Ab initio calculations of the structure of p-shell nuclei

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Tomography of light nuclei at an EIC
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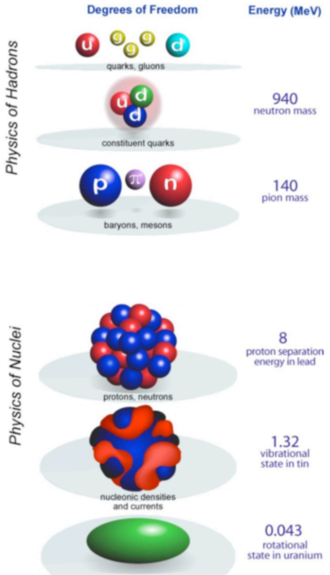
Introduction



- Perturbative QCD at GeV scales
- Hadron physics: Nonperturbative QCD
  relativistic quantum field theory
- NN systems: 2 nucleons or 6 quarks?
  quantum mechanics or field theory?
  relativistic or not ?
- Few-nucleon systems ($A = 3, 4$)
  nonrelativistic quantum mechanics,
  Faddeev–Yakubovsky equations
- Nuclear Structure of *p*-shell nuclei
  'not-so-few-but-not-too-many-body'
  computationally challenging
- Quantum many-body systems,
  density functional theory,
  semi-classical methods, . . .

Computational Challenges

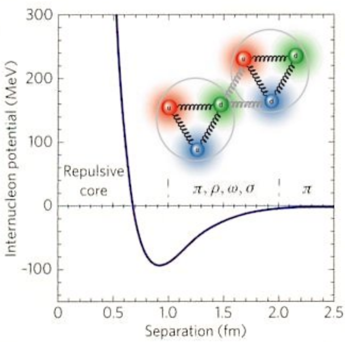
- Self-bound quantum many-body problem, with $3A$ degrees of freedom in coordinate (or momentum) space, as well as spin degrees of freedom
- Strong interactions, with both short-range and long-range pieces
- Not only 2-body interactions, but also intrinsic 3-body interactions and possibly 4- and higher N-body interactions
- Uncertainty quantification for calculations needed
  - for comparisons with experiments
  - for comparisons between different methods
- Sources of numerical uncertainty
  - statistical and round-off errors
  - systematical errors inherent to the computational method
    - Configuration Interaction methods: finite basis space
    - Monte Carlo methods: sensitivity to the trial wave function
    - Lattice Simulations: finite volume and lattice spacing
  - uncertainties in the nuclear interactions

Nuclear Interactions

$$\hat{\mathbf{H}}_{\rm rel} = \hat{\mathbf{T}}_{\rm rel} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

Nuclear interaction not well-determined

- In principle calculable from QCD
- Constrained by (fitted to) experimental (scattering) data



Alphabet of realistic NN potentials

- Argonne potentials (AV18 + . . .)
- Bonn potentials
- Chiral EFT interactions
  - Δ-less
  - Δ-full
  - pion-less
- Daejeon16 (based on Idaho-N^{3}LO)
- . . .

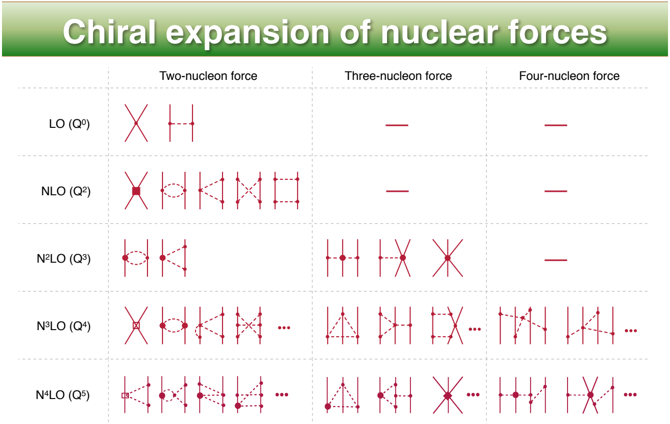
Most NN potentials need 3N forces for agreement with data for nuclei

NN Potential and Scattering Data

- Typically, cross-section data converted to phase-shifts
- NN potentials fitted to phase-shifts
  - propagation of experimental uncertainties?
  - fitted up to what energy?
- Experimental cross-section data for *pp* and *pn* scattering, but not for *nn* scattering
  - analysis in terms of isoscalar $T = 0$ and isovector $T = 1$ channels
- NN scattering data constrain only the on-shell NN potential, but not the off-shell behavior
  - many NN potentials describe NN scattering data, but differ for $A > 2$
  - some give good description of
    - binding energies & spectra (may need 3NFs)
    - select electroweak observables (may need corrections beyond IA)
  - wave functions not unique (unitary transformations)
- Additional (physics) input
  - chiral effective field theory
  - select observables from light nuclei (which?)
  - more or less suitable for intended computational framework

