Skyrme density functional description of the double magic $^{78}\text{Ni}$ nucleus

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Abstract

We calculate the single particle spectrum of the double magic nucleus $^{78}\text{Ni}$ in a Hartree-Fock approach using the Skyrme density-dependent effective interaction containing central, spin-orbit and tensor parts. We show that the tensor part has an important effect on the spin-orbit splitting of the proton $1f$ orbit which may explain the survival of magicity so far from the stability valley. We confirm the inversion of the $1f5/2$ and $2p3/2$ levels at the neutron number 48 in the Ni isotopic chain expected from previous Monte Carlo shell model calculations and supported by experimental observation.

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I. INTRODUCTION

Since more than a decade there is a growing interest into the neutron- or proton-rich nuclei far from the stability valley and into the evolution of nuclear shells in these regions. In particular $^{78}\text{Ni}$ was expected to be one of the most neutron-rich doubly magic nucleus. Its half-life time of 122.2(5.1)ms \cite{1} and the prediction of a first excited state above 2 MeV \cite{2} were a hint of stability of the $Z = 28$ and $N = 50$ shells. The recent experiments of in-beam $\gamma$-ray spectroscopy at the Radioactive Isotope Beam Factory of RIKEN producing the nucleus $^{79}\text{Cu}$ \cite{3}, indicated that the gaps at $Z = 28$ and $N = 50$ remain large, which is a clear sign of stability. At the same time the production of copper isotopes $^{75-79}\text{Cu}$ at the CERN-ISOLDE facility supports the doubly magic character of $^{78}\text{Ni}$ \cite{4}. The magnetic dipole and the electric quadrupole moments of $^{78,29}\text{Cu}$ and other Cu isotopes, measured using the CRIS experiment at the CERN-ISOLDE facility suggests that the magicity of $Z = 28$ and $N = 50$ is restored towards $^{78}\text{Ni}$ \cite{5}.

The shell structure and the existence of magic numbers are a consequence of the spin-orbit interaction \cite{6,7}. Since 2005 there is much concern about the role of the tensor force in the shell evolution and the structure of exotic nuclei, both in the framework of the shell model \cite{8,11} and the Hartree-Fock Skyrme energy density functionals \cite{12}.

In a mean field approach, which leads to a one-body potential containing a central part and a spin-orbit part, the origin of the spin-orbit interaction can be clearly understood. 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 both from the exchange part of the central two-body force and from the tensor force \cite{13-15}.

In an early work \cite{13} we estimated the contribution of the tensor part of the Skyrme interaction to the Hartree-Fock spin-orbit splitting in several spin-saturated magic nuclei and adjusted the strength of the tensor force such as to obtain a good global fit.

In Ref. \cite{16} we extended the previous study to exotic nuclei, most of which were unknown in 1977 and tried to shed a new light on the previous results. We presented results for single particle levels of Sn isotopes, $N = 82$ isotones and Ca isotopes, where the tensor force considerably improves the agreement with the experiment when its parameters are properly chosen.

About ten years ago the Ni isotopes were analyzed in Ref. \cite{17}. There it was claimed
that the currently used central and spin-orbit parts of the Skyrme energy density functional are not flexible enough to allow for the presence of large tensor terms. However, ten years later, in Ref. [18], based on the energy density functional of the Skyrme interaction with a tensor term and including the effect of unpaired nucleons on the superfluid properties of nuclei, the $\beta$-decay of $^{72-80}$Ni isotopes were calculated and found that the $\beta$-decay half-lives of these neutron-rich nuclei were in reasonable good agreement with the experiment.

With this incentive, here we calculate the single particle spectrum of $^{56-78}$Ni isotopes in order to better understand the role of the tensor part and the behaviour of the gap in the proton $1f$ shell. We found that there is an inversion of the $1f5/2$ and $2p3/2$ levels at $N = 48$ consistent with the experimental proposal of Ref. [3] and shell model calculations. We have analyzed the behaviour of the neutron $1g9/2$ subshell in the Ni isotopic chain. Agreement was found with recent shell model calculations which predicted that the size of the shell gap at $N = 50$ is smaller than that at $N = 45$ [19].

