Ground-state electromagnetic moments of calcium isotopes

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Background: The neutron-rich calcium isotopes have gained particular interest as evidence of closed-shell structures has recently been found in two exotic nuclei, at N = 32 and N = 34. Additionally, the study of such neutron-rich systems has revealed new aspects of nuclear forces, in particular regarding the role of three-nucleon forces.

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Purpose: We study the electromagnetic properties of Ca isotopes around the neutron number N=32.

Methods: High-resolution bunched-beam collinear laser spectroscopy was used to measure the optical hyperfine spectra of the $^{43-51}$ Ca isotopes.

Results: The ground-state magnetic moments of 49,51 Ca and quadrupole moments of 47,49,51 Ca were measured for the first time, and the 51 Ca ground-state spin I=3/2 was determined in a model-independent way. Our experimental results are compared with state-of-the-art shell-model calculations using both phenomenological interactions and microscopic interactions derived from chiral effective field theory.

Conclusions: The results for the ground-state moments of neutron-rich isotopes are in excellent agreement with predictions of interactions derived from chiral effective field theory including three-nucleon forces. Lighter isotopes illustrate the presence of particle-hole excitations of the 40 Ca core in their ground state. Our results provide a critical test of modern nuclear theories, and give direct answer to the evolution of ground-state electromagnetic properties in the Ca isotopic chain across three doubly closed-shell configurations at N=20, 28, 32 of this unique system.

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The existence of doubly magic nuclei has played a key role in our understanding of nuclear structure. Doubly magic nuclei have been the basis to develop the shell model, and are an ideal probe to test our knowledge of nuclear interactions by comparing experimental data with shell-model predictions [1,2]. Such shell-model calculations depend on the effective Hamiltonian used, a suitable valence space to capture the low-energy degrees of freedom, and consistent effective operators. Although effective charges and *g* factors are widely used in shell-model calculations, they are not completely understood. Furthermore, their orbital [3] and valence-space [4] dependence and connection to two-body currents (meson-exchange currents), known to be important for magnetic moments in light nuclei [5], are under discussion.

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Having a closed proton shell, Z=20, and two naturally occurring doubly magic isotopes, 40 Ca and 48 Ca, the calcium isotopic chain has always been considered a prime benchmark for nuclear structure, both from a theoretical [6] and an experimental perspective [7]. Recently, special attention has turned to the evolution of the structure beyond N=28, where additional shell closures have been suggested at N=32 [8] and N=34 [9]. These neutron-rich calcium isotopes have also gained exceptional interest from the theoretical side [10–14], as their properties reveal new aspects of nuclear forces, in particular regarding the role of three-nucleon (3N) forces [10,11] (for a review on 3N forces see [15]).

Spectroscopic properties in the Ca region are well described by phenomenological shell-model interactions, such as KB3G [16] and GXPF1A [17]. These interactions start from a 40 Ca core and two-nucleon (NN) forces and refit part of the interactions to experimental data in the pf shell, to compensate for neglected many-body effects (both due to 3N and many-body correlations) [2]. Normal and superdeformed bands in 40 Ca have been understood as due to particle-hole excitations of protons and neutrons from the sd shell into the pf orbits, and have been well described

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using the SDPF.SM shell model interaction starting from a virtual ²⁸Si core [18]. These calculations showed that the ⁴⁰Ca ground state is very correlated. In the last years, valence-shell interactions have been derived from NN and 3N forces based on chiral effective field theory [10], fitted only to few-nucleon systems. Investigating the reliability of these microscopic NN + 3N interactions is a matter of general interest as they have direct implications for the modeling of astrophysical systems [19]. The NN + 3N interactions provide a good description of the shell structure and the spectra of neutron rich calcium isotopes in an extended valence space $(fpg_{9/2})$ [14]. The electric quadrupole (E2) transitions obtained from both phenomenological and microscopic interactions exhibit good agreement using the neutron effective charge: $e_n = 0.5e$. On the other hand, phenomenological interactions and NN + 3Ndisagree in effective nucleon g factors needed to reproduce the magnetic (M1) transition strengths [14].

Despite the remarkable differences, both phenomenological and microscopic NN+3N interactions give a similar description of neutron separation (binding) energies and low-lying excitation energies of Ca isotopes from N=22 up to N=32 [8,9,20]. As illustrated in [21], such observables might however be insensitive to cross-shell correlations. Therefore, there is a need to measure additional observables like electromagnetic moments, which further test the above models and might provide a deeper insight to developing improved shell-model interactions.

