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Auxiliary field diffusion Monte Carlo calculations of magnetic moments of light nuclei with chiral EFT interactions

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We calculate the magnetic moments of light nuclei ($A < 20$) using the auxiliary field diffusion Monte Carlo method and local two- and three-nucleon forces with electromagnetic currents from chiral effective field theory. For all nuclei under consideration, we also calculate the ground-state energies and charge radii. We generally find a good agreement with experimental values for all of these observables. For the electromagnetic currents, we explore the impact of employing two different power counting schemes, and study theoretical uncertainties stemming from the truncation of the chiral expansion order-by-order for select nuclei within these two approaches. We find that it is crucial to employ consistent power counting schemes for interactions and currents to achieve a systematic order-by-order convergence.

Introduction— Electromagnetic (EM) phenomena are of great importance in nuclear physics both as external probes into the structure of atomic nuclei and to understand certain internal observables. From high-energy electron scattering that explores nuclear distributions [1–3] to EM transition strengths that reveal details of nuclear structure [4–6], it is crucial to have a robust theoretical description of both strong and EM forces in nuclear-physics systems. One instance of their union manifests in the magnetic moment of an atomic nucleus. Magnetic moments are fundamental properties of nuclei which interact with atomic electrons and give rise to the hyperfine structure in electronic spectra which can be used as a powerful tool to test quantum electrodynamics and nuclear structure. Additionally, nuclear magnetic moments provide a compelling test of both nuclear many-body methods and the construction of nuclear interactions and EM currents in a low-energy framework.

The nuclear magnetic moment is the vector that defines the strength and direction of the magnetic field created by an atomic nucleus. In a simple independent-particle model, the magnetic moment can be computed from the sum of individual nucleon magnetic moments and contributions from nonzero orbital angular momenta of protons. For a more realistic description, this model is greatly complicated in two ways: correlations in the nuclear wave function and inter-nucleon EM currents. The former can be handled by quantum many-body methods such as the quantum Monte-Carlo (QMC) [7] method, while the latter can be handled in a consistent way by including higher-order contributions from an EM current derived from chiral effective field theory (EFT)[8–13].

Chiral EFT provides a framework for modeling the interactions both among constituent nucleons and with external probes in terms of an expansion in powers of the relevant momentum scale (Q) over the chiral breakdown scale (Λ). Retaining a finite number of terms in the chiral expansion allows one to study nuclear systems using a systematically improvable yet tractable model of the in-

teractions. Additionally, theoretical uncertainties can be systematically estimated by analyzing the order-by-order convergence of the expansion [15, 16]. In this expansion, the lowest order term in Q/Λ is referred to as the leading order (LO) term, the second lowest order term as next-to-leading order (NLO), the third lowest order term as next-to-next-to-leading order (N²LO), and so on.

In this letter, we employ local interactions and EM currents from chiral EFT and use them to compute the magnetic dipole moments of light nuclei with the auxiliary

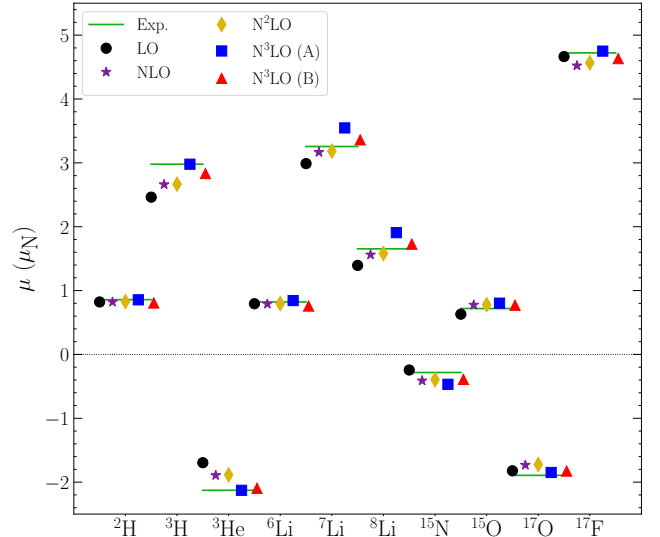


FIG. 1: AFDMC results for the magnetic moments for all nuclei studied in this work. We show the experimental values (green lines) and results with the EM current at LO (black points), NLO (purple stars), N²LO (yellow diamonds), and N³LO (blue squares for scheme A and red triangles for scheme B; see text for details), while keeping the interaction fixed to be the N²LO_{E1} interaction with $R_0 = 1.0$ fm [14]. The uncertainties for each experimental value and for the Monte Carlo statistics are indiscernible on this scale.

