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Remodelling the spin-orbit term of Skyrme energy density functionals

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Abstract. We review the Skyrme interaction as first used by Vautherin and Brink in the Hartree-Fock (HF) formalism to construct the energy density functional and more specifically, the two-body spin-orbit term. Problems with this term were already pointed out by Skyrme himself and have been discussed in the past years by other authors. We present examples where existing Skyrme parametrizations are unable to properly describe spin-orbit splittings in nuclei. We also discuss possible options that allow for more flexibility in the spin-orbit dependent terms of the energy density functional and of the self-consistent mean field potential. Focusing in particular on the recently measured spectroscopic factors in germanium and selenium isotopes, we show that using different neutron and proton spin-orbit coupling constants, together with pairing and deformation, greatly improves the agreement with experiment. Results on spectroscopic factors, rms radii and other collective and single-particle properties of germanium and selenium isotopes obtained with the new and old parametrizations of the constrained HF(Sk3)+BCS potential are shown.

1. Introduction
The occupation probabilities of the active shells of ⁷⁴,⁷⁶Ge and ⁷⁶,⁷⁸Se have been recently measured by Schiffer et al. [1] (for neutrons) and by Kay et al. [2] (for protons). Within a spherically symmetric description, these active shells are 1p⁹/₂, 1p⁷/₂, 0f⁵/₂, 0g⁹/₂. One of the reasons for measuring these occupations lies on their relevance for the theoretical description of the double beta decay of ⁷⁶Ge going to ⁷⁶Se, which is one of the best studied processes of this type. The measured occupations were not reproduced by previous theoretical mean-field or shell-model calculations. Attempts to improve the agreement were made by increasing the binding energy of the 0g⁹/₂ level, thus increasing the corresponding occupation probability and eventually reaching the experimental value. This energy shifting has been performed by hand in some cases and, in some other cases, the single-particle energies used are not available in the literature [3, 4, 5, 6]. In this work we have modified the nucleon-nucleon interaction to improve the agreement with experimental data. One of our most successful trials, as will be shown later on, consisted of changing the nucleon spin-orbit interactions. Indeed, in the past it was already pointed out that the Skyrme interactions do not reproduce properly the spin-orbit splittings in some nuclei, especially concerning neutron states, and that a more flexible spin-orbit interaction is required [7].

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The central potential reads:

$$U_t^{so}(r) = t_0[(1 + \frac{1}{2}x_0)\rho - (x_0 + \frac{1}{2})\rho t_0] + \frac{4}{3}t_3(\rho^2 - \rho^2 t_2) - \frac{1}{8}(3t_1 - t_2)\nabla^2\rho$$

$$+ \frac{1}{16}(3t_1 + t_2)\nabla^2\rho t_2 + \frac{1}{16}(t_2 - t_1)\rho t_2 - \frac{1}{8}W_0(\nabla \cdot \vec{J}) + \nabla \cdot \vec{J} + \frac{1}{2}W_0(\nabla \cdot \vec{J}) + V_C(r)\delta_{t_2} + \frac{1}{2}$$

and the spin-orbit potential reads:

$$\tilde{S}_t^{so}(r) = \frac{1}{2}W_0(\nabla \rho + \nabla \rho t_2) + \frac{1}{8}(t_2 - t_1)\tilde{J}_t$$

(2)

The subscript $t_2$ is the third component of the isospin and stands for protons when $t_z = +1/2$ and for neutrons when $t_z = -1/2$. These potentials take part, together with an effective mass $m^*$, in the one-body Schrödinger-like equation for the Hartree-Fock single particle energies and wave functions with Skyrme interactions [8],

$$\left[-\frac{\hbar^2}{2m^*_t}\frac{\nabla^2}{\nabla} + U_t^{so}(r) - i\tilde{S}_t^{so}(r)(\nabla \times \sigma)\right] \Phi^{(t_z)} = e^{(t_z)}\Phi^{(t_z)}$$

(3)

We are concerned here with the terms in both one-body potentials containing the spin-orbit strength $W_0$:

$$U_t^{so}(W_0; r) = -\frac{1}{2}W_0(\nabla \cdot \vec{J}) + \nabla \cdot \vec{J}_t$$

$$\tilde{S}_t^{so}(W_0; r) = \frac{1}{2}W_0(\nabla \rho + \nabla \rho t_2)$$

(4)

In order to modify the spin-orbit strength separately for protons and for neutrons, different values can be given when computing the potentials corresponding to the protons and to the neutrons ($W_{t_2} \neq W_{-t_2}$):

$$U_{t_2}^{so}(W_{t_2}; r) = -\frac{1}{2}W_{t_2}^{U}(\nabla \cdot \vec{J}) + \nabla \cdot \vec{J}_{t_2}$$

$$\tilde{S}_{t_2}^{so}(W_{t_2}; r) = \frac{1}{2}W_{t_2}^{S}(\nabla \rho + \nabla \rho t_2)$$

