

Reexamination of the $N = 50$ and $Z = 28$ shell closure

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Recent experiments performed in neutron-rich copper isotopes have revealed a crossing in the nucleus ^{75}Cu between the $3/2^-$ and $5/2^-$ levels, which correspond to the ground state and the first excited state in isotopes with mass number below $A = 75$. Due to the strong single-particle character of these states, this scenario can be investigated through the analysis of the proton spectrum provided by mean-field models in nickel isotopes with neutron numbers between $N = 40$ and $N = 50$. In this work, we show that the aforementioned crossing is mainly driven by the mean field provided by the effective nucleon-nucleon and spin-orbit interactions. We also analyze the impact of the tensor interaction and find that in some mean-field models it is essential to reproduce the crossing of the $2p_{3/2}$ and $1f_{5/2}$ proton single-particle levels, as in the case of the SAMi-T Skyrme force and the DIM Gogny interaction, whereas in other cases, as for example the SLy5 Skyrme force, a reasonable tensor force appears to be unable to modify the mean-field enough to reproduce this level crossing. Finally, in the calculations performed with the so-called simple effective interaction (SEI), it is shown that the experimental data in nickel and copper isotopes considered in this work can be explained satisfactorily without any explicit consideration of the tensor interaction.

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Effective nuclear mean field models are usually fitted to reproduce as well as possible the structure and properties of nuclei along the stability valley. However, modern facilities, such as *Système de Production d'Ions Radioactifs Accélérés en Ligne* (SPIRAL) at Grand Accélérateur National d'Ions Lourds (GANIL), *Isotope Separator On Line Device* (ISOLDE) at Conseil Européen Pour la Recherche Nucléaire (CERN), the *Facility for Antiprotons and Ion Research* (FAIR) at *Gesellschaft für Schwerionenforschung* (GSI), and the *Facility for Rare Isotope Beams* (FRIB) at Michigan State University (MSU), are delivering many new experimental data about exotic nuclei near the drip lines. Of particular relevance are the changes observed in the nuclear shell structure where new phenomena, such as the disappearance of the standard magic numbers 20 and 28 for neutrons and the emergence of new magic numbers at $N = 14, 16, 32,$ and $34,$ may occur in neutron-rich nuclei (see Ref. [1] and references therein). These new magic numbers appear due to the imbalance of

neutron and protons, which strongly modify the spin-orbit potential that in turn determines the shell structure.

A region of experimental interest nowadays is around the magic numbers $Z = 28$ and $N = 50$, where measurements of the decay properties in Co, Ni, Cu, and Zn reveal the magic character of the nucleus ^{78}Ni [2–4], which is also confirmed by the precise measure of the nuclear spin and dipole and quadrupole moments in neutron-rich Cu-isotopes [5,6] and by the γ -ray spectroscopy in ^{79}Cu [1]. The experimental results also show an inversion of the spin of the ground state of neutron-rich copper isotopes from $3/2^-$ to $5/2^-$, which takes place beyond ^{73}Cu [7]. Large-scale shell-model calculations reported in Ref. [8] show that in copper isotopes with neutron number larger than $N = 40$ the $3/2^-$ and $5/2^-$ states have an important single-particle character, although coexisting with other states of collective nature. It is not guaranteed that this characteristic can be translated to the Hartree-Fock (HF) orbitals discussed below because beyond mean-field correlations may play a non-negligible role in the renormalization of single-particle propagators. In particular, particle-vibration coupling is known to have a potentially strong effect on single-particle orbitals in odd nuclei. However, as we are concerned about the behavior as a function of the interaction of the orbitals, most of these effects are going to be similar in all the considered cases. More recent shell-model calculations [9] also predict the double-magic character of the nucleus