field diffusion Monte Carlo (AFDMC) method [7, 17, 18]. In Fig. 1, we compare the calculated magnetic moments to experimental data and generally find good agreement. To bolster these results, we also compute the corresponding ground-state energies and charge radii. We then explore different power counting (PC) schemes for the chiral expansion of the EM currents and address the consistency between these and nuclear interactions. Low-energy constants introduced by the EM currents at N³LO are constrained by two different fits to data. Additionally, we compute results order-by-order and use those to estimate theoretical uncertainties for both PC schemes.

Methods— We treat nuclei as a collection of A point-like interacting nucleons of average mass m described via the non-relativistic intrinsic Hamiltonian

$$H = \sum_i -\frac{\nabla_i^2}{2m} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk}. \quad (1)$$

Here, the first term describes the kinetic contribution to the Hamiltonian, and V_{ij} and V_{ijk} are the nucleon-nucleon (NN) and three-nucleon (3N) potentials, respectively, the former of which also includes the Coulomb force. The NN interactions we use in this work were derived in Refs. [19, 20] and the 3N interactions in Refs. [14, 21] and are based on a local formulation of chiral EFT. Chiral EFT is a systematic theory for nuclear forces describing interactions in terms of a systematic momentum expansion [22, 23]. It enables an improvement of interactions order-by-order and enables theoretical uncertainty estimates [15, 16]. The interactions employed here are derived within Weinberg PC [24, 25] but other PCs have been introduced in the past, see, e.g., Refs. [26–33]. Local interactions from chiral EFT [34] have been successfully applied to QMC calculations of various nuclear systems [35]. Here, we perform AFDMC calculations of the magnetic moment using the local chiral NN and 3N interactions with cutoff $R_0 = 1.0$ fm up to N²LO using the $E1$ parametrization for the 3N forces (N²LO_{E1}) [14]. These interactions have been used to study the ground-state properties of various atomic nuclei up to ¹⁶O [14, 18, 36–41], few neutron systems [42, 43], and neutron-star matter [14, 44–49].

With the Hamiltonian in hand, as the first step, we optimize the variational trial wave function of the form

$$|\Psi_T\rangle = [F_C + F_2 + F_3]|\Phi\rangle_{J^\pi, T}, \quad (2)$$

where F_C accounts for all the spin- and isospin-independent correlations, and F_2 and F_3 are NN and 3N correlations linear in spin- and isospin-pairs as described in Ref. [7]. The term $|\Phi\rangle_{J^\pi, T}$ is taken to be a shell-model-like state with total angular momentum J , parity π , and total isospin T describing the target nucleus. Its wave function consists of a sum of Slater determinants ($\mathcal{D}$)

constructed using single-particle orbitals:

$$\langle RS|\Phi\rangle_{J^\pi, T} = \sum_n c_n \left(\sum \mathcal{C}_{JT} \mathcal{D}\{\phi_\alpha(\mathbf{r}_i, s_i)\} \right)_{J^\pi, T}, \quad (3)$$

where $\mathbf{r}_i$ are the spatial coordinates of the nucleons and s_i represent their spins. Each single-particle orbital ϕ_α consists of a product of a radial function $\varphi(r)$ and an appropriate spherical harmonic coupled to the spin and isospin states. The determinants are coupled with Clebsch-Gordan coefficients ($\mathcal{C}_{JT}$) to total J and T , and the c_n are variational parameters multiplying different components having the same quantum numbers. The radial functions $\varphi(r)$ are obtained by solving for the eigenfunctions of a Wood-Saxon well, and all parameters are chosen by minimizing the variational energy as described in Ref. [50]. Then, using the AFDMC algorithm, the ground-state wave function is projected out by evolving the variational wave function with the time-propagation operator in imaginary time,

$$|\Psi(\tau)\rangle = \lim_{\tau \rightarrow \infty} e^{-(H-E_0)\tau} |\Psi_T\rangle. \quad (4)$$

More details on the AFDMC method for nuclear systems are given in Refs. [7, 17, 35].