Nuclear Interactions from Chiral Effective Field Theory

- Controlled power series expansion in $Q = \max(p, M_\pi)/\Lambda_B \sim 0.3$
  - average momentum p-shell nuclei up to $\sim$ 200 MeV based on $\langle \hat{\mathbf{T}}_{\rm rel} \rangle$
- Hierarchy for many-body forces $V_{NN} \gg V_{NNN} \gg V_{NNNN}$



- Question: How to fit Low-Energy Constants (LECs)?

No-Core Configuration Interaction Approach

Barrett, Navrátil, Vary, *Ab initio no-core shell model*, PPNP69, 131 (2013)

Given a Hamiltonian operator

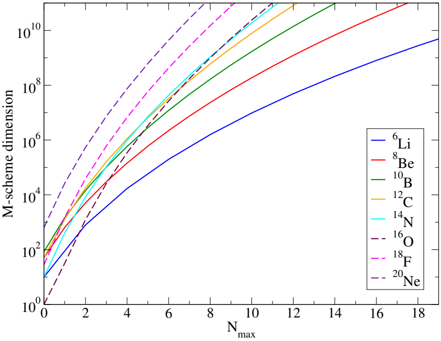
$$\hat{\mathbf{H}} \quad = \quad \sum_{i<j} \frac{(\vec{p}_i - \vec{p}_j)^2}{2\, m\, A} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

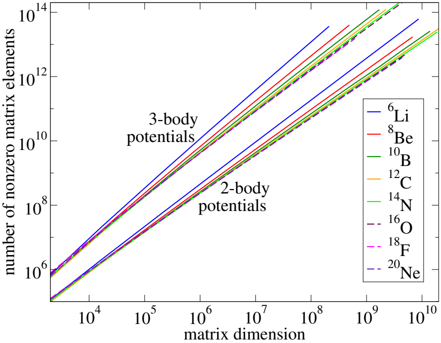
solve the eigenvalue problem for wave function of A nucleons

$$\hat{\mathbf{H}}\, \Psi(r_1, \ldots, r_A) \quad = \quad \lambda\, \Psi(r_1, \ldots, r_A)$$

- Expand wavefunction in basis states $|\Psi\rangle = \sum a_i |\Phi_i\rangle$
- Express Hamiltonian in basis $\langle\Phi_j|\hat{\mathbf{H}}|\Phi_i\rangle = H_{ij}$
- Diagonalize Hamiltonian matrix H_{ij}
- Use wavefunction for evaluating observables
- Complete basis $\longrightarrow$ exact result
- In practice: truncate basis, extrapolation to complete basis
  - truncation error, extrapolation uncertainties
- Computational challenge
  - construct large $(10^{10} \times 10^{10})$ sparse symmetric matrix H_{ij}
  - obtain lowest eigenvalues & -vectors

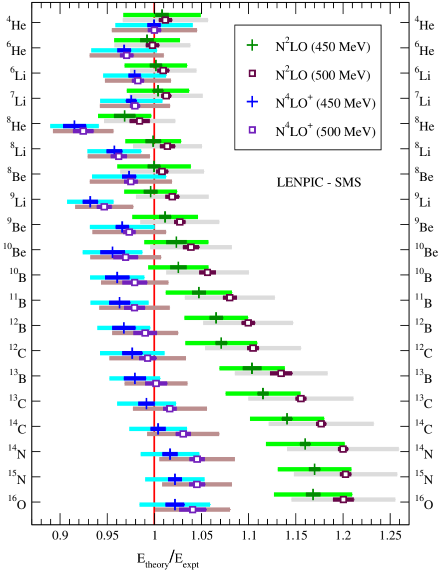
Main Challenge





- Increase of basis space dimension with increasing A and N_{max}
  - need calculations up to at least $N_{max} = 8$, preferably $N_{max} = 10$ for meaningful extrapolation and numerical error estimates
- More relevant measure for computational needs
  - number of nonzero matrix elements
  - current limit 10^{14} (Cori @ NERSC, Theta @ ALCF)