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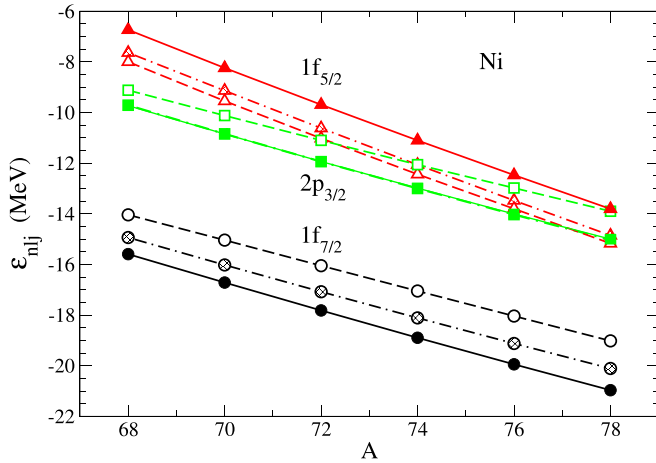


FIG. 1. Proton single-particle levels around the Fermi level for Ni isotopes from $A = 68$ to $A = 78$ computed with the Skyrme forces SAMi-T [17] (dashed line) and SLy5 with the tensor part fitted in Refs. [19] (solid line) and [20] (dash-dotted line), respectively.

^{78}Ni , which, however, shows the phenomenon of shape coexistence.

At the mean field level, Ni isotopes are spherical with a deep minimum as a function of quadrupole deformation as can be seen in the online database [10] for the Gogny D1S interaction. We have checked that the behavior is qualitative and quantitatively similar with the other forces discussed below. The Cu isotopes show a similar behavior except for two shallow deformed minima around the spherical configuration [10] consequence of the polarization effect of the unpaired proton. The crossing of the $2p_{3/2}$ and $1f_{5/2}$ single-particle proton levels in neutron-rich Ni isotopes can be understood in terms of a strong tensor interaction, which is attractive between the neutron $1g_{9/2}$ and proton $1f_{5/2}$ levels and repulsive between $1g_{9/2}$ and $2p_{3/2}$ levels [11]. The microscopic nucleon-nucleon interaction contains a tensor contribution, whose most important component is related to the tensor-isospin channel. In this case, the long-range behavior of the tensor force is dominated by the exchange of a single pion [12,13], which is longer than the ranges of all the remaining contributions to the nucleon-nucleon interaction.

In the case of Skyrme forces, a tensor interaction, which is zero range and momentum dependent in configuration space, was proposed long ago [14]. The question raised on the validity of the use of the zero-range tensor force in Ref. [15] is clarified later on in the work by Brink and Stancu [16], where they have shown that the momentum dependence of the zero-range tensor force [14] simulates the same effect as the finite-range tensor interaction. With Skyrme forces, the use of a tensor term seems unavoidable to reproduce the position of the $2p_{3/2}$ and $1f_{5/2}$ single-particle proton levels in the Ni isotopic chain beyond neutron number $N = 40$ [16] observed experimentally in Refs. [2,4,5,7] and interpreted theoretically with Monte Carlo shell model calculations [8,9]. In Fig. 1, we show the single-particle energies of the $1f_{7/2}$, $2p_{3/2}$, and $1f_{5/2}$ proton levels along the Ni isotopic chain with neutron number in the range $N = 40$ – 50 obtained with the Skyrme

interaction SAMi-T that includes tensor terms [17]. This force predicts the crossing between the $2p_{3/2}$ and $1f_{5/2}$ proton levels in the nucleus ^{72}Ni . However, it should be pointed out that the incorporation of tensor terms in the Skyrme interaction may not be sufficient to reproduce the crossing of the $2p_{3/2}$ and $1f_{5/2}$ single-particle proton levels in neutron-rich Ni isotopes. For example, this appears to be the case of the Skyrme interaction SLy5 [18] including tensor terms, which fails to reproduce the proton level crossing in Ni isotopes, as can be seen in Fig. 1. This is surprising as this force was fitted to reproduce the relative energies of proton (neutron) single-particle levels in some isotopic (isotonic) chains [19] determined experimentally in Ref. [21]. A reparametrization of the tensor part of the SLy5 interaction has been proposed recently [20] by fitting the the neutron $1f$ spin-orbit splitting for the nuclei ^{40}Ca , ^{48}Ca , and ^{56}Ni to the experimental data. Again, this parametrization of the tensor force does not predict the crossing of the aforementioned levels, which can be seen in the same figure.