(5)

Another possibility is to assign a different strength for the proton density term and for the neutron density term within each potential (no matter if it is for protons or for neutrons):

$$U_{t_2}^{so}(W_{t_2}; r) = -W_{t_2}^{U}\nabla \cdot \vec{J}_{t_2} - \frac{1}{2}W_{t_2}^{U}\nabla \cdot \vec{J}_{-t_2}$$

$$\tilde{S}_{t_2}^{so}(W_{t_2}; r) = W_{t_2}^{S}\nabla \rho t_2 + \frac{1}{2}W_{-t_2}^{S}\nabla \rho - t_2$$

(6)

In the previous expressions there is also the possibility of using different values of the spin-orbit strength for the term in the central potential and for the term in the spin-orbit potential ($W_{t_2}^{U} \neq W_{t_2}^{S}$).

It is worth recalling here that the spin-orbit interaction is relativistic in origin. The Dirac equation can be written in Schrödinger form as [9]:

$$\begin{bmatrix} i\alpha \cdot \nabla - \beta[m + V_S] + E - V_V - V_C \end{bmatrix} \Phi = 0 \Rightarrow \left[-\frac{\nabla^2}{2m} - V_D\right] \phi = E'\phi$$

(7)
with \( V_D = W_C + W_{SO} \hat{\sigma} \cdot \vec{l} \), where

\[
W_{SO} = \frac{1}{2m} \frac{1}{rA} \frac{\partial A}{\partial r}
\]

(8)

with \( A = E + m + V_S - V_V - V_C \). As can be seen in these expressions, the spin-orbit interaction term containing \( \hat{\sigma} \cdot \vec{l} \) arises from the relativistic equation and is proportional to the derivative of the nuclear potentials \( V_S, V_V, V_C \). An equivalent structure, this time involving the nuclear density, can be found in the term of the Schrödinger equation (Eq. 3) containing the Skyrme spin-orbit potential:

\[
i \vec{S}^\text{so} \cdot (\vec{\nabla} \times \hat{\sigma}) \sim \frac{\partial \rho}{\partial r} \left[ i(\hat{\sigma} \cdot \hat{r})(\hat{\sigma} \cdot \vec{p}) - \vec{\nabla} \cdot \hat{\sigma} \right] = \frac{1}{r} \frac{\partial \rho}{\partial r} \hat{\sigma} \cdot \vec{l}
\]

(9)

since the spin-orbit potential, as shown in Eq. 4, is \( \vec{S}^\text{so} \sim \vec{\nabla} \rho \sim \frac{\partial \rho}{\partial r} \). This dependence on the radial derivative of the nuclear density makes the spin-orbit interaction particularly sensitive to the details of the nucleon distributions, especially in the surface, where the derivatives take larger values. Whereas the proton distribution is accurately known using charged lepton probes, the one for neutrons suffers from large uncertainties. Great experimental and theoretical efforts are currently aimed at improving this situation.

3. Results for the Ge-Se region

In this work we use a deformed Hartree-Fock (HF) mean field with Sk3 Skyrme interaction and pairing correlations within BCS approximation to obtain the single-particle wave functions \( \Phi_i \), energies \( e_i \) and occupation probabilities \( v^2_i \) in the ground state of the isotopes under study. The axially-deformed HF single-particle wave functions \( \Phi_i \) can be expanded in an axially-deformed harmonic oscillator basis (more convenient to solve the HF equations for deformed nuclei as it converges faster) or in a spherical harmonic oscillator basis:

\[
\Phi_i(\vec{r}) = \sum_{n\rho n_\Lambda \Sigma} k^i_{n\rho n_\Lambda \Sigma} \psi_{n\rho n_\Lambda \Sigma}(\vec{r}) = \sum_{nlj} c^i_{nlj} \phi_{nljm}(\vec{r})
\]

(10)

The valence shell occupation probabilities \( V^2_{nlj} \), corresponding to spherical single-particle wave functions, to be compared with the experimental values are:

\[
V^2_{nlj} = \sum_i c^i_{nlj} v^2_i
\]

(11)

where the summation through the single-particle states \( i \) should contain those states lying within an energy range around the Fermi level equivalent to the excitation energy range considered in the experiments.

We perform different HF+BCS calculations in a search for a better agreement between our results and the experimental data in the region \( 74-78 \) Ge-Se. In particular, we carry out constrained HF+BCS calculations with different quadrupole deformations, and we also vary the strength of the spin-orbit interaction \( W_{so} \) for neutrons in the Skyrme one-body potentials as described in Eqs. 6. The strength for protons has been kept constant (with the usual value of the Sk3 parametrization), and we have used the same values of the strengths in the central and the spin-orbit potentials.

