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Quantum Monte Carlo calculations of (electro)magnetic structure in light nuclei

Garrett King

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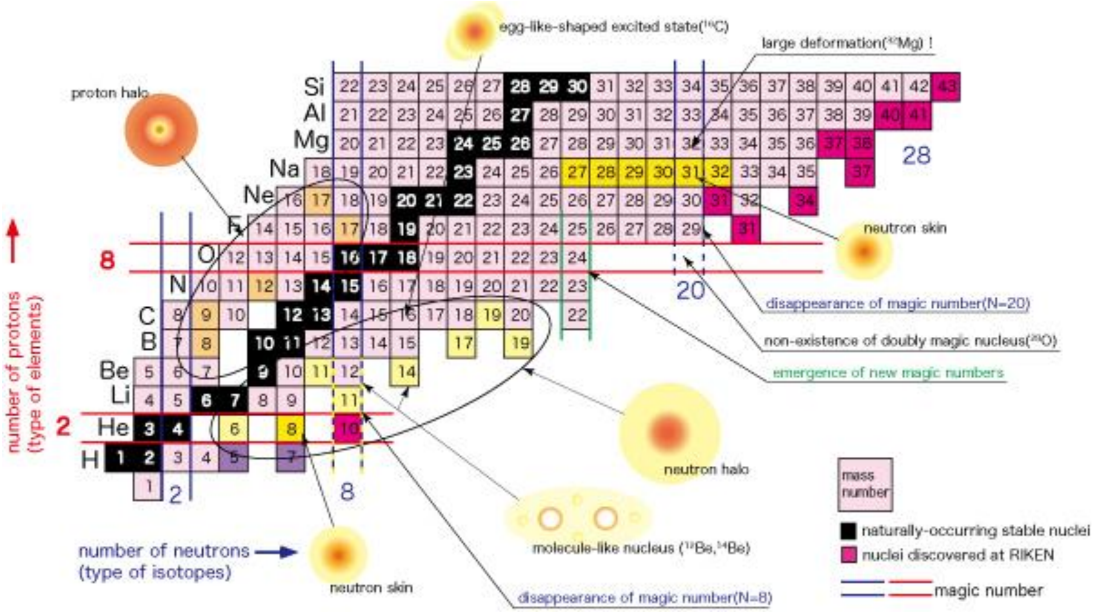
Motivation



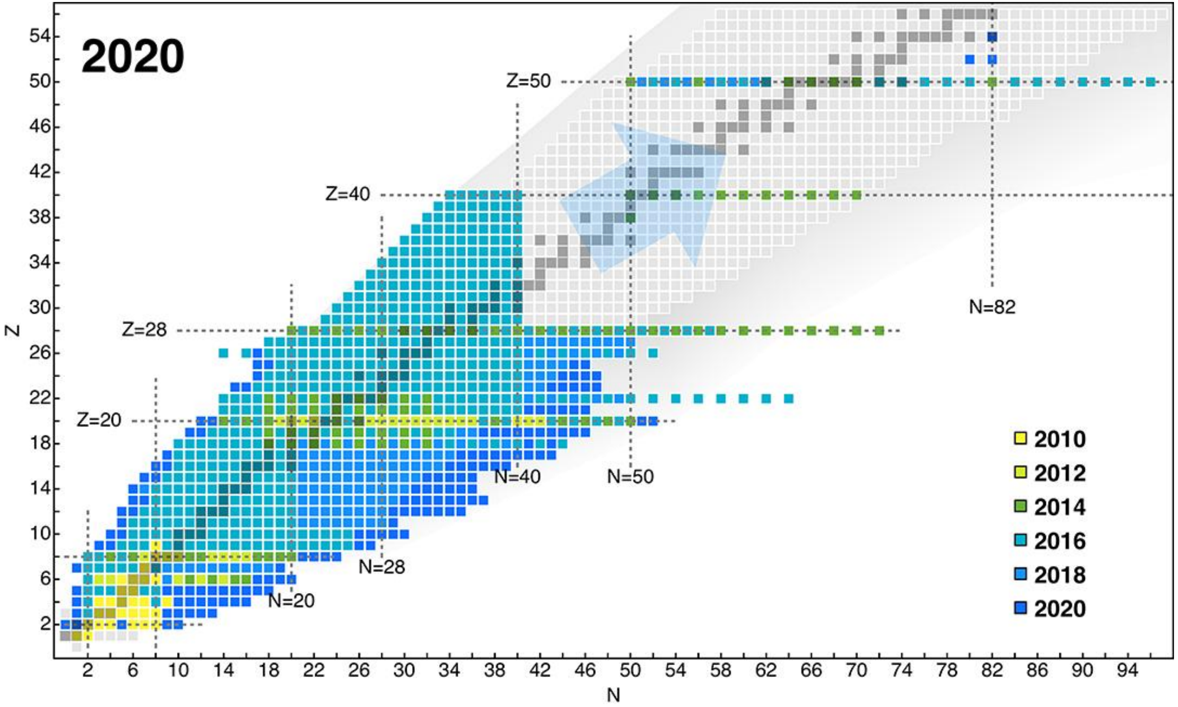
https://www.nishina.riken.jp/research/nucleus_e.html

RIB facilities are probing the limits of nuclear existence

Combined with electron probes, can answer fundamental questions:

- How does structure change near the limit of stability?
- What role does clustering play in exotic systems?
- What is the nature of the nuclear force?