The standard parametrizations of the Gogny force [22] of the D1 family, namely D1S [23], D1N [24], and D1M [25], predict that, for increasing neutron number, the energy gap between the $2p_{3/2}$ and $1f_{5/2}$ single-particle proton levels in neutron-rich Ni isotopes decreases and almost vanishes in the magic nucleus ^{78}Ni . This can be seen in the upper panel of Fig. 2 that displays the single-particle energies of the proton levels $1f_{7/2}$, $2p_{3/2}$, and $1f_{5/2}$ of the nuclei between ^{68}Ni and ^{78}Ni computed with the D1M interaction. In this panel, we show the full HF result calculated in coordinate space (see Ref. [28] and references therein) and the one obtained using the so-called quasilocal density functional theory (QLDFT) [27], where the exchange energy is written as a local density functional with the help of the semiclassical one-body density matrix including \hbar^2 corrections [29]. From this figure, we can conclude that the QLDFT single-particles energies agree very accurately with the full HF ones. If a tensor contribution is included in the Gogny force [26,28,30], the HF+BCS calculation performed with the D1MTd interaction in neutron-rich Ni isotopes predicts the same eigenvalues for the $2p_{3/2}$ and $1f_{5/2}$ proton levels in the nucleus ^{74}Ni . The same result can be obtained using QLDFT if a tensor contribution is included. Unlike the calculations reported in Refs. [26,28,30], we include in the QLDFT functional a zero-range tensor force as the one used in Skyrme interactions [14]. The predictions of the HF+BCS calculation using the D1MTd parametrization are compared in the lower panel of Fig. 2 with those provided by the QLDFT with D1M supplemented by a zero-range tensor force with parameters $\alpha_T = -52.08 \text{ MeV fm}^5$ and $\beta_T = 215.83 \text{ MeV fm}^5$ (see Refs. [16,20] for the definition of these parameters). The tensor term used for the D1MTd interaction has been defined as

$$V_T(1, 2) = \left[V_{T1} + V_{T2} \frac{[1 + \boldsymbol{\tau}(1) \cdot \boldsymbol{\tau}(2)]}{2} \right] S_{12} \times \exp[-(\mathbf{r}_1 - \mathbf{r}_2)^2 / \mu_T^2], \quad (1)$$

where S_{12} is the traditional tensor operator and $\boldsymbol{\tau}(i)$ is the isospin operator. The specific values of the parameters are $V_{T1} = -230 \text{ MeV}$, $V_{T2} = 180 \text{ MeV}$, and $\mu_T = 1.0 \text{ fm}$, and

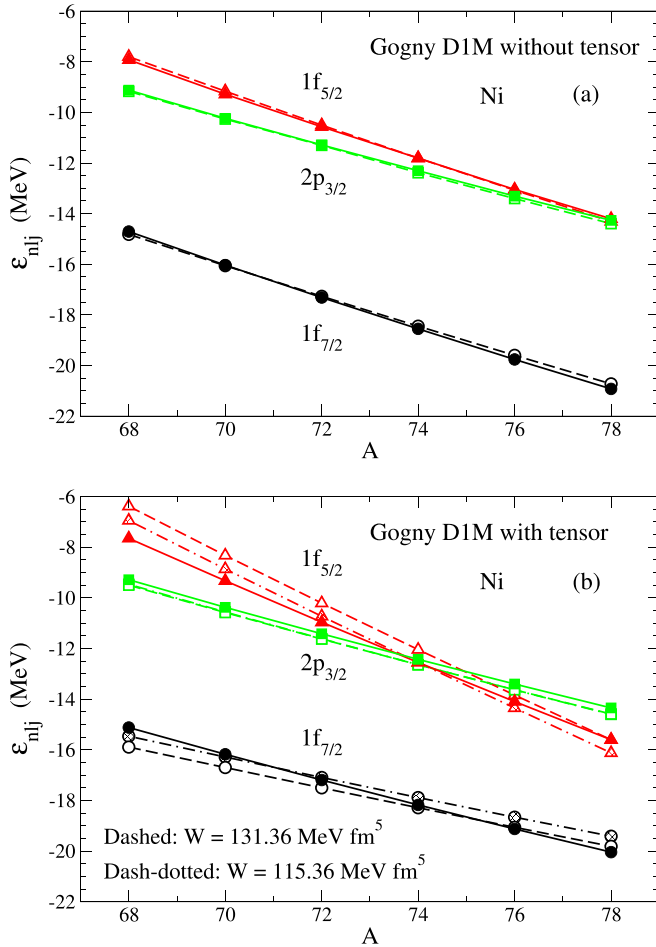


FIG. 2. Same as Fig. 1 but computed with the DIM Gogny force without (upper panel) and with (lower panel) tensor terms. Solid lines are obtained from the HF calculation of Ref. [26] using the D1MTd interaction. Dashed and dashed-dotted lines are computed within the QLDFT approximation described in Ref. [27].