Magnetic moments and g factors, $g = \mu/(I\mu_N)$, of isotopes near shell closures are very sensitive to the occupancy of particular orbitals by valence particles (or holes). The quadrupole moments on the other hand are directly sensitive to nuclear shell structure [22]. While the terms *closed shell* or *magic number* may lack a rigid definition, the electromagnetic moments provide a more direct probe of the structure involved including cross-shell effects [23,24].

In this Rapid Communication, we report the first measurements of the quadrupole moment of the closed shell -1 isotope 47 Ca, and the quadrupole and magnetic moment of the closed-shell +1 isotope 49 Ca. Also the magnetic and quadrupole moments of 51 Ca, having a single-hole with respect to the new N=32 subshell closure, are presented, as well as its ground state (g.s.) spin. The experimental data are compared to shell-model calculations using phenomenological interactions, and to calculations including 3N forces based on chiral effective field theory.

At ISOLDE, CERN, exotic Ca isotopes were produced from nuclear reactions induced by a high-energy proton beam (1.4 GeV; pulses of 2 μ C typically every 2.4 s) impinging on a uranium carbide target. High selectivity for the Ca reaction products was accomplished by laser ionization [25]. Ions were extracted from the ion source and accelerated up to 30 keV or 40 keV to be mass separated, after which they were injected into the ISOLDE radiofrequency quadrupole (RFQ) beam cooler, ISCOOL [26]. Ions were trapped for

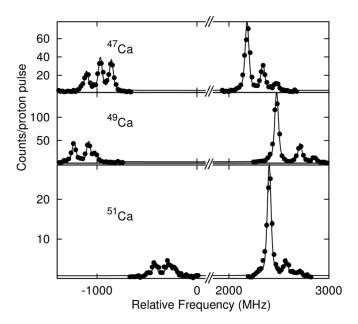


FIG. 1. Examples of hfs spectra measured for the Ca isotopes in the 393 nm $4s^2S_{1/2} \rightarrow 4p^2P_{3/2}$ ionic transition. The lines show the fit with a Voigt profile. Frequency values are relative to the centroid of ⁴³Ca.

approximately 50 ms, and extracted bunches of 5 μ s temporal width were distributed to a dedicated beam line for collinear laser spectroscopy experiments (COLLAPS). At COLLAPS, the ion beam was superimposed with a continuous wave (CW) laser beam from a frequency-doubled Ti:Sa laser, providing a 393-nm laser wavelength to excite the 4s $^2S_{1/2} \rightarrow 4p$ $^2P_{3/2}$ transition in Ca⁺. The laser frequency was locked to a Fabry-Perrot interferometer, which was in turn locked to a polarization-stabilized HeNe laser, reducing the laser frequency drift to <10 MHz per day.

By changing the ion velocity, and thereby Doppler tuning the laser frequency in the ion rest frame, hyperfine structure (hfs) components could be scanned. Fluorescence photons were detected by a set of four photomultipliers (PMT) at the end of the beam line (see Refs. [27,28] for details). By only accepting signals from the PMT while the ion bunch passed in front of them, background from scattered laser light and PMT dark counts was reduced by a factor of $\sim 10^4$. Sample hfs spectra measured during the experiment are shown in Fig. 1. The magnetic hfs constants, $A(^2S_{1/2})$, $A(^2P_{3/2})$, and quadrupole hfs constants, $B(^2P_{3/2})$, were extracted from the fit of Voigt profiles to the experimental spectra by using a χ^2 -minimization technique as explained, e.g., in Ref. [29]. The values are listed in Table I. Only ⁴³Ca has been studied before in this ionic transition, and our values are in agreement within 1.1 standard deviations. For 41Ca and 45Ca, two measurements of the quadrupole hfs constants have been reported in the atomic level system, both relative to that of ⁴³Ca [30,31], yielding the ratios $B(^{41}\text{Ca})/B(^{43}\text{Ca}) = 1.63(1)$, and $B(^{45}\text{Ca})/B(^{43}\text{Ca}) = -0.94(27)$. The *B*-factor ratio equals the ratio of the quadrupole moments. Thus we can compare the ratio of our B values, measured in the ionic system

¹A previous value for the magnetic moment of ⁴⁹Ca was suggested from a partial measurement of its hfs and assuming a value for its unknown isotope shift [52].

TABLE I. Hyperfine structure values obtained from the fit to the experimental data compared to previous measurements.