Motivation



H. Hergert, J. Front. Phys. 8 (2020)

The reach of many-body approaches has also expanded greatly in the last decade

We can now study nuclei that intersect with the frontiers probed by experiment

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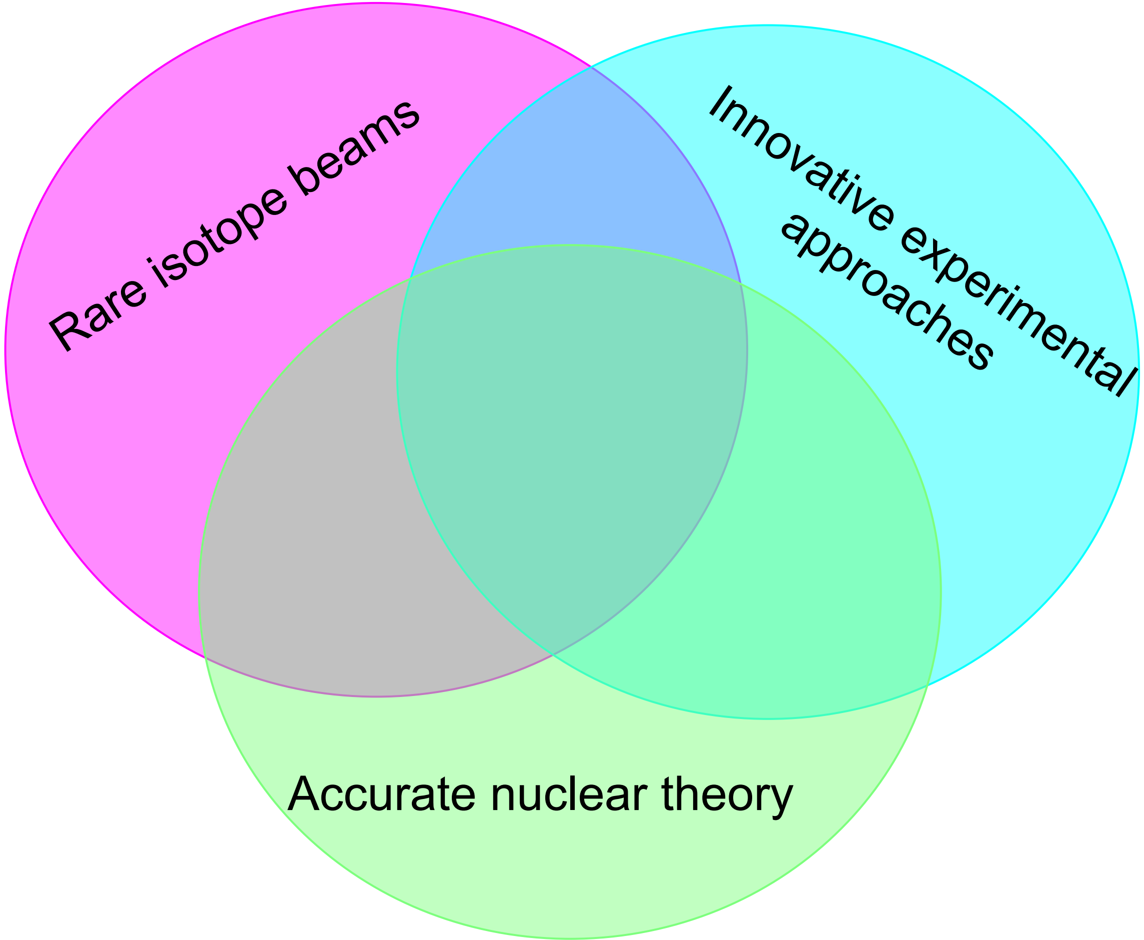
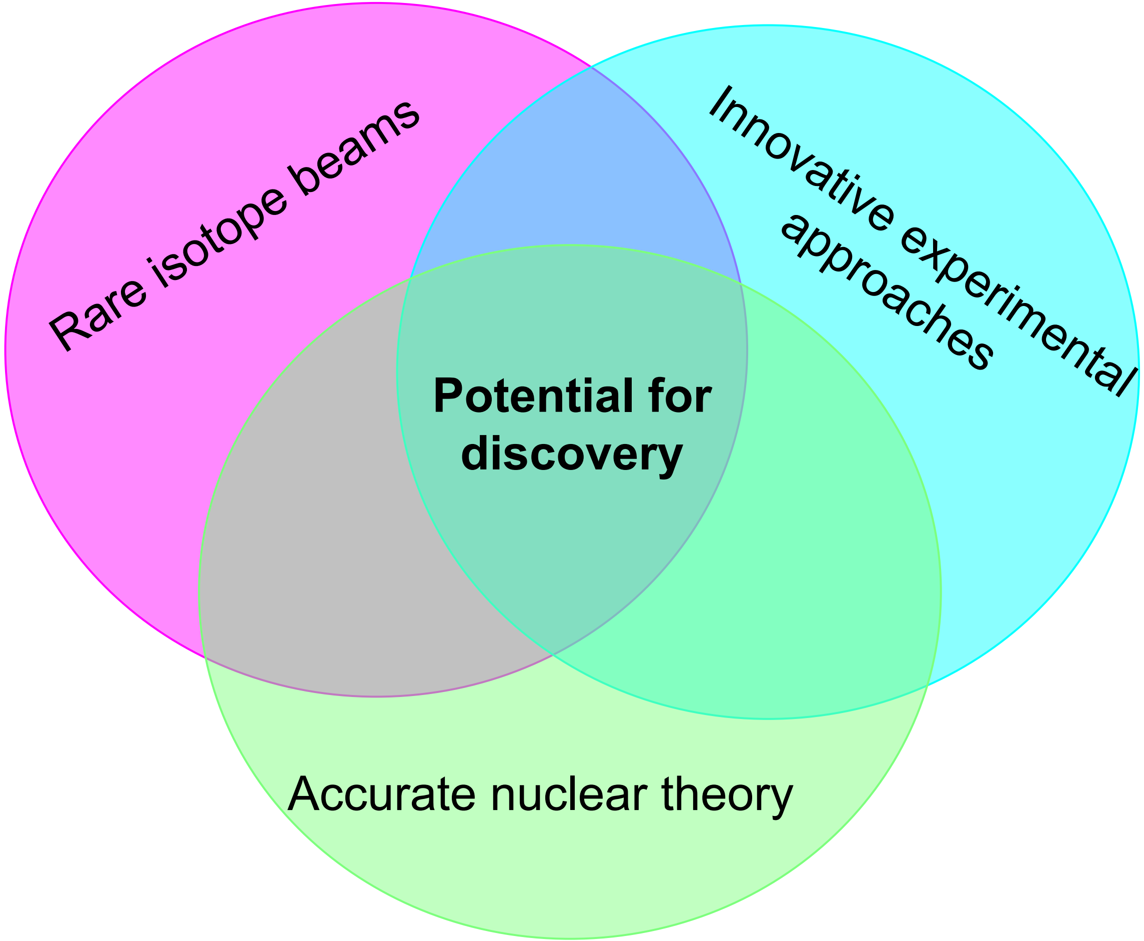
Motivation



Rare isotope beams
Innovative experimental approaches
Accurate nuclear theory

Motivation



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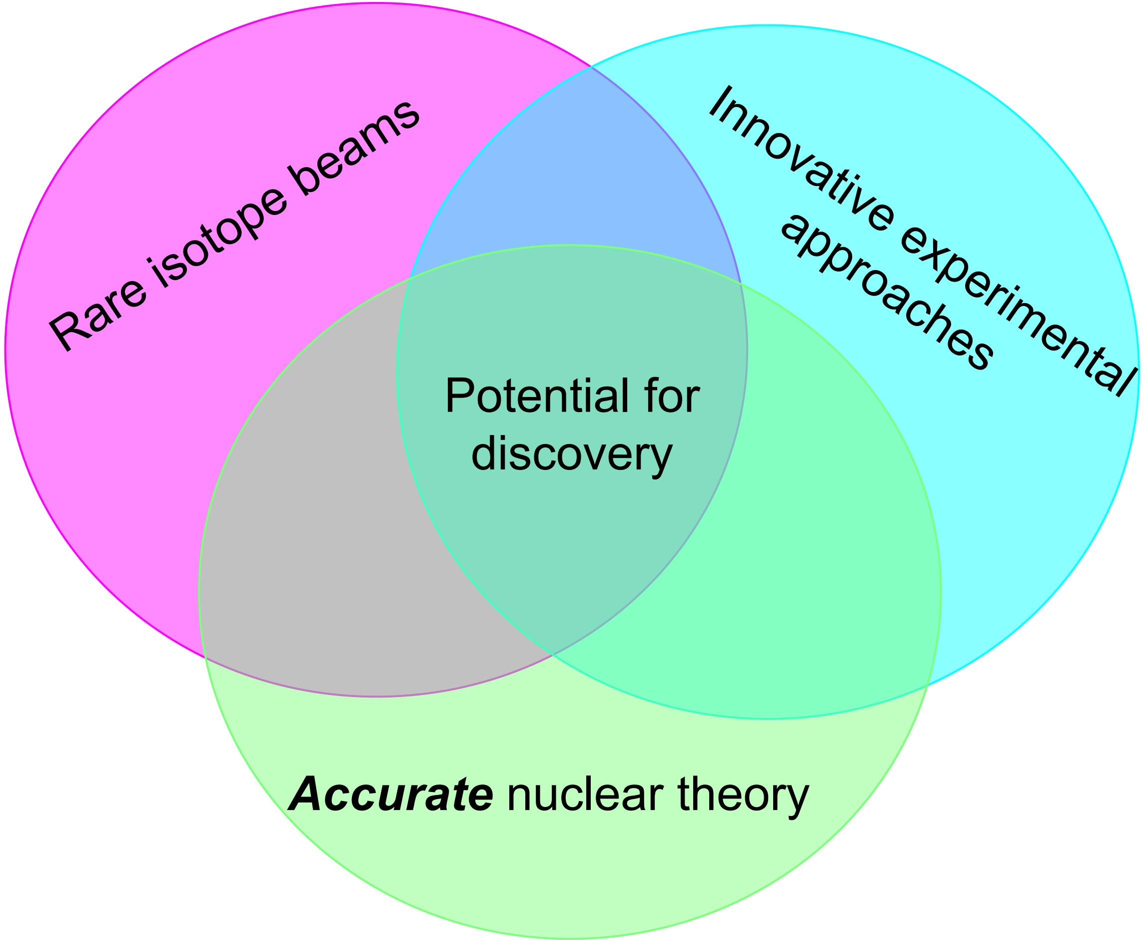
Motivation

