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Shell quenching in ^{78}Ni: A hint from the structure of neutron-rich copper isotopes

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Recent progress in experimental techniques allows us to study very exotic systems like neutron-rich nuclei in the vicinity of ^{78}Ni. The spectroscopy of this region can nowadays be studied theoretically in the large scale shell model calculations. In this work, we perform a shell model study of odd copper nuclei with $N = 40$–50, in a large valence space with the ^{48}Ca core, using a realistic interaction derived from the CD-Bonn potential. We present the crucial importance of the proton core excitations for the description of spectra and magnetic moments, which are for the first time correctly reproduced in theoretical calculations. Shell evolution from ^{68}Ni to ^{78}Ni is discussed in detail. A weakening of the $Z = 28$ gap when approaching the $N = 50$ shell closure, suggested by the experimental evidence, is confirmed in the calculations.

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The region of nuclei toward the ^{78}Ni is nowadays one of the most extensively studied in both experiment and theory. The doubly closed ^{78}Ni, with an unusual proton to neutron ratio, lies between two regions: of the light nuclei, where experimental evidence for changing magic numbers far from stability is well established [1], and of heavy ones, where no quenching of the known spin-orbit shell closures has been so far observed. The weakening of the $Z = 28$ gap when approaching the $N = 50$ shell closure has been suggested, e.gfor example, by Otsuka in Ref. [2] due to the proton-neutron part of the nuclear force, which has an opposite action on protons in the $f_{7/2}$ and $f_{5/2}$ orbitals while filling the neutron $g_{9/2}$ shell. Previous shell model (SM) calculations [3,4] have also revealed the possibility of a weakening of this shell closure.

A related subject of a great experimental interest is the so-called monopole migration in the copper isotopes and the competition of single-particle and collective modes at low excitation energies [5–7]. A decade ago a sudden drop of the $5/2^-$ level in ^{73,71}Cu was observed [8], giving a hint that this state may become the ground state of ^{75}Cu. Such a scenario may be expected concerning a strong attractive monopole interaction between protons and neutrons occupying the $f_{5/2}$ and $g_{9/2}$ orbitals, respectively. The recent measurements of magnetic moments in the copper chain [7] established experimentally the inversion of $5/2^-$ and $3/2^-$ levels in ^{75}Cu. In the same work, the authors pointed out that, however in the available shell model calculations this inversion is present between ^{73}Cu and ^{79}Cu [9–11], it is not followed by a rapid lowering of the first excited $1/2^-$ level observed in experiment. Therefore, *some important physics mechanism is either omitted or underestimated in the recently developed shell model interactions*.

In this work we show that the $Z = 28$ proton gap is eroded in neutron-rich nuclei, thus the physics part which is missing in all previous shell model calculations is not related to the interaction itself, but rather to the lack of proton core excitations excluded in valence spaces based on the ^{56}Ni core used up to now in SM calculations in this region of nuclei. The SM calculations presented here for the copper isotopic chain are performed in the valence space containing all orbitals necessary for the description of the nuclear structure in this region, that is, $f_{7/2}$, $f_{5/2}$, $p_{3/2}$, $p_{1/2}$ for protons and $f_{5/2}$, $p_{3/2}$, $p_{1/2}$, $g_{9/2}$ for neutrons. Such a valence space allows for simultaneous proton excitations from the $f_{7/2}$ orbital to the rest of the pf shell and neutron excitations across the $N = 40$ harmonic oscillator shell closure. At the same time, the spurious center of mass excitations are excluded as the $J^\pi = 1^-$ couplings are not possible within this set of single-particle orbits. This type of a model space has been previously used in the shell model study of Coulomb excitation in ^{68}Ni [12]. An effective interaction derived from a realistic nucleon-nucleon CD-Bonn potential, corrected empirically in its monopole part to reproduce a large set of nuclear data, has been employed. This work continues the development of the interaction but with a special emphasis on the properties of neutron-rich nuclei between $N = 40$ and $N = 50$ shell closures. We present in detail the results for odd copper isotopes: spectra, magnetic moments, composition of the wave functions, from which we draw conclusions on the underlying shell structure in the vicinity of the doubly magic ^{78}Ni. The calculations are performed using the ANTOINE shell model code [13]. Exact diagonalization in the model space has been achieved for nuclei with $N = 42$–50; for ^{69}Cu truncated calculation allowing 8p-8h excitations across $Z = 28$ and $N = 40$ gaps is presented. Maximal dimensions of the matrices treated here reach 7×10^8.

