# Electromagnetic moments of scandium isotopes and N = 28 isotones in the distinctive 0f7/2 orbit postprint

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## Abstract

The electric quadrupole moment of $^{49}$Sc was measured by collinear laser spectroscopy at CERN-ISOLDE to be $Q_{rms} = -0.159(8)$~$e$b, and a nearly tenfold improvement in precision was reached for the electromagnetic moments of $^{47,49}$Sc. The single-particle behavior and nucleon-nucleon correlations are investigated with the electromagnetic moments of $Z = 21$ isotopes and $N = 28$ isotones as valence neutrons and protons fill the distinctive $0f_{7/2}$ orbit, respectively, located between magic numbers, 20 and 28. The experimental data are interpreted with shell-model calculations using an effective interaction, and textit{ab-initio} valence-space in-medium similarity renormalization group calculations based on chiral interactions. These results highlight the sensitivity of nuclear electromagnetic moments to different types of nucleon-nucleon correlations, and establish an important benchmark for further developments of theoretical calculations.

## Full Text

## Preamble

Electromagnetic moments of scandium isotopes and N = 28 isotones in the distinctive 0 f7/2 orbit

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## Abstract

The electric quadrupole moment of $^{49}$Sc was measured by collinear laser spectroscopy at CERN-ISOLDE to be $Q_s = -0.159(8)$ eb, achieving a nearly tenfold improvement in precision for the electromagnetic moments of $^{47,49}$Sc. The single-particle behavior and nucleon-nucleon correlations are investigated through electromagnetic moments of $Z = 21$ isotopes and $N = 28$ isotones as valence neutrons and protons fill the distinctive $0f_{7/2}$ orbit, respectively, located between the magic numbers 20 and 28. The experimental data are interpreted using shell-model calculations with an effective interaction and ab-initio valence-space in-medium similarity renormalization group calculations based on chiral interactions. These results highlight the sensitivity of nuclear electromagnetic moments to different types of nucleon-nucleon correlations and establish an important benchmark for further developments of theoretical calculations.

Keywords: Collinear laser spectroscopy, Electromagnetic moments, Nucleon-nucleon correlation, Ab-initio calculation

## 1. Introduction

Since its establishment by Mayer and Jensen [?, ?], the nuclear shell model (SM) and the concept of magic numbers have played an essential role in our understanding of nuclear structure as a quantum many-body system [?]. The independent-particle SM assumes non-interacting valence nucleons outside a spherical core and can reasonably describe properties of near-magic nuclei [?, ?], such as their ground-state spins and electromagnetic moments. Deviations of observed properties from this model are attributed to residual nucleon-nucleon (NN) interactions between valence nucleons and to interactions between valence nucleon(s) and the core. Moments of nuclei with clear single-particle orbit configurations, measured with sufficient precision across a long range of isotopes, serve as sensitive probes of different aspects of the residual interaction that can be included in large-scale SM calculations. While effective interactions were traditionally determined empirically for specific model spaces [?], recent years have witnessed the emergence of more realistic interactions rooted in QCD, including two- and three-body forces derived through chiral effective field theory ($\chi$EFT) [?].

More quantitatively, within the independent-particle SM, the magnetic moment for a single particle (SP) occupying a shell-model orbit—the so-called "Schmidt moment"—depends only on the angular momentum $j$ and the free nucleon magnetic moments [?]. It should thus remain constant as odd nucleons fill an orbit [?, ?]. Deviations from Schmidt moments may be broadly attributed to two possible causes: configuration mixing and meson-exchange currents through the two-body magnetic-moment operator [?, ?]. The quadrupole moment, on the other hand, serves as a good indicator of collective effects in the nucleus [?, ?]. The single-particle quadrupole moment of a nucleon depends on the angular momentum $j$ and the mean-square charge radius of the orbit occupied by the unpaired valence nucleon. As nucleons are added to an orbit, the seniority scheme of the independent-particle SM predicts that quadrupole moments should follow a linear increase with the number of valence particles in the SM orbit, crossing zero at half filling [?]. Such experimental linear trends have been observed in Pb (Cd) isotopes as neutrons fill the $\nu i_{13/2}$ ($\nu h_{11/2}$) orbit [?, ?] and in $N = 82$ ($N = 126$) isotones as protons fill the $\pi g_{7/2}$ ($\pi h_{9/2}$) orbit [?, ?]. However, as these orbits are closely embedded among others in the shell, scattering of nucleons among several orbits may result in the zero-crossing of the linear trend occurring away from half filling. A rather unexpected and not yet explained deviation from such linear trend was recently observed in Sn isotopes [?].

