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

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(Received 29 March 2018; published 6 June 2018)

We calculate the single-particle spectrum of the double magic nucleus ^{78}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 that 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.

DOI: 10.1103/PhysRevC.97.064304

I. INTRODUCTION

For more than a decade there has been a growing interest in the neutron- or proton-rich nuclei far from the stability valley and in the evolution of nuclear shells in these regions. In particular ^{78}Ni was expected to be one of the most neutron-rich doubly magic nuclei. Its half-life time of 122.2(5.1) ms [1] and the prediction of a first excited state above 2 MeV [2] were a hint of the stability of the $Z = 28$ and $N = 50$ shells. The recent experiments of in-beam γ-ray spectroscopy at the Radioactive Isotope Beam Factory of RIKEN producing the nucleus ^{79}Cu [3] have 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 $^{75-79}$Cu at the CERN-ISOLDE facility supports the doubly magic character of ^{78}Ni [4]. The magnetic dipole and the electric quadrupole moments of $^{78}_{29}$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}Ni [5].

The shell structure and the existence of magic numbers are a consequence of the spin-orbit interaction [6,7]. Since 2005 there has been 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 [8–11] and the Hartree-Fock Skyrme energy density functionals [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 [13–15].

In an early work [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 so as to obtain a good global fit.

In Ref. [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. [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 β decay of $^{72-80}$Ni isotopes was calculated and it was found that the β-decay half-lives of these neutron-rich nuclei were in reasonably good agreement with the experiment.

With this incentive, here we calculate the single-particle spectrum of $^{56-78}$Ni isotopes to better understand the role of the tensor part and the behavior of the gap in the proton $1f$ shell. We find 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 analyze the behavior of the neutron $1g9/2$ subshell in the Ni isotopic chain. Agreement is found with recent shell-model calculations that 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 Sec. III we note the relation to a long-range tensor force. In Sec. IV we introduce the parameters. In Sec. 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.

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II. THE TENSOR PART OF THE SKYRME INTERACTION

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

$$\begin{aligned} V_T = {} & \tfrac{1}{2}T\{[(\vec{\sigma}_1\cdot\vec{k}')(\vec{\sigma}_2\cdot\vec{k}') - \tfrac{1}{3}k'^2(\vec{\sigma}_1\cdot\vec{\sigma}_2)]\delta(\vec{r}_1-\vec{r}_2) \\ & + \delta(\vec{r}_1-\vec{r}_2)[(\vec{\sigma}_1\cdot\vec{k})(\vec{\sigma}_2\cdot\vec{k}) - \tfrac{1}{3}k^2(\vec{\sigma}_1\cdot\vec{\sigma}_2)]\} \\ & + U\{(\vec{\sigma}_1\cdot\vec{k}')\delta(\vec{r}_1-\vec{r}_2)(\vec{\sigma}_2\cdot\vec{k}) \\ & - \tfrac{1}{3}(\vec{\sigma}_1\cdot\vec{\sigma}_2)[\vec{k}'\cdot\delta(\vec{r}_1-\vec{r}_2)\vec{k}]\}. \end{aligned} \tag{1}$$

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 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 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 $q = n$ and p stands for neutrons and protons, respectively. One has [14]

$$\begin{aligned} J_q = {} & \frac{1}{4\pi r^3}\sum_k n_{q,k}(2j_{q,k}+1) \\ & \times\left[j_{q,k}(j_{q,k}+1) - \ell_{q,k}(\ell_{q,k}+1) - \tfrac{3}{4}\right]R^2_{q,k}(r), \end{aligned} \tag{2}$$

where k runs over all occupied neutron or proton states, $R_k(r)$ 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]

$$\Delta W_n = (\alpha J_n + \beta J_p)\vec{\ell}\cdot\vec{s}, \tag{3}$$

$$\Delta W_p = (\alpha J_p + \beta J_n)\vec{\ell}\cdot\vec{s}, \tag{4}$$

with

$$\alpha = \alpha_T + \alpha_c, \;\; \beta = \beta_T + \beta_c. \tag{5}$$

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

$$\alpha_c = \tfrac{1}{8}(t_1 - t_2) = 61.25 \text{ MeV fm}^5, \quad \beta_c = 0, \tag{6}$$

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. (1), one has

$$\alpha_T = \tfrac{5}{12}U, \quad \beta_T = \tfrac{5}{24}(T+U). \tag{7}$$

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

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

The additional contributions from Eqs. (3) and (4) imply that when β 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 δ function in the internucleon separation multiplied by momentum-dependent terms. However, 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 δ-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] that leads to a simplified form for a short-range tensor interaction. On the other hand we have 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 ℓ could be expressed as a product of the short-range expression given by Eq. (7) of Ref. [16] and the suppression factor $S^Y \approx 0.147$, which is almost constant for nuclei with mass number $A \geqslant 48$. The suppression is only slightly larger, i.e., $S^Y \approx 0.16$, for nuclei near ^{28}Si. Thus the short-range formulas (3) and (4) with constants α and β should give qualitatively good results for a Yukawa one-pion-exchange potential. One should clearly see a difference between a zero-range tensor interaction and the tensor Skyrme interaction that 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-Schrieffer (HF + BCS) approach.

