Reduction of SO in $^{34}\text{Si}$: weak binding or density-depletion effect?

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The reduction of the neutron spin-orbit splitting $2p_{3/2} - 2p_{1/2}$ between the $^{41}\text{Ca}$ and $^{35}\text{Si}$ isotones is a unique feature throughout the chart of nuclides, as the spin-orbit splitting usually increases with $A$. Moreover, its way of decrease, gradual between $^{41}\text{Ca}$ and $^{35}\text{Si}$ or abrupt between $^{37}\text{Si}$ and $^{33}\text{Si}$, as well as its origin, caused by the weak binding energy of the $p$ states or by the sudden central proton density depletion in $^{35}\text{Si}$, are subject of debate. The results reported here using the self-consistent Covariant Energy Functional calculations with the DD-ME2 parametrization rather point to an abrupt, local decrease in $^{35}\text{Si}$, and to the large dominance of the central density depletion effect. It is concluded that weak binding, central density depletion as well as correlations must be taken into account to fully evaluate the amplitude and causes of this spin-orbit reduction.

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**Introduction**- The spin-orbit (SO) force, which results from the coupling of the particle orbital momentum $\ell$ and its intrinsic spin value $s$, plays an important role in quantum systems [1]. In analogy with atomic physics, this force was introduced empirically in atomic nuclei in 1949 [2] to account for shell gaps and magic numbers that could not be explained otherwise. In a simplified version, it can be written as $-V_{s\ell} \frac{\partial \rho(r)}{\partial r} \vec{\ell} \cdot \vec{s}$, where $\rho(r)$ is the density distribution of the nucleons. The scalar product lifts the degeneracy between the $\ell + s$ and $\ell - s$ spin-orbit partners, the latter being the least bound. The resulting SO splitting $\epsilon_{\text{SO}}$ is of the order of the nucleon binding energy and scales approximately with $24.5/n$ ($\ell+1/2$) $A^{-0.597}$ [3], as shown in Fig. 1 with $n$ the number of nodes in the wave function and $A$ the atomic mass of the nucleus. This relation just considers the bulk variation of the SO force and not any local effect of two-body forces induced by the occupancy of certain orbitals. More realistic versions of this force can be found for mean field [4] and relativistic mean field theories in [5, 6]. They usually differ by their isospin dependence [7] but their common feature is their density dependence, which implies a SO reduction for weakly bound orbitals having a more shallow density distribution (e.g. [5, 6]), as well as for orbits probing the interior of a nucleus with a central density depletion (e.g. [4, 8, 11]). Although shell-model calculations do not have an explicit density-dependent two-body matrix elements, the lack of occupation of low-$\ell$ orbits also induces a central density depletion [12]. However, the proper long-tail behavior of the loosely bound orbits’ wave function cannot be properly treated in a Harmonic Oscillator basis, as shell models does [12].

The $3/2^-$ and $1/2^-$ states in $^{35}\text{Si}$, coming from the SO partners of the $2p_{3/2}$ and $2p_{1/2}$ SO orbits, fulfill these two conditions of being potentially sensitive to the weak binding effect and to the nuclear density depletion. Indeed, while the $7/2^-$ ground state of $^{35}\text{Si}$ is bound by 2.470(40) MeV, the $3/2^-$ and $1/2^-$ spin-orbit partners are bound by only 1.560 and 0.426 MeV, respectively, according to Ref. [14]. Moreover, the proton density distribution of $^{35}\text{Si}$ exhibits, as for $^{34}\text{Si}$, a significant central depletion. This is due to the lack of two $1/2^-$ protons [10], which, with their $\ell = 0$ angular momentum, usually occupy to some extent the center of the nucleus. It follows that the reduction of the $2p_{3/2} − 2p_{1/2}$ splitting, that is observed in $^{35}\text{Si}$ in comparison with $N = 21$ isotones (see Fig. 1), could be caused by the two effects. The experimental and theoretical works of Refs. [8, 11, 13] point out that the central density depletion is the major cause of the SO reduction, while the work of Kay et al. [17] find that the

**FIG. 1:** Evolution of the SO splitting $2\epsilon_{\text{SO}}/(2\ell + 1)$ as a function of the numbers of nodes $n$ of the waves function and as a function of the atomic mass $A$. This representation, derived in Ref. [8] for $p, d, f, g, h, i$ orbits with $n = 1 - 3$, is meant to show the global SO trend and not to provide exact values. Recent results obtained from the studies of $^{133}\text{Sn}$ [15], $^{132}\text{In}$ [16] and $^{35}\text{Si}$ [14] have been added. It is seen that the $^{35}\text{Si}$ data point strongly deviates from the expected trend.
full SO reduction can be explained by the effect of weak binding energy.