In the next Section we recall the original form of the tensor part of the Skyrme interaction. In Section III we remind the relation to a long range tensor force. In Section IV we introduce the parameters. In Section V we present the calculated single particle spectra of Ni isotopes with $N = 40 - 50$ and compare the results with other studies. The last section is devoted to conclusions.

II. THE TENSOR PART OF THE SKYRME INTERACTION

As in Ref. [13], in the configuration space the tensor interaction has the following form

$$V_T = \frac{1}{2}T\{[\sigma_1 \cdot \vec{k}'(\sigma_2 \cdot \vec{k}') - \frac{1}{3}k'^2(\sigma_1 \cdot \sigma_2)]\delta(r_1 - r_2)$$

$$+\delta(r_1^* - r_2^*)[(\sigma_1 \cdot \vec{k})(\sigma_2 \cdot \vec{k}) - \frac{1}{3}k^2(\sigma_1 \cdot \sigma_2)]\}$$

$$+U\{(\sigma_1 \cdot \vec{k}')\delta(r_1 - r_2^*)(\sigma_2 \cdot \vec{k}) - \frac{1}{3}(\sigma_1 \cdot \sigma_2)[k'^2 \cdot \delta(r_1^* - r_2^*)\vec{k}].$$

(1)

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

The parameters of the Skyrme interaction without tensor force were originally determined in Hartree-Fock calculations to reproduce the total binding energies and charge radii of closed-shell nuclei [14]. Further extensive calculations were made later [15]. 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. [13] 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.

Both the central exchange and the tensor interactions give contributions to the binding energy and the spin-orbit single particle potential to be added to the usual spin-orbit interaction. First we need to introduce the spin density $J_q$ where $q = n, p$ stands for neutrons and protons respectively. One has [14]

$$J_q = \frac{1}{4\pi r^3} \sum_k n_{q,k}(2j_{q,k} + 1)(j_{q,k}(j_{q,k} + 1) - \ell_{q,k}(\ell_{q,k} + 1) - \frac{3}{4} R_{q,k}^2(r),$$

where $k$ runs over all occupied neutron or proton states, $R_{q,k}(r)$ is the radial single particle wave function and $n_{q,k}$ is the occupation probability. When the orbit is completely filled one has $n_{q,k} = 1$.

In terms of $J_q$ the additional contribution of the central and tensor parts to the spin orbit potential is [13]

$$\Delta W_n = (\alpha J_n + \beta J_p) \tilde{\ell} \cdot \tilde{s}$$

$$\Delta W_p = (\alpha J_p + \beta J_n) \tilde{\ell} \cdot \tilde{s}$$

with

$$\alpha = \alpha_T + \alpha_c, \quad \beta = \beta_T + \beta_c.$$  

For the Skyrme SIII interaction used in the present work the parameters of the central exchange part are [15]

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

where $t_1$ and $t_2$ are two of the Skyrme interaction parameters. In terms of the tensor parameters $T$ and $U$ introduced in Eq. (11) one has

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

Equations (3) and (4) imply that the mechanism invoked by Otsuka et al. [8, 9, 11] 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 $\beta \neq 0$. In the Skyrme energy density approach this mechanism is very simple.
The usual spin-orbit single particle potential resulting from the two-body spin-orbit is

$$V_{so} = W_0 \frac{1}{r} \left( \frac{d\rho}{dr} + \frac{dp}{dr} \right) \vec{\ell} \cdot \vec{s} \quad \text{with} \quad \frac{dp}{dr} < 0.$$  \hspace{1cm} (8)

The additional contributions from Eqs. (3) and (4) imply that when $\beta$ is positive the neutron (proton) spin-orbit splitting is reduced as protons (neutrons) fill a $j = l + 1/2$ level because $J_{p(n)} > 0$.

It is worth mentioning that with the Skyrme density formalism, one can easily study the combined contribution of the central exchange (6) and tensor (7) nucleon-nucleon interactions to the spin-orbit potential.

### III. THE RELATION TO A LONG RANGE TENSOR FORCE

Otsuka et al. [8] have pointed out that the nucleon-nucleon tensor force has a rather long range, reason for which the use of an energy density part due to the tensor force in the Skyrme approach may not be justified.