Have a great opportunity for experimental and theory communities to identify interesting cases

In order to learn from experimental advances, we need ***accurate*** theory



Outline

01

Microscopic description of nuclei

- Many-body problem
- Quantum Monte Carlo
- The Norfolk Model

02

Electron scattering

- Theory
- Connection to QMC

03

Results for light nuclei

- Magnetic moments
- Form factors
- Radii

04

Outlook and Conclusion

- Going beyond light nuclei

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Microscopic description of nuclei

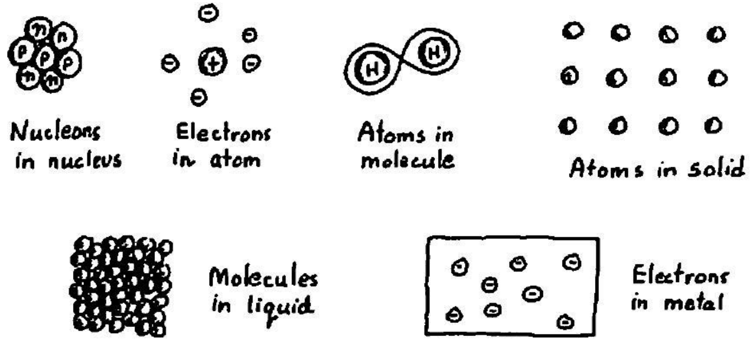
The quantum many-body problem

Modeling physical phenomena in a system with many bodies interacting amongst themselves

$$H = \sum_i T_i + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

Interaction generates *correlations* in solution of the Schrödinger equation

$$H|\Psi\rangle = E|\Psi\rangle$$



Mattuck, "A Guide to Feynman Diagrams in the Many-Body Problem", McGraw-Hill

The quantum many-body problem

Wave function of ***A* nucleons** containing information about ***coordinates*, *spins*, *and isospins***

$$\Psi(r_1, r_2, \ldots, r_A; s_1, s_2, \ldots, s_A; t_1, t_2, \ldots, t_A)$$

$$\dim(\Psi) = 3A \times 2^A \times \frac{A!}{N!Z!}$$

Turn to numerical approaches; In this talk, **Quantum Monte Carlo** which can address **A≲14**

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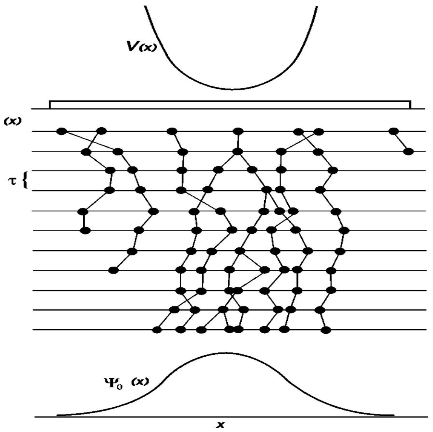
Quantum Monte Carlo

Solving the many-body problem using random sampling to compute integrals

Variational MC wave function $|\Psi_T\rangle = \mathcal{F}|\Phi\rangle$ contains model wave function and many-body correlations optimized by minimizing:



$$E_V = \min\left\{\frac{\langle\Psi_T|H|\Psi_T\rangle}{\langle\Psi_T|\Psi_T\rangle}\right\} \geq E_0$$

Green's function MC improves by ***removing excited state contamination and gives the exact ground state***

$$\lim_{\tau\to\infty} e^{-(H-E_0)\tau}\Psi_V = \lim_{\tau\to\infty} e^{-(H-E_0)\tau}\left(c_0\psi_0 + \sum_{i=1}^{N} c_i\psi_i\right) \to c_0\psi_0$$

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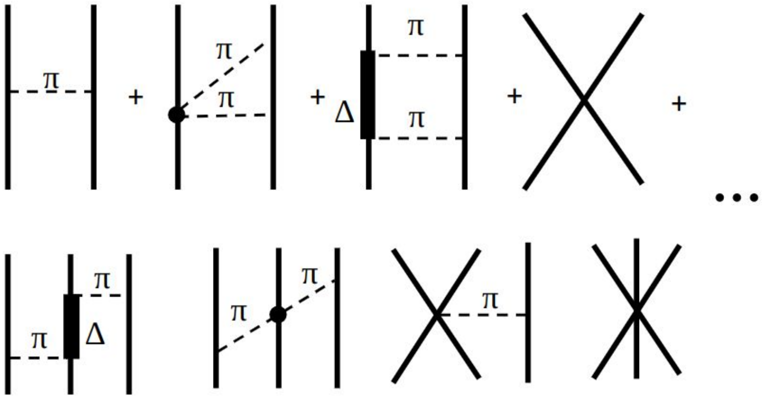
Foulkes et al. Rev. Mod. Phys. 73, 33 (2001)

Chiral Effective Field Theory



Procedure to obtain NN interaction rooted in the underlying symmetry of Quantum Chromodynamics

Separation of scales: Nucleon momentum $Q \sim m_\pi \sim m_N - m_\Delta$ vs. heavier mesons at the scale $\Lambda \sim 1$ GeV

Heavy degrees of freedom integrated out

Low-energy constants (LECs) subsume the underlying QCD

Weinberg, van Kolck, Ordóñez, Epelbaum, Hammer, Meißner, Entem, Machleidt, …

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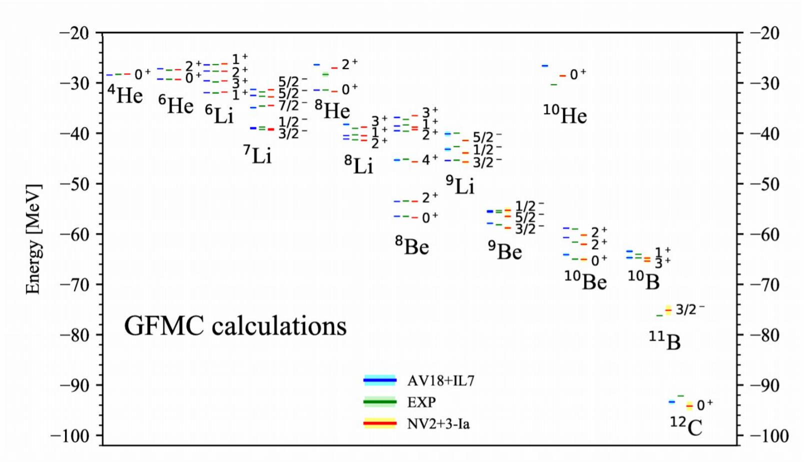
The Norfolk (NV2+3) interaction

$$H = \sum_i K_i + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$



Derived in χEFT with pion, nucleon, and delta degrees of freedom by **Piarulli et al. [PRL 120, 052503 (2018)]**

NV2 contains 26 unknown LECs in contacts, two more from the NV3

Eight model classes arrived at from different procedures to constrains the unknown LECs

