study the contribution of finite range tensor forces, even if the range is that of the one-pion exchange force. Shell gaps are mainly determined by the spin-orbit splitting of the states with highest $l$ in any shell and our study is restricted to these states. The spin-orbit splitting is less important in states with lower $l$ because it is hidden by pairing effects and other forms of configuration mixing.

In section 3 of this paper we derive an expression for the leading contribution of the
tensor force to the Skyrme energy density functional using some results from the paper of Negele and Vautherin [14] on the density matrix expansion method. Section 4 presents some numerical calculations which show that the main effect of a longer range interaction is to introduce a suppression factor which is almost constant for all nuclei with mass number greater than $A \sim 28$. The conclusion is that the Skyrme energy functional with the tensor force is adequate to describe the evolution of shell effects.

II. CONTRIBUTION OF A SHORT RANGE TENSOR FORCE

The Skyrme parametrization of a short range tensor force leads to a contribution to the energy density

$$\Delta H_T(r) = \frac{1}{2} \alpha [J^2_n(r) + J^2_p(r)] + \beta J_n(r)J_p(r)$$

(1)

where the $J_q(r)$ ($q = n, p$) are spin-orbit densities and $\alpha$ and $\beta$ are parameters defined in the next section. They represent the combined effect of the tensor plus central exchange interactions. If the radial wave functions depend only on the orbital angular momentum $l$ and not on $j$ then the spin-orbit densities are zero if both components of a spin-orbit doublet are filled. Then the energy density (1) brings contributions only to spin unsaturated nuclei. Thus $H_T(r)$ would be almost zero in $^{40}$Ca which is an orbital double closed shell nucleus. It would be large for $^{208}$Pb which has spin unsaturated shells for both neutrons and protons. The energy functional (1) leads to a simple modification of the single particle spin-orbit potential for both protons and neutrons (see next section).

The purpose of the present section is to derive the form of $H_T(r)$ for a short range tensor interaction. We focus on the contribution of the neutron-proton interaction. The starting point is a two-body tensor potential

$$V_T(r) = v_T(r) \, \tau_1.\tau_2 \left[ \frac{1}{3r^2} (\sigma_1, \mathbf{r})(\sigma_2, \mathbf{r}) - \sigma_1.\sigma_2 \right]$$

(2)

like the one arising from one-pion exchange. The effect of the isospin dependence in Eq. (2) is to make $\beta \approx 2\alpha$. An interaction with no isospin dependence would have $\beta = 0$.

According to Negele and Vautherin [14] the expectation value of the tensor interaction with Hartree-Fock wave functions is

$$\langle V_T^{np} \rangle = -\int d^3r_1 d^3r_2 v_T(r_1 - r_2) |\bar{\rho}_n(r_1, r_2).\bar{\rho}_p(r_1, r_2)|$$

(3)
The expressions for the \(nn\) and \(pp\) contributions are similar but are each multiplied by a factor 1/2 from the isospin dependence of (2). Negele and Vautherin give a factorization of the spin-density matrices for spherical nuclei in which sub-shells are either completely full or completely empty. It is

\[
\vec{\rho}(r_1, r_2) = i(r_1 \times r_2)\rho_1(r_1, r_2)
\]

where

\[
\rho_1(r_1, r_2) = \pm \sum_{njl} \frac{1}{2\pi r_1 r_2} R_{njl}(r_1) R_{njl}(r_2) P'_l(\cos \Theta).
\]

(5)

\(P'_l\) is the derivative of the Legendre polynomial \(P_l\), \(\Theta\) is the angle between the directions of \(r_1\) and \(r_2\) and the ± sign in Eq. (5) stands for \(j = l \pm \frac{1}{2}\). For a short range interaction \(\Theta \approx 0\) in Eq. (5) and \(P'_l(\cos \Theta) \approx l(l+1)/2\). This is the origin of the spin-orbit splitting factor in Eq. (6) of Ref. [3]

\[
(2j + 1)[j(j + 1) - l(l + 1) - 3/4] = \pm 2l(l + 1) \quad \text{if} \quad j = l \pm 1/2.
\]

(6)

If the radial wave functions \(R_{njl}(r)\) are the same for \(j = l \pm 1/2\) then the contribution of a particular \(l\)-level to \(\rho_1(r_1, r_2)\) vanishes if both \(j\)-components are either completely occupied or completely empty.