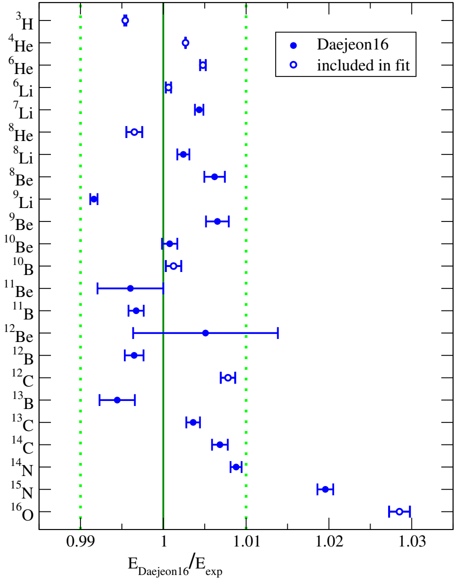
Binding Energies with LENPIC-SMS chiral EFT



PRC103, 054001 (2021); PRC, in press;
Frontiers, to be submitted this week

- NN potential up to N^{4}LO$^+$
- 3NFs at N^{2}LO
- SRG evolved to improve numerical convergence
- LECs fitted to
  - NN scattering data
  - ^{3}H binding energy
  - Nd scattering
- Parameter-free predictions
- Error bars
  - numerical uncertainty
  - chiral EFT uncertainty from Bayesian analysis

Binding energies with Daejeon16

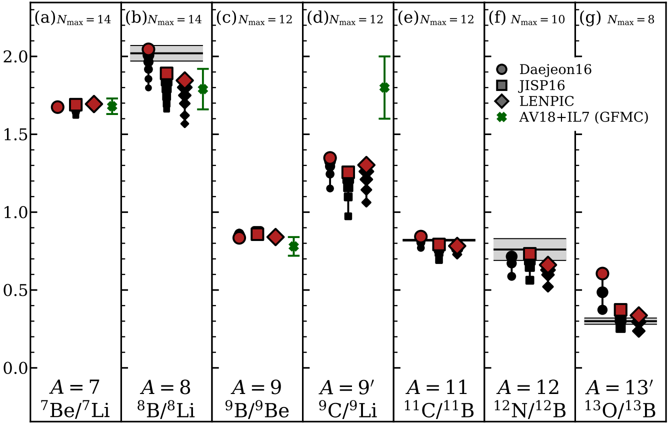


(PM, Shin, Caprio, Vary, in preparation)

- NN interaction, based on SRG evolved chiral EFT, using phase-equivalent transformations to fit select *p*-shell nuclei
- Ground state energies agree with experiment to within 1% for all *p*-shell nuclei up to A=14
- Correct J^π for ^{10}B (fitted)
- Parity inversion ^{11}Be
- Correct J^π for ^{12}B

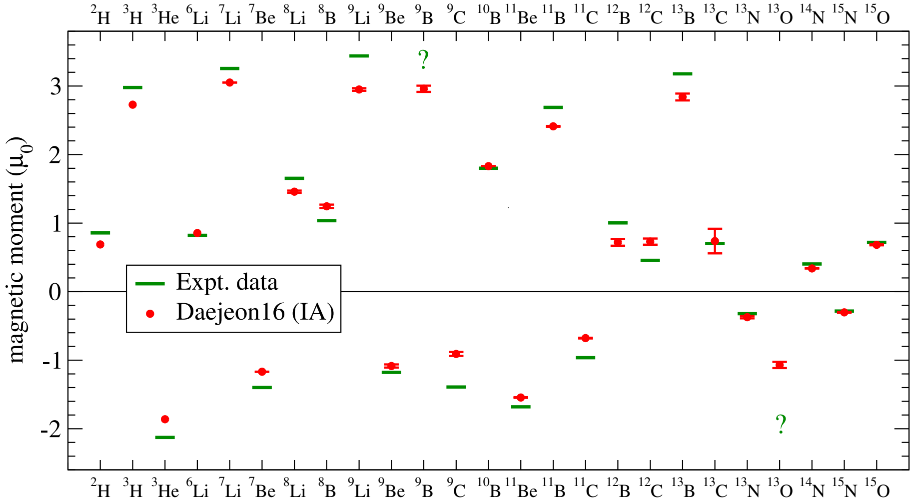
Ratio of Quadrupole Moments

Caprio, Fasano, PM, McCoy, PRC104, 034319 (2021)