Shell gaps are mainly determined by the spin-orbit splitting of the states with the 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.

The conclusion is 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 constants α and β are a good approximation to the contribution of the tensor forces to the energy density. Values of α and β can be taken to be constant for states with maximum l in nuclei with $A \geqslant 48$ even for forces with a range of the one-pion-exchange potential.

In Ref. [13] we searched for sets of parameters α and β that 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 MeV fm$^5 \leqslant \alpha \leqslant 0$ and $0 \leqslant \beta \leqslant 80$ MeV fm^5 and the 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 the $N = 82$ isotones that were analyzed using a HF + BCS approach based on the Skyrme interaction SLy5 [23] 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 the values $\alpha_T = -180$ MeV fm^5 and $\beta_T = 120$ MeV fm^5, or equivalently $\alpha = -118.75$ MeV fm^5 and $\beta = 120$ 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 $Z = 28$ and $N = 50$ 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 αJ_p is negative ($\alpha < 0$ and $J_p > 0$) as seen from Eq. (2). For $N > 40$ both terms in Eq. (4) contribute. Because 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).

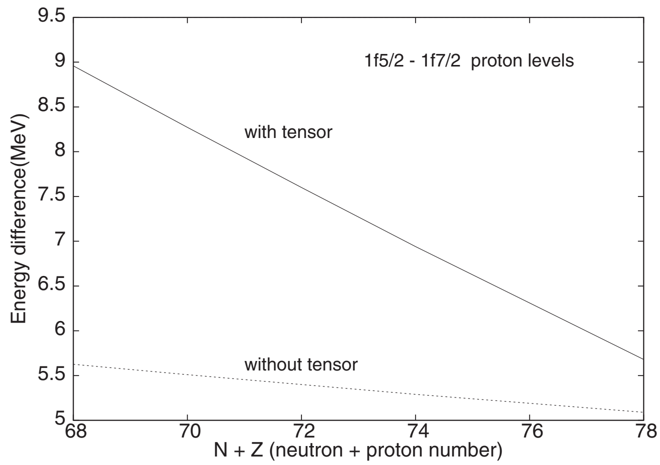

FIG. 1. Proton single-particle energy difference between the unoccupied $1f5/2$ level and the occupied $1f7/2$ level in Ni isotopes ($Z = 28$, $N = 40$–50) from the Skyrme SIII interaction without and with tensor force of parameters $\alpha = -118.75$ MeV fm^5 and $\beta = 120$ MeV fm^5 [Eqs. (5)].

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 semimagic structure at $N = 50$ to a collective structure at $N = 52$. The explanation is that $Z = 28$ is a weak submagic 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}Ni but exhibit a well-deformed prolate band at low excitation energy [2]. Therefore, there is hope that the single-particle properties are not perturbed by complicated correlations that 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 was found to be due to quadrupole correlations.

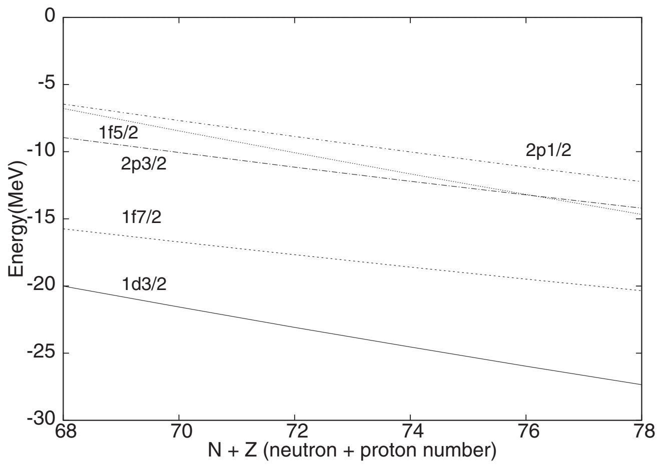

FIG. 2. Proton single-particle energies of Ni isotopes ($Z = 28$, $N = 40$–50) around the Fermi sea obtained with the Skyrme SIII interaction with the tensor force parameters $\alpha = -118.75$ MeV fm^5 and $\beta = 120$ MeV fm^5.