have been chosen to reproduce the energy values of the first 0^- states for the nuclei ^{16}O , ^{40}Ca , and ^{48}Ca . It is important to note that this tensor term is added in a perturbative way, in the sense that no other terms of the Gogny interaction (central and density-dependent terms) have been modified and then, in this approximation, no interplay effect can be expected between tensor terms and other central ones, as, for example, the $\sigma\sigma\tau\tau$ part, as it was argued by Otsuka *et al.* in Ref. [11] in a more general context. The DIST2 interaction, based on the DIS Gogny force and including a perturbative tensor term [26], also predicts the same level crossing in Ni isotopes as D1MTd.

The nice agreement between both results points out, along with Ref. [16], that the main effects of the tensor interaction can be very well reproduced by using a zero-range tensor force similar to that associated to the Skyrme forces [14]. It should be pointed out that when the tensor force is added in the QLDFT functional the parameters of the interaction should be readjusted. Here, in order to estimate the impact of the additional tensor force on the binding energies and single-particle spectra in a simple way, we refit the strength of the spin-orbit

force to keep the binding energy of the nucleus ^{208}Pb equal to the original value predicted by the DIM force. This implies that the spin-orbit strength changes from the original DIM value 115.36 to 131.36 MeV fm^5 when the zero-range tensor force is included in the QLDFT functional. With this change, the binding energy of the nucleus ^{78}Ni increases by almost 1.5%, while the crossing of the $2p_{3/2}$ and $1f_{5/2}$ levels is slightly modified but still predicting the crossing of the two first proton single-particle excited states in passing from ^{74}Ni to ^{76}Ni .

In this work, we would like to note the fact that, in spite of the results discussed until now, the tensor interaction may not be necessary to reproduce the crossing between the $2p_{3/2}$ and $1f_{5/2}$ single-particle proton levels in neutron-rich Ni isotopes. This is the case, for instance, with the so-called simple effective interaction (SEI), which was first proposed for symmetric and asymmetric nuclear matter studies in Ref. [31] and extended later on to finite nuclei in Refs. [32,33]. This effective interaction contains a single finite-range term with a form factor $f(r)$ of Gauss or Yukawa type and two zero-range terms, one of them density dependent with an additional factor to avoid a supraluminous behavior [34]. Thus, the SEI reads

$$\begin{aligned}
 V_{\text{eff}} = & t_0(1 + x_0 P_\sigma)\delta(\vec{r}) \\
 & + \frac{t_3}{6}(1 + x_3 P_\sigma)\left(\frac{\rho(\vec{R})}{1 + b\rho(\vec{R})}\right)^\gamma \delta(\vec{r}) \\
 & + (W + BP_\sigma - HP_\tau - MP_\sigma P_\tau)f(\vec{r}). \quad (2)
 \end{aligned}$$

Nine of the eleven parameters of SEI are fitted to reproduce empirical constraints and microscopical results in nuclear and neutron matter obtained with realistic interactions. In particular, it is demanded that the nuclear mean-field in symmetric nuclear matter at saturation density vanishes for a kinetic energy of the incident nucleon of 300 MeV, a value extracted from the optical model fit to the nucleon-nucleus scattering data at intermediate energies. This constraint allows us to determine, for a given value of the exponent γ , the strength of the exchange energy and the range of the form factor in an unambiguous way. One of the two free parameters, namely x_0 , is fixed from the spin-up spin-down splitting of the effective mass in polarized neutron matter [33]. Finite nuclei calculations require, in addition, to consider the spin-orbit interaction, which is chosen of zero range as in the case of Skyrme or Gogny forces [35]. The t_0 parameter of SEI and the strength of the spin-orbit interaction W_0 are fitted within the QLDFT to reproduce the binding energies of the magic nuclei ^{40}Ca and ^{208}Pb . To deal with open-shell nuclei, we introduce a density-dependent pairing force proposed by Bertsch and Esbensen [36] without any adjustable parameter and treat the pairing correlations within an improved BCS approach [37] (see Refs. [32,33] for further details). In Ref. [32], we have analyzed the binding energies of 161 even-even spherical nuclei using the QLDFT formalism. This study was enlarged to 620 even-even spherical and deformed nuclei described at HFB level using SEI [38]. These studies performed in finite nuclei show that, on the one hand, the binding energies obtained in the QLDFT approximation with this parametrization of SEI are in excellent agreement with the corresponding full HFB