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Electroweak charge and current operators

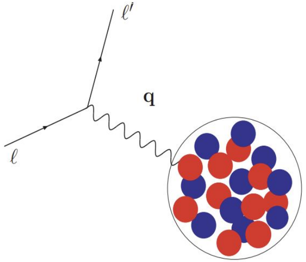
Need electromagnetic and weak current operators to study decays

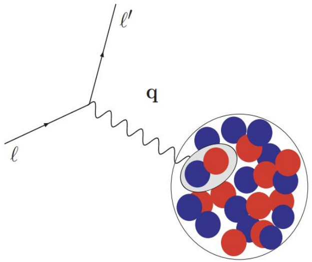
Schematically:

$$\rho = \sum_{i=1}^{A} \rho_i + \sum_{i<j} \rho_{ij} + \ldots$$

$$\mathbf{j} = \sum_{i=1}^{A} \mathbf{j}_i + \sum_{i<j} \mathbf{j}_{ij} + \ldots$$

External field interacts with single nucleons and correlated pairs of nucleons

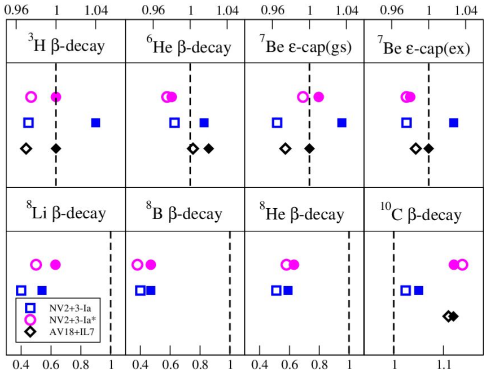




Pastore et al. PRC 80, 034004 (2009), Pastore et al. PRC 84, 024001 (2011), Piarulli et al. PRC 87, 014006 (2013), Schiavilla et al. PRC 99, 034005 (2019)

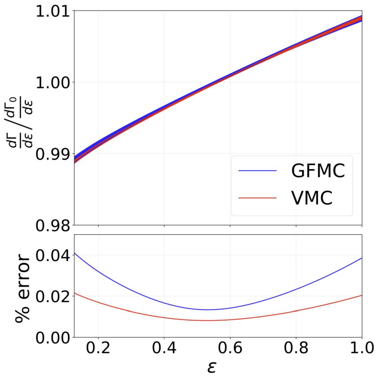
Low-to-moderate energy electroweak structure

Decay rates



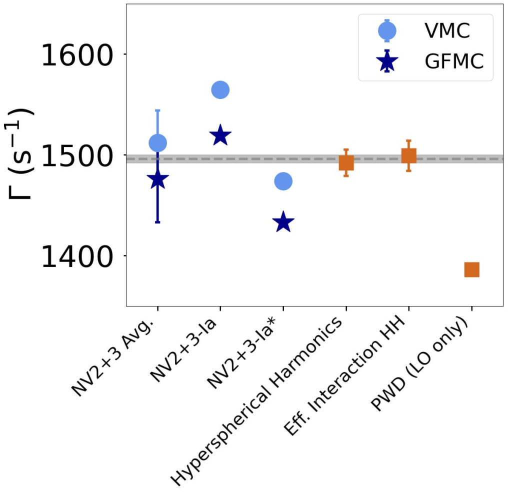
King et al. PRC 102, 025501 (2020)

Decay spectra



King et al. PRC 107, 015503 (2022)

Captures



King et al. PRC 105, L0425 (2022)

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Electron scattering

Cross section

$$\frac{d\sigma}{d\Omega} = 4\pi\sigma_M f_{\mathrm{rec}}^{-1} \left[\frac{Q^4}{q^4} F_L^2(q) + \left(\frac{Q^2}{2q^2} + \tan^2\theta_e/2 \right) F_T^2(q) \right]$$

In elastic scattering:

$$F_T^2(q) = F_M^2(q) = \frac{1}{2J_i+1} \sum_{L=1}^{\infty} |\langle J_f || M_L(q) || J_i \rangle|^2$$

$$F_L^2(q) = \frac{1}{2J_i+1} \sum_{L=0}^{\infty} |\langle J_f || C_L(q) || J_i \rangle|^2$$

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Cross section

$$\frac{d\sigma}{d\Omega} = 4\pi\sigma_M f_{\rm rec}^{-1} \left[\frac{Q^4}{q^4} F_L^2(q) + \left(\frac{Q^2}{2q^2} + \tan^2\theta_e/2\right) F_T^2(q)\right]$$

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Sensitive to single particle structure

$$F_L^2(q) = \frac{1}{2J_i+1}\sum_{L=0}^{\infty} |\langle J_f || C_L(q) || J_i\rangle|^2$$

Sensitive to density, collectivity

Cross section

$$\frac{d\sigma}{d\Omega} = 4\pi\sigma_M f_{\text{rec}}^{-1} \left[\frac{Q^4}{q^4} F_L^2(q) + \left(\frac{Q^2}{2q^2} + \tan^2\theta_e/2\right) F_T^2(q)\right]$$

In elastic scattering:

$$F_T^2(q) = F_M^2(q) = \frac{1}{2J_i+1} \sum_{L=1}^{\infty} \left|\langle J_f || M_L(q) || J_i \rangle\right|^2 \qquad F_L^2(q) = \frac{1}{2J_i+1} \sum_{L=0}^{\infty} \left|\langle J_f || C_L(q) || J_i \rangle\right|^2$$

QMC is used to compute reduced multipoles

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Computation of reduced multipoles

Reduced multipoles are defined by **[Carlson and Schiavilla RMP 70 (1998)]**:

$$\langle J_f M | \rho^\dagger(q) | J_i M \rangle = (-1)^{J_i - M} \sum_L \sqrt{4\pi} (-i)^L P_L(\cos\theta) c^M_{J_f J_i L} C_L(q) \,,$$

$$\langle J_f M | \hat{\mathbf{e}}^*_\lambda \cdot \mathbf{j}^\dagger(q) | J_i M \rangle = (-1)^{J_i - M + 1} \sum_{L \geq 1} \sqrt{8\pi^2} \frac{(-i)^L}{\sqrt{2L+1}} Y^*_{LM}(\theta, \phi) c^M_{J_f J_i L} M_L(q)$$

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$$\langle J_f M|\hat{e}^*_\lambda \cdot \mathbf{j}^\dagger(q)|J_i M\rangle = (-1)^{J_i-M+1}\sum_{L\geq 1} \sqrt{8\pi^2}\frac{(-i)^L}{\sqrt{2L+1}} Y^*_{LM}(\theta,\phi) c^M_{J_f J_i L} M_L(q)$$

Calculable with QMC techniques

Invert system of equations with as many independent choices of q as allowed multipolarities

