Ab initio description of open-shell nuclei



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Ab initio approach

A-body Hamiltonian $H = T + V^{2N} + V^{3N} + ... + V^{AN}$ $H = T + V^{2N} + V^{3N} + ... + V^{AN}$ $H = T + V^{2N} + V^{3N} + ... + V^{AN}$ $H = T + V^{2N} + V^{3N} + ... + V^{AN}$ $H = T + V^{2N} + V^{3N} + ... + V^{AN}$ $H = T + V^{2N} + V^{3N} + ... + V^{AN}$ $H = T + V^{2N} + V^{3N} + ... + V^{AN}$ $H = T + V^{2N} + V^{3N} + ... + V^{AN}$ $H = T + V^{2N} + V^{3N} + ... + V^{AN}$ $H = T + V^{2N} + V^{3N} + ... + V^{AN}$

Solve many-body Schrödinger equation in a controlled, systematically improvable way



Open-shell nuclei

● Approximate / truncated methods capture correlations via an expansion in ph excitations
○ Reference states respects symmetries of H → works well in closed-shell systems

• Open-shell nuclei are **(near-)degenerate** with respect to ph excitations



 $\Sigma^{11}[ADC(3)] \longrightarrow$

 $\underbrace{\operatorname{Set} up}_{\Sigma(\omega) = \Sigma(\infty) + \Sigma^{\operatorname{dyn}}(\omega)}$



• Hamiltonians

○ NN+3N(400) (~2010)	[Entem & MacHleidt 2003, Navrátil 2007, Roth et al. 2012]
• NNLO _{sat} (2015)	[Ekström <i>et al.</i> 2015] $\{ \Psi^{\text{eff}}\rangle, E \approx E^{\text{brok}}\}$
○ NN+3N(lnl) (2018)	[Entem & Machleidt 2003, Navrátil 2018]
	$\{ \Psi^{\text{eff}}\rangle, E = E^{\text{rest}}\}$

Energy systematics: binding energies

• First objective: ab initio calculations as a **diagnostic tool** for the development of Hamiltonian



• Total energies E(N, Z)



Energy systematics: S_{2n}

• Two-neutron separation energies $S_{2n}(N,Z) \equiv |E(N,Z)| - |E(N-2,Z)|$



Energy systematics: gaps & magic numbers

• Neutron gaps $\Delta_{2n}(N,Z) \equiv S_{2n}(N,Z) - S_{2n}(N+2,Z)$



Energy systematics: pairing gaps



Charge radii & density distributions



Charge radii & density distributions



One-nucleon addition / removal spectra





Spectra of K isotopes

• Interesting g.s. spin inversion and re-inversion in K spectra

Laser spectroscopy COLLAPS @ ISOLDE $1/2^{+}$ 3/2+ 2522 Energy (keV) 5 [Papuga et al. 2013] 1371 4 E(1/2⁺ - 3/2⁺) [MeV] 980 3 561 474 359 2 ⁴⁹K ³⁷K ⁵¹K ³⁹K ⁴¹K ⁴⁵K ⁴⁷K ⁴³K 7 0 Exp. 6 Experiment N3LO -1 5 E(1/2⁺ - 3/2⁺) [MeV] - NN+3N(lnl)-2 4 51 49 43 47 53 55 37 39 41 45 3 AK 2 0 Recent experiment confirms -1 NN+3N(lnl) prediction for ⁵¹K and ⁵³K [Papuga et al. 2014] -2 [Sun et al. submitted, 2019] 37 45 47 49 51 53 55 39 41 43 AK

Electron and neutrino scattering

• Next-generation neutrino experiments (e.g. DUNE) make use of liquid-argon TPCs

• Modelling neutrino-40Ar cross section crucial

 \circ Impulse approximation the neuron for the numbers represent upper limits or the neuron for t argon. On the other hand, the differences between the rethe range for the uncertainties that vary between different sults for argon and carbon indicate significant differences kinematical regions. in the ground-state properties of these nuclei, which are relevant in the context of MC simulations for DUNE. 1.7% - 2.9%1. Total statistical uncertainty 2. Total systematic uncertainty 1.8% - 3.0%0.3%a. Beam charge & beam energy 1.0 0.4% - 1.0%b. Beam offset x & y60 c. Target thickness and boiling effect 0.7%Motivated e-scattering d. HRS offset x & y + optics 40e. Acceptance cut $(\theta, \phi, dp/p)$ 0.6% - 1.2%0.8 experiments @JLAB 0.6% - 2.4%alorimeter & Čerenkov cutsrons 50 0.01% - 0.03%S(p,E) [fm⁻³ MeV⁻¹] 0.6 1.3% $\mathrm{f}(\psi)$ **Radiative & Coulomb corrections** 1.0%h 40 0.4 (JLab, k_F=240 MeV 30 σ_{en} LNF, k_{F} =375 Me • 0.2 $(JLab, k_F = 245)$ • 20 JLab, k_F=220 M 0.0 0 -1.00-0.250.00 -0 10 0.5 N=24-28 Z=18 0 FIG. 3. (color online). Comprise 22 between the Zee 22 func-0 tion of the second kind, $f(\psi)$, obtained from E12-14-012 data 1.5 $\frac{d^2 \mathbf{d}}{d\Omega dE'}$ on Ar, Ti, and C. The k_F of C is fixed to the value obtained -10 by Moniz *et al.* [34] while the data analysis of Ti and Ar -15 2 MeV/]/ sets k_F at 240 MeV and 245 MeV, respectively. The circles 2.0 1.8 1.6 2.2 are the Ar data from LNF [11], which turn out to prefer an E' (GeV) inconsistently higher value of k_F .

FIG. 2. (color online). Comparison of Ar(e, e') cross section

To further elucidate the differences between the argon, titanium, and carbon cross sections, in Fig. 3, we show

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• Application to **electron and neutrino scattering**

• Good reproduction of JLAB data [Dai *et al.* 2018 & 2019]

• Small contribution from final-state interactions

 \circ Approximation ${}^{40}Ar_{[n]} \leftrightarrow {}^{48}Ti_{[p]}$ validated

• To be included next: 2B currents

Conclusions

• Considerable progress in ab initio calculations of (open-shell) mid-mass nuclei

Many-body approaches

 \circ Complementary methods \rightarrow benchmarks

 \circ Systematic calculations up to $A \sim 100$

• Frontiers: doubly open-shell & heavy nuclei

Hamiltonians

- Good quality, but not for all observables
- Strong activity ongoing, new developments
- Long-term: full assessment of uncertainties