A	I^{π}	$A(^2S_{1/2})$ (MHz)	$A(^{2}P_{3/2})$ (MHz)	$B(^{2}P_{3/2})$ (MHz)	Ref.
43	7/2-	-806.87(42) -806.40207160(8) -805(2)	-31.10(30) -31.9(2) -31.0(2)	-4.2(1.3) -6.7(1.4) -6.9(1.7)	[32] [33] [34]
45 47 49 51	7/2 ⁻ 7/2 ⁻ 3/2 ⁻ 3/2 ⁻	-811.99(44) -860.96(28) -1971.02(30) -1499.22(94)	-31.43(19) -33.33(13) -75.98(11) -58.15(54)	3.1(1.0) 12.68(96) -5.53(40) 5.4(1.8)	

 $B(^{45}\text{Ca})/B(^{43}\text{Ca}) = -0.74(31)$, to the latter value. They are in agreement within the error bars.

The nuclear spin, I, is required to calculate each peak position in the minimization procedure. Since a different set of hfs constants is found for a given spin, the ratio, $R = A(^2P_{3/2})/A(^2S_{1/2})$, can be used to determine the correct spin for each isotope, as this ratio should be a constant over the entire isotopic chain (neglecting a possible small hyperfine anomaly). As can be seen from Fig. 2, the ratio R remains constant along the Ca isotopes up to 49 Ca, using the earlier determined g.s. spins in the fitting procedure. For 51 Ca we assumed three possible spins for its ground state and only when I = 3/2 is used, the ratio of the fitted hfs parameters is consistent with those from the other isotopes. Thus I = 3/2 is the g.s. spin of 51 Ca, confirming earlier tentative assignments [35,36], and in agreement with expectations from the shell model.

Magnetic moments were extracted from the lower state magnetic hfs constants, $A = \mu_I B_0/(IJ)$, where B_0 is the magnetic field produced by the electrons at the nucleus, and J is the electronic total angular momentum. Since high-precision

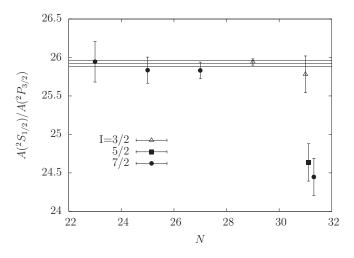


FIG. 2. Ratio between the hfs constants $A(^2P_{1/2})$ and $A(^2P_{3/2})$. The continuous line shows the average value $A(^2S_{1/2})/A(^2P_{3/2}) = 25.92(3)$. Hyperfine structure spectra of 51 Ca were fitted assuming different g.s. spin values of I = 3/2, 5/2, 7/2.

values of $A(^2S_{1/2}) = -806.40207160(8)$ MHz [32] and $\mu = -1.3173(6)$ [37] are known for 43 Ca, this isotope was used as a reference to calculate the other magnetic moments from the measured A values. The results are shown in Table II, where we compare our data to earlier reported values for 45 Ca and 47 Ca.

Quadrupole moments, Q, were obtained from the quadrupole hfs constant, $B = eQV_{JJ}$, with e the electron charge, and V_{JJ} the electric field gradient (EFG) produced by the electrons at the nucleus, the latter being isotope independent. To extract quadrupole moments from the measured hfs B parameters, a calculated value for the EFG, $eV_{IJ} =$ 151.3(7) MHz/b, was taken from atomic-physics calculations based on relativistic coupled-cluster theory (RCC) [40]. Independent values calculated from many-body perturbation theory (MBPT) [43,44] agree with the value from RCC within 3%. The extracted quadrupole moments are shown in Table II. The deviation of our value for ⁴³Ca from the literature values is attributed to the low statistics of our data for this isotope combined with a poorly resolved hyperfine splitting in the excited state. Note however that our ratio of the ⁴⁵Ca to ⁴³Ca quadrupole moment is consistent with the value measured in the atomic system.

Since the g factors are sensitive to the valence-particle configuration, it is illustrative to study their evolution along the Ca isotopic chain. The horizontal lines in Fig. 3 show the effective single-particle values ($g_{\rm eff}^{\nu}=0.8g_{\rm free}^{\nu}$) for the different shell-model orbits. The isotope ³⁹Ca (N=19) has a g factor close to the $d_{3/2}$ effective single-particle value, confirming the hole nature of this isotope. Once the $d_{3/2}$ orbit is filled, the fairly constant g-factor values from N=21 up to N=27 are in agreement with that of an odd neutron in the $f_{7/2}$ orbital.

As expected, the measured g factor of 49 Ca is close to the effective single-particle value of the $p_{3/2}$ orbit, and a similar value would be expected for 51 Ca. However, a deviation from this value is observed, indicating an appreciable contribution from the mixing with configurations due to neutron excitations across N=32, which seems to contradict the closed-shell nature of N=32. The isotope 51 Ca is an exceptional case for testing different shell-model interactions as excitations across N=32 can be of M1-type (from $p_{3/2}$ into $p_{1/2}$) and therefore even a one percent mixing of those configurations in the wave function is sufficient to induce a $\sim 20\%$ change of the g factor [46].

