PHYSICAL REVIEW C **85**, 051301(R) (2012)

Three-body forces and persistence of spin-orbit shell gaps in medium-mass nuclei: Toward the doubly magic ^{78}Ni

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(Received 27 January 2012; published 7 May 2012)

We present state-of-the-art shell-model calculations in a large model space (pf for protons, $fpgd$ for neutrons), which allows us to study simultaneously excitations across the $Z = 28$ and $N = 50$ shell gaps. We explore the region in the vicinity of ^{78}Ni, which is a subject of intense experimental investigations. Our calculations correctly account for the known low-lying excited states in this region, including those which may correspond to cross-shell excitations. We observe the minimum of the $N = 50$ mass gap at $Z = 32$ consistent with experimental data and its further increase toward $Z = 28$, indicating a robustness of the $N = 50$ gap in ^{78}Ni. The evolution of the $N = 50$ gap along the nickel chain is shown to bear similarities to what is known in oxygen and calcium chains, providing a new opportunity for the studies of three-body monopole effects in medium-mass nuclei.

DOI: 10.1103/PhysRevC.85.051301 PACS number(s): 21.60.Cs, 21.30.−x, 21.45.Ff, 23.20.Lv

The search for the breaking of shell closures known at the stability valley when going toward the drip lines is one of the problems of contemporary nuclear structure studies. Recent decades have provided many cases of unexpected shell erosions, ^{42}Si being a famous example [1], and of appearances of deformed intruders in supposedly semimagic nuclei known as the phenomena of *islands of inversions* [2,3]. The issue of the occurrence of shell quenching in connection with astrophysical scenarios has been widely debated, in particular for $N = 50$ and $N = 82$ around the r-process waiting points [4–7].

Experimental progress allows for the study of more and more exotic systems, including the nuclear structure toward the still unknown, possibly doubly magic nucleus ^{78}Ni. The region around it is interesting for several reasons: very neutron rich nuclei play an important role in r-process nucleosynthesis, and ^{78}Ni is one of its possible waiting points [8–10]. From the nuclear structure point of view, ^{78}Ni, with the largest N/Z ratio in a doubly magic nucleus, represents a unique possibility of exploring the properties of very neutron-rich nuclei. The evolution of the $N = 50$ gap between ^{68}Ni and ^{78}Ni may be due to the repulsive character of the effective three-body force, in analogy to what has been found in oxygen and calcium chains [11,12]. Thus, constraining its size is of paramount importance for future developments and tests of state-of-the-art effective interactions with the inclusion of many-body forces, as well as for validation of empirical *universal monopole* interactions, such as those proposed in Refs. [13–15]. The knowledge of single-particle energies of ^{78}Ni is also crucial for shell-model studies which utilize this nucleus as a core [16–20] and which allow exploration of the properties of $A = 80$–90 neutron-rich nuclei, including those lying on the r-process path.

Though a lot of experimental evidence in this region has been accumulated, the data, or to be precise the conclusions drawn by different authors, seem contradictory. The possibility of the weakening of the $N = 50$ closure has been anticipated, e.g., in Refs. [21–23], while the contrary has been deduced by other authors, e.g., in Refs. [24–26]. One should notice, however, that experimentally it is still not possible to reach ^{78}Ni itself and since the shell effects manifest themselves suddenly at the shell closures, while being hindered by correlations in semimagic nuclei, it is not possible to conclude firmly on the rigidity of ^{78}Ni based on the currently available data alone. To shed light on the physics of this nucleus one needs a theory capable of reproducing the spectroscopic details of the region and robust enough to extrapolate to the yet unknown regions. As crucial information about the underlying shell evolution can be extracted from the structure of odd nuclei, the large-scale shell model, currently the only nuclear theory model treating on the same footing even and odd systems, is a tool of choice to explore the shell evolution in the vicinity of ^{78}Ni.