When the interaction \(V_T(r)\) has a sufficiently short range the \(\langle V_{np}^{\text{np}}\rangle\) simplifies to

\[
\langle V_{np}^{\text{np}}\rangle = \frac{\pi}{6} \int d^3 r J_n(r) J_p(r) \int v(s)s^4 ds.
\]

(7)

where

\[
J_q(r) = 2r \rho_{nq}(r, r)
\]

(8)

which is the spin-orbit density in Eq. (6) of Ref. [3]. Equation (6) shows that \(J_q(r) > 0\) when the lower component of a spin-orbit doublet is being filled and goes to zero when both components are filled.

III. A FINITE RANGE SUPPRESSION FACTOR

The analysis in the present section shows that, for a tensor interaction with a range of the order of the one pion exchange interaction and for single particle states with the largest \(l\) for a given \(A\), the effect of the finite range interactions is to multiply Eq. (7) by a simple suppression factor which is almost the same for any pair of nuclei with mass number greater
than $A = 28$. As a consequence one should be able to parametrize the contribution of a
tensor force to the energy density by the simple form in Eq. (1) with values of $\alpha$ and $\beta$
which are constant for all nuclei.

We start with Eq. (3) and make a change of variables in the expression for $\langle V_{\text{np}}^T \rangle$
is
$$\langle V_{\text{np}}^T \rangle = 4\pi^2 \int \int v_T(s)(r^2 - s_r^2/4)\rho_{1n}(\mathbf{r}_1, \mathbf{r}_2)\rho_{1p}(\mathbf{r}_1, \mathbf{r}_2) \sin^3 \Theta dr ds d\Theta. \quad (9)$$
where $r_1 = r + s_r/2$, $r_2 = r - s_r/2$ and $\Theta$ is the angle between $\mathbf{r}_1$ and $\mathbf{r}_2$. There are three
other angles which have been integrated out to give a factor $8\pi^2$. The factor $|\mathbf{r}_1 \times \mathbf{r}_2|^2 = (r^2 - s_r^2/4)^2 \sin^2 \Theta$. The distance $|s|$ between the points $\mathbf{r}_1$ and $\mathbf{r}_2$ is
$$|s|^2 = |\mathbf{r}_1 - \mathbf{r}_2|^2 = s_r^2 + 4(r^2 - s_r^2/4)\sin^2(\Theta/2) = s_r^2 + s_\perp^2 \quad (10)$$
In the following equations, including Eq. (13), $r^2 - s_r^2/4$ has been replaced by $r^2$. The error
is small because $s \sim a = 1.2$ fm and the important values of $r$ lie in the range 2.5 - 5.8 fm
(see Table 1).

Bellow we calculate the expectation values of $V_T$ by approximating the Yukawa form
factor of the nucleon-nucleon spin-orbit potential by a Gaussian $v_T(s) = V_0 \exp(-s^2/a^2)$
with $a = 1.2$ fm [9]. This is because the integral separates approximately into a radial part
and angular part for the Gaussian interaction. The calculations are made with oscillator
wave functions with $\hbar\omega = 40A^{1/3}$ MeV The corresponding oscillator length parameter is
$b = 1.021A^{1/6}$ fm.

Using Eq. (10) one can see that the expression for the angle part of the integral in Eq.
(9) can be written as
$$I(l, l', r/a) = 8N(l, r/a)N(l', r/a) \int \exp \left(-2r^2/a^2 (1 - \mu)\right) P_l^l(\mu)P_{l'}^{l'}(\mu)(1 - \mu^2)d\mu. \quad (11)$$
where $\mu = \cos \Theta$. The normalization factors
$$N(l, r/a) = \frac{r^2}{a^2l(l + 1)}$$
are chosen so that $I(l, l', r/a) \rightarrow 1$ when $r >> a$. The deviation of $I(l, l', r/a)$ from unity
measures the effect of the finite range of the interaction. The radial wave functions of states
with maximum $l$ in any shell have one peak with a maximum at $R$. Table I shows values of
$I(l, l', R/a)$ for a range of mass numbers $A$ and $l$-values, where $R$ is calculated for oscillator
wave functions in the standard potential. When $l \neq l'$ it is chosen to be the average of the
peak positions for the two $l$-values.
A l R(fm) z = R/a I(l, l', z) X(l, l', z) S_r
28 2 2.52 2.10 0.642 0.556 0.829 0.53
48 3 3.37 2.81 0.553 0.525 0.851 0.47
90 4 4.23 3.60 0.527 0.521 0.874 0.46
132 4.5 4.87 4.06 0.514 0.529 0.886 0.46
208 5.6 5.83 4.86 0.509 0.526 0.901 0.46

Table 1: The reduction factor $S$ for various values of $A$ and $l$.