The $0f_{7/2}$ orbit, located between magic numbers 20 and 28, forms a unique example in the nuclear chart where a single orbit is well isolated from its neighbors. One can expect that electromagnetic moments of isotopes with valence protons and neutrons in the $0f_{7/2}$ orbit—such as the $N = 28$ isotones and

$Z = 21$ isotopes—would serve as excellent probes to experimentally verify the single-particle nature and correlations. In addition, the moments of $N = 28$ magic isotones would potentially offer an ideal platform to explore the seniority properties of the independent-particle SM [?] and the influence of E2 and M1 correlations. The electromagnetic moments of isotopes with such simple configurations are also needed to validate recent progress in ab-initio many-body methods and microscopic interactions derived from $\chi$EFT. These methods have been continuously improved to interpret nuclear masses and radii [?, ?, ?] but have so far only scarcely been applied to magnetic and quadrupole moments, two other basic properties of the atomic nucleus [?, ?, ?]. This letter presents precise measurements of the unstable nuclei $^{47,49}$Sc, yielding the first quadrupole moment for $^{49}$Sc. This provides key data for the systematics of nuclear moments associated with the $0f_{7/2}$ orbit and facilitates investigation of single-particle behavior and NN correlations. The experimental data are compared with shell-model calculations and valence-space in-medium similarity renormalization group (VS-IMSRG) calculations [?, ?] based on $\chi$EFT interactions [?, ?].

## 2. Experimental Method

Due to conflicting data on magnetic moments from different measurement methods [?, ?], as will be discussed further in Sec. 3, two collinear laser spectroscopy (CLS) setups—COLLAPS and CRIS—were adopted for this study. This allows the moments of Sc isotopes to be determined unambiguously from both atomic and ionic hyperfine structure (hfs). Details on both setups can be found in Refs. [?, ?, ?]. In brief, the Sc isotopes were produced by impinging 1.4-GeV protons onto a Ta-foil target at ISOLDE-CERN and resonantly ionized with RILIS [?]. The ions were accelerated up to 40 keV, mass separated, and cooled for 100 ms (or 10 ms) in a linear Paul trap [?]. The Sc ions were released as bunches of $ $5-µs temporal length and sent to either the COLLAPS or CRIS setup.

At COLLAPS, the ion bunch was collinearly overlapped with a frequency-doubled continuous-wave Ti:Sapphire laser at 364.3 nm to match the Doppler-shifted $3d4s\ {}^{3D}_{1} \rightarrow 3d4p\ {}^{3F}_{2}$ ionic transition. The laser frequency was stabilized by a wavemeter, which was calibrated in real time by a diode laser locked to one hyperfine component of the $^{87}$Rb atom. The ion velocity was tuned to probe the resonant excitation. Photomultiplier tubes were used to record fluorescence photons emitted from the laser-excited Sc ions as a function of scanning voltage to obtain the hfs spectrum. At CRIS, the ion bunches (100 Hz) were neutralized using potassium vapor and then overlapped in time and space with two 100-Hz pulsed lasers at 246.8 nm and 532 nm, respectively. The first frequency-tripled narrow-band laser was used to resonantly excite the atoms via the $3d4s^2\ {}^{2D}_{3/2} \rightarrow 3d4s5p\ {}^{2P^0}_{1/2}$ transition, and the subsequent frequency-doubled Nd:YAG laser ionized them. The resonantly ionized ions were deflected from the beam and recorded by an ion detector as a function of laser frequency detuning to obtain the hfs spectrum [?].