Recently, we have addressed the problem of the possible quenching of the $Z = 28$ gap in the shell-model framework, using a large valence space containing pf orbitals for protons and $pf_{5/2}g_{9/2}$ orbitals for neutrons [27]. In this Rapid Communication we present calculations that are performed in an even larger model space, which contains pf-shell orbitals for protons and $f_{5/2}$, p, $g_{9/2}$, $d_{5/2}$ orbitals for neutrons, allowing thus for simultaneous excitations across $Z = 28$ and $N = 50$ gaps. The detailed spectroscopy of $N = 49$–50 nuclei and the evolution of the neutron $N = 50$ gap with the proton number between ^{78}Ni and ^{86}Kr and with the neutron number between ^{68}Ni and ^{78}Ni is discussed.

The effective interaction used in this work is based on realistic G matrices with a number of experimental constraints taken into account to improve the properties of the monopole part of the Hamiltonian, as commonly practiced in the shell model [28]. A detailed description of this effective interaction can be found in Ref. [3]. In this work, however, we have introduced additional monopole adjustments with respect to Ref. [3], in order to constrain the proton gap evolution from ^{68}Ni to ^{78}Ni [27]. To probe reliability of such an interaction, we investigate the low-lying states of even-even $N = 50$ nuclei between ^{78}Ni and ^{84}Se, as well as even-odd $N = 49$ isotones between ^{79}Zn and ^{85}Kr, which correspond to cross-shell excitations. We discuss also the evolution of neutron shells along the nickel chain and provide predictions for the structure of ^{78}Ni. The calculations are performed using the m-scheme code ANTOINE [28,29].

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TABLE I. Experimental vs theoretical excitations energies and calculated occupation numbers in the wave functions of low-lying excited states in ^{82}Ge. Given in bold are the neutron occupancies in the states corresponding to the 1p-1h excitations across the $N = 50$ shell gap.

Expt.		Theor.		Protons			Neutrons	
J^π	E (MeV)	J^π	E (MeV)	$f_{7/2}$	$f_{5/2}$	p	$g_{9/2}$	$d_{5/2}$
0^+	0.0	0^+	0.0	7.64	3.74	0.41	9.65	0.37
2^+	1.35	2^+	1.40	7.77	3.73	0.33	9.60	0.42
4^+	2.28	4^+	2.21	7.84	3.79	0.23	9.6	0.36
$(5^+, 6^+)$	2.93	5^+_1	3.17	7.59	3.61	0.50	**8.53**	**1.48**
(6^+)	3.23	6^+_1	3.37	7.59	3.62	0.49	**8.57**	**1.44**
		5^+_2	4.22	7.79	3.01	0.81	9.52	0.49
		6^+_2	4.32	7.82	3.04	1.02	9.64	0.37

Let us start the discussion with a reminder of the current status of experimental knowledge on the structure of $N = 49$ and $N = 50$ isotones. In the low-lying spectra of $N = 49$ nuclei one observes the low-lying negative parity states corresponding to the holes in the $p_{1/2}$ orbital, as well as positive parity states, among which the lowest excited $5/2^+$ may correspond to a 1p-1h excitation across the $N = 50$ gap, and can be thus addressed in our model space which encompasses the $d_{5/2}$ neutron orbital. The systematics of $5/2^+$ states in $N = 49$ isotones is known up to ^{81}Ge (four protons away from ^{79}Ni) but experimental data should be soon available as far as ^{79}Zn (two protons away from ^{79}Ni) [30]. The states corresponding to the excitations across the $N = 50$ gap serve as a perfect test for its size in our interaction in the vicinity of ^{78}Ni. In the spectra of even-even nuclei, 1p-1h excitation can form the first excited $5^+, 6^+$ states. They are known experimentally up to ^{82}Ge and the relatively low excitation energy of these states at $Z = 32$ has lead the authors of Ref. [22] to anticipate the possible weakening of the $N = 50$ closure. We start thus the presentation of our results with the example of ^{82}Ge. In Table I we show the spectra calculated in our approach compared to experimental data for the case of ^{82}Ge and the wave functions of the calculated levels. The known energy levels $2^+, 4^+$ are reproduced with great accuracy, and theoretical counterparts for the experimental candidates of $5^+, 6^+$ spins are located within 200 keV. The first excited $2^+, 4^+$ states are clearly of a proton nature. In contrast, it is seen that the lowest calculated $5^+, 6^+$ levels correspond indeed to the 1p-1h excitations to the $\nu d_{5/2}$ orbital, as proposed in Ref. [22]. The second calculated $5^+, 6^+$ states, located at around 4 MeV, are again of proton nature, having nearly the same occupations of the neutron $g_{9/2}, d_{5/2}$ orbitals as the ground state.