Here, we will use the AFDMC method to calculate the magnetic moments of the nuclei ²H, ³H, ³He, ⁶Li, ⁷Li, ⁸Li, ¹⁵N, ¹⁵O, ¹⁷O, and ¹⁷F. For these nuclei, we show the binding energies per nucleon and the charge radii without theoretical uncertainties in Fig. 2. Overall, our calculations follow the trends of the experimental data. For the binding energies, we observe a slight underbinding consistent with the results of Ref. [38] for which all results agree with experiment within theoretical uncertainties. For the charge radii, on the other hand, we find a very good description of experimental values. The magnetic moment (μ) is calculated from the mixed expectation value of VMC and DMC wave functions (see Ref. [18] for more details) for the magnetic form factor F_M ,

$$F_M(q; \tau) \approx -i \frac{2m}{q} \left[2 \frac{\langle \Psi_T | j_y(q\hat{x}) | \Psi(\tau) \rangle}{\langle \Psi_T | \Psi(\tau) \rangle} - \frac{\langle \Psi_T | j_y(q\hat{x}) | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \right], \quad (5)$$

in the limit of zero external momentum, $\mu = F_M(0; \tau)$.

Electromagnetic current contributions — We study magnetic moments by employing two different PCs for EM currents that are consistent with Weinberg PC for nuclear interactions: the Pisa [12, 51] and Bochum [13] PCs. In the Pisa PC, ratios of momenta to the nucleon mass are counted similar to ratios of momenta to the breakdown scale (Λ_b) so that $\frac{Q}{m} \sim \frac{Q}{\Lambda_b}$. The coordinate-space leading-order (LO) and next-to-leading order (NLO) contributions to the EM currents for the