In this Letter, we wish to discuss the role of these two competing effects. We shall first briefly summarize the work of Kay et al., then present another experimental viewpoint to address the decrease in SO splitting in the $N = 21$ isotones, before showing the results of two different theoretical approaches, each of them having more self-consistency, as compared to the work of Ref. [17].

SO reduction due to weak binding- Kay et al. [17] have determined a gradual decrease of the SO splitting from $^{41}$Ca to $^{35}$Si, shown with black open circles in Fig. 2 by collecting the single-particle and single-hole strength of $3/2^-$ and $1/2^-$ states available in all studied nuclei. They added some error bar to their experimental values to take into account some unobserved strength. They have used a one-body Woods-Saxon (WS) potential with a fixed spin-orbit amplitude to reproduce the $2p_{3/2} - 2p_{1/2}$ splitting in $^{41}$Ca, and the WS potential depths were adjusted in each $N = 21$ isotope to match the binding energy of the weakly bound $2p_{3/2}$ orbital. They calculated the energy of the $2p_{1/2}$ and determined the corresponding SO splittings, shown in the orange band of Fig. 2. From the good agreement between the experimental and calculated trends, they affirm that simple geometrical effects on loosely bound $p$ states can fully account for a gradual reduction of the neutron $2p_{3/2} - 2p_{1/2}$ splitting between $^{41}$Ca and $^{35}$Si, without any need for a modification of the spin-orbit coupling.

An important remark is that, by applying a constant SO amplitude of about 2 MeV to the weakly bound $2p_{3/2}$ orbital at 1.560 MeV in $^{35}$Si, the $2p_{1/2}$ orbital becomes unbound by about 500 keV. In their calculation, this orbital is therefore extremely sensitive to the effect of coupling to continuum. Solving the Shrödinger for the $2p_{1/2}$ orbital makes it bound, which results in a very significant apparent change of the $2p_{3/2} - 2p_{1/2}$ splitting. If, as will be discussed in the following, the SO amplitude is reduced by the central density depletion, the $2p_{1/2}$ orbital would become more bound as compared to the use of a constant SO interaction and less sensitive to the effect of weak binding.

Evolution of SO splitting in the $N = 21$ isotones- Kay et al. [17] collected the single-particle and single-hole strength available in all studied nuclei to deduce a decrease of the $2p_{3/2} - 2p_{1/2}$ SO splitting in the $N = 21$ isotones. However, the amplitude of this apparent reduction could not be firmly quantified from the determination of single-particle energies, as this information could never be obtained experimentally [18]. Moreover, the available experimental information on single-particle or single-hole strongly differs between the $N = 21$ isotones. Many $3/2^-$ and $1/2^-$ states are observed in $^{41}$Ca, while fewer and fewer are observed when $Z$ decreases until reaching $^{35}$Si, in which only one $3/2^-$ and one $1/2^-$ states have been observed in $^{14}$. Kay et al. added error bars to their single-particle energy differences of Fig. 2 to partly consider this effect.

By using the $p$ fragments ($3/2^-$ and $1/2^-$) that are populated with the largest $(d,p)$ spectroscopic factor instead, the SO splitting $\Delta E$ of Fig. 2 (shown with red filled triangles) remains remarkably constant between $^{41}$Ca, $^{39}$Ar and $^{37}$S at a value around 2 MeV (with only 0.5% variation), and decreases suddenly to 1.134 MeV in $^{35}$Si. This trend differs then completely from that of a gradual decrease.

Being aware of the fact that these dominant fragments carry some amount of correlations, this evolution was compared to shell model [13] and ab initio calculations [11], in which correlations are taken into account. A clear correlation between the depletion in the $s_{1/2}$ orbital, predicted in [12] [19] and quantified in [10], and the reduction of the spin-orbit splitting between $^{37}$Si and $^{35}$Si, is found in [9] [11] [13]. This is at variance with Ref. [17], in which this reduction is gradual and solely attributed to a progressive decrease of the neutron binding energy, independently of the occupied proton orbitals.

It is also very instructive to notice that the presently discussed reduction of the $p$ SO splitting with $A$, would it be gradual or sudden, is opposite to the global trend predicted by Mairle [3] (green stars in Fig. 2), that has been derived from the study of SO splitting throughout the

![FIG. 2: Evolution of the $p_{3/2} - p_{1/2}$ or $3/2^- - 1/2^-$ splitting, $\Delta SO$, for the $N = 21$ isotones. Black open circles (with estimated error bars) correspond to the centroid of the single-particle strength derived in [17], in which WS calculations were made (orange band). Green stars correspond to the systematics of Ref. [3]. Red filled triangles are obtained using the energy difference between the $3/2^-$ and $1/2^-$ states having the dominating spectroscopic factor value, when populated by the $(d,p)$ reaction. Blue squares correspond to DDME2 calculations of the $3/2^-$ and $1/2^-$ states shifted upwards by 340 keV (see text). Some symbols have been slightly shifted to the left or right to be better distinguished.](image-url)
chart of nuclides (see Fig. 1). This significant discrepancy is extremely rare, but it proves that physics exist beyond the global increase of SO splitting with decreasing A, likely in specific two-body forces and in effects due to the proximity of the continuum, for the least bound states.