In Fig. 1 we present the systematics of lowest excited $5^+, 6^+$ states from $Z = 28$ to $Z = 36$ compared to the known experimental data, which probes the evolution of the gap when moving away from $Z = 32$. Our calculations match well the decreasing trend observed from Kr to Ge, but the increase of the excitation energy is predicted toward Ni. In addition, we present in the same figure the systematics of the calculated and experimentally known $5/2^+$ states in $N = 49$ isotones. These states are correctly reproduced and, similarly to the case of even-even nuclei, the increase of the $5/2^+$ is observed toward Ni. In both systematics a minimum appears around $Z = 32$. Such a minimum however does not reflect any changes in the spherical mean-field in these nuclei. This is illustrated in Figs. 1(b) and 2. The former shows the correlated gap, i.e., the gap obtained from binding energies

$$\Delta = BE(Z, N + 1) + BE(Z, N - 1) - 2BE(Z, N). \quad (1)$$

The latter is the shell-model prediction for the evolution of the effective single-particle energies (ESPE). The ESPE are obtained as the differences of energies of closed shell and closed shell ± 1 particle configurations which, by definition, contain no correlations [28]. Thus the splitting of the ESPE defines the uncorrelated shell gap and allows us to separate the spherical mean-field from correlation effects contained in Δ. One should also add that the ESPE represent schematically the evolution of the monopole field in nuclei, which is not an observable itself. In particular, it assumes a given filling ordering scheme, which in reality is broken by the residual interaction, but for many years the monopole Hamiltonian has been used successfully to investigate and visualize the shell evolution in nuclei.

It is seen in Fig. 2 that there is no clear variation of the ESPE between ^{78}Ni and ^{86}Kr. At the same time, the gap calculated from shell-model masses varies from 4.7 MeV in ^{78}Ni to only 3.6 MeV in ^{82}Ge and then increases again toward ^{86}Kr as shown in Fig. 1(b). This indicates that the

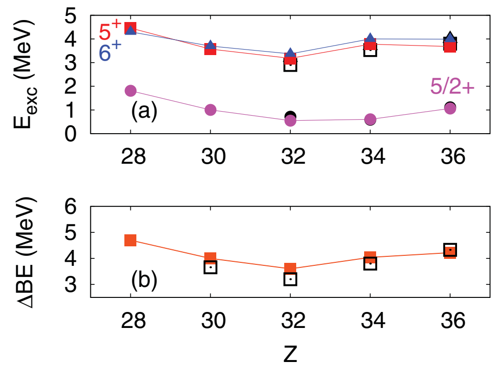

FIG. 1. (Color online) Systematics of the low-lying 1p-1h states in $N = 50$ and $N = 49$ isotones (a) and the evolution of the $N = 50$ gap calculated from masses (b). Color symbols stand for shell-model (SM) results; black (open) symbols represent the experimental data from Refs. [7,31,32].