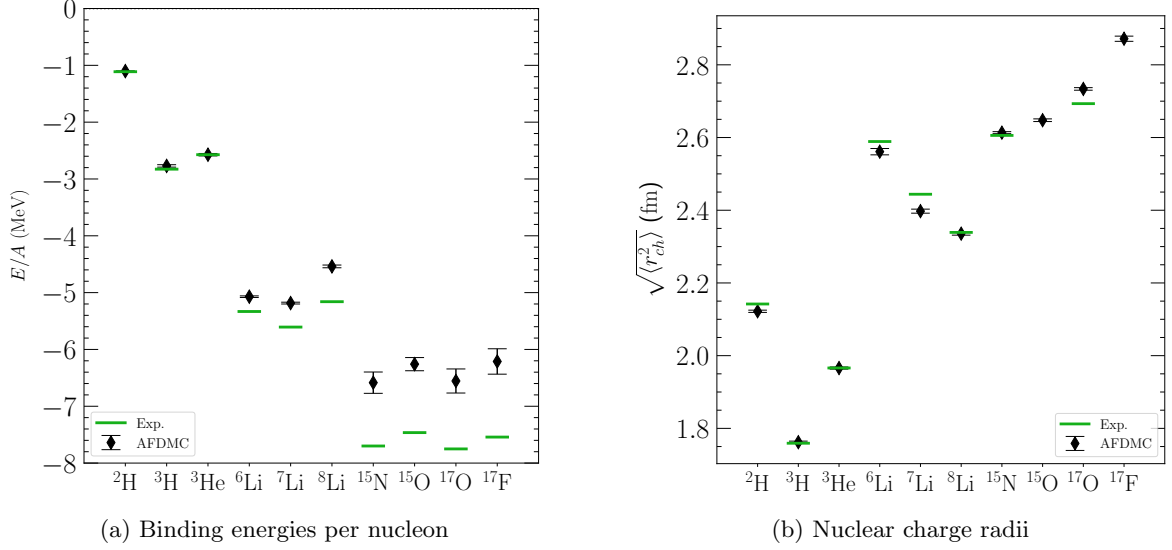


FIG. 2: Binding energies per nucleon (a) and nuclear charge radii (b) estimated using AFDMC (black diamonds) and the experimentally determined values (green lines denoted “Exp.”) for all nuclei studied in this work. Binding energies are calculated from a transient unconstrained path evolution for the $\text{N}^2\text{LO}_{\text{E1}}$ interaction with $R_0 = 1.0$ fm, while the charge radii are estimated using AFDMC using a constrained-path extrapolation. (See [18] for discussion on (un)constrained estimates.) There is no available experimental data for the charge radii of ^{15}O and ^{17}F . The indicated errors represent the standard error arising from the statistical uncertainty of the Monte Carlo estimate, and do not include the theoretical uncertainty arising from the truncation of the chiral expansion.

Pisa PC are given in Eqs. (2.1) and (2.3) of Ref. [51] and in momentum space in Ref. [12]. In contrast, the Bochum PC counts $\frac{Q}{m} \sim \frac{Q^2}{\Lambda_b^2}$. As a consequence, the lowest-order contributions to the electromagnetic vector current appear at NLO in the Bochum PC. The total contribution to the EM current operators at NLO is identical between the Bochum and the Pisa PCs and is equal to the sum of the LO single-nucleon operators and the one-pion-exchange (OPE) NLO contributions of Ref. [51].

At N^2LO , there are several differences between both PCs. First, relativistic corrections proportional to $1/m^2$ appear at N^2LO in the Pisa PC while the same contribution appears at N^4LO in the Bochum PC. Second, the Pisa PC explicitly includes intermediate excitations of the Δ isobar. The corresponding N^2LO operator is proportional to an equivalent operator contribution at N^3LO in a Δ -less PC. The term at N^2LO is assumed to be significantly larger than that at N^3LO which is subsequently omitted in Ref. [51]. Because we employ a Δ -less Hamiltonian, we omit this structure at N^2LO , and restore the saturated operator structure at N^3LO . As a result, Eq. (2.9) of Ref. [51] is modified: first, the term proportional to $\tau_{z,i}$ appears at N^3LO (weighted by the πN LEC d_8), and the operator proportional to $(\boldsymbol{\tau}_i \times \boldsymbol{\tau}_j)_z$ appears at N^3LO but with a different multiplicative factor. We therefore retain the term proportional to $(\boldsymbol{\tau}_i \times \boldsymbol{\tau}_j)_z$ at N^3LO and make the substitution of its prefactor

$$\frac{g_A h_A \mu_{\Delta} m_{\pi}^4}{36\pi m m_{\Delta} f_{\pi}^2} \rightarrow \frac{g_A^4 m_{\pi}^4}{512\pi^3 f_{\pi}^4}$$

We discuss our treatment of the Δ -saturated N^3LO term proportional to $\tau_{i,z}$ in the next section. Finally, we employ the commonly utilized phenomenological Sachs form factors instead of EM currents arising from the chiral expansion of these form factors which is only slowly converging [13, 51, 52]. As a consequence, there is no EM current contribution at N^2LO in the Bochum PC.

Two nucleon, pion-nucleon, and electromagnetic LECs— At N^3LO in both the Bochum and Pisa PCs, there appear three types of low-energy constants (LECs). First, there are NN contact LECs which already appear in the NLO nuclear interaction (C_2 , C_4 , C_5 , and C_7). These LECs are associated with the particular parameterization of the nuclear interaction used in Ref. [8] which includes both local and nonlocal operators in momentum space. Here, instead, the Hamiltonian employed for the imaginary time propagation includes a different set of purely local operators expressed in configuration space [20], described by a different set of NN contact LECs. We can employ the Fierz rearrangement freedom [53] in order to relate the LECs appearing in the EM currents (C_i [54]) to our interaction LECs (C'_i):

$$C_2 = -4(C'_2 + 3C'_4 + C'_7), \quad (6a)$$

$$C_4 = -4(C'_2 - C'_4 - C'_7), \quad (6b)$$

$$C_5 = -C'_5, \quad (6c)$$

$$C_7 = -8C'_7. \quad (6d)$$

The C'_i were determined from fits to NN scattering data [20]. Details on the mapping between the LECs

identified via the Fierz rearrangement are provided in the Supplemental Material [55].