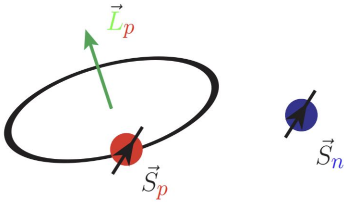
Results in light nuclei

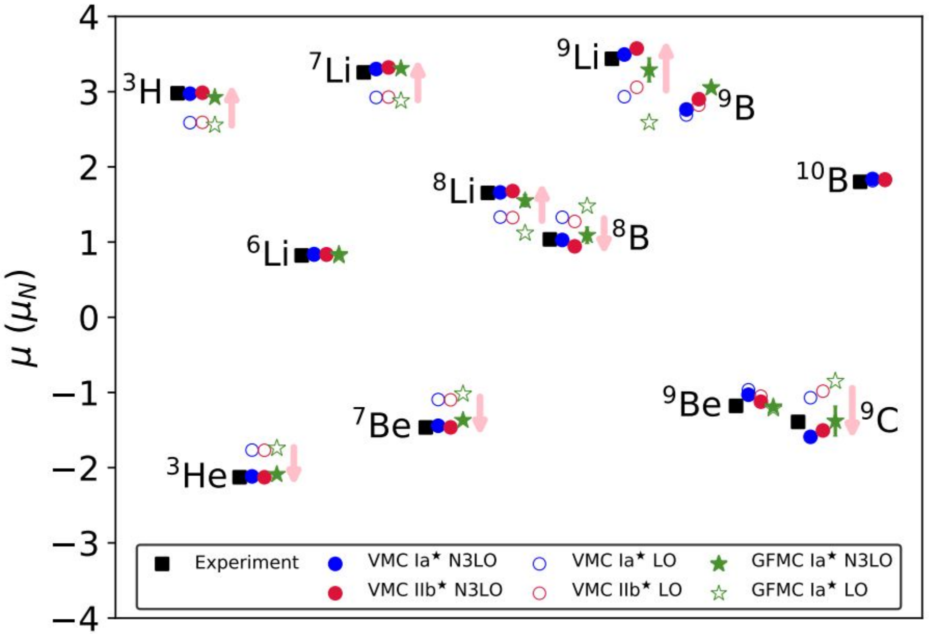
Chambers-Wall et al., arXiv:2407.03487 (*Accepted PRL*),
Chambers-Wall et al., arXiv:2407.04744 (*Accepted PRC*)

Magnetic moments

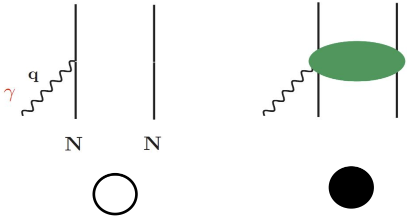
One-body picture:

$$\mu^{LO} = \sum_i (L_{i,z} + g_p S_{i,z}) \frac{1+\tau_{3,i}}{2} + g_n S_{i,z} \frac{1-\tau_{3,i}}{2}$$





Two-body currents can play a large role (up to ~33%) in describing magnetic dipole moments



Two-body dynamics: VMC magnetic densities

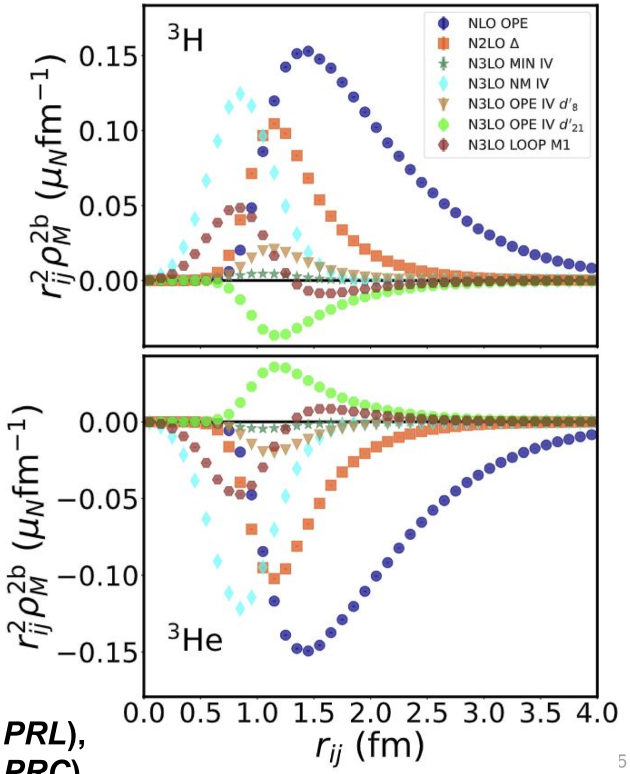
QMC allows one access to the two-body dynamics involved in process

Ex: $$\mu^{2b} = \int dr_{ij} 4\pi r_{ij}^2 \rho_M^{2b}(r_{ij})$$

Understand the importance of contributions to matrix elements, multipoles

Not limited to zero momentum transfer

NV2+3-IIb*



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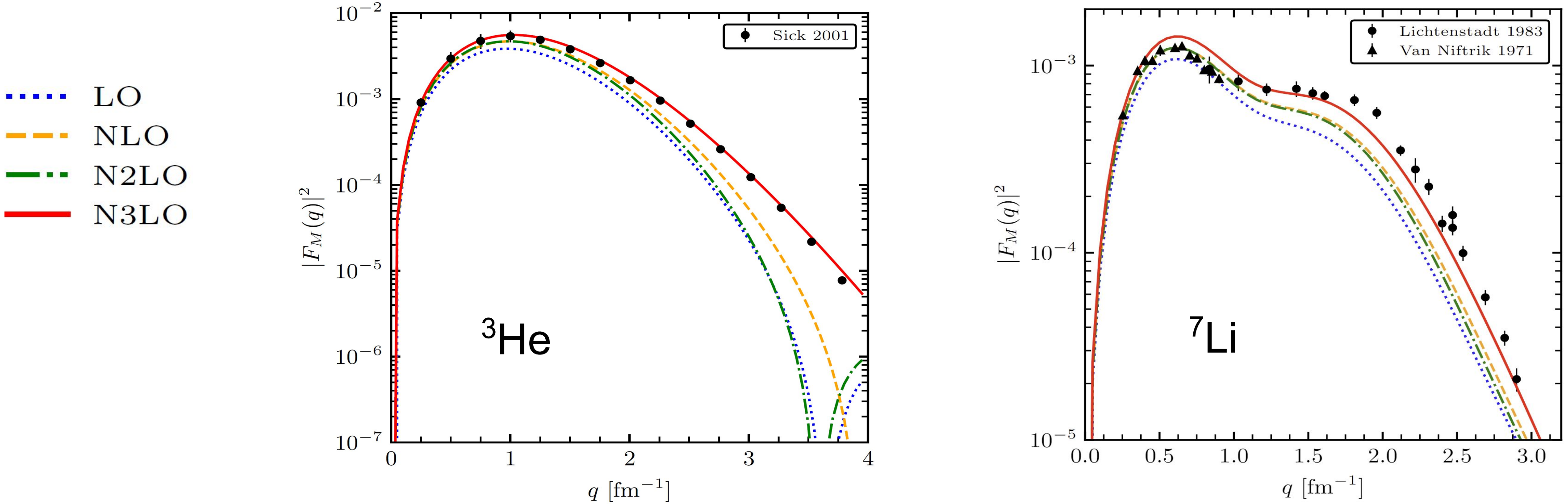
Chambers-Wall et al., arXiv:2407.03487 (*Accepted PRL*), Chambers-Wall et al., arXiv:2407.04744 (*Accepted PRC*)