The measured and calculated magnetic moments of the Ca isotopes are shown in the upper panel of Fig. 4. A 40 Ca core is assumed in the calculations with the GXPF1A and KB3G phenomenological interactions, as well as for the calculations with the microscopic NN + 3N interaction. To investigate the effect of breaking the 40 Ca core we also compare to a large-scale shell model calculation using the phenomenological interaction SDPF.SM starting from a virtual 28 Si core. For the KB3G and GXPF1A interactions, neutrons were allowed to occupy the pf shell, while an extended valence space including the $0g_{9/2}$ orbital ($pfg_{9/2}$ space) was used for the NN + 3N calculations. Excitations of neutrons and protons from the upper sd shell into the pf shell are allowed with the SDPF.SM interaction. Bare spin and orbital

TABLE II. Quadrupole and magnetic moments obtained from the measured hfs constants (Table I). The magnetic moments were obtained using the reference isotope 43 Ca, with $A({}^{2}P_{3/2}) = -806.40207160(8)$ MHz [32]. Quadrupole moments were extracted using the calculated electric field gradient, $eV_{JJ} = 151.3(7)$ MHz/b [40]. Data are compared to calculations using the NN + 3N interaction.

A	$\mu(\mu_N)$	$\mu(\mu_N) \\ (NN+3N)$	Q (b)	Q (b) $(NN + 3N)$	Ref.
41	-1.594781(9)				[38]
			-0.080(8)		[31]
43		-1.56	-0.028(9)	-0.0246	This work
	$-1.3173(6)^{a}$				[37]
			-0.043(9)		[33]
			-0.049(5)		[31]
			-0.0408(8)		[39]
			-0.0444(6)		[40]
45	-1.3264(13)	-1.45	+0.020(7)	+0.0252	This work
	-1.3278(9)				[41]
	. ,		+0.046(14)		[31]
47	-1.4064(11)	-1.38	+0.084(6)	+0.0856	This work
	-1.380(24)				[42]
49	-1.3799(8)	-1.40	-0.036(3)	-0.0422	This work
51	-1.0496(11)	-1.04	+0.036(12)	+0.0425	This work

^aReference value.

g factors were used in all theories to calculate the magnetic moments

The disagreement between the shell-model calculations starting from a 40 Ca core and the experimental magnetic moments of 41,43,45 Ca suggests that nucleon excitations across the sd shell are important in the vicinity of N=20. Indeed, large-scale shell model calculations using the SDPF.SM interaction are closer to the experimental values. These calculations include up to 6p-6h for 41 Ca, 4p-4p for 43 Ca, and 2p-2p for the other isotopes. A similar conclusion on the importance of cross-shell correlation across N=20 was obtained from experimental $g(2^+)$ factors and B(E2) values of 42,44 Ca [47,48] as well as the calcium isotope shifts [49]. For the heavier Ca isotopes, all theoretical calculations describe

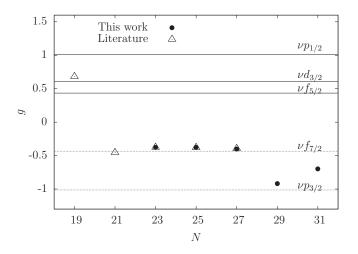


FIG. 3. Measured g factors compared with literature values and effective single-particle values (lines) using $g_s^{\nu} = -3.041$ and $g_l^{\nu} = 0.0$ ($g_{\rm eff}^{\nu} = 0.8 g_{\rm free}^{\nu}$). The magnetic moment of ³⁹Ca was taken from Ref. [45]. The experimental error bars are smaller than the symbols.