Next, there are contributions to the EM currents from the $N^3\text{LO}$ pion-nucleon and $N^4\text{LO}$ pion-pion Lagrangians which are proportional to the d_i and l_i LECs, respectively. All except three terms proportional to the πN LECs vanish in the $q \rightarrow 0$ limit, and do not contribute to the evaluation of nuclear magnetic moments. The three which contribute are proportional to d_8 , d_9 and d_{21} . Here, we chose to exclude all operators proportional to d_i , as these LECs are of higher order compared to the employed nuclear Hamiltonians.

Finally, there arise two unknown purely EM LECs that must be fit to experimental data. These are called L_1 and L_2 in Ref. [13] or d_1^S and d_1^V in Ref. [51], respectively. We fit these two unknown EM LECs using two prescriptions, hereafter denoted scheme A and scheme B. In scheme A, we have fit the unknown LECs to reproduce the experimental values of the magnetic moments of ^3H and ^3He . For scheme B we have performed a linear least squares fit of the two LECs to the entire data set for the magnetic moments. Using the naming convention of Ref. [51], we find the LEC values for scheme A to be $d_1^S = -0.09596 \pm 0.0018$ and $d_1^V = -0.11085 \pm 0.00099$ with a χ^2 per degree-of-freedom (DOF) of 0.48078. For scheme B we find $d_1^S = -0.03958 \pm 0.0035$ and $d_1^V = -0.06420 \pm 0.0028$ with a χ^2 per DOF of 1.5035.

Results— In Fig. 1, we show AFDMC results for the magnetic moments at each order in the EM current expansion as expressed in Ref. [51], omitting the terms proportional to the d_i LECs as detailed above. For all calculations, we fix the nuclear interaction to be the $N^2\text{LO}_{\text{E1}}$ Hamiltonian and include all contributions to the EM currents up to the specified order. None of these results include theoretical uncertainty estimates. As a simple measure of the convergence, we consider the absolute difference between the estimated and experimental magnetic moments averaged across all nuclei at each order in the EM currents. This difference is 0.18 at LO, 0.13 at NLO, 0.13 at $N^2\text{LO}$, and 0.08 (0.09) at $N^3\text{LO}$ in scheme A (B). Generally, the order-by-order convergence is reasonable for all nuclei and we reproduce experimental data well.

We note that $N^3\text{LO}$ contributions seem to be larger than expected based on lower-order contributions, which was also observed in $A = [2, 3]$ systems in Ref. [51]. To highlight this, in Fig. 3 we show the contribution of each order in the expansion for the EM currents to the total magnetic moments in the Pisa PC. We find a nearly universal large size of the $N^3\text{LO}$ contribution, particularly with respect to the relativistic corrections at $N^2\text{LO}$, with most nuclei displaying $\mathcal{O}(\mu^{\text{NLO}}) \sim \mathcal{O}(\mu^{\text{N}^3\text{LO}})$. This feature is independent of the fitting scheme.

Next, we study the systematic uncertainty of the magnetic moments arising from the truncation of the chiral expansion in both PCs for ^6Li , ^7Li , ^8Li , and ^{15}N . For this, we perform AFDMC calculations of the magnetic

