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Phys. Rev. Lett. 117, 172501 — Published 17 October 2016
DOI: 10.1103/PhysRevLett.117.172501
Structure of $^{78}$Ni from first principles computations

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Doubly magic nuclei have a simple structure and are the cornerstones for entire regions of the nuclear chart. Theoretical insights into the supposedly doubly magic $^{78}$Ni and its neighbors are challenging because of the extreme neutron-to-proton ratio and the proximity of the continuum. We predict the $J^\pi = 2^+$ state in $^{78}$Ni from a correlation between the $J^\pi = 2^+$ state in $^{48}$Ca using chiral nucleon-nucleon and three-nucleon interactions. Our results confirm that $^{78}$Ni is doubly magic, and the predicted low-lying states of $^{79,80}$Ni open the way for shell-model studies of many more rare isotopes.

Introduction – Doubly magic nuclei, i.e. nuclei with closed proton and neutron shells, play a most important role in nuclear physics [1]. They are more strongly bound than their neighbors, exhibit simple regular patterns, and are the cornerstones for our understanding of nuclear structure in entire regions of the Segré chart. In recent years, experiments and theory have made considerable progress in uncovering the evolution of shell structure in rare isotopes of oxygen [2–12], calcium [13–20], and tin [21,22].

The supposedly doubly magic nucleus $^{78}$Ni (with neutron number 50 and proton number 28) has been the focus of considerable experimental and theoretical efforts [24–30]. This nucleus is also of astrophysical relevance because it is in the region of the $r$-process path. Reliable theoretical predictions for $^{78}$Ni and its neighbors are challenging [31,32], because of the extreme neutron-to-proton ratio and the proximity to the neutron dripline. The large isospin brings to the fore smaller aspects of the nuclear interaction that are poorly constrained in $\beta$ stable nuclei, while for weakly bound and unbound nuclear states it is necessary to include coupling to the particle continuum. We address these challenges as follows: We employ a set of interactions [33,34] from chiral effective field theory (EFT) [35–37]. These interactions consist of nucleon-nucleon ($NN$) and three-nucleon forces (3NFs) [38,39]. They reproduce properties of nuclei with mass numbers $A = 2, 3, 4$ nuclei well, but differ in binding energies, radii, and spectra of medium-mass nuclei [40]. We include continuum physics by employing the Berggreen basis [41,42] which treats bound-, resonant- and non-resonant scattering states on equal footing. The Berggren basis has been extensively used in the Gamow-shell-model and coupled-cluster computations of weakly bound and unbound nuclear states, see for example [43–46]. Finally, using these ingredients we solve for the structure of $^{78}$Ni and its neighbors using coupled-cluster theory [47,56], see Refs. [57,58] for recent reviews. For the computation of $J^\pi = 2^+$ excited states in $^{48}$Ca and $^{78}$Ni we use an implementation of the equation-of-motion (EOM) coupled-cluster method that properly accounts for two-particle-two-hole (2p-2h) excitations.

As a key indicator of the $^{78}$Ni structure, we focus on the energy of the first excited $J^\pi = 2^+$ state. This $2^+$ state is at about 1 MeV of excitation energy in $^{70,72,74,76}$Ni, reflecting a softness regarding (a collective) quadrupole vibration. In contrast to these semi magic nuclei, the nucleus $^{68}$Ni exhibits a soft subshell closure (at neutron
Finally we focus on the neighbors of \( ^{78}\text{Ni} \) and \( ^{80}\text{Ni} \) from this Letter. For \( ^{78}\text{Ni} \) the red shaded area gives the predicted range for the \( 2^+_1 \) state obtained by correlating relevant observables; details are given below. The predicted range for the \( 2^+_1 \) state in \( ^{78}\text{Ni} \) is considerably higher than for its neighbors – indicating that this nucleus is doubly magic. This is the main result of this Letter. The red bar marks the result obtained with the interaction “1.8/2.0(EM)” from Ref. [33], which is singled out because it accurately reproduces the binding energy interaction “1.8/2.0(EM)” from Ref. [33], which is singled out because it accurately reproduces the binding energy of \( ^{78}\text{Ni} \), as well as the nuclei \(^{4}\text{He}, ^{16}\text{O}, \) and \(^{40,48}\text{Ca} \).