A striking observation about the table is that $I(l, l', R/a)$ with $a = 1.2$ fm is remarkably constant for the closed shell nuclei $^{48}$Ca, $^{90}$Zr, $^{132}$Sn and $^{208}$Pb when the length parameter of the potential, $a = 1.2$ fm. It is significantly larger for $^{28}$Si. The same situation holds for $a = 1.4$ fm.

The values of $I$ in the table were calculated by numerical integration. Numerical calculations show that $I(l, l, r/a)$ varies a lot with $r/a$ for fixed $l$. The dependence on $l$, $l'$, $r$ and $a$ can be understood by the following simple approximation

$$I(l, l, r/a) \approx X(l, l, r/a) = \left[ \frac{4r^2/a^2}{l(l+1) + 4r^2/a^2} \right]^2 \tag{12}$$

which is accurate to within 5% for $a = 1.2$ fm except for $A = 28$ where the error is 15%. The approximation $X(l, l, R/a)$ is almost constant because $l(l+1)R^2/a^2$ is almost constant for all the nuclei considered.

The effects of the finite range on the radial integral in Eq. (9) involves the ratio $S_r$ of integrals

$$\int ds R_a(r + s/2)R_a(r - s/2)R_b(r + s/2)R_b(r - s/2) \exp(-s^2/a^2). \tag{13}$$
calculated exactly and in the short range approximation. At the average position $R$ of the maxima of the radial wave functions these integrals can be approximated by Gaussians. The finite range of the interaction multiplies the short range approximation by the factor

$$S_r \approx \left[ \frac{1}{1 + a^2/b^2} \right]^{1/2} \tag{14}$$

where $b$ is the oscillator length parameter. A full numerical calculation of this suppression factor agrees with this simple formula to an accuracy of better than 1%. The total suppression
factor $S$ is the product of $I(l,l',R/a)$ and $S_r$. Values of $S$ and $S_r$ are also shown in Table 1. The constancy of $S$ and the validity of the approximation (1) depend on the value of $a$. It is very good for $a \leq 1.2$ fm but fails when $a > 1.8$ fm. It is very near 0.46 for nuclei with $A \geq 48$, but larger for lighter nuclei.

IV. THE TENSOR PART OF THE SKYRME INTERACTION

The parameters of the Skyrme interaction were originally determined in Hartree-Fock calculations to reproduce the total binding energies and charge radii of closed-shell nuclei [4]. Further extensive calculations were made later [5]. Several improved parameter sets were found. They differ mainly through the single particle spectra. In the present paper as in our previous work, we shall use the parameter set SIII which gives good overall single particle spectra. In Ref. [3] a tensor force was added and a range of its strength was found such as to maintain a good quality of the single particle spectra of $^{48}$Ca, $^{56}$Ni, $^{90}$Zr and $^{208}$Pb.

As in Ref. [3], in the configuration space the tensor interaction has the following form

$$V_T = \frac{1}{2} T \{ [(\vec{\sigma}_1 \cdot \vec{k})(\vec{\sigma}_2 \cdot \vec{k'}) - \frac{1}{3} k'^2 (\vec{\sigma}_1 \cdot \vec{\sigma}_2)] \delta(\vec{r}_1 - \vec{r}_2)$$

$$+ \delta(\vec{r}_1 - \vec{r}_2) [(\vec{\sigma}_1 \cdot \vec{k})(\vec{\sigma}_2 \cdot \vec{k}) - \frac{1}{3} k^2 (\vec{\sigma}_1 \cdot \vec{\sigma}_2)] \delta(\vec{r}_1 - \vec{r}_1') \}$$

$$+ U \{ [ (\vec{\sigma}_1 \cdot \vec{k'}) \delta(\vec{r}_1 - \vec{r}_2)(\vec{\sigma}_1 \cdot \vec{k}) - \frac{1}{3} (\vec{\sigma}_1 \cdot \vec{\sigma}_2)[\vec{k'} \cdot \delta(\vec{r}_1 - \vec{r}_2)\vec{k}]. \}$$

The parameters $T$ and $U$ measure the strength of the tensor force in even and odd states of relative motion.

V. RESULTS

The analysis in Sections 2 and 3 show that the simple form (1) is a good approximation to the contribution of the tensor forces to the energy density. Values of $\alpha$ and $\beta$ can be taken to be constant for states with maximum $l$ in nuclei with $A \geq 48$ even for forces with a range of the one pion exchange potential.