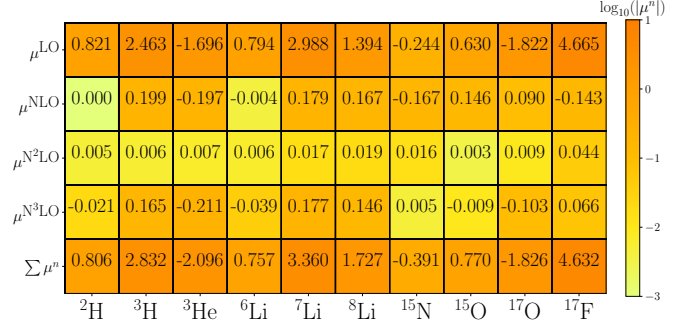


FIG. 3: Contributions to the magnetic moment at each order in the chiral expansion of the nuclear EM current for each nucleus considered. We show results for the Pisa PC [51] but the sum of the LO and NLO results is equivalent to the NLO contribution in the Bochum PC. $N^2\text{LO}$ only includes the $1/m^2$ relativistic correction while the $N^3\text{LO}$ results are obtained by using the LECs fit in scheme B. The number appearing in each cell represents the MC estimate of the contribution, while the color of the cell represents the logarithm of the magnitude of the contribution to guide the eye.

moments order-by-order in the chiral expansion for *both* the nuclear interaction Hamiltonian and the electromagnetic current operators, i.e., the Hamiltonian now also varies from order to order. We use the simple prescription introduced in Ref. [15] and for the Pisa PC, the theoretical uncertainty at each order is found using the following recursive expressions:

$$\delta(\mu_{\text{LO}}^{\text{LO}}) = Q|\mu_{\text{LO}}^{\text{LO}}|, \quad (7)$$

$$\delta(\mu_{\text{LO}}^{\text{NLO}}) = \max\left\{Q|\mu_{\text{LO}}^{\text{NLO}} - \mu_{\text{LO}}^{\text{LO}}|, Q\delta(\mu_{\text{LO}}^{\text{LO}})\right\}, \quad (8)$$

$$\delta(\mu_{\text{NLO}}^{\text{N}^2\text{LO}}) = \max\left\{Q|\mu_{\text{NLO}}^{\text{N}^2\text{LO}} - \mu_{\text{NLO}}^{\text{NLO}}|, Q\delta(\mu_{\text{NLO}}^{\text{NLO}})\right\}, \quad (9)$$

$$\delta(\mu_{\text{N}^2\text{LO}}^{\text{N}^3\text{LO}}) = \max\left\{Q|\mu_{\text{N}^2\text{LO}}^{\text{N}^3\text{LO}} - \mu_{\text{N}^2\text{LO}}^{\text{N}^2\text{LO}}|, Q\delta(\mu_{\text{N}^2\text{LO}}^{\text{N}^2\text{LO}})\right\}, \quad (10)$$

where we take $Q = m_\pi/\Lambda$, and $\Lambda = 500$ MeV corresponding to our cutoff choice of $R_0 = 1.0$ fm [20]. In the above expressions superscripts denote the order in the expansion of the currents, and subscripts denote the order in the nuclear interaction Hamiltonian. In estimating the uncertainty, we systematically increase the order of the expansion by powers of (Q/Λ) , but because of the differences in counting powers of $1/m$ in the Pisa PC, some care is needed. At LO, the magnetic moment is calculated using both the Hamiltonian and the EM currents at LO in the Pisa PC. Because the nuclear interactions are suppressed by $(Q/\Lambda)^2$ at NLO relative to LO but only by $(Q/\Lambda)^1$ in the Pisa PC, next we calculate the result matching LO interactions with the NLO currents. We include this step in our uncertainty estimate as $\delta\mu_{\text{LO}}^{\text{NLO}}$, and refer to this combination as LO* in Fig. 4. At NLO, the

magnetic moments are calculated with the NLO Hamiltonian and the N²LO currents, while at N²LO they are calculated with the N²LO Hamiltonian and the N³LO currents.

Similarly, we estimate the truncation uncertainty in the Bochum PC for the EM currents, which is more consistent with the employed interaction Hamiltonian. Because the LO and N²LO contributions to the magnetic moments vanish in this PC, effectively only the NLO contribution is employed. Then, order-by-order changes in the magnetic moments arise from the nuclear interactions and the theoretical uncertainty estimate is given by

$$\delta(\mu_{\text{NLO}}^{\text{NLO}}) = Q|\mu_{\text{NLO}}^{\text{NLO}}|, \quad (11)$$

$$\delta(\mu_{\text{N}^2\text{LO}}^{\text{NLO}}) = \max\left\{Q|\mu_{\text{N}^2\text{LO}}^{\text{NLO}} - \mu_{\text{NLO}}^{\text{NLO}}|, Q\delta(\mu_{\text{NLO}}^{\text{NLO}})\right\}. \quad (12)$$