In Fig. 1 we show the active-shell energies obtained in the HF+BCS calculation for protons and neutrons in \( ^{76}\text{Ge} \) and \( ^{76}\text{Se} \) for different prolate deformations and for different strengths of the spin-orbit interaction for neutrons in the Skyrme one-body potentials (starting with the original Sk3 value of 120 MeV fm\(^3\)). The main effect of the deformation is the loss of degeneracy
in the states with different angular momentum projection, but it is apparent that some of the states get more bound while other get less bound in such a way that the overall shift of the whole \(nlj\) set is very small. On the contrary, the modification of the spin-orbit strength for neutrons has a strong effect on the energies of some of the states under consideration. In Fig. 2 we show the occupation probabilities of the active shells again for different deformation parameters and neutron spin-orbit strengths. In agreement with the previous figure, it shows that the quadrupole deformation hardly changes the relative occupation probabilities of the \(lj\) shells, whereas the strength of the spin-orbit interaction has a much stronger effect on them. The experimental occupations are shown as dotted lines in the figure, and the theoretical results get closer to them only when the spin-orbit interaction is modified.

Once the increase of the neutron spin-orbit interaction has been shown to improve the agreement with experimental occupations in \(^{76}\text{Ge}\) and \(^{76}\text{Se}\), the question arises of the effect of this modification on the bulk properties of the isotopes in this region. Indeed, the parameters of the Skyrme interactions are fitted to reproduce some of these bulk properties in a given set of nuclei, and a modification of any of the Skyrme parameters without an overall refitting of the rest may give rise to deviations. To illustrate this effect we show in Tables 1 and 2 the binding energies and charge radii, respectively, of the isotopes \(^{74,76}\text{Ge}\) and \(^{76,78}\text{Se}\) obtained from a HF+BCS calculation for two values of the neutron spin-orbit interaction (the original one in Sk3 force, 120 MeV fm\(^5\), and 200 MeV fm\(^5\)) and for two nuclear shapes (spherical, \(\beta = 0\), and...
Figure 2. Theoretical single-particle occupations in the active shells of $^{76}$Ge and $^{76}$Se. Left: evolution of occupations for different deformation parameters $\beta$ (0, 0.10, 0.16, 0.20). Right: evolution of occupations for different values of the spin-orbit strength of neutrons $W_n$ (120, 160, 200, 240 MeV fm$^5$). The horizontal dotted lines indicate the experimental values.

Table 1. Binding energies in MeV of $^{74,76}$Ge and $^{76,78}$Se from a HF+BCS calculation (different nuclear shapes and neutron spin-orbit strengths) together with experimental data.

<table>
<thead>
<tr>
<th></th>
<th>$W_n=120$ MeV fm$^5$</th>
<th>$W_n=200$ MeV fm$^5$</th>
<th>EXP.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Spherical</td>
<td>$\beta$ exp.</td>
<td>Spherical</td>
</tr>
<tr>
<td>$^{74}$Ge</td>
<td>-641.42</td>
<td>-642.28</td>
<td>-655.57</td>
</tr>
<tr>
<td>$^{76}$Ge</td>
<td>-657.32</td>
<td>-658.58</td>
<td>-674.22</td>
</tr>
<tr>
<td>$^{76}$Se</td>
<td>-657.26</td>
<td>-658.01</td>
<td>-669.97</td>
</tr>
<tr>
<td>$^{78}$Se</td>
<td>-675.69</td>
<td>-676.91</td>
<td>-691.37</td>
</tr>
</tbody>
</table>

the experimental deformations [10]).

Concerning the binding energies, we get a 0.5% underestimation in the calculation with the usual Sk3 force and a 2% overestimation in the calculation with the increased neutron spin-orbit strength. As for the charge radii, the results with larger spin-orbit strength agree better with the experimental values. Further comparison between these new calculations and experimental data has been carried out for single- and double-beta decay strength distributions of $^{76}$Ge and $^{76}$Se [13] finding once again a nice agreement.
Table 2. Charge radii in fm of $^{74,76}$Ge and $^{76,78}$Se from a HF+BCS calculation (different nuclear shapes and neutron spin-orbit strengths) together with experimental data.

<table>
<thead>
<tr>
<th></th>
<th>$W_n=120\ \text{MeV} \ \text{fm}^5$</th>
<th>$W_n=200\ \text{MeV} \ \text{fm}^5$</th>
<th>EXP.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Spherical $\beta$ exp.</td>
<td>Spherical $\beta$ exp.</td>
<td>[12]</td>
</tr>
<tr>
<td>$^{74}$Ge</td>
<td>4.108</td>
<td>4.109</td>
<td>4.080</td>
</tr>
<tr>
<td>$^{76}$Ge</td>
<td>4.121</td>
<td>4.118</td>
<td>4.096</td>
</tr>
<tr>
<td>$^{76}$Se</td>
<td>4.165</td>
<td>4.171</td>
<td>4.140</td>
</tr>
<tr>
<td>$^{78}$Se</td>
<td>4.176</td>
<td>4.175</td>
<td>4.153</td>
</tr>
</tbody>
</table>

Acknowledgments
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