Equation (1) shows that the tensor term of the Skyrme interaction contains a $\delta$-function in the internucleon separation multiplied by momentum dependent terms. But 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 [8], this interaction has the same effect as a finite size interaction, due to its momentum dependence.

In Ref. [16] we have shown that the expressions (3) and (4), can be used to study the contribution of finite range tensor forces. We have used a factorization of the spin-density matrix for spherical nuclei introduced by Negele and Vautherin [20] which lead to a simplified form for a short range tensor interaction. On the other hand we considered a tensor interaction with a range of the order of the one pion exchange potential and calculated the ratio of the two contributions, say $S_Y$. In this way we have shown that the exact matrix elements of the one-pion exchange tensor potential for orbits with the largest $\ell$ could be expressed as a product of the short range expression given by Eq. (7) of Ref. [16] and a suppression factor $S_Y \approx 0.147$ which is almost constant for nuclei with mass number $A \geq 48$. It is only slightly larger, i.e. $S_Y \approx 0.16$ for nuclei near $^{28}\text{Si}$. Thus the short range formulae (3) and (4) with constant $\alpha$ and $\beta$ should give qualitatively good results for a Yukawa one-pion exchange potential. One should clearly make a difference between a zero-range tensor
FIG. 1: Proton single particle energy difference between the unoccupied $1f5/2$ level and the occupied $1f7/2$ level in Ni isotopes ($Z = 28$, $N = 40 - 50$) from the Skyrme SIII interaction without and with tensor force of parameters $\alpha = -118.75$ MeV fm$^5$, $\beta = 120$ MeV fm$^5$, Eqs. (5).

interaction and the tensor Skyrme interaction which is in fact finite range, as subsequently stressed in Ref. [21].

Interestingly, in Ref. [22] a reduction of the strength of the pion exchange tensor force from experimental nucleon-nucleon scattering was found necessary to get closer to experiment for Ca and Sn isotopic chains in a relativistic Hartree-Fock + Bardeen Cooper Schriffer (HF + BCS) approach.

Shell gaps are mainly determined by the spin-orbit splitting of the states with highest $l$ in any shell and our study was 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.

The conclusion was that the Skyrme energy functional with the tensor force is adequate to describe the evolution of shell effects.
IV. PARAMETERS

The considerations of the previous sections show that the simple forms (3) and (4) with constant $\alpha$ and $\beta$ are 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.

In Ref. [13] we searched for sets of parameters $\alpha$ and $\beta$ which simultaneously fit absolute values of single particle levels in the closed shell nuclei $^{48}$Ca, $^{56}$Ni, $^{48}$Zr and $^{208}$Pb. There we found that the common optimal values were located in a right angled triangle with the sides $-80 \text{ MeV fm}^5 \leq \alpha \leq 0$, $0 \leq \beta \leq 80 \text{ MeV fm}^5$ and hypotenuse $\alpha + \beta = 0$. In Ref. [16] these constraints were relaxed because we tried to analyze single particle energies of some nuclei far from the stability line. Our choice was guided by the recent results of Ref. [12] on the $Z = 50$ isotopes and $N = 82$ isotones which were analyzed in a HF + BCS approach based on the Skyrme interaction SLy5 with refitted values of $T$ and $U$ plus a pairing force.

In the present paper we still use the SIII version of the Skyrme interaction [15] for comparison with the previous work. We maintain the conditions $\alpha < 0$ and $\beta > 0$ which are not inconsistent with the previous findings [13]. In Ref. [16] we found that that the 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 $\beta = 120 \text{ MeV fm}^5$, gave a reasonably good fit to $Z = 50$ isotopes and $N = 82$ isotones. These values are similar to the ones fitted by Brown et al. [10].