VMC magnetic form factors

NV2+3-IIb*



Two-body effects to N3LO needed to describe data up to q ~ 600 MeV

Minimal model dependence in total form factor for 3 A 10

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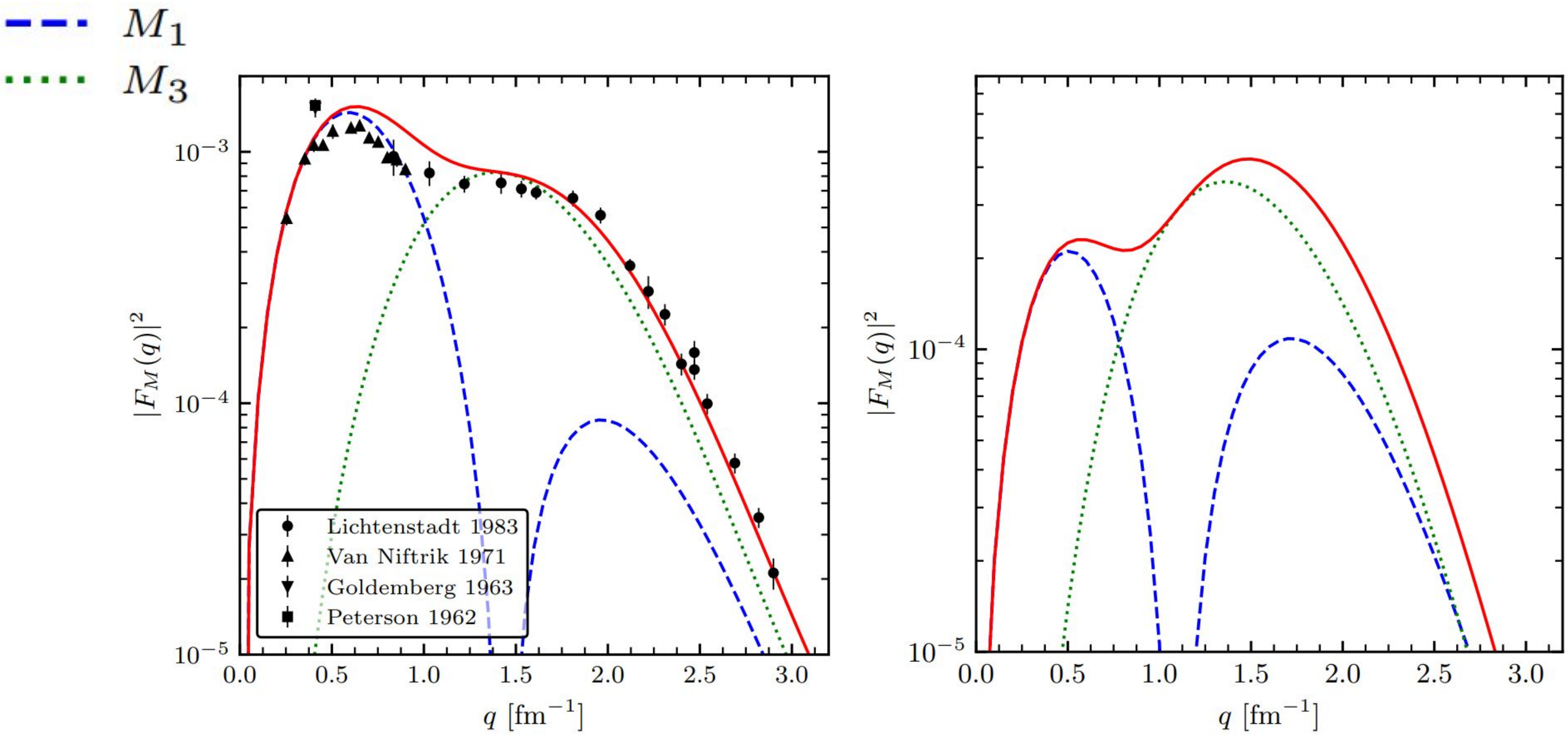
Chambers-Wall et al., arXiv:2407.03487 (*Accepted PRL*),
Chambers-Wall et al., arXiv:2407.04744 (*Accepted PRC*)

Magnetic form factors for mirror nuclei



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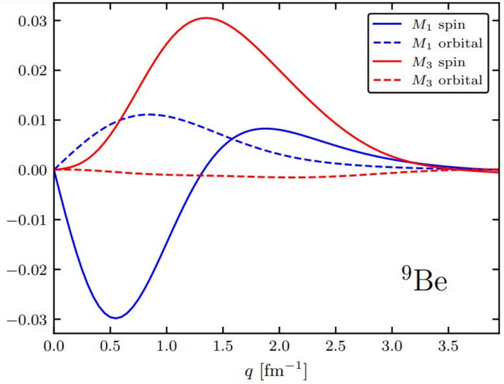
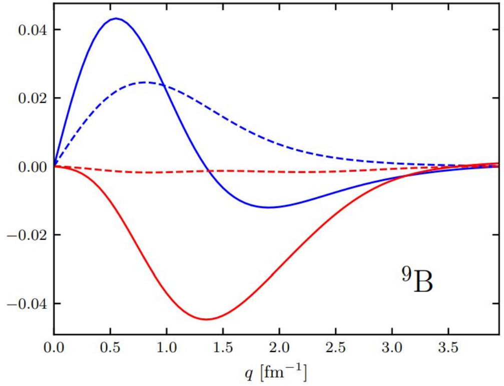
Chambers-Wall et al., arXiv:2407.03487 (*Accepted PRL*),
Chambers-Wall et al., arXiv:2407.04744 (*Accepted PRC*)

Spin-orbit interference in M1





Orbital contribution generates positive contribution to M1

Spin can be positive or negative, depending on single particle structure

Minimal contribution orbital contribution to M3

Destructive interference between spin and orbit present in nuclei with smaller M1 peak than M3

Chambers-Wall et al., arXiv:2407.03487 (*Accepted PRL*), Chambers-Wall et al., arXiv:2407.04744 (*Accepted PRC*)

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Magnetic radii

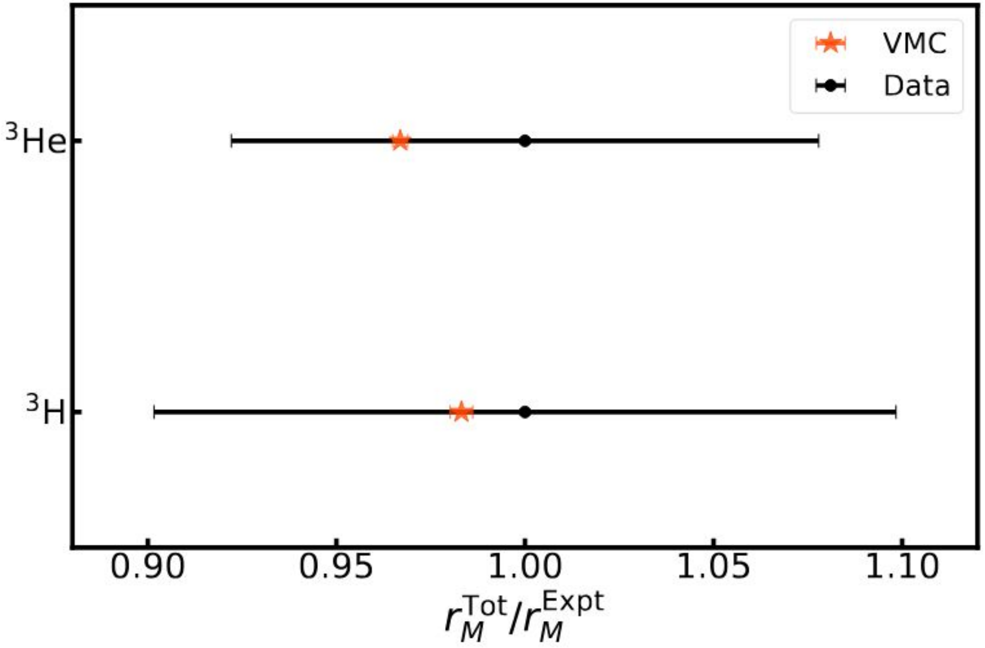
Extracted from low-momentum transfer behavior of form factor

Accounts for two-body correlations, finite size/nucleon level corrections via form factors

Limited data for magnetic radii, but good agreement where possible

Uncertainty is statistical, form factor dependence may also be important

NV2+3-IIb*



$$-i\frac{2m}{q\mu}\langle JJ|\mathrm{j}_y(q\hat{\mathbf{x}})|JJ\rangle \approx 1-\frac{1}{6}r_M^2q^2+\mathcal{O}(q^4)$$