Both the central exchange and the tensor interactions give contributions to the spin-orbit single particle potential to be added to the spin-orbit interaction. The additional contribution are [3]
\[ \Delta W_n = (\alpha J_n + \beta J_p) \vec{\ell} \cdot \vec{s} \]  

(16)

\[ \Delta W_p = (\alpha J_p + \beta J_n) \vec{\ell} \cdot \vec{s} \]  

(17)

with \( \alpha = \alpha_T + \alpha_c \) and \( \beta = \beta_T + \beta_c \). For the Skyrme SIII interaction the parameters of the central exchange part are [5]

\[ \alpha_c = \frac{1}{8}(t_1 - t_2) = 61.25 \text{ MeV fm}^5, \quad \beta_c = 0, \]  

(18)

where \( t_1 \) and \( t_2 \) are two of the Skyrme interaction parameters. In terms of the tensor parameters \( T \) and \( U \) one has

\[ \alpha_T = \frac{5}{12}U, \quad \beta_T = \frac{5}{24}(T + U). \]  

(19)

Equations (16) and (17) imply that the mechanism invoked by Otsuka et al. is intrinsic to the Skyrme energy density formalism. These equations show that the filling of proton (neutron) levels influences the spin-orbit splitting of neutron (proton) levels whenever \( \beta \neq 0 \). The normal spin-orbit single particle potential is

\[ V_{so} = W_0 \frac{1}{r}(\frac{d\rho}{dr} + \frac{d\rho_0}{dr}) \vec{\ell} \cdot \vec{s} \quad \text{with} \quad \frac{d\rho}{dr} < 0. \]  

(20)

When \( \beta \) is positive the neutron (proton) spin-orbit splitting is reduced as protons (neutrons) fill a \( j = l + 1/2 \) level because \( J_{p(n)} > 0 \). This effect is clearly seen in Fig. (4) of Otsuka et al. [7].

In Ref. [3] we searched for sets of parameters \( \alpha \) and \( \beta \) which simultaneously fit absolute values of single particle levels in the closed shell nuclei \(^{48}\text{Ca}, ^{56}\text{Ni}, ^{48}\text{Zr}\) and \(^{208}\text{Pb}\). We found that the common optimal values were located in a right angled triangle with sides \( \alpha = -80, \beta = 80 \) and hypotenuse \( \alpha + \beta = 0 \). Here we relax these constraints and try to analyze single particle energies some nuclei far from the stability line. The experimental data did not exist in 1977 when we discussed the global fit for closed shell nuclei [3]. Our present choice of parameters is guided by the recent results of Ref. [10] on the \( Z = 50 \) isotopes and \( N = 82 \) isotones which were analyzed in a HF + BCS approach based on the Skyrme interaction SLy5 [15] with refitted values of \( T \) and \( U \) plus a pairing force. To see whether or not one can obtain the correct trend in the evolution of single particle levels we look at energy
differences between them. These differences can give a clear indication of the formation of closed shells from the size of the gaps. Absolute values of single particle energies depend not only on the tensor, but also on other parts of the Skyrme interaction. Here we are not concerned with making the best fits to absolute energies.

In the present paper we still use the SIII version of the Skyrme interaction [5] for comparison with the previous work. We maintain the conditions $\alpha < 0$ and $\beta > 0$ but take values outside the triangle found before which are not inconsistent with the previous findings [3]. We show that values $\alpha_T = -180 \text{ MeV fm}^5$ and $\beta_T = 120 \text{ MeV fm}^5$, or equivalently $\alpha = -118.75 \text{ MeV fm}^5$ and $\beta = 120 \text{ MeV fm}^5$, give a reasonably good fit to $Z = 50$ isotopes and $N = 82$ isotones. These values are similar to the ones fitted by Brown et al. [8] in a recent paper. For a more general orientation we also discuss the role of this parametrization on Ca isotopes.

We conclude this section with some remarks on $^{208}\text{Pb}$ and $^{90}\text{Zr}$. The proton $h_{11/2}$ and neutron $i_{13/2}$ in $^{208}\text{Pb}$ are filled and $J_p$ and $J_n$ are both positive with comparable magnitudes. Because $\alpha \approx -\beta$ we have $\Delta W_n \approx \Delta W_p \approx 0$ and the tensor forces hardly change the spin-orbit splitting. The situation is different for $^{90}\text{Zr}$. There $J_p = 0$ and the effect of the tensor forces is to increase the spin-orbit splitting for neutrons and reduce it for protons. The shell gaps for protons and neutrons are both increased significantly and the stability of the double closed shell at $^{90}\text{Zr}$ is enhanced.