This Letter is organized as follows. We briefly summarize the Hamiltonian and model-spaces that are input to the calculations of neutron-rich nickel isotopes. We discuss an implementation of three-particle-three-hole corrections to coupled-cluster computations of excited states. Using these theoretical ingredients we compute the first \( ^2\text{p} \) state in the doubly magic \( ^{48}\text{Ca} \) and in \( ^{78}\text{Ni} \) from a family of chiral \( NN \) and \( 3NFs \). From an observed correlation between the energies of the \( 2^+_1 \) states in \( ^{40}\text{Ca} \) and \( ^{78}\text{Ni} \) we obtain a range for the latter. We discuss the relevance of \( 2p-2h \) excitations in this state. We also give predictions for other low-lying states in \( ^{78}\text{Ni} \). Finally we focus on the neighbors of \( ^{78}\text{Ni} \) and present predictions for low-lying states in \( ^{77,79,80}\text{Ni} \).

**Hamiltonian and model-space** – Our coupled-cluster calculations start from the intrinsic Hamiltonian

\[
\hat{H} = \sum_{i<j} \left( \frac{(p_i - p_j)^2}{2mA} + \hat{V}_{NN}(i,j) \right) + \sum_{i<j<k} \hat{V}_{3N}(i,j,k). \tag{1}
\]

We compute the Hamiltonian (1) using interactions from Refs. [33,34]. The interactions of Ref. [33] are based on similarity-renormalization-group (SRG) [61] transformations of \( NN \) interactions from chiral EFT augmented with leading \( 3NFs \) from chiral EFT. Here, the low-energy constants of the \( 3NFs \) are adjusted to data from nuclei with mass numbers \( A = 3, 4 \). These interactions yield saturation points for nuclear matter around the empirical value [33], and they yield radii and binding energies in calcium isotopes scattered around data [40]. The interaction \( NNLO_{\text{sat}} \) of Ref. [34] by construction yields accurate radii and binding energies in light nuclei and isotopes of oxygen. It extrapolates well to calcium isotopes [40] and \( ^{56}\text{Ni} \) [62], and within uncertainties reproduces the empirical saturation point in symmetric nuclear matter. We employ these interactions to study systematic sensitivities because a full-fledged propagation of uncertainties is not yet possible [63]. The five interactions used in this Letter have different cutoffs and three different sets of pion-nucleon constants, i.e. they also differ in the long-range part of the nuclear interaction. They are truly different parametrizations of chiral EFTs that describe \( A = 2, 3, 4 \) nuclei about equally well, but differ in medium-mass nuclei [40], see also Ref. [63].

We use a Hartree-Fock basis constructed from a harmonic oscillator basis of up to 15 major oscillator shells. To compute weakly bound and unbound states in \( ^{78}\text{Ni} \) we construct a Gamow-Hartree-Fock basis [46,65] by including a Berggren basis for relevant partial waves and follow Ref. [62] for inclusion of \( 3NFs \). For \( ^{48}\text{Ca} \) we use the same model-spaces that were employed in Ref. [40], while for the neutron-rich nickel isotopes we perform the calculations at the oscillator frequency \( h\omega = 16 \text{ MeV} \) which yields the minimum in energy for the largest model-space that we consider. We use the normal-ordered two-body approximation [67,68] for the \( 3NF \) with the additional three-body energy cut \( E_{3\max} = N_1 + N_2 + N_3 \leq 16 \). Here \( N_i = 2n_i + l_i \) refers to the oscillator shell of the \( i \)th particle.