The ratio of the QMC estimate of the magnetic moment to the experimentally determined value for the selected nuclei is shown in Fig. 4 for both the Pisa and Bochum PCs. For all nuclei, we observe a systematic behavior within the Bochum PC. However, for ¹⁵N, the calculations seem to predict a magnetic moment 40% above the experimental value. For the Pisa PC, we observe a (scheme dependent) systematic convergence for ⁶Li, ⁷Li and ⁸Li. In contrast, for ¹⁵N the order-by-order results are less systematic. We also observe that for both fitting schemes, the N²LO estimate lies outside the estimated error band for NLO for ⁶Li, ⁷Li and ⁸Li.

This highlights that consistent PCs for interactions and currents need to be employed. It might also point to a systematic underestimate of the characteristic momentum scale Q for these nuclei, and a more detailed investigation into the one- and two-nucleon momentum distributions in these nuclei is warranted. The choice of fitting scheme for the N³LO EM LECs also produces some variance in the estimated values of the magnetic moments but this variance is of the same order as the theoretical uncertainty at NLO.

Discussion and conclusions— We performed AFDMC calculations of the magnetic moments of several light nuclei with nuclear interactions and EM currents derived from chiral EFT and found agreement with experiment. These results are supported by comparing supplementary AFDMC calculations of the ground-state binding energies and charge-radii to experiment as well. Additionally, we explored the two prevalent PCs for the chiral EM currents and the order-by-order convergence of the magnetic moments.

While our accurate magnetic moment results are valuable in verifying the different components of these *ab initio* calculations, our uncertainty analysis indicates that the consistency between employed nuclear interactions and EM currents is crucial: Our results for the consistent PC shows a more natural order-by-order convergence pattern. This is also supported by the prominence of the N³LO EM contributions to the calculated magnetic

moments, and more work is necessary to study the convergence up to N³LO in a consistent PC. Furthermore, ensuring that the corresponding continuity equation is fulfilled is crucial [13]. Future work to derive consistent currents for the interactions used in AFDMC is important. Given the significance of uncertainty quantification for this task, it is key to properly estimate momentum scales that are being used. Employing uncertainty quantification tools based on Gaussian Processes [16] might be beneficial for this task.

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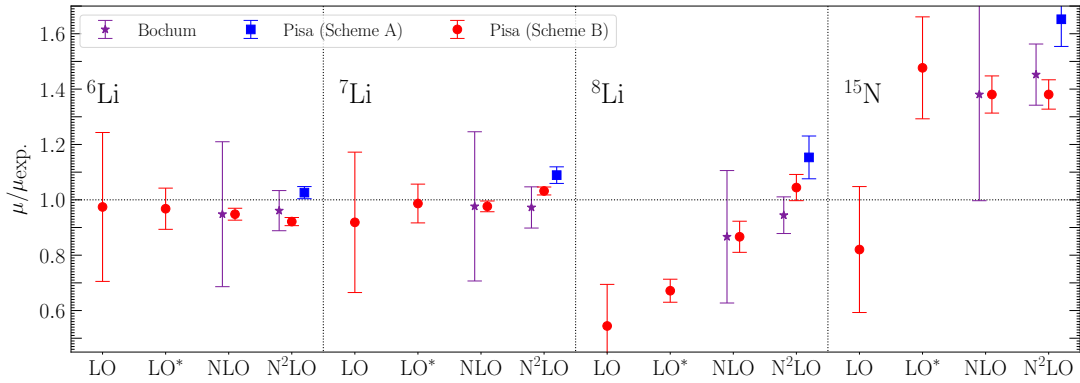


FIG. 4: Order-by-order contributions to the magnetic moment relative to the experimental value for the indicated nuclei. The abscissa labels indicate the order in the chiral expansion for the nuclear interaction Hamiltonian. The estimates labeled LO* are calculated using the LO nuclear interactions and the NLO EM current operators.

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