A. Sn isotopes

Fig. 1 shows the HF results for the proton single particle energy difference between $1h_{11/2}$ and $1g_{7/2}$ in Sn isotopes ($Z = 50, N = 64-82$) with and without tensor force. One can see that the effect of the tensor force is indeed important. The experimental pattern is satisfactorily reproduced with this simple approach. In the more sophisticated HF+BCS calculations of Ref. [10] the theoretical results beyond $^{126}\text{Sn}$ are better. However in that region the experimental situation is less certain because the corresponding values have been assigned using methods which are less sensitive to the single particle nature of the levels [16]. For the double magic nucleus $^{132}\text{Sn}$ the effect of the tensor force and of the central exchange part cancels out because $J_p \approx J_n$. For isotopes with $Z = 56-62$ the comparison with the experiment is not possible because the $1h_{11/2}$ level becomes unbound in these calculations.
FIG. 1: The proton single particle energy difference between $1_{11/2}$ and $1_{7/2}$ in Sn isotopes ($Z = 50$, $N = 64-82$) calculated without and with tensor force $\alpha = -118.75$ MeV fm$^5$, $\beta = 120$ MeV fm$^5$. Data points are from Ref. [16]. Solid dots give information from transfer reactions. Open circles are obtained from methods less sensitive to the single particle nature.

B. $N = 82$ isotones

In Fig. 2 we present neutron single particle energy differences between $1_{13/2}$ and $1_{9/2}$ in $N = 82$ isotones calculated with and without tensor force and compare them with data from Ref. [16]. Again the role of the tensor force is considerable, bringing down the energy difference $e(1_{13/2}) - e(1_{9/2})$ close to the best known experimental values. For $Z \leq 50$ and for $Z \geq 70$ the $1_{9/2}$ level becomes unbound both with and without tensor force.

C. Ca isotopes

As the Skyrme interaction SIII was fitted to closed shell nuclei it has the peculiarity that the central exchange interaction produces some undesirable effects in the middle of a shell. The predicted single particle levels have the wrong order when compared with the experimental levels and the wrong levels are occupied [5]. This happens in the absence of the tensor interaction, but when a tensor interaction with adequate parameters is added the problem is solved. In particular the parameters $\alpha = -118.75$ and $\beta = 120$ remove this
FIG. 2: The neutron single particle energy difference between $1i_{13/2}$ and $1h_{9/2}$ in $N = 82$ isotones calculated with and without tensor force. Data points are from Ref. [16]. Solid dots give information from transfer reactions. Open circles are obtained from methods less sensitive to the single particle nature.

FIG. 3: The proton single particle energies in Ca isotopes relative to $1d_{3/2}$ level, calculated with tensor force ($nlj + T$): $\alpha = -118.75$ MeV fm$^5$, $\beta = 120$ MeV fm$^5$ and without tensor force ($nlj$): $\alpha = 61.25$ MeV fm$^5$, $\beta = 0$. Data points are from Ref. [12]: solid dots for $1d_{5/2}$ and stars for $2s_{1/2}$. 
anomaly in $^{50}$Ca. The reason is a considerable increase of the spin-orbit in the $1f$ shell which shifts the $1f_{3/2}$ above the $1p$ levels. However the anomaly persists for $\alpha = 0$ and $\beta = 80$ located at the edge of the above mentioned triangle.

In addition, from Fig. 3 one can see that the effect of the tensor interaction is important and improves the spin-orbit splitting in the $1d$ shell. In the $2s_{1/2}$ shell the trend is correct but the theoretical results are above the experimental points, with or without tensor. The pattern is quite similar to that obtained in Ref. [6] in a shell model approach. Note that in that approach only the triplet odd interaction was included in the analysis.

VI. CONCLUSIONS

The short range approximations for the contribution of a tensor force to the spin-orbit splitting in nuclei was studied in sections 2 and 3. It was shown that the short range formulae (1), (16) and (17) should give qualitatively good results in nuclei with $A \geq 48$ and for states with maximum $l$ even for potentials with the range of the one-pion exchange potential.

We have made a new fit to the parameters $\alpha$ and $\beta$ in the parametrization (16) and (17) of the tensor contribution to the spin-orbit coupling using data on $Z = 82$ isotopes and $N = 82$ isotones. The tensor force makes a dramatic difference to the single particle energy difference between the $h_{11/2}$ and $g_{7/2}$ single particle levels. A similar situation holds for the energy difference between the $i_{13/2}$ and $h_{9/2}$ single particle levels in $N = 82$ isotones. In both cases the calculation with the addition of the tensor force give a good description of the experimental data. The case with Ca isotopes is similar to $^{90}$Zr. The tensor force reduces the spin-orbit splitting for protons and increases it for neutrons. This brings the order of single particle into a better agreement with experiment.