the experimental value rather well (see Fig. 4), indicating that from N = 27 and beyond, the assumption of a rigid ⁴⁰Ca core works well. Especially, the calculations with the NN + 3N interaction give a very good agreement for ^{47,49,51}Ca. Considering that from the measured g factor a mixed ground state wave function is expected (Fig. 3), the excellent agreement for the microscopic calculations, which are not fitted to this mass region, is remarkable. The fact that the calculated values for the phenomenological KB3G and GXPF1A lay on opposite side of the experimental value is due to the different contributions of $(p_{1/2})^2(p_{3/2})^1$ and $(p_{1/2})^1(p_{3/2})^2$ configurations. Certainly, the magnetic moment is highly sensitive to matrix elements involving the $p_{3/2}$ - $p_{1/2}$ spin-orbit partners. The ratio of $(p_{1/2})^1(p_{3/2})^2$ to $(p_{3/2})^3$ configurations in 51 Ca is a measure for these cross-shell excitations across N = 32: it is almost twice larger with NN + 3N and GXPF1A (3.5% and 4.0%, respectively) than in KB3G (2.0%). Larger cross-shell excitations reduce the absolute value of the magnetic moment. On the other hand, due to stronger pairing, the NN + 3N and KB3G interactions have a two times larger ratio of $(p_{1/2})^2(p_{3/2})^1$ over $(p_{1/2})^1(p_{3/2})^2$ configurations than GXPF1A, 1.6 and 1.9 compared to 0.9. These cross-shell excitations increase the absolute value of the magnetic moment.

In the lower panel of Fig. 4, the experimental and calculated quadrupole moments are shown. The theoretical results assume neutron and proton effective charges, $e_n = 0.5e$ and $e_p = 1.5e$, respectively (protons in the valence space are allowed for the SDPF.SM interaction only). All interactions exhibit in general a good description of the experimental quadrupole moments. The only deviation exists for N = 27, where KB3G and GXPF1A slightly disagree with the experimental value, while NN + 3N and SDPF.SM agrees nicely. The agreement between calculated and experimental values also confirms the values of effective charges used around N = 20 [18,49], and more recently around N = 28 [50]. Earlier studies of $N \sim Z$

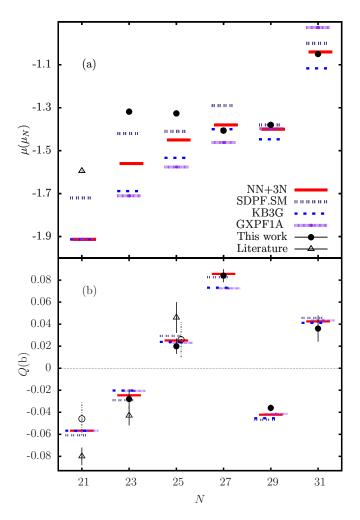


FIG. 4. (Color online) Measured magnetic and quadrupole moments of Ca isotopes. Results are compared with theoretical predictions from phenomenological interactions (KB3G, GXPF1A, SDPF.SM) and calculations including three-nucleon forces (NN+3N). Experimental literature values (empty triangles) are given in Table II. The open circles show the values calculated from the ratios $B(^{41}\text{Ca})/B(^{43}\text{Ca}) = 1.63(1), \ B(^{45}\text{Ca})/B(^{43}\text{Ca}) = -0.94(27)$ [31] and relative to our value of $Q(^{43}\text{Ca})$.

isotopes, where the $f_{7/2}$ orbital is dominant, suggested values of $e_n = 0.8e$ and $e_p = 1.15e$ [51], opening a discussion on the possible orbital dependence of the effective charges in the pf shell [3].

In summary, bunched-beam collinear laser spectroscopy was used to measure the hfs spectra in the Ca II resonance transition from ^{43–51}Ca. Our results allowed a direct g.s. spin determination for ⁵¹Ca. The quadrupole moments of ^{47,49,51}Ca, and magnetic moments of ^{49,51}Ca were measured for the first time. We compared these results with new shell-model calculations using a microscopic interaction derived from chiral effective field theory, including NN + 3N forces, and fitted only to isotopes up to mass A = 4. Comparison was also made with existing and new calculations using phenomenological interactions. Large discrepancies among the measured magnetic moments and the calculated values using a 40 Ca core were observed around N=20. Large-scale shell model calculations in the sd-pf valence space are required to reproduce better the observed magnetic moments. Further developments of microscopic interactions in the complete sd-pf valence space for both protons and neutrons are needed to provide a consistent description for all observables of Ca isotopes from below N = 20 up to above N = 32. For $N \ge 27$, the calculations with NN + 3N forces derived from chiral effective field theory provide excellent agreement for both the magnetic and quadrupole moments. Through the gradual filling of the $f_{7/2}$ and $p_{3/2}$ orbits, our results provide a comprehensive study of the basic ingredients employed in shell-model calculations over a wide range of neutrons. At the level of precision of our experimental results, the g.s. quadrupole moments do not reveal any orbital dependence of the effective charges. The larger difference in calculated magnetic moments compared to electric quadrupole moments highlights the need of improved theoretical calculations, e.g., including two-body currents from chiral effective field theory, that compared to the present measurements may provide new insights on the magnetic operator and effective g factors.

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