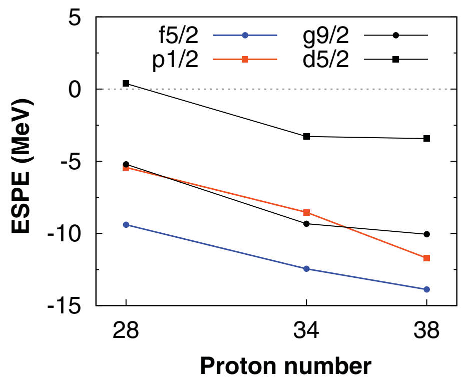

FIG. 2. (Color online) Evolution of the neutron effective single-particle energies with the proton number at $N = 50$.

correlation effects lead to a minimum in the mass gap at $Z = 32$, which explains the observed pattern of the excited states; but at the same time no indication for the weakening of the spherical gap toward ^{78}Ni is found. One should note that the majority of other microscopic models used in nuclear structure calculations fail to reproduce the $N = 50$ gap size and trend in the experimentally known region, and deviate substantially in their predictions toward ^{78}Ni (See Fig. 4 of Ref. [32]).

One of the key issues in nuclear structure is knowledge of the shell closure formation in nuclei. For a long time, it was not understood why nucleon-nucleon (NN) realistic interactions fail to reproduce spin-orbit shell closures, such as those in ^{48}Ca and ^{56}Ni. A deeper insight came when the importance of the monopole field was emphasized in the mechanism of shell drift [33] and later, when the connection with missing three-nucleon monopole forces in nuclear structure calculations was suggested [34]. The evolution of such gaps can be placed in a general context of fundamental problems of nuclear structure: when the largest orbit in a major shell fills, it binds itself and contributes to the binding of the largest orbits in neighboring shells in a way that NN forces fail to reproduce. As the largest orbit in the oscillator shell n is the one that is expelled to become an intruder in an orbit $n - 1$, it follows that the pure two-body forces are unable to produce the spin-orbit shell closures at N, $Z = 14$, 28, 50, 82, and 126. Only recently the first attempts of shell-model (SM) calculations with effective three-body forces based on the chiral next-to-next-to-leading order potential became available [11,12], for the time being exclusively in the $T = 1$ channel. These calculations suggest that at least some of the missing repulsion between $d_{5/2}$ and $s_{1/2}$ orbitals in oxygen and between $f_{7/2}$ and $p_{3/2}$ orbitals in calcium can be gained by including the three-body contribution of two valence and one core particles in the two-body matrix elements. If the three-body effects can explain the spin-orbit shell closures observed experimentally in $Z = 8$ isotopes ($n = 1$ harmonic oscillator shell closure) and $Z = 20$ isotopes ($n = 2$), one could search for similar effects at $Z = 40$ ($n = 3$) around ^{80}Zr. However, the proton shell closure appears as well at $Z = 28$, making the next place in the Segrè chart available for such studies already between ^{68}Ni and ^{78}Ni, where the neutron $N = 50$ shell closure may appear due to the filling of the $g_{9/2}$ orbital.

We would like to discuss now the $g_{9/2}$-$d_{5/2}$ splitting along the nickel chain. In Fig. 3 we show the evolution of neutron effective single- particle energies in the region considered in this work, in comparison to analogous ESPE in sd and fp shells obtained with empirical interactions: USDb [35] and LNPS [3]. In addition, the ESPE obtained with V_{lowk} effective interactions with 2.0 fm^{-2} cutoff based on charge-dependent Bonn potentials [36] are plotted for each case. For transparency, only the first two orbits in a harmonic oscillator shell are plotted, and we arbitrarily normalized the starting energy of the large shell to zero. Apparently, with empirical interactions a shell gap is created when filling the large orbit, leading to 14, 28, and 50 closures in the subsequent shells. The behavior given by the realistic force is incompatible with empirical ESPE, and, in particular, there is nearly no variation of the gap with the filling of the large orbital. Additionally, the V_{lowk} forces predict degeneracy (sd, pf) or even inversion (gd) of the $f_{7/2}$-$p_{3/2}$, $d_{5/2}$-$s_{1/2}$, and $g_{9/2}$-$d_{5/2}$ orbitals, inconsistent with their experimental ordering at $N = 8$, 20, and 40 [37]. As has been shown in Refs. [11,12], the inclusion of the effective three-body forces in sd and fp shells can separate the single-particle levels and provide at least a part of the repulsion necessary to pull apart the orbitals with the filling of the large shell. Thus the nickel chain offers another possibility for state-of-the-art derivations of the three-body monopole interactions, the present work providing a precious benchmark for such studies. It has to be noted that this qualitatively analogous behavior of the $N = 50$ gap has not been imposed in our model but results solely