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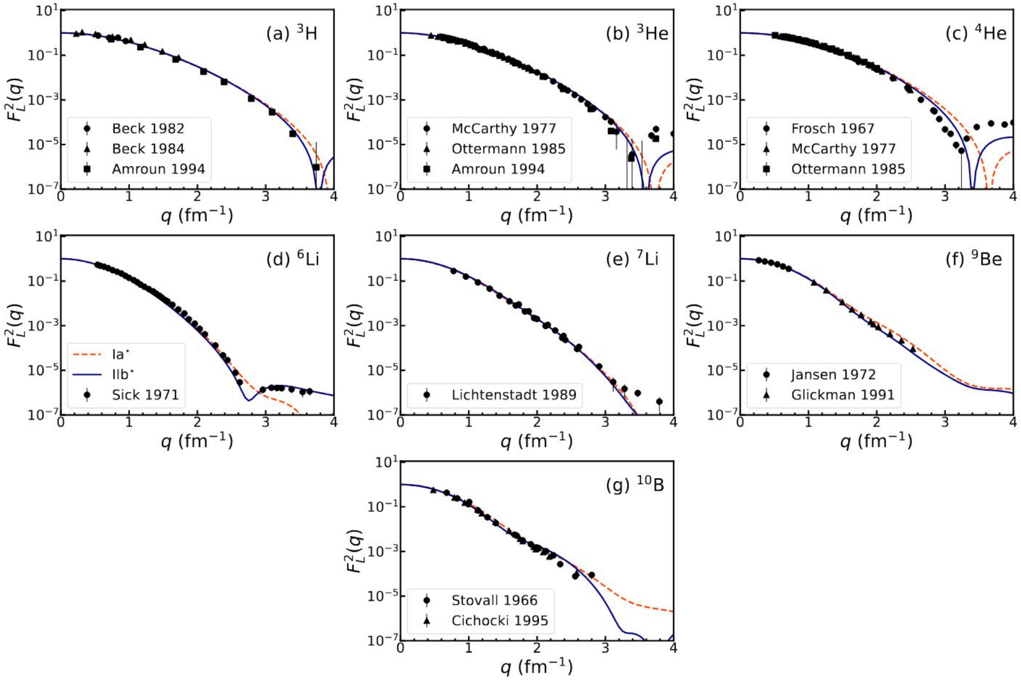
King et al., *in preparation*

Longitudinal form factors



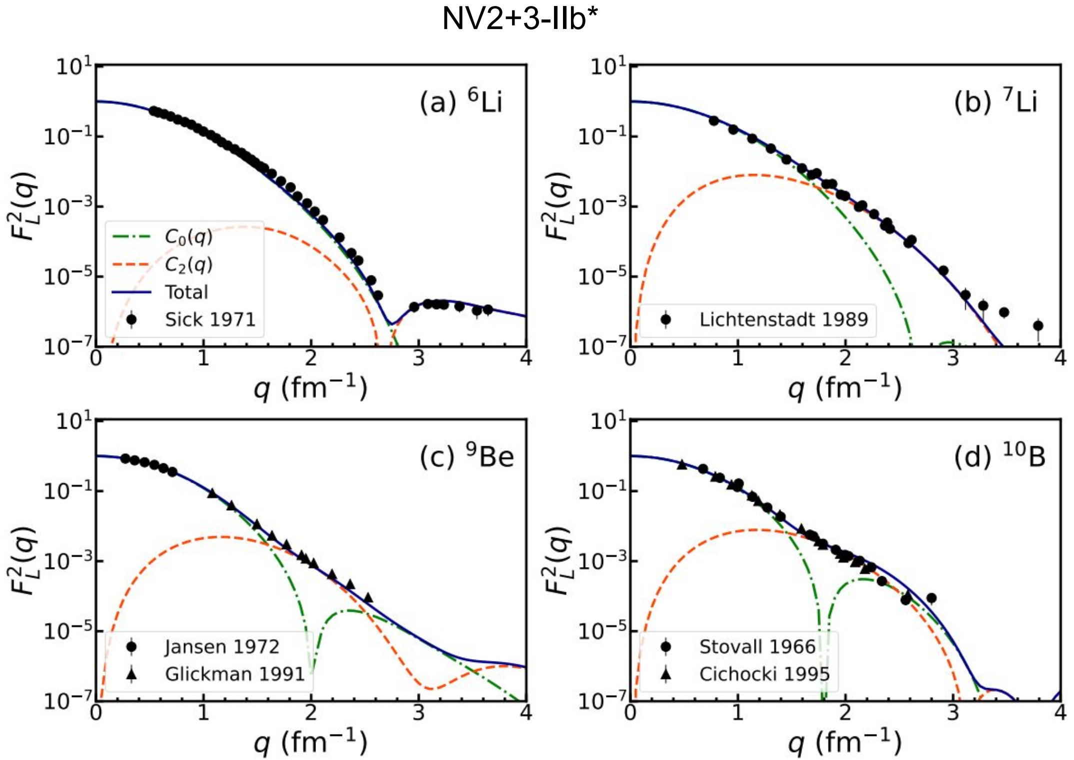
Calculation of longitudinal form factors similarly possible

Sensitive to nuclear model around the breakdown scale (q ~ 2.5 fm^{-1})

Excellent agreement at low energies

King et al., arXiv:2408.16909

Higher-order multipoles



C2 necessary to explain the data at moderate momentum transfer

C4, C6 have small enough effect in ^{10}B that we can neglect them

Sensitive to the density and shape of the system

Reproducing distinct features in charge densities could be test of nuclear models

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King et al., arXiv:2408.16909

Charge radii

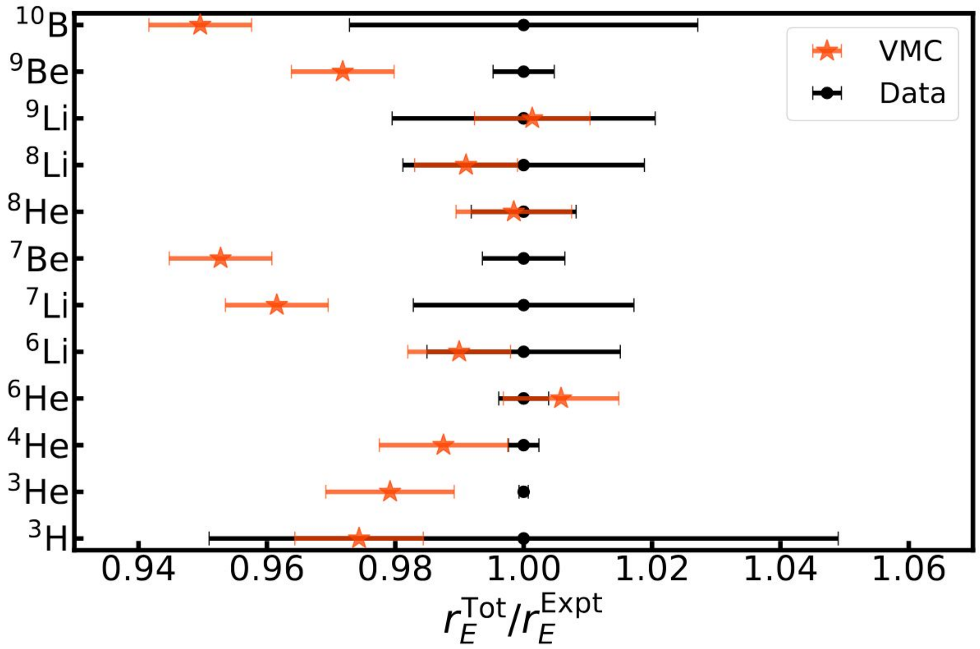
Agreement of ~5% or better across the board