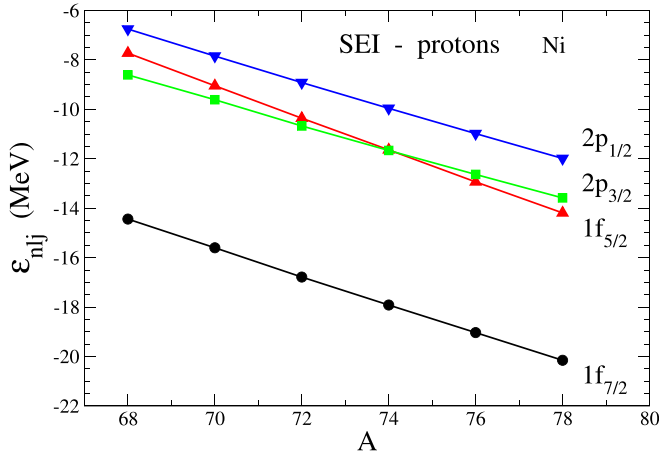


FIG. 3. Same as Fig. 1 but computed with the SEI model discussed in Ref. [32].

results and, on the other hand, that the rms deviations predicted by this set for the binding energies and charge radii of 620 even-even nuclei are similar to those found using Skyrme and Gogny effective forces. We also point out that the single-particle energies computed with the SEI parametrization used in this work are in reasonable agreement with the experimental values and describe the spectrum of ^{208}Pb as good or better than other effective mean-field models (see in this respect Fig. 8 of Ref. [32]). The mean-field predicted by SEI is also able to predict, without any additional modification, the kinks in the isotopic shifts of charge radii in ^{208}Pb , ^{210}Pb , and ^{212}Pb , which are not predicted by Skyrme or Gogny forces with an isospin-independent spin-orbit interaction (see Ref. [32] for a more detailed discussion).

In Fig. 3, we display the proton single-particle levels around the Fermi level for Ni isotopes with $N = 40$ – 50 computed using the SEI parametrization of Ref. [32]. It can be seen that the splitting between the $1f_{5/2}$ and $1f_{7/2}$ proton levels decreases in passing from $N = 40$ to $N = 50$ by 0.75 MeV, which is about one-half of the proton gap reduction found in large-scale shell-model calculations [39]. This reduction is due to the strong $1f_{5/2}$ - $1g_{9/2}$ proton-neutron attraction combined with the $1f_{7/2}$ - $1g_{9/2}$ repulsion, which increases when the occupation of the $1g_{9/2}$ level grows [11,40,41]. A similar effect, but less pronounced, also happens with the $2p_{3/2}$ - $2p_{1/2}$ proton gap, which is reduced by 0.26 MeV in passing from ^{68}Ni to ^{78}Ni . As explained in detail in Refs. [11,40,41], these changes in the single-particle energies are due to the monopole contributions of the original interaction, which includes central, spin-orbit, and eventually tensor contributions. As a result of the mentioned evolution of the Ni proton levels with neutron number in SEI, this interaction leads to the crossing between the $2p_{3/2}$ and $1f_{5/2}$ proton levels in neutron-rich Ni isotopes at $N = 46$, in agreement with the experimental observation.