## 3. Experimental Results

Example hfs spectra of $^{49}$Sc measured with both methods are shown in Fig. 1 and analyzed using the $\chi^2$-minimization approach in SATLAS [?]. The extracted magnetic and quadrupole hfs parameters ($A$ and $B$) are summarized in Tab. 1 and show good agreement with literature values [?, ?, ?].

The magnetic moments ($\mu$) of $^{46,47,49}$Sc were extracted using the atomic parameter, ionic $\mu = \mu_{45} I A/(I_{45} A_{45})$ with the re-evaluated $\mu(^{45}\text{Sc})$ [?]. The final $\mu$ measured with COLLAPS were calculated as the weighted average of the two sets of magnetic moments, taking into account the correlation between $A(^{3D}_{1})$ and $A(^{3F}_{2})$. As presented in Tab. 2, the magnetic moments measured with the two CLS methods are in excellent agreement with each other. The quadrupole moments ($Q_s$) are obtained from the larger $B(^{3F}_{2})$ parameters using $Q_s = Q_{s,45} B/B_{45}$ with the most recent recommended value of $Q_s(^{45}\text{Sc})$ [?]\$.

Table 1 presents the hfs constants $A$ and $B$ of the $^{3D}_{1}$ and $^{3F}_{2}$ ionic states, and $A$ of the $^{2D}_{3/2}$ atomic level, given in MHz. Table 2 presents the newly-measured electromagnetic moments of Sc isotopes along with literature values [?, ?, ?, ?, ?, ?, ?]. The new results for $^{47,49}$Sc are more precise than those from atomic-beam magnetic resonance (ABMR) and nuclear magnetic resonance (NMR) experiments [?, ?]. A systematic deviation of \$ \$2% is found between the magnetic moments of $^{43,47,49}$Sc measured using CLS and those measured using NMR [?] or ABMR [?]. The magnetic moments of $^{43,47}$Sc were measured in one ABMR experiment [?], and the $^{49}$Sc magnetic moment was obtained via NMR and determined relative to the $^{47}$Sc ABMR moment [?], which links all these moments. The magnetic moments measured with CLS were obtained from three independent experiments at IGISOL [?], COLLAPS, and CRIS (this work), using four ionic and one atomic states, and are all in excellent agreement. The $^{46}$Sc magnetic moment was, however, measured in another independent ABMR experiment [?], which is in excellent agreement with the CLS results. This indicates that the discrepancy between the newly measured $^{43,47,49}$Sc magnetic moments and those from ABMR/NMR methods can all be traced back to one particular ABMR experiment [?].

## 4. Discussion

Our measurements provide key experimental data for the systematic investigation of magnetic and quadrupole moments of $Z = 21$ isotopes and $N = 28$ isotones when valence nucleons fill the unique $f_{7/2}$ orbit, as presented in Fig. 2. Particularly, the first $Q_s$ measurement of the short-lived $^{49}$Sc is essential to validate the simple seniority scheme of the independent-particle SM (see Fig. 2(d) and discussion below).

As presented in Figs. 2(a, b), both magnetic and quadrupole moments of $^{41-49}$Sc ($Z = 21$, even $N = 20 - 28$) exhibit identical parabolic trends, approaching the single-particle values for a proton in the $\pi f_{7/2}$ orbit at the neutron magic numbers 20 and 28. This points to the rather pure single-particle character of $^{41,49}$Sc and the doubly-magic nature of $^{40,48}$Ca. Note that the single-particle moments are calculated using an effective $g$-factor of $g_{\text{eff}} = 0.9g_{\text{free}}$ and an effective charge of $e_\pi = 1.5e$ to compensate for possible missing core excitations. The deviation of the magnetic moment of $^{43-47}$Sc ($N = 22, 24, 26$) from the Schmidt line indicates an enhancement of NN correlation as more neutrons/holes are added to the $f_{7/2}$ orbit. The single proton outside the $^{40}$Ca and $^{48}$Ca cores induces an oblate core polarization for $^{41,49}$Sc (sketches on the top of Fig. 2), leading to a negative $Q_s$ (Fig. 2(b)). This core polarization effect is maximized around mid-shell where more particles/holes appear in the $\nu f_{7/2}$ orbit, but a more precise measurement of the $^{43}$Sc quadrupole moment should confirm the expected quadratic trend for these quadrupole moments.