**Woods-Saxon calculations** - The one-body Woods-Saxon (WS) potential approach has certainly a relatively good predictive power between mirror nuclei, once one of the nucleus has a well established structure. An example of this remarkable predictive power can be found in Ref. [20] in which the profound reordering of the levels between $^{16}\text{N}$ and the unbound $^{16}\text{F}$ can be nicely explained. However, when changing nuclei, this predictive power is lost as this method is not self-consistent, i.e. the density distribution or the shape of the mean field potential does not change consistently as different orbitals are occupied, when moving from one nucleus to another. Therefore, a normalization of the depth of the WS potential had to be made in order to get the $2p_{3/2}$ orbit at the correct binding energy for each $N=21$ isotope [17]. Using this method, the evolution of the $2p_{3/2}$ binding energy, one of the member of the SO splitting, is not predicted but fixed.

It is however possible to use this simple potential approach to access to the influence of the central depletion on the energy of the orbits. We have performed calculations with the WS potential of Ref. [17] ($r_0 = 1.28$ fm, $a = 0.63$ fm, $V_{cs} = 6$ MeV), except that it was modified to take into account the existence of a central density depletion, due to the lack of a certain fraction of $2s_{1/2}$ protons. The shape of the depletion to be applied to the potential well was determined consistently from the calculation of the $2s_{1/2}$ wave function. The spin-orbit potential has been derived accordingly, as shown in Fig. 3. The calculated $2p_{3/2} - 2p_{1/2}$ SO splitting is found to be of 1.8 MeV, under the assumption of no central depletion at an hypothetical binding energy of 6 MeV for the $2p_{3/2}$ orbit. This splitting is reduced to 1.35 MeV when applying the central density depletion of Fig. 3. It further decreases to 0.91 MeV from the effect of the weak binding, when assuming that the $2p_{3/2}$ orbit is bound by 1.8 MeV (the experimental value of $^{35}\text{Si}$). In contrast with Ref. [17], we find that adding a central depletion in $^{35}\text{Si}$, which corresponds to add some self-consistency to the WS approach, the SO splitting is reduced by about 50% from the central depletion and 50% from the weak binding. This shows that, when not considering the proton depletion into account, as in [17], the effect of the continuum is clearly overestimated.

**Relativistic mean field calculations** - In order to judge the combined effects of a central proton density depletion (induced by the removal of $2s_{1/2}$ protons) and of the weak neutron binding energy, in inducing a reduction of the $p$ SO splitting between $^{37}\text{Si}$ and $^{35}\text{Si}$ ($\DeltaSO$), we use a Covariant Energy Density Functional (CEDF) calculation with the DD-ME2 parametrization [21]. The relativistic mean-field equations are solved in a large size box in order to obtain the correct asymptotic behavior of the orbitals.

A first way to evaluate the $2p_{3/2} - 2p_{1/2}$ SO splitting in the $N=21$ isotones is via the calculation of the 1-neutron removal energy $E(Z,N = 21) - E(Z,N = 20)$ where $E(Z,N)$ is the binding energy of the $(Z,N)$ nucleus. In the present CEDF calculations, the odd-N nuclei are computed within the so-called equal filling approximation [22, 23]. After calculating the removal energies for the $N=21$ systems in the $3/2^-$ and $1/2^-$ states, the $2p_{3/2} - 2p_{1/2}$ SO splittings, $E_{1/2^-}(Z,N = 21) - E_{3/2^-}(Z,N = 21)$, are displayed in Table I. Energies have globally been shifted upwards by 340 keV in Fig. 2 to match the experimental value in $^{41}\text{Ca}$.  