Let us start the discussion with the shell evolution as obtained in the SM calculations, which is crucial for understanding of the observed nuclear structure in this region. The proton effective single-particle energies (ESPE) evolving with filling of subsequent neutron orbitals are traced in Fig. 1. Two experimental constraints have been taken into account in the monopole corrections of the interaction that lead to the ESPE shown in this figure: the sizes of the gaps at $N = 40$ and at $N = 50$. While the size of the proton gap in ^{68}Ni is well established (5.8 MeV from binding energy differences), the corresponding gap in ^{78}Ni can be now inferred indirectly from the recently measured $B(E2; 2^+ \rightarrow 0^+)$ transition rate in ^{80}Zn [14]. Because ^{80}Zn has a closed neutron shell ($N = 50$) and two protons above the $Z = 28$ shell closure, one expects its first excited 2^+ state to be of a predominantly proton character. We obtain in our calculations with a standard polarization

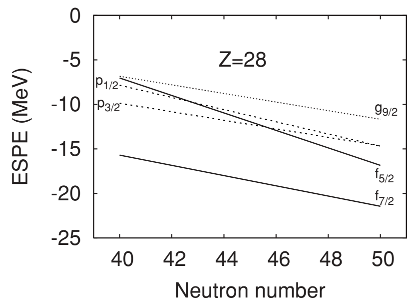

FIG. 1. Evolution of proton effective single-particle energies between ^{68}Ni and ^{78}Ni.

charge of 0.5 e the transition probability of 143 e^2 fm^4, in good agreement with the experimental value of 150(32) e^2 fm^4. The calculated correlated gaps amount to 5.7 and to 5.0 MeV in ^{68}Ni and ^{78}Ni, respectively. The corresponding reduction of the gaps in ESPE, observed in Fig. 1, is from 5.8 MeV in ^{68}Ni (the gap between $f_{7/2}$ and $p_{3/2}$ orbits) to 4.6 MeV (between $f_{7/2}$ and $f_{5/2}$ orbits) in ^{78}Ni. The reduction of the proton gap points to the necessity of taking into account the proton core excitations when approaching the neutron shell closure. One should notice, however, our prediction of a larger gap as compared to that of Ref. [15], where the value of 3.5 MeV has been deduced from the systematics. The rigidity of the gaps in ^{78}Ni is an important issue for the astrophysics because this nucleus is one of the waiting points in the r-process. Future experiments, especially mass measurements, will hopefully allow for precise verification of the size of the gaps in ^{78}Ni.

The resemblance of the proton ESPE in Fig. 1 to the ones calculated in Ref. [2] using a schematic tensor force is conspicuous, indirectly giving evidence for the role of the first-order tensor effects in the monopole drift, as noticed in Refs. [2,16]. In addition to the reduction of the gap between spin-orbit partners $f_{7/2}$ and $f_{5/2}$, a second important feature is observed in the proton ESPE, that is, the rapidly descending $f_{5/2}$ orbital that crosses the $p_{3/2}$ orbital in the middle of the shell. This single-particle level crossing should manifest itself in the low spin structure of copper isotopes, which have only one proton above the $f_{7/2}$ proton orbital. As mentioned, a sharp decrease in the energy of the first excited $5/2^-$ level between $N = 40$ and $N = 50$ was considered as an indication for monopole migration [8,17] and recent measurements established that $5/2^-$ becomes the ground state in ^{75}Cu [7]. The SM calculations presented in the same work, performed assuming a ^{56}Ni core, revealed a considerable deficiency in reproducing both the collectivity of the $1/2^-$ state and the systematics of the magnetic moments. We show in the following that this ill behavior is the effect of the truncation of the valence space, which eliminates the important proton degrees of freedom.