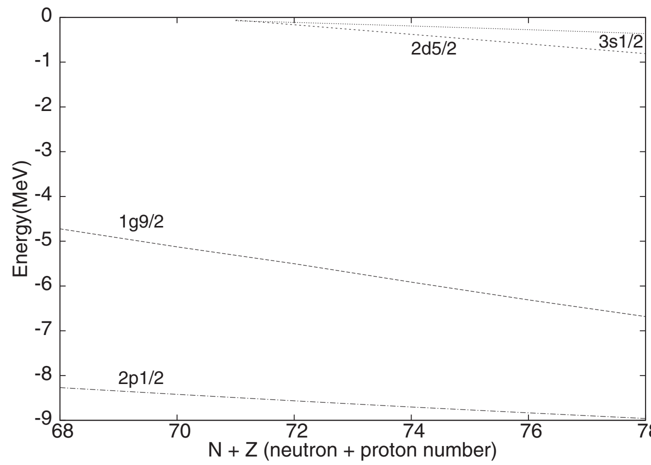

FIG. 4. Neutron single-particle energies of Ni isotopes ($Z = 28$, $N = 40$–50) around the Fermi sea from Skyrme SIII interaction with tensor force parameters T and U giving $\alpha = -118.75$ MeV fm^5 and $\beta = 120$ MeV fm^5.

As mentioned in Sec. II the additional contribution brought by the tensor interaction to the spin-orbit is given by Eq. (4). There the product βJ_n is positive because the parameter β 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 αJ_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}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 the 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}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 the tensor is included. A fine-tuning of the tensor parameters α_T and β_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 $pfg9/2d5/2$ 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.

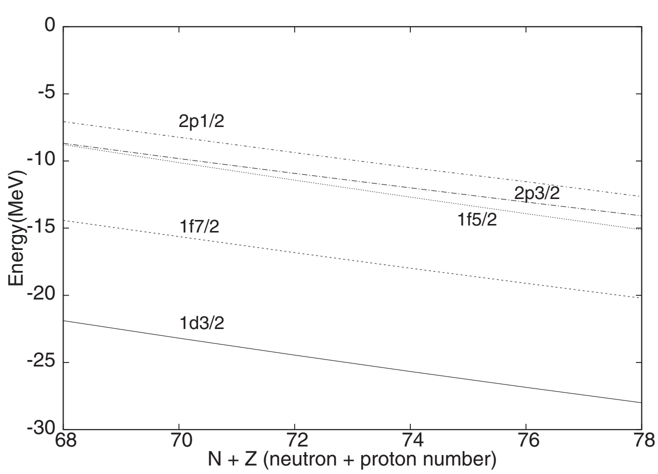

FIG. 3. Proton single-particle energies of Ni isotopes ($Z = 28$, $N = 40$–50) around the Fermi sea obtained from the Skyrme SIII interaction without tensor force, $\alpha_T = 0$ and $\beta_T = 0$ [see Eqs. (7)].

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 being 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 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 the tensor. Our Eqs. (3) and (4) are consistent with such an interpretation about the role of the tensor force.

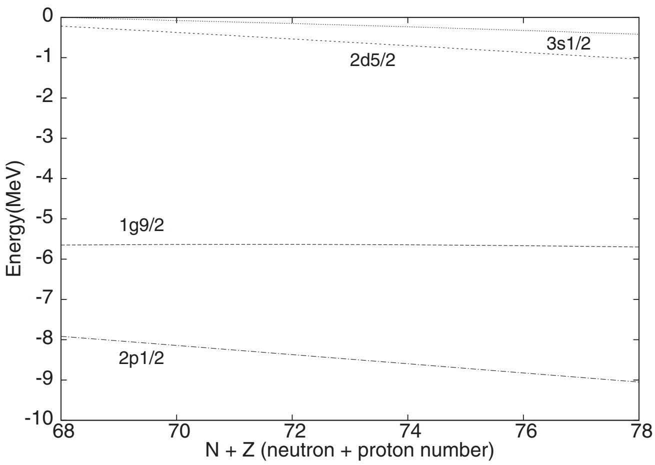

FIG. 5. Neutron single-particle energies of Ni isotopes ($Z = 28$, $N = 40$–50) around the Fermi sea calculated with the Skyrme SIII interaction without tensor force, $\alpha_T = 0$ and $\beta_T = 0$ [see Eqs. (7)].

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. Figure 4 shows the result with the tensor force. One can notice the presence of an increasingly large gap between the occupied $1g9/2$ level and the unoccupied $2d5/2$ level when $N > 44$ that takes the value of 5.87 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 Mev at $N = 40$ to 4.66 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 neutron spectra for the Ni isotopic chain $Z = 28$ and $N = 40$–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 $1f5/2$ and $2p3/2$ proton levels around $N = 48$. This supports the doubly magic character of ^{78}Ni as observed in recent experiments [3,4] and the conclusion of Ref. [3] that ^{79}Cu can be described as a ^{78}Ni core plus a valence proton. Our calculations are in agreement with large-scale shell-model calculations that include a tensor interaction, as for example those of Ref. [19]. The single-particle spectra present a large gap for both 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.

ACKNOWLEDGMENTS

We thank Ileana Guiasu for a careful reading of the manuscript. F.S. acknowledges support from the Fonds de la Recherche Scientifique-FNRS under Grant No. 4.4501.05.

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