![FIG. 3: Woods-Saxon (WS potential) and spin-orbit interaction](image)

**TABLE I: 2p_{3/2}−2p_{1/2} SO splittings evaluated by subtracting the binding energies of the N = 21 nuclei in the state 3/2^- and 1/2^- (ΔSO odd column) or by subtracting the energies of the 2p_{1/2} and the 2p_{3/2} orbitals in the N = 20 systems (ΔSO even column).**

| Isotope | ΔSO odd (MeV) | ΔSO even (MeV) |
|---------|---------------|----------------|
| Si      | 0.72          | 0.76           |
| S       | 1.51          | 1.64           |
| Ar      | 1.50          | 1.67           |
| Ca      | 1.66          | 1.71           |

Another way of computing the evolution of $2p_{3/2} - 2p_{1/2}$ SO splitting is by subtracting the energies of the $2p_{1/2}$ and $2p_{3/2}$ orbitals in the even-even $N = 20$ systems. Indeed, according to the Koopmans’ theorem [21], the one-neutron removal energies of the odd nuclei are close to the Hartree-Fock single-particle energies calculated in the even-even system $(Z,N = 20)$. As can be seen in
FIG. 4: Evolution of the binding energy $\epsilon$ of the $p_{3/2}$ (square symbols) and $p_{1/2}$ (round symbols) in $^{36}$S (violet) and $^{34}$Si (green) as a function of the relative change of the potential depth $\delta V_0$.

(see Table I), both methods yield similar results, hereby supporting the correlation between the depletion in the $s_{1/2}$ orbital and the reduction of the SO splitting between $^{37}$Si and $^{35}$Si. The slight differences come from the fact that the Koopmans’ theorem neglects the rearrangement of the neutron orbitals when going from the \(N\) to the \(N+1\) system.

The second method is more convenient to track the impact of the weak neutron binding energy on the $2p_{3/2} - 2p_{1/2}$ SO splitting. To this end, we introduce an artificial change in the depth of the self-consistent confining potential $\delta V_0$, as compared to $\delta V_0=0$ taken in Table I. As shown in Fig. 4, the major reduction of the SO interaction at large $\delta V_0$ is caused by the depletion in the proton $2s_{1/2}$ orbital between $^{36}$S and $^{34}$Si. Lowering the depth of the confining potential first shifts the single particle energies to weaker binding energies according to a linear law, displayed by dashed lines. The proximity to the continuum induces a departure from the linear behavior, as in [17]. At a binding energy $\epsilon$ of -460 keV (-1.69 MeV), that is the experimental value in $^{35}$Si ($^{37}$S), the calculated SO gap amounts to about 0.93 (2 MeV).

The effect of the continuum is measured by comparing the spin-orbit gap calculated when the proximity to the continuum is fully taken into account to that of the extrapolated linear evolutions. As expected, the binding energy of the $2p_{1/2}$ in $^{35}$Si displays a significant departure from the linear law, viz. the SO gap evolves from 1.03 MeV, neglecting the proximity of the continuum, to 0.93 MeV (10% more) when the continuum is correctly taken into account.

Conclusions- When using the self-consistent Covariant Energy Density Functional calculations with the DDME2 parametrization, it is found that the $2p_{3/2} - 2p_{1/2}$ SO splitting remains almost constant in the \(N=21\) isotones between $^{41}$Ca (\(Z=20\)) and $^{37}$S (\(Z=16\)) and drops suddenly at $^{35}$Si (\(Z=14\)). This drop is mainly caused by the depletion of the proton $2s_{1/2}$ orbital between $^{37}$S and $^{35}$Si, to which 10% adds from the lingering of the weakly bound $2p$ orbits in $^{35}$Si. A similar conclusion has been derived from the shell-model + WS calculations of Ref. [25], in which the main reduction factor is caused by 2-body LS forces that induce an attractive (repulsive) interaction between the protons in the $2s_{1/2}$ and the neutrons in the $2p_{3/2}$ ($2p_{1/2}$) orbitals, to which an additional 8% is due to the proximity of the continuum.

We also have shown in the present work that adding a central density depletion to a simple WS potential induces a further SO reduction, as compared to the work of Kay et al. [17], in which only the effect of weak binding was considered. Therefore, neglecting the central density depletion leads to an overestimation of the weak binding energy effect on the SO reduction.

Our results are at variance with those of Kay et al. who proposed that “the proximity of the threshold can explain the (full) reduction of the splitting between these (neutron $2p_{3/2} - 2p_{1/2}$ spin-orbit partners)” and that “this effect must be taken into account before other explanations are considered”. We have demonstrated in the present work, complementary Refs. [9] [11] [13] [25], that all effects, including those induced by realistic nuclear forces, correlations, and the proximity of the continuum, must be taken into account on the same footing to reach a complete understanding of the SO splitting in the \(N=21\) isotones, as well as for the neutron $1f_{7/2} - 2p_{3/2}$ splitting. This latter \(N=28\) gap also exhibits significant changes between $^{40}$Ca and $^{34}$S which has dramatic consequences on the evolution of shell structure between $^{48}$Ca and $^{32}$Si [20].

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