The low-lying level systematics in coppers is shown in Fig. 2. Our SM calculations reproduce correctly the change of the ground state in ^{75}Cu and, moreover, the pronounced lowering of the $1/2^-$ level that we obtain at the same excitation energy as the $3/2^-$ level. One should note that the ordering of these two levels has not been uniquely established in the experiment so far [6]. The collective nature of the $1/2^-$

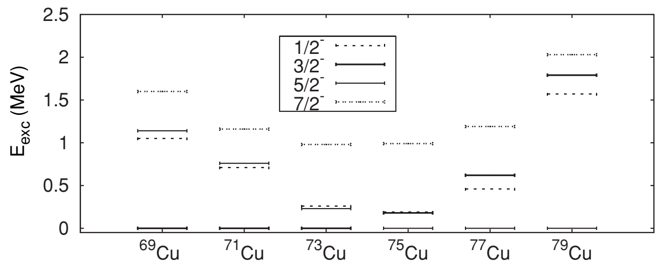

FIG. 2. Low-lying levels in copper isotopes resulting shell model calculations.

level can be deduced from experimental $B(E2; 1/2^- \rightarrow 3/2^-)$ transition rates, which reach around 20 W.u. in ^{71,73}Cu compared with $B(E2; 5/2^- \rightarrow 3/2^-)$ transition rates of about 4 W.u. in the same nuclei. The electromagnetic transition rates calculated in our model have been recently published in another work [6] and appear to agree fairly with the known experimental values, which together with the results for magnetic moments presented later in this article confirm the realistic character of the calculated wave functions.

In Fig. 3 the proton occupations of the single-particle orbitals in the lowest calculated states are depicted. In the case of the $7/2^-$ state, the number of holes in the $f_{7/2}$ orbit is reported. It is apparent from the figure that the nature of the low-lying states evolves a lot with the filling of the neutron $g_{9/2}$ orbital.

It is also worth noticing that the excitations through the neutron gap are unblocked at $N = 40$. In the calculations of Ref. [12] it was pointed out that the $N = 40$ harmonic oscillator shell is not a rigid shell closure and that ^{68}Ni has a mixed character of a superfluid and closed-shell nucleus in its ground state, with an extra occupancy of the $\nu g_{9/2}$ orbital of 1.19. This additional occupancy is then lowered in heavier nickels due to the Pauli blocking and the same behavior is observed here in copper isotopes for which the extra occupancies of the $g_{9/2}$ orbital are listed in Table I.

One can now see from Fig. 3 and Table I that at the neutron shell closure $N = 40$ the occupancy of the $p_{3/2}$ orbital is close to 1.0 and the extra occupancy of the neutron $g_{9/2}$ orbit is 0.84: this information confirms the single-particle character of the $3/2^-$ level, which has the $\pi p^1_{3/2} \otimes \nu 0^+$ structure. This is no longer the case for $1/2^-$ and $5/2^-$ states whose neutron occupancies resemble those of the 2^+ state in ^{68}Ni [12], and the occupancies of the proton single-particle orbitals ($p_{1/2}$ in $1/2^-$ and $f_{5/2}$ in $5/2^-$) are much lower. The $3/2^-$

TABLE I. The extra occupancy of the neutron $g_{9/2}$ orbital in the low-lying states in neutron-rich copper isotopes.

A	$1/2^-$	$3/2^-$	$5/2^-$	$7/2^-$
69	2.15	0.87	2.27	2.21
71	0.98	0.60	1.11	0.44
73	0.42	0.37	0.52	0.21
75	0.18	0.17	0.23	0.09
77	0.05	0.05	0.12	0.02
79	0.0	0.0	0.0	0.0