**Method** – We employ the coupled-cluster singles-doubles (CCSD) approximation in an angular momentum coupled representation and compute the similarity-transformed Hamiltonian \( \hat{H} \) (see Refs. [58,69] for details). We include triple excitations perturbatively using the \( \Lambda-\text{CCSD(T)} \) method [70] for the computation of the ground-state energy. The excited \( 2^+_1 \) state is computed with the EOM coupled-cluster method in the EOM-CCSD [71] and EOM-CCSD(T) approximations [72]. EOM-CCSD has been shown to be accurate for states that are dominated by \( 1p-1h \) excitations [57]. In this Letter we go beyond the standard EOM-CCSD approach and include corrections from \( 3p-3h \) excitations perturbatively using the EOM-CCSD(T) approach. EOM-CCSD(T) capture the dominant \( 2p-2h \) excitations in the computation of the \( 2^+_1 \) state in \( ^{48}\text{Ca} \) and \( ^{78}\text{Ni} \). This method generalizes the \( \Lambda-\text{CCSD(T)} \) approach for the ground-state energy and requires the solution of both the left and right EOM-CCSD eigenvalue problem, with a non-iterative \( 3p-3h \) correction computed perturbatively. The computational cost is considerably larger than for \( \Lambda-\text{CCSD(T)} \) since we are considering a non-scalar excitation. In quantum chemistry applications, EOM-CCSD(T) is an economical and accurate correction to EOM-CCSD [73]. Excited states in neighboring nuclei \( ^{77,79,80}\text{Ni} \) are computed as generalized \( mp-nh \) excited states [69,74,75] of \( \hat{H} \). Details of this approach are presented in the review [58] and in the supplementary information of Ref. [40].

**Results** – To probe the quality of the EOM-CCSD(T) approximation, and for a comparison with data, we also compute the \( 2^+_1 \) excited state in \( ^{48}\text{Ca} \). For the computation of the \( 2^+_1 \) state in \( ^{78}\text{Ni} \), we employ the same interactions but choose lower model space frequencies to minimize the ground-state energies.

Figure 2 shows that the excitation energy of the \( 2^+_1 \) state in \( ^{48}\text{Ca} \) and \( ^{78}\text{Ni} \) are strongly correlated. The error bars on the individual data points estimate uncertainties from the method and model-space truncation. We estimate the model-space uncertainty from enlarging the
model space from $N = 12$ to $N = 14$ which is less than 200 keV for all employed interactions. For the method we include 10% of the triples correlation energy as an uncertainty estimate. We take the average from all interactions and give a combined uncertainty on the $2^+_1$ state in $^{48}\text{Ca}$ and $^{78}\text{Ni}$. A linear fit to the data points, and an encompassing diagonal uncertainty band is also shown. The thin horizontal line marks the known energy of the $2^+_1$ state in $^{48}\text{Ca}$. The interaction NNLO sat, which accurately reproduces charge radii in $^{48}\text{Ca}$, yields an excitation energy that is too low. We also note that the origin of the correlation between the $2^+_1$ states in $^{48}\text{Ca}$ and $^{78}\text{Ni}$ depicted in Fig. 2 is not understood theoretically. While several such correlations have been reported (and exploited) in the literature, see, e.g., Refs. [40, 76, 77], only few have been understood [78]. In the supplemental material [79] we show that the correlation reported in Fig. 2 is nontrivial. The spectroscopy of $^{78}\text{Ni}$ was recently measured at RIBF, RIKEN [80], and it will be interesting to compare our theoretical result with data.

For $^{78}\text{Ni}$, the convergence of the ground-state energy with respect to the size of the model space is slow for most of the employed interactions, and we are only able to achieve convergence for the softest interaction “1.8/2.0 (EM)” of Ref. [33]. For this interaction the computed binding energy is 637(4) MeV which agrees with the value 641 MeV extracted from systematic trends. The $E_{3\text{max}}$ truncation used for the 3NF is the dominant uncertainty, and the estimated error of 4 MeV comes from increasing $E_{3\text{max}}$ from 14 to 16 [79]. We note that the convergence is improved for energy differences. Figure 3 shows the convergence of the energy of the $2^+_1$ state in $^{48}\text{Ca}$ and $^{78}\text{Ni}$ with increasing size of the model space, obtained for the interaction “1.8/2.0 (EM)”. The convergence is qualitatively similar for the other interactions, and the difference between the $N = 12$ and $N = 14$ spaces entered the uncertainties presented in Fig. 2. Further details on the convergence are presented in the supplemental material [79].

We note that the interaction “1.8/2.0 (EM)” describes the $2^+_1$ state in $^{48}\text{Ca}$ and the binding energies for a variety of nuclei remarkably well. For example, the computed binding energies for $^4\text{He}$, $^{16}\text{O}$ and $^{40,48}\text{Ca}$ are 28.2 MeV, 128 MeV, 348 MeV, and 419 MeV, respectively; they are close to the corresponding experimental binding energies of 28.2 MeV, 128 MeV, 342 MeV, and 416 MeV.