For the $N = 28$ isotonic sequence with (odd) protons filling the $\pi f_{7/2}$ orbit from Sc ($Z = 21$) to Co ($Z = 27$), the magnetic moment is expected to be constant from the independent-particle SM ("Schmidt value," Fig. 2(c)). However, experimental values follow a characteristic linear deviation from the single-particle value. This phenomenon can be explained by increasing cross-shell proton excitations to the upper $f_{5/2}$ spin-orbit partner when the $\pi f_{7/2}$ orbit is being filled [**?**, **?**]. A minor mixing of this M1-excitation into the odd-proton wave function may impact the magnetic moment [**?**]. Thus, the magnetic moment ($\mu$) of an isotone with $n$ protons ($\pi f^n_{7/2}$) follows a linear trend proportional to $n$ and a constant $\delta\mu$ that relates to the M1 spin-flip matrix element: $\mu(\pi f^n_{7/2}) = \mu(^{49}\text{Sc}) + (n-1)\delta\mu$. As a result, a fraction of such orbit mixing in $^{55}$Co induces the observed reduction of its $\mu$ relative to $\mu(^{49}\text{Sc})$, further emphasizing the relatively "pure" single-particle nature of $^{49}$Sc.

In the extreme independent-particle SM, the seniority scheme allows an estimation of the spectroscopic quadrupole moment of isotones with odd protons ($n$) filling an orbit $j$ [**?**, **?**]:

$$Q_{s.p.}(j) = \frac{2n-2}{2j-2} Q_{s.p.}(j)$$

leading to a linear increase proportional to $Q_{s.p.}(j)$, the single-particle quadrupole moment for a proton in orbit $j$ [**?**, **?**, **?**]. This linear trend of $Q_s$ is expected to cross zero when orbit $j$ is half filled. The single proton outside the doubly-magic $^{48}$Ca core induces an oblate core polarization for $^{49}$Sc (negative $Q_s$), whereas a prolate shape is predicted with a positive $Q_s$ for $^{55}$Co (due to a hole inside the doubly-magic $^{56}$Ni), as schematically presented on the top of Fig. 2. With the addition of this precise measurement of $Q_s$ for $^{49}$Sc, a linear trend can then be unambiguously determined from the available experimental $Q_s$ of $N = 28$ isotones, crossing zero at the half-filling of the $\pi f_{7/2}$ orbit (Fig. 2(d)), representing a textbook example for the independent-particle SM picture. It is worth noting that the proton cross-shell excitations, which strongly affect the magnetic moments (M1 correlations) (Fig. 2(c)), have no notable effect on the quadrupole moments (E2 correlations).

Naturally, one would expect large-scale SM calculations to provide a good description of these nuclear moments. However, as shown in Figs. 2(a, c), the SM calculation using the GXPF1A effective interaction ($^{40}$Ca core and $pf$ model space) [?] does not reproduce well the trend of magnetic moments for heavier scandium isotopes and systematically underestimates those of the $N = 28$ isotones. This may suggest a missing polarization effect of the $^{40}$Ca core, requiring an effective interaction with a valence space that includes $sd$ and $pf$ shells optimized for the calcium region. While interactions exist for protons and neutrons in the $sd - pf$ model space (e.g., SDPF-U [?] and SDPF-MU [?]), these have been developed for isotopes with $Z = 8 - 20$ (namely in the $sd$-shell) to properly account for neutron $sd - pf$ shell excitations in neutron-rich isotopes.