The experimental results in Cu isotopes suggest that the crossing between the $2p_{3/2}$ and $1f_{5/2}$ proton levels take place in the nucleus ^{75}Cu , which implies that the ground state of

^{79}Cu has spin parity $5/2^-$ [1]. In the same nucleus, it is also found that the first excited state has spin parity $3/2^-$ and lies 656 keV above the ground state. The nature of the low-lying levels in Cu isotopes with neutron numbers beyond $N = 40$ have been investigated by means of Coulomb excitation with radioactive beams [7]. These experimental results reveal that at very low excitation energy collective and single-particle levels coexist. The $3/2^-$ and $5/2^-$ levels are of particular interest and their excitation energies can be easily estimated from the single-particle energies computed with a mean-field model. The QLDFT calculation of ^{78}Ni with the SEI model without adding any extra tensor term predicts that the excitation energy of the $3/2^-$ level is 607 keV, to be compared with the value 656 keV, extracted from the analysis of experimental data [1], and 294 keV obtained in the shell-model calculations reported in Ref. [1]. The analysis of the experimental data of ^{79}Cu also suggests another excited state $1/2^-$ 1511 keV above its ground state, while the excitation energy is 1957 keV according to shell-model calculations and it is predicted at 2203 keV by the SEI calculation in ^{78}Ni . The level structure of the nucleus ^{77}Cu has been investigated in Ref. [4]. The ground state is also $5/2^-$ and the first excited state $3/2^-$ lies 293 keV above the ground state while the shell-model prediction is 184 keV. This experimental scenario is also described, at least qualitatively, by the SEI calculations carried out in ^{76}Ni , where the ground state is predicted to be $5/2^-$ and the first excited state, $3/2^-$, is placed 301 keV above it.

A slightly more accurate estimate about the single-particle properties of neutron-rich Cu isotopes can be obtained by performing mean-field calculations of odd ^{69}Cu - ^{75}Cu isotopes with blocking in the uniform filling approximation [42]. Although these nuclei are slightly deformed [10], we neglect the deformation effects in our estimate of the energies of the ground state and the first excited state. The results of our investigations using the SEI model are collected in Table I together with the experimental energies extracted from Fig. 3 of Ref. [1]. The SEI model predicts that the crossing between the $3/2^-$ and $5/2^-$ single-particle states occurs for the nucleus ^{75}Cu , in agreement with the experimental findings. The excitation energies of the first excited level $5/2^-$, in isotopes between ^{69}Cu and ^{75}Cu , and $3/2^-$, for ^{77}Cu and ^{79}Cu , predicted by the SEI model are in nice agreement with the experimental data. We have repeated this analysis but using the DIM and DIMTd Gogny forces in full HF calculations. Using the DIMTd interaction, the experimental spin parity of the ground state is predicted correctly and the experimental energy of the first excited state is qualitatively reproduced (see the column of results for DIMTd in Table I). On the other hand, using the DIM force the crossing of the ground and first excited states is not predicted and the energy of the first excited state follows a downward trend, in disagreement with the experimental results.

There is not much experimental information available concerning the neutron single-particle levels in neutron-rich Ni isotopes between ^{68}Ni and ^{78}Ni [16]. The SEI predicts that the gap between the $1g_{9/2}$ and $2d_{5/2}$ neutron levels remains practically constant for all the neutron-rich isotopes considered, pointing out that the SEI model maintains the

TABLE I. Ground-state spin and energy of neutron-rich odd Cu isotopes predicted by the SEI model used in this work. The energy of the first excited state E^* is shown for the SEI model and for the HF calculation in a simple IPM approximation using the D1M and D1MTd Gogny forces. Notice that D1M predicts $3/2^-$ as spin parity of the ground state of the nuclei ^{77}Cu and ^{79}Cu . The experimental energies are also reported for comparison. Also notice that according to the experimental results of Ref. [5], the spin parity of the ground state of the nucleus ^{75}Cu is $5/2^-$ and the first excited state $3/2^-$ lies 62 keV above.