- Ratio's of mirror $\mathcal{Q}$s similar with different interactions
  - exceptions: ^{9}C/^{9}Li with AV18+IL7 and ^{13}O/^{13}B with Daejeon16
  - naively, $\mathcal{Q} \approx 0$ because of closed proton shell in ^{13}O
- Reasonable agreement with available data

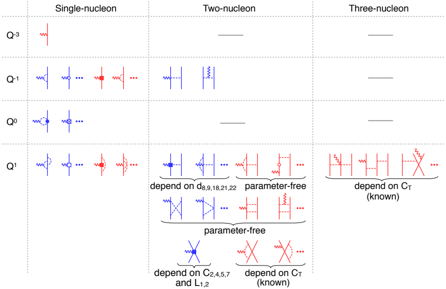
Magnetic Moments thoughout *p*-shell with Daejeon16

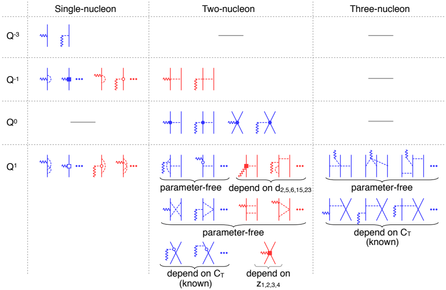


- Deviation from data agree with expected MEC corrections
- Nontrivial to construct consistent M1 corrections due to PETs

Electroweak Operators from Chiral EFT

figures from Epelbaum, arXiv:1908.09349





em charge and current operators; **axial** charge and current operators

- Chiral EFT two-body corrections to M1 operator at NLO
- Two- and three-body corrections to charge operator at N^3LO
- Leading two-body corrections corrections to axial charge at NLO
- Leading two-body corrections corrections to axial current at N^2LO

Introduction Nucleon-Nucleus Scattering

- Spectator expansion of multiple scattering theory
  - ordering of the scattering process according to the number of active target nucleons interacting directly with the projectile nucleon
- Generally restricted to leading-order term:
  projectile interacts directly with only one target nucleon
  - believed to be applicable in the 50 $\sim$ 200 MeV projectile energies
  - need one-body density of target nucleus
- Note: unclear what the actual expansion parameter is
  (assuming the spectator expansion has a well-defined expansion parameter . . .)
- Until recently
  - use realistic NN potential
  - purely phenomenological, local, one-body density
- Recent development
  - use one-body density from ab initio nuclear structure calculation
  - use same NN interaction for structure and scattering
  - consistency:
    also restricted to NN-only interactions in structure calculation

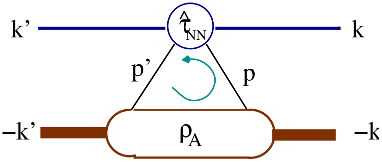
Leading-order spectator expansion for NA scattering

Effective (optical) potential

$$\widehat{U}(q, \mathcal{K}_{NA}, \epsilon) = \sum_{\alpha=n,p} \sum_{K_s} \int d^3\mathcal{K}\, \eta(q, \mathcal{K}, \mathcal{K}_{NA}) \;\; \hat{\tau}_{\alpha}^{K_s} \left(q, \frac{1}{2} \left(\frac{A+1}{A} \mathcal{K}_{NA} - \mathcal{K} \right); \varepsilon \right)$$
$$\rho_{\alpha}^{K_s} \left(\mathcal{K} - \frac{A-1}{A} \frac{q}{2}, \mathcal{K} + \frac{A-1}{A} \frac{q}{2} \right)$$

with $\eta(\ldots)$ the Moller factor, relating the NN frame to the NA frame
$\hat{\tau}_{n,p}^{K_s}$ the NN amplitude between projectile and target nucleon ($K_s = 0, 1$)
$\rho_{n,p}^{K_s}$ the (nonlocal) one-body density of the target ($K_s = 0, 1$) and

$$q = p' - p \qquad \mathcal{K} = \frac{1}{2}(p' + p)$$
$$\mathcal{K}_{NA} = \frac{A}{A+1} \left[(k' + k) + \frac{1}{2}(p' + p) \right]$$



One-Body Densities

One-Body Density for A-body wave function $|\Psi\rangle = |AJM\lambda\rangle$

$$\rho_{sf}(\vec{r},\vec{r'}) = \langle AJM\lambda| \sum_{i=1}^{A} \delta^3(\vec{r_i}-\vec{r})\delta^3(\vec{r_i'}-\vec{r'}) |AJM\lambda\rangle$$