Let us discuss the effect of $2p$-$2h$ excitations in the $2^+_1$ excited state of $^{48}\text{Ca}$ and $^{78}\text{Ni}$. Table I shows results for this state using the EOM-CCS, EOM-CCSD and EOM-CCSD(T) approximations for the interactions used in this work. We find that that the inclusion of perturbative $3p$-$3h$ excitations in EOM-CCSD(T) reduces the excitation energy by 1-2 MeV for all interactions when compared to the corresponding EOM-CCSD results. The triples corrections for the $2^+_1$ state in both $^{48}\text{Ca}$ and in $^{78}\text{Ni}$ amounts to about 20% of the EOM-CCSD correlation energy (defined as the difference between the EOM-CCS and EOM-CCSD excitation energies). In coupled cluster theory, one could conservatively assume that $4p$-$4h$ contributions are again of the order of 20% of the

![Graph](image_url)
3p-3h correction, yielding uncertainty estimates that are within the uncertainties shown in Fig. 2. We note that the role of 3p-3h excitations in the computation of the 2^+ state in both 48Ca and in 78Ni is considerably larger than the role of 3p-3h excitations in the ground-state. For the ground-state of closed (sub-)shell nuclei the triples correlation energy typically amounts to about 10% of the CCSD correlation energy, see Ref. [81] for an example. We also note that the role of correlations beyond 1p-1h is larger than in RPA calculations based on Skyrme-Hartree-Fock because those yield much less correlated wave functions (cf. Ref. [82] for a recent application to nickel isotopes.)

<table>
<thead>
<tr>
<th>Interaction</th>
<th>48Ca</th>
<th>78Ni</th>
</tr>
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<tbody>
<tr>
<td>1.8/2.0 (EM)</td>
<td>10.5</td>
<td>3.8</td>
</tr>
<tr>
<td>2.0/2.0 (EM)</td>
<td>11.3</td>
<td>3.6</td>
</tr>
<tr>
<td>2.2/2.0 (EM)</td>
<td>12.0</td>
<td>3.3</td>
</tr>
<tr>
<td>2.0/2.0 (PWA)</td>
<td>12.0</td>
<td>3.7</td>
</tr>
<tr>
<td>NNLOsat</td>
<td>14.8</td>
<td>3.2</td>
</tr>
</tbody>
</table>

TABLE I. Results for the excitation energy (in MeV) of the 2^+ state in 48Ca and 78Ni computed in the EOM-CCS (denoted by 1p-1h), EOM-CCSD (denoted by 2p-2h) and EOM-CCSD(T) (denoted by 3p-3h) approximations. The interactions labeled (EM) and (PWA) are taken from Ref. [33] and NNLOsat is from Ref. [31].

Our analysis shows that 2p-2h excitations are significant for the 2^+ state in 48Ca and 78Ni, and that a precise description of this state therefore requires EOM-CCSD(T). This finding is somewhat surprising, because the collective 2^+_n state is usually thought of as a coherent superposition of 1p-1h excitations [33]. However, a simple shell-model argument suggests that 2p-2h excitations should yield significant corrections. In the doubly-magic 48Ca for instance, no 1p-1h excitations of protons near the Fermi surface can generate a 2^+ state, as one need at least 2p-2h excitations from the sd shell to the pf shell to yield a 2^+ state. Following the same reasoning, a computation of the electric quadrupole transition in 48Ca will have significant 2p-2h contributions since this observable measures mostly the excitations of protons. Similarly, we find that for 78Ni 2p-2h excitations of neutrons near the Fermi surface have significant contributions to the low-lying 2^+_n state. In the naive shell-model picture the gn/2 orbital is the last filled neutron shell with s1/2, d5/2, d3/2, g7/2 shells being the next unoccupied orbitals closest to the Fermi surface. A 2^+ state near the Fermi surface can be generated via 1p-1h excitations of neutrons from the gn/2 to the d5/2, g7/2 orbitals, but 2p-2h excitations are necessary to utilize the low-lying s1/2 and d3/2 orbitals. As shown in Tab. I, the effect of 2p-2h excitations from the gn/2 to the s1/2 and d3/2 orbitals is significant in the 2^+_n state of 78Ni. As we will see below the 1/2^+_n state is actually the lowest state in 78Ni.