V. NI ISOTOPES

The shell gaps of the proton and neutron single particle spectra obtained in the present Hartree Fock calculations with the Skyrme energy density functional can give an indication of the double magic character of $^{78}$Ni as observed in the recent experimental investigation of the stability of $Z = 28$, $N = 50$ shells [3,4]. Also one can study the compatibility with large scale shell model calculations. An important issue is to find out to what extent the tensor part of the Skyrme interaction influences the stability in the case of $^{78}$Ni. For example, Fig. 1 shows the evolution of the proton gap $e(1f5/2) - e(1f7/2)$ in Ni isotopes ($Z = 28$, $N = 40-50$) with and without tensor force. One can see that the effect of the tensor force is indeed important.
In both cases there is a decrease of the gap with the increase of the neutron number. At \( N = 40 \) the gap is maximum because \( J_n = 0 \), so that only the first term in Eq. 4 contributes to the spin-orbit part. The gap is positive because \( \alpha J_p \) is negative (\( \alpha < 0 \) and \( J_p > 0 \)) as seen from the definition. For \( N > 40 \) both terms in Eq. 4 contribute. As they have opposite signs due to \( \beta > 0 \), the second term reduces the contribution from the first and makes the gap smaller with increasing \( N \), i.e. with \( n_{q,k} \) in Eq. 2.

The decrease in the proton gap is compatible with the large scale shell model calculation results, mentioned in Ref. 4, where from the effective single particle energies it is found that the proton gap is reduced from 6.7 MeV at \( N = 40 \) to 4.9 MeV at \( N = 50 \) i.e. by 1.8 MeV, due to the strong \( 1f5/2 - 1g9/2 \) proton-neutron attractive interaction, contained in the spin-orbit and the tensor parts. Note the recent experimental results shown in Fig. 3 of Ref. 24 attest for the first time that the proton-neutron correlations are strong enough for a rapid change from the semi-magic structure at \( N = 50 \) to a collective structure at \( N = 52 \). The explanation is that \( Z = 28 \) is a weak sub-magic structure, as a consequence of the repulsive nature of the tensor force between the proton \( 1f7/2 \) and the fully occupied neutron \( 1g9/2 \).

In our case the reduction is of 3.28 MeV with tensor and 0.54 MeV without tensor. Thus the result with the tensor part included in the Skyrme interaction is closer to the large scale shell model results. It is useful to note that large-scale shell model calculations including the full \( pf \) shells for the protons and the full \( sdg \) shells for neutrons preserve the doubly magic nature of the ground state of \( ^{78}\text{Ni} \) but exhibits a well deformed prolate band at low excitation energy. Therefore, there is hope that the single particle properties are not perturbed by complicated correlations which appear to be important across \( Z = 28 \) and \( N = 50 \) as seen from Fig. 3 of Ref. 4 describing the two-neutron separation energies. Accordingly the evolution of the two-neutron shell gap as a function of the proton number seems to be an important observable for the strength of a shell as seen from Fig. 5 of the same paper. There is a peak at each neutron magic number. The overall behavior was explained in Ref. 25 using a mean field calculation where the peaked structure is found to be due to quadrupole correlations.

As mentioned in Section 11 the additional contribution brought by the tensor interaction to the spin-orbit is given by Eq. 11. There the product \( \beta J_n \) is positive because the parameter \( \beta \) is positive in these calculations and \( J_n \) is positive because the neutron \( 1g9/2 \) is filled so
that the proton spin-orbit splitting is reduced at $N = 50$, because $\alpha J_p$ is negative, thus weakening the $N = 50$ magic number. Such a weakening has been noticed in Ref. [3] in relation to the experimental analysis of the $^{79}\text{Cu}$ spectroscopy.

A. Proton single particle spectrum

Comparing Figs. 2 and 3 one can see the effect of the tensor force on the proton single particle levels around Fermi sea. The important difference is that while the levels $1f5/2$ and $2p3/2$ cross at $N = 48$ when the tensor is included, they never cross beyond $N = 40$ when the tensor is removed. The crossing is compatible with Fig. 3 of Ref. [3] where experimental systematics of the first $3/2^-$ and $5/2^-$ states of copper isotopes for $N = 40$ to 50 are indicated. The experiment suggests that the crossing takes place at $N = 46$ so that the ground state of $^{79}\text{Cu}$ should have a spin value of $5/2$. Our results with the tensor interaction support the proposal of Ref. [3]. The experimental excited state $3/2^-$, (see Fig. 2 of Ref. [3] for the proposed level scheme) lies at 656 keV above the ground state while in our case it lies at 470 keV when tensor is included. A fine tuning of the tensor parameters
FIG. 3: Proton single particle energies of Ni isotopes \((Z = 28, N = 40 - 50)\) around the Fermi sea obtained from the Skyrme SIII interaction without tensor force, \(\alpha_T = 0, \beta_T = 0\), see Eqs. (7).