Nucleus	Spin parity	Energy (SEI) (MeV)	Energy (exp) (MeV)	E^* (SEI) (keV)	E^* (exp) (keV)	E^* (D1M) (keV)	E^* (D1MTd) (keV)
^{69}Cu	$3/2^-$	-598.59	-599.97	794	1215	1199	1635
^{71}Cu	$3/2^-$	-612.93	-613.09	544	537	952	1048
^{73}Cu	$3/2^-$	-625.76	-625.51	282	263	719	458
^{75}Cu	$3/2^-$	-637.49	-637.13	72	62	499	123
^{77}Cu	$5/2^-$	-648.38	-647.42	246	295	264	692
^{79}Cu	$5/2^-$	-658.19	-656.65	525	660	61	1257

magic character of the neutron number $N = 50$. This fact is in agreement with a similar finding reported in Ref. [16], which for the case of the Skyrme III interaction including a tensor contribution predicts an enhancement of the neutron gap between the $1g_{9/2}$ and $2d_{5/2}$ levels in passing from ^{68}Ni to ^{78}Ni , reinforcing the magic character of the neutron number $N = 50$.

In summary, in this work we wanted to underline that the effect of the monopole component of the central part of the nucleon-nucleon interaction is actually relevant and may modify the behavior of the single-particle levels along isotopic or isotonic chains in a quite considerable extension, masking the monopole effects coming from the spin-orbit and tensor parts of the nucleon-nucleon interaction. To highlight these facts, we consider exotic nickel isotopes between ^{68}Ni and ^{78}Ni because different measurements performed in copper isotopes suggest a crossing between the unoccupied $2p_{3/2}$ and $1f_{5/2}$ single-particle proton levels that occurs when the neutron number is $N = 46$. It has been claimed in earlier literature [16] that using Skyrme forces including a zero-range tensor term the aforementioned crossing can be reproduced. This is true for some particular forces, as for example the Skyrme III interaction used in Ref. [16] or in the recently reported SAMi-T force [17]. However, in the particular case of the SLy5 interaction [18], the crossing between the $2p_{3/2}$ and $1f_{5/2}$ proton levels does not seem to be reproduced by adding tensor terms [19,20], which were fitted to reproduce other observables sensitive to the tensor force but not to the crossing of proton levels in neutron-rich Ni isotopes. This is a first indication that the monopole effects from the tensor force may not be enough to reproduce the aforementioned crossing. It also suggests that in the case of the SLy5 interaction the central and spin-orbit components of the mean field are not well suited to reproduce the crossing of the proton levels in neutron-rich Ni isotopes. Another interesting example is provided by the finite-range D1M Gogny interaction [25]. This Gogny force, as well as the D1S one [23] widely used as a benchmark for pairing and deformation properties in finite nuclei [10], predicts that the single-particle energies of the $2p_{3/2}$ and $1f_{5/2}$ proton levels almost coincide for the nucleus ^{78}Ni , implying that the monopole contribution of the central and spin-orbit

parts of the nucleon-nucleon interaction are not enough for yielding the crossing in the right place. However, the right crossing can be achieved by adding a tensor force [26,28,30]. We have repeated this study of neutron-rich nickel isotopes described by the D1M Gogny force by using the QLDFT formalism instead of HF in coordinate space. We have seen that the QLDFT energy levels coincide almost perfectly with the ones obtained at HF level, at least for the Ni isotopes analyzed here. We have included in the QLDFT formalism a zero-range tensor term as the one used in Skyrme interactions [14], finding again a very good agreement with the HF calculation that includes a finite-range tensor force. As a last example, we discuss the predictions of QLDFT calculations obtained with the SEI interaction used in Refs. [32,33], which does not contain tensor terms. In this case, the crossing of the $2p_{3/2}$ and $1f_{5/2}$ proton levels in the nickel isotopic chain takes place at the nucleus ^{74}Ni without any modification of the interaction and its parameters. We have refined the SEI predictions by performing mean-field calculations along the ^{69}Cu - ^{79}Cu isotopic chain including blocking in the uniform filling approach and neglecting deformation effects. These calculations predict that the ground state and the first excited state are $3/2^-$ and $5/2^-$, respectively, for isotopes lighter than ^{75}Cu where the crossing takes place, in agreement with the compilation of experimental data of Fig. 3 of Ref. [1]. The spin parity of the ground state and first excited state of the nuclei ^{77}Cu and ^{79}Cu are predicted to be $5/2^-$ and $3/2^-$, respectively, also in agreement with the experimental data. In addition, our estimate also reproduces the energies of the first excited state of copper isotopes in the range ^{69}Cu - ^{79}Cu to quite satisfactory extent.

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