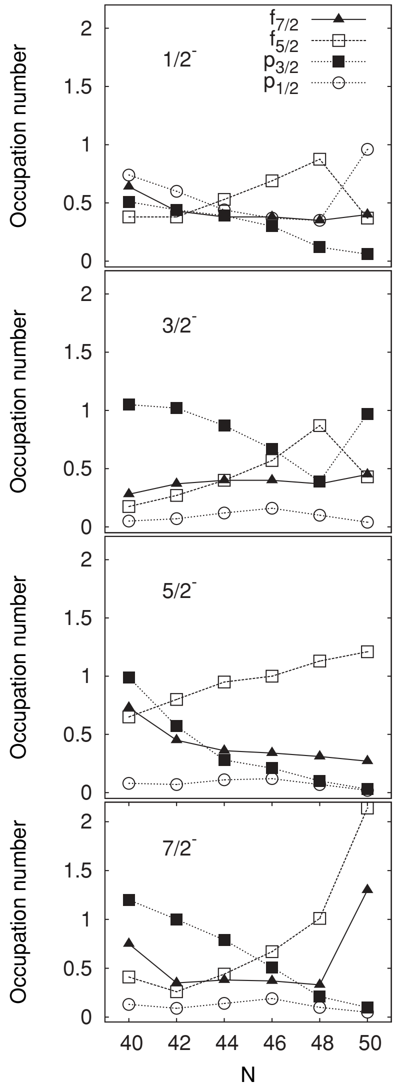

FIG. 3. Occupation of proton single-particle levels in the lowest calculated levels along the copper chain. In the case of the $f_{7/2}$ orbital the number of holes is plotted.

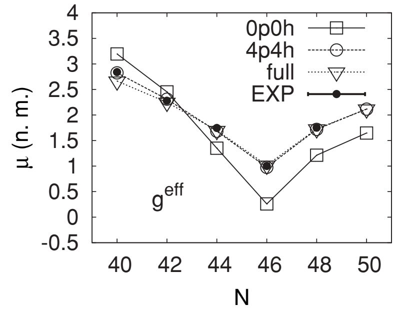

FIG. 4. Experimental (solid symbols) and theoretical (open symbols) magnetic moments of neutron-rich copper isotopes ($Z = 29$). SM calculations are shown without (0p0h) and with configuration mixing at the 4p4h level and in a full space calculation.

state loses, however, its single-particle character very quickly with the filling of the $g_{9/2}$ shell. Similarly, the $1/2^-$ level gains in collectivity with increasing neutron number, and the occupation of the $p_{1/2}$ drops twice when the middle of the shell is reached, to be enhanced again closer to the $N = 50$ closure. One observes that the sudden lowering of the $7/2^-$ state between ^{69}Cu and ^{71}Cu is also due to its change of the proton structure from $\sim$70% of a single-hole structure to a more collective one. Interestingly, the behavior of the hole number in the $f_{7/2}$ orbital in the $7/2^-$ level resembles the parabolic trend of the $p_{1/2}$ particles in the $1/2^-$ state. Finally, one observes that the occupation of the $f_{5/2}$ orbital in the lowest $5/2^-$ increases linearly when the neutron shell is filled. This behavior reflects clearly the crossing of the single-particle levels caused by the difference in the strength of the $V_{g_{9/2}\text{-}p_{3/2}}$ and $V_{g_{9/2}\text{-}f_{5/2}}$ proton-neutron interactions.

Finally, let us show the impact of the core excitations on the description of magnetic moments. In Fig. 4, the experimental data from Refs. [7,18] are plotted in comparison to calculated values. Three theoretical curves are shown: without configuration mixing (0p0h), allowing for four particle-four holes excitations (4p4h), and a full space diagonalization calculation (or 8p8h in the case of ^{69}Cu). A standard effective $M1$ operator is used in the calculation with the quenching factor 0.75 of the spin g factors and orbital g factors equal to 1.1 for protons and -0.1 for neutrons [19–21].

One can see that the magnetic moments are converged basically at the 4p4h level and that the agreement with experiment is excellent when particle-hole excitations are allowed, contrary to the 0p0h case. It could come as a surprise that the improvement in our model is maximal in the middle of the shell, where the proton $f_{5/2}$, $p_{3/2}$ single-particle orbitals cross and a $5/2^-$ level becomes the single-particle-like ground state. Nonetheless, one should bare in mind that in our model the attractive $f_{5/2}$-$g_{9/2}$ monopole interaction tends to purify the single-particle nature of the $5/2^-$ state and the occupancy of the $f_{5/2}$ shell increases when correlations are taken into account.