Expand One-Body Density in terms of tensors of rank $K \leq 2J$

$$\rho_{sf}(\vec{r},\vec{r'}) = \sum_{ll'K} (-1)^{J-M} \begin{pmatrix} J & K & J \\ -M & 0 & M \end{pmatrix} \mathcal{Y}^{*l'l}_{K0}(\hat{r},\hat{r}')\, \rho_{ll'K}(r,r')$$

$$\rho_{ll'K}(r,r') = \sum_{njn'j'} \hat{j}\hat{j}'(-1)^{l'+l+j+\frac{1}{2}+K} \begin{Bmatrix} l' & l & K \\ j & j' & \frac{1}{2} \end{Bmatrix} R_{n'l'}(r')R_{nl}(r) \langle AJM\lambda||(a^\dagger_{nljm}\tilde{a}_{n'l'j'm})^{(K)}||AJM\lambda\rangle$$

with $(a^\dagger_{nljm}\tilde{a}_{n'l'j'm})^{(K)}$ one-body operator of rank K and $a_{nljm} = (-1)^{j-m}\,\tilde{a}_{nlj-m}$

- Reduced One-Body Density Matrix elements (OBDME) of rank K $\langle AJM\lambda||(a^\dagger_{nljm}\tilde{a}_{n'l'j'm})^{(K)}||AJM\lambda\rangle$ from ab initio NCSM calculations
- NCSM wavefunctions contain c.m. contributions ('space-fixed') which can be removed using Talmi-Moshinsky transformations

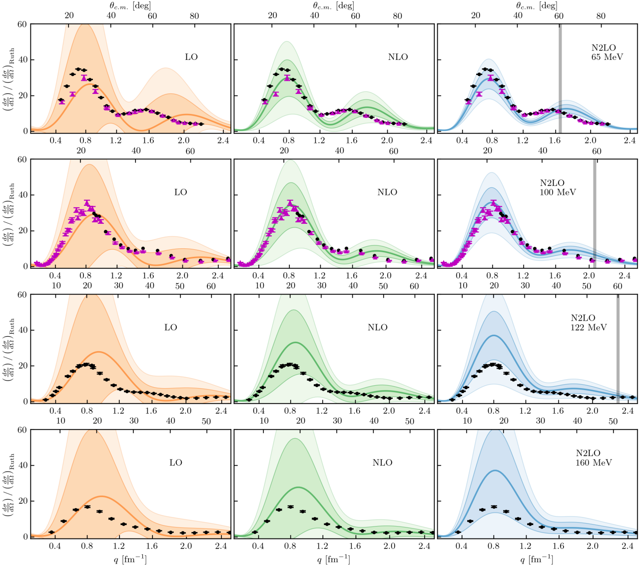
Burrows, Baker, Elster, Webbner, Launey, PM, Popa, PRC102, 034606 (2020)

LENPIC SCS with chiral uncertainties

- Interaction
  - LENPIC SCS: LO, NLO, and N^2LO (NN-only)
- Same interaction in structure and scattering calculation
  - no SRG evolution, no 3NFs
- Results for ^{4}He, ^{12}C, ^{16}O
  - at energies for which data exist
- Pointwise chiral EFT uncertainty estimates for total cross-sections
- Correlated uncertainty estimates for differential cross-sections, analyzing power A_y, and spin rotation function Q
- Expansion parameter $Q = p/\Lambda_b$
  with $\Lambda_b = 600$ MeV for regulator $R = 1.0$ fm
  - confirmed by checking posteriors

Baker, McClung, Elster, PM, Weppner, Burrows, Poppa, arXiv:2112.02442 (in press)
Baker, Burrows, Elster, Launey, PM, Popa, Weppner, Frontiers, submitted

Differential cross section, $^{12}C(p,p)^{12}C$



Concluding remarks

- NCCI approach powerful tool for ab initio nuclear structure
  - Binding energies agree with experiments
    - LENPIC NN + 3NF chiral EFT interactions
      can quantify EFT truncation uncertainties
    - Daejeon16 (based on chiral N^3LO NN potential)
  - Electroweak observables need chiral EFT corrections
    ('Meson Exchange Currents')
  - Provide one-body densities as input for NA scattering calculations
  - Could also be useful for EIC analyses ?
- Caveats
  - Neither NN (and 3NFs) nor nuclear wave functions are unique
  - Be aware: unitary transformations are often used in
    nuclear CI calculations to improve numerical convergence
    - Physical observables are invariant under
      consistent transformations of both operators and wavefunctions
  - If nucleon properties are modified in nuclei, then we should
    use modified LECs instead of free-space LECs in chiral EFT ?