Shell closures manifest themselves in several observables. Besides the energy of the 2^+_n state, separation energies also yield valuable information. For the computation of other low-lying states in 78Ni and its neighbors 77,79,80Ni, we limit ourselves to the “1.8/2.0 (EM)” interaction because this interaction yields converged results with respect to the model space and accurate energies. For 78Ni, we employed a Berggren basis for the s1/2, d5/2 and d3/2 partial waves because of the proximity of the continuum. For the g7/2 partial wave we use the harmonic-oscillator basis, because the large centrifugal barrier reduces the impact of the coupling to the continuum. The resulting spectra are shown in Fig. 4 relative to the ground-state energy of 78Ni. For 78Ni we predict low-lying 1^+_1, 3^+_1, 4^+_1 excited states all below the neutron-emission threshold. The ratio of the excited 4^+_1 state with the 2^+_n state is 1.2, which is consistent with 78Ni being a doubly magic nucleus. Due to the high computational cost the 1^+_1, 3^+_1, 4^+_1 excited states in 78Ni were computed with N = 12; the triples correlation energy for the 4^+_1 state was well converged for N = 10. The theoretical result for the neutron-separation energies in 78,79Ni are S_n ≈ 4.5 MeV and S_p ≈ 1 MeV, respectively, which are consistent with 5450(950) keV and 1650(1130) keV from systematics [84]. For 79Ni we find that the inclusion of the continuum impacts the level ordering and lowers the 1/2^+_n state by about 1 MeV, the 5/2^+_n state by about 0.5 MeV, and the unbound 3/2^+_n state by about 0.7 MeV, as compared to a calculation in the harmonic oscillator basis.

The 1/2^+_n ground-state of 79Ni is quasi-degenerate with the 5/2^+_n state. This finding mirrors the results of Refs. [15,62,85], where the inclusion of continuum effects also impacted the energies and level ordering of unbound states in the neutron-rich calcium isotopes 53,55,61Ca. The ground-state of 80Ni is bound by 2 MeV with respect to 78Ni, thereby setting the neutron dripline beyond 80Ni. This is consistent with mean-field surveys [86]. The two-neutron separation S_{2n}(80Ni) ≈ 2 MeV is significantly smaller than the estimate S_{2n}(78Ni) = 8600(950) keV [51] – consistent with expectations for a doubly magic nucleus. The 2^+_n state in 80Ni is computed to be 0.7 MeV above its ground state. The combined results of this study – a relatively high-lying 2^+_n state in 78Ni, the marked difference of neutron-separation energies between 79Ni and 78Ni, and of two-neutron separation energies between 80Ni and 78Ni, respectively, indicate the strength of the shell closure at neutron number 50.

Conclusions – We presented first-principles computations of the structure of 78Ni and its neighbors. Correlating the 2^+_n energies in 78Ni and 48Ca leads to the prediction 2.1 MeV ≲ E(2^+_n) ≲ 3.1 MeV for the energy of the 2^+_n state in 78Ni. Neutron separation energies and two-neutron separation energies confirm the picture of the shell closure at neutron number 50, and the theoretical results put the neutron dripline beyond 80Ni. We also
FIG. 4. (Color online) Low-lying states in $^{77-80}$Ni with respect to the ground-state of $^{78}$Ni computed with the interaction “1.8/2.0 (EM)” of Ref. [33]. The ground states are shown in black, while excited states are shown in red.

We thank Kai Hebeler for providing us with matrix elements in Jacobi coordinates for the three-nucleon interaction at next-to-next-to-leading order. This work was supported by the Office of Nuclear Physics, U.S. Department of Energy, under grants DE-FG02-96ER40963, DESC0008499 (NUCLEI SciDAC collaboration), and the Field Work Proposal ERKBP57 at Oak Ridge National Laboratory (ORNL). Computer time was provided by the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. This research used resources of the Oak Ridge Leadership Computing Facility located at ORNL, which is supported by the Office of Science of the Department of Energy under Contract No. DE-AC05-00OR22725.


[79] “Supplemental material.”