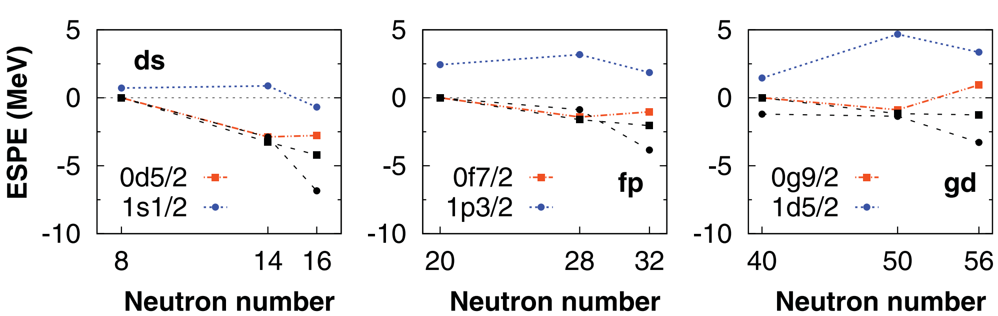

FIG. 3. (Color online) Evolution of the neutron effective single-particle energies with neutron filling in sd, fp, and gd shells. Only orbitals of interest are plotted between which the spin-orbit gap is created. Color lines correspond to empirical interactions and black lines to realistic V_{lowk} interactions; see text for more details.

from the spectroscopic description of the island of inversion around ^{64}Cr studied in Ref. [3] and of $N = 49$–50 isotones.

Finally, let us comment on the structure of ^{78}Ni itself, resulting from the shell-model calculations. Its ground state is calculated to have 79% of the closed shell configuration, the largest value in the whole nickel chain (around 60% of closed shell is found in pf calculations in ^{56}Ni with various interactions and only 50% in ^{68}Ni, here or in previous SM studies [3,38]). The first 2^+ state in ^{78}Ni is predicted at nearly 4 MeV, a value analogous to the 2^+ state of its "big sister" ^{132}Sn. This first excited state is of a neutron nature, having 1.35 particle in the $d_{5/2}$ orbital (0.16 particle in the 0^+ state). The gaps estimated from calculated mass differences in ^{78}Ni are 4.7 MeV for neutrons and 5.0 MeV for protons. These prediction appears much more robust than recent extrapolations from two-neutron separation energies of ground and isomeric states [39].

In summary, we have performed large-scale shell-model calculations in the $\pi(fp)$-$\nu(fpgd)$ model space in the vicinity of ^{78}Ni. We have studied the evolution of the $N = 50$ shell gap due to the proton-neutron interaction between ^{86}Kr and ^{78}Ni. The calculations point to a minimum of the mass gap in ^{82}Ge consistent with data and its increase toward ^{78}Ni. We predict the location of the first excited $5/2^+$ in ^{79}Ni at nearly 2 MeV and a high-lying 2^+ (4 MeV) in ^{78}Ni. We thus conclude on the robustness of both $Z = 28$ and $N = 50$ gaps in ^{78}Ni. The evolution of the $N = 50$ gap due to the $T = 1$ interaction is shown to be analogous to what has been attributed to the action of the effective three-body forces in oxygen and calcium chains, providing a new opportunity for exploring further the three-body effects in medium-mass nuclei. The developments of this work open a possibility of microscopic evaluations of (n, γ) cross sections around $A = 80$, where due to the low level density statistical approaches cannot be employed.

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