We further investigate the influence of proton M1 and E2 correlations in the $pf$ model space on the moments of $N = 28$ isotones by performing calculations for protons in a gradually extended model space, as shown in Fig. 3. For consistency with the VS-IMSRG calculation, neutron excitations across $N = 28$ are intentionally blocked in the SM calculations. As presented in Fig. 3 (upper panel), proton excitations to the $\pi f_{5/2}$ orbit clearly drive the linearly increased deviation of $\mu$ from the Schmidt value from $^{49}$Sc to $^{55}$Co, and this is captured well in both theories. On the contrary, these proton M1-excitations have nearly negligible impact on the $Q_s$ moments (Fig. 3, lower panel). The SM GXPF1A calculations for magnetic and quadrupole moments without neutron excitations across $N = 28$ (Fig. 3, right panel) show better agreement with experimental data compared to SM results performed in the full model space (Fig. 2(c, d)). This suggests that neutron excitations across $N = 28$, which in turn correlatively induce proton excitations across $Z = 28$, are overestimated in the full SM calculations (Fig. 2), and that even a small portion of these excitations leads to a notable change of $\mu$ as discussed above, supporting the "pure" single-particle character of $^{49}$Sc. In other words, the $N = 28$ shell gap seems to be underestimated in the GXPF1A shell model interaction.

It is worth noting that there is a substantial difference between the performance of the theories for the $N = 28$ isotones (Figs. 2(c, d) and Fig. 3) and that for the $Z = 21$ isotopes (Figs. 2(a, b)). Both SM and VS-IMSRG calculations give a good description of the systematic trends of moments for $N = 28$ isotopes when odd protons fill the $f_{7/2}$ orbit (Figs. 2(c, d) and Fig. 3). This benchmarks the significant progress of ab initio calculations for describing electromagnetic moments of simple cases with magic neutron number ($N = 28$) and valence protons outside the doubly-magic $^{48}$Ca core. For $^{41-49}$Sc isotopes, where enhanced NN correlations are induced by additional neutrons/holes in the $f_{7/2}$ orbit and possible polarization effects of the $^{40}$Ca core, the theories are much less successful in describing their electromagnetic moments. This instead provides a systematic quantification of their deviations from experimental data along the entire isotopic chain, motivating further development of interactions and many-body methods when encountering more complicated correlations.

With advances in many-body methods and NN+3N forces from $\chi$EFT [?], first-principles calculations of electromagnetic properties of medium-mass nuclei are now possible using VS-IMSRG [?, ?, ?, ?], with first applications in the *sd* shell [?, ?, ?, ?, ?, ?, ?]. Here, we use two chiral interactions for the first time in the $pf$ space: NNLOsat [?] and ΔNNLOGO(394) [?]; the latter explicitly includes Δ(1232)-isobars and has so far only been tested for charge radii and binding energies [?, ?]. In this work, the VS-IMSRG calculation follows the same procedure as in Ref. [?], with an increased $E3_{\mathrm{max}} = 22$ truncation on storage of 3N matrix elements [?]. We decouple a $pf$-shell valence-space Hamiltonian above a $^{40}$Ca core (or $^{48}$Ca core for $N = 28$ isotones), and the E2 and M1 operators are consistently transformed by the VS-IMSRG [?] to produce consistent effective valence-space operators. Final energies and transition rates are obtained with the KSHELL code [?].

We emphasize that only bare nucleon charges and free $g$-factors are used here, which is fundamentally different from the SM GXPF1A calculation where $g_{\mathrm{eff}} = 0.9g_{\mathrm{free}}$, $e_\pi = 1.5e$, and $e_\nu = 0.5e$ have been used. Similar to the SM calculation, both chiral interactions (ΔNNLOGO and NNLOsat) result in a clear underestimation of the magnetic moments of $^{45,47,49}$Sc and a systematic underestimation of magnetic moment trends for the $N = 28$ isotones, as shown in Figs. 2(a, c). We note that the new ΔNNLOGO interaction gives a somewhat better description along the Sc isotopic chain, which may benefit from the inclusion of the Δ(1232)-isobar degree of freedom.