Model successful for He and Li isotopes, less so for Be

Same framework could be used for radioisotopes in the future

Uncertainty is statistical, form factor dependence may also be important

NV2+3-IIb*



$$\frac{1}{Z}\langle JJ|\rho(q\hat{\mathbf{z}})|JJ\rangle \approx 1 - \frac{1}{6}r_E^2 q^2 + \mathcal{O}(q^4)$$

King et al., *in preparation*

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Outlook: Beyond light nuclei

Auxiliary Field Diffusion Monte Carlo

Use the single particle basis: $\langle S|\Psi\rangle \propto \xi_{\alpha_1}(s_1)\,\xi_{\alpha_2}(s_2)\ldots\,\xi_{\alpha_A}(s_A)$

Advantage of a polynomial scaling with A

Technically more complicated to operate on wave function

Cost is a simpler correlation structure in the wave function

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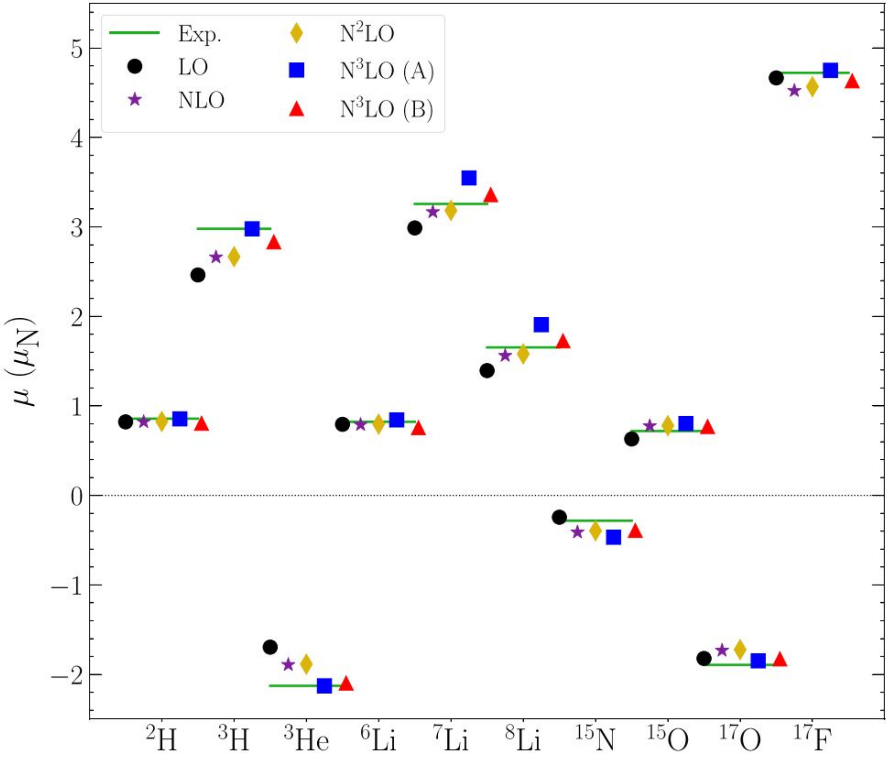
Lonardoni *et al.*, PRC 97, 044318 (2018)

Recent progress in AFDMC for EM properties

Applied to the study of low momentum transfer observable – magnetic moments

Future work to push elastic electron scattering to A ≲ 20



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Martin *et al.*, PRC 108, L031304 (2023)

Conclusions

Accurate many-body calculations plus χEFT is a powerful way to understand the impact of the nuclear dynamics on electromagnetic structure

Two-body physics plays an important role in describing experimental data

Framework developed for QMC calculations of form factors, cross sections

Outlook: Push VMC and GFMC to study A=11-14 nuclei, incorporate the framework in AFDMC for heavier systems, collaboration with experimentalists and other many-body theorists in the future

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JLab+ODU: Gnech, Schiavilla

Funding from DOE/NNSA Stewardship Science Graduate Fellowship

SSGF
STEWARDSHIP SCIENCE GRADUATE FELLOWSHIP

Additional slides

Variational Monte Carlo

Slater determinant of nucleons in s- and p-shell coupled to the appropriate quantum numbers

Pair correlation operator encoding appropriate cluster structure

Two- and three-body correlation operator to reflect impact of nuclear interaction at short distances

Optimize when you minimize:

$$E_V = \frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} \geq E_0$$

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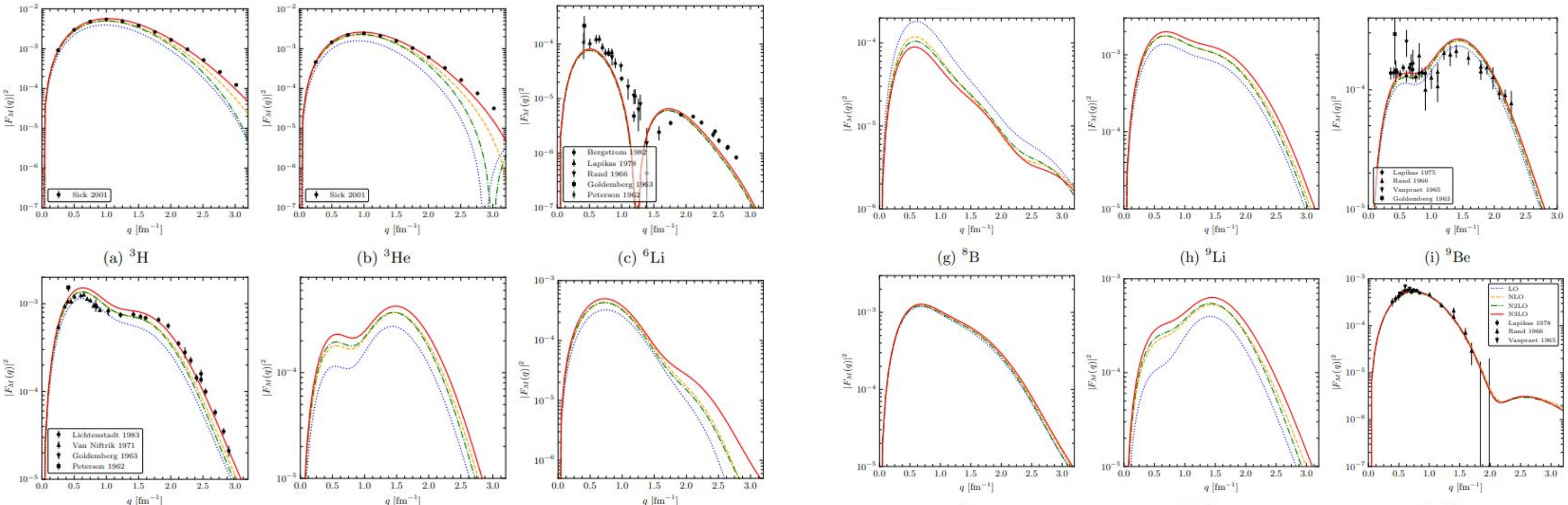
Carlson et al. Rev. Mod. Phys. 87, 1607 (2015)

Magnetic form factors 3≤A≤10



(a) ^{3}H (b) ^{3}He (c) ^{6}Li (g) ^{8}B (h) ^{9}Li (i) ^{9}Be

(d) ^{7}Li (e) ^{7}Be (f) ^{8}Li (j) ^{9}B (k) ^{9}C (l) ^{10}B

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