\(\alpha_T\) and \(\beta_T\) of Eq. (7) may improve the agreement with the experiment, which is beyond the present purpose. The Monte Carlo shell-model calculations in the \(pf/g9/2d5/2\) model space with an A3DA Hamiltonian \(^26\) performed in Ref. \(^3\) give an excitation energy of 294 keV for the \(3/2^-\) level and 1957 keV for the \(1/2^-\) level while for the latter we obtain 2440 keV. The second excited level experimental of \(^{79}\)Cu is placed at 1511 keV. Its structure seems to be more complicated.

On the other hand our findings agree with the proton single particle energies calculated within a shell model with an A3DA Hamiltonian including minor corrections, which predict that the inversion of \(1f5/2\) and \(2p3/2\) levels in the Nickel chain does not take place before \(N = 48\), as seen from Fig. 4 of Ref. \(^19\), very much similar to ours. The interpretation is again as due to the tensor force. The probability of a state to have a single particle structure is convincingly high in the calculated low lying spectrum of \(^{77}\)Cu. The lowest \(3/2^-\) appears at 184 keV, somewhat smaller than the experimental value of 293 keV.

An inversion of in the proton occupation of the \(1f5/2\) and \(2p3/2\) levels in the Nickel chain is also observed in Fig. 4 of Ref. \(^4\), in this case between \(N = 44\) and \(N = 46\). The explanation given there is the effect of a strong \(1f5/2 - 1g9/2\) proton-neutron attractive interaction whose main active components are the spin-orbit and tensor. Our Eqs. (3) and
FIG. 4: Neutron single particle energies of Ni isotopes (Z = 28, N = 40 - 50) around the Fermi sea from Skyrme SIII interaction with tensor force parameters $T$ and $U$ giving $\alpha = -118.75 \text{ MeV fm}^5$, $\beta = 120 \text{ MeV fm}^5$.

(4) are consistent with such an interpretation about the role of the tensor force.

B. Neutron single particle spectrum

Although not much experimental information is available, the neutron single particle levels of Ni isotopes with $N = 40 - 50$ around the Fermi sea have been calculated. Fig. 4 shows the result with the tensor force. One can notice the presence of an increasingly large gap between the occupied $1g9/2$ and the unoccupied $2d5/2$ levels when $N > 44$ which takes the value of $5.87 \text{ MeV}$ for the neutron number $N = 50$. Note that at $N = 40$ the level $2d5/2$ is unbound. Thus the stability with increasing $N$ is larger and larger when tensor interaction is included at variance with the hint of possible weakening of the magic number $N = 50$ mentioned in Ref. (2). Such a weakening appears only when there is no tensor contribution, see Fig. 5 where the gap decreases from $5.43 \text{ MeV}$ at $N = 40$ to $4.66 \text{ MeV}$ at $N = 50$. Note that when the tensor is missing the level $1g9/2$ remains practically constant from $N = 40$ to $N = 50$. 
VI. CONCLUSIONS

We have performed Hartree-Fock calculations for the single particle proton and neutrons spectra for the Ni isotopic chain \( Z = 28, N = 40 - 50 \) by using the Skyrme energy density functional with the a previously determined parametrization including a tensor term. We have found that the tensor term is crucial in obtaining the inversion of the \( 1f_{5/2} \) and \( 2p_{3/2} \) proton levels around \( N = 48 \). This supports the doubly magic character of \(^{78}\text{Ni}\) as observed in recent experiments \cite{3,4} and the conclusion of Ref. \cite{3} that \(^{79}\text{Cu}\) can be described as a \(^{78}\text{Ni}\) core plus a valence proton. Our calculations are in agreement with large scale shell model calculations which include a tensor interaction, as for example those of Ref. \cite{19}. The single particle spectra present a large gap both for protons and neutrons the size of which is increased and governed by the tensor force. The Skyrme energy density functional remains a simple, reliable and predictive approach to study the evolution of nuclear shells far from the stability valley.
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