In Figs. 2(b, d), the quadrupole moments are compared with calculated moments from these theories. While the SM GXPF1A calculations follow reasonably well the general trend of $Q_s$ as a function of $N$, the VS-IMSRG calculations largely underestimate the experimental absolute values of quadrupole moments for $Z = 21$ isotopes (Fig. 2(b)). A similar underestimation was already seen for calculated E2 matrix elements in lighter Mg isotopes [?, ?], which is likely due to missing higher-order collective excitations in the VS-IMSRG calculation at the IMSRG(2) level, as discussed in Refs. [?, ?]. Further theoretical studies are needed to understand the origin of missing E2 correlations in the ab-initio calculations. For the $N = 28$ isotones, as shown in Fig. 2(d), the characteristic symmetric linear trend of $Q_s$ when filling the proton $\pi f_{7/2}$ orbit is captured remarkably well by both theories. The smaller slope of the calculated trend using the ab-initio interaction reflects only a small underestimation of the single-particle quadrupole moment for a proton (particle or hole) in the $f_{7/2}$ orbit (no effective charges are used here). With the GXPF1A effective interaction, the slope is overestimated, which points to either too large an effective proton charge or an overestimated value for the single-particle quadrupole moment. This can be further investigated by blocking neutron excitations across $N = 28$.

## 5. Summary and Conclusion

In summary, electromagnetic moments of $^{47,49}$Sc were measured with improved precision and accuracy, including the first electric quadrupole moment $Q_s$ of the $^{49}$Sc isotope. A systematic investigation of electromagnetic moments has been performed for $N = 28$ isotones and $Z = 21$ isotopes with valence nucleons filling the $f_{7/2}$ orbit. Thanks to the unique location of this orbit in the SM scheme, the sensitivity of electromagnetic moments to nucleon-nucleon M1 and E2 correlations has been probed. Particularly, the seniority scheme of the independent-particle SM is experimentally confirmed based on the $Q_s$ of $^{49}$Sc and its $N = 28$ isotones, providing a textbook example. This study serves as a benchmark for state-of-the-art theoretical models, especially ab initio VS-IMSRG calculations using microscopic interactions derived from $\chi$EFT.

At experimental precision, none of the theories used in this work satisfactorily reproduces the magnetic moment trends along the $Z = 21$ isotopic chain or their absolute values for the $N = 28$ isotones. In particular towards $N = 28$, all magnetic moments are largely underestimated, which may suggest that neutron M1 excitations to the $f_{5/2}$ orbit are too pronounced in the models. As for the quadrupole moments, the trend along the $Z = 21$ isotopic chain is reasonably reproduced by the SM GXPF1A calculations, although the absolute value towards $N = 28$ is clearly overestimated, suggesting that E2 excitations to the $p_{3/2}$ orbit are also overestimated. Together with the underestimated magnetic moments, this points to too small an $N = 28$ gap in the GXPF1A interaction. The linear trend of $Q_s$ observed for $N = 28$ isotones is well described with the SM GXPF1A, but the absolute single-particle quadrupole moment (or the effective charge) is overestimated, as the slope is too steep.

With the ab-initio interactions, the quadrupole moments of $Z = 21$ isotopes are largely underestimated, pointing to missing E2 correlations when opening the neutron shell between $N = 20$ and 28. Nevertheless, the linear trend of quadrupole moments along $N = 28$ isotones is very well captured, and the slope is only slightly less steep than observed, illustrating that the single-particle quadrupole moment (without use of effective charge) is well reproduced by the ab-initio theory.

The present work highlights the progress made in advanced nuclear theory and paves the way for a coherent description of basic nuclear properties with further development of nuclear interactions and many-body methods, such as a more proper effective SM interaction for the calcium region in the $sd{-}pf$ model space, VS-IMSRG approach with all operators truncated at the three-body level and decoupling a cross-shell Hamiltonian, as well as inclusion of meson-exchange currents.

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