One should also stress that the calculations with the ^{56}Ni core [7] reproduce experimental values only in ^{69}Cu and ^{75}Cu, where the ground states ($3/2^-$ and $5/2^-$, respectively) calculated in our model reveal the most clean, single-particle-type of structure. This observation proves the necessity of the proton core excitations that allow for mixing of proton configurations, apparently inevitable for a realistic composition of the calculated wave functions. Let us acknowledge, in passing, the very insightful role of the measurements of the magnetic moments for the understanding of the nuclear structure and testing in detail the calculated wave functions.

In Fig. 5 we distinguish also the proton and neutron contributions from the orbital and spin parts to the ground-state magnetic moments obtained in full SM calculations with effective g factors presented in Fig. 4. The most important message of this decomposition is that the magnetic moments are clearly dominated by the proton components. The magnetic moment of the $5/2^-$ state ($N = 46$–50) arises from a destructive superposition of a smaller negative proton spin part and a large proton orbital part. The magnetic moment of the $3/2^-$ state ($N = 40$–44) consists of positive, nearly equal proton spin and orbital components. The neutron spin and orbital

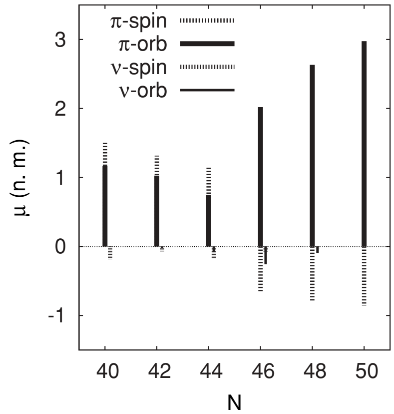

FIG. 5. Proton and neutron contributions from orbital and spin components to the magnetic moments of the ground states of copper isotopes.

components remain negative all along the chain but, as stated, their total contribution to the magnetic moment is negligible.

Finally, let us comment on the g factors used in the calculations. The need of effective g factors in the SM studies is well understood as ones performs calculations in a limited model space where an *effective* operator needs to act. While the effective Hamiltonians for the model spaces are derived nowadays in a perturbative scheme [22,23], the effective transition operators are introduced in a bare form with a renormalization factor, for the sake of simplicity. It has been shown in Refs. [19–21] that spin operators are to be quenched by a factor 0.75, as only ~70% of the Gamow-Teller (GT) strength resides in the model space, while the other 30% rests outside [20]. The enhancement of the orbital g factors has been proven necessary to redistribute the orbital strength in sd, pf, and gds shells [24–26]. In Fig. 6 we show, however, the calculations with the bare g factors for an explanatory purpose: One sees that though the discrepancies between theory and experiment are now larger (as expected) the correct systematics preserves and the agreement between experiment and theory improves the same way as in Fig. 4, once the particle-hole excitations are allowed. This result rules out any speculation whether the correct reproduction of the experimental systematics may be related to a specific choice of the gyromagnetic factors in the particular case of $^{69-77}$Cu.

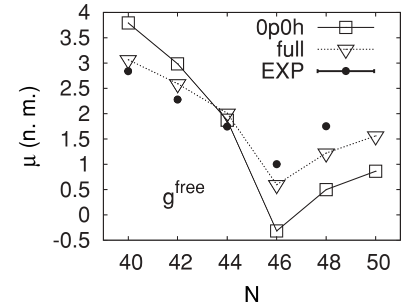

FIG. 6. Magnetic moments calculated with bare g factors. Full space diagonalization results (open triangles) are compared with the ones without configuration mixing (open squares) and available experimental data (solid circles).

In conclusion, we have presented SM calculations in an enlarged model space outside the ^{48}Ca core for the copper isotopic chain. A correct systematics of the low-lying levels and magnetic moments have been obtained for the first time in SM calculations. This appeared due to the inclusion of proton degrees of freedom omitted in previous SM calculations in limited valence spaces outside the ^{56}Ni core. We have also discussed the underlying proton shell evolution between ^{68}Ni and ^{78}Ni. The calculations have indicated that the $Z = 28$ shell closure gets reduced by about 0.7 MeV when filling the neutron $g_{9/2}$ orbital. This implies that the proton core excitations are an indispensable ingredient in understanding the structure of neutron-rich nuclei toward ^{78}Ni.

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