Ab initio description of open-shell nuclei

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○ Barbieri, Rocco, VS
  arXiv:1907.01122
**Ab initio approach**

\[ H = T + V_{2N} + V_{3N} + ... + V_{AN} \]

\[ H |\Psi_k^A\rangle = E_k^A |\Psi_k^A\rangle \]

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

**Hamiltonian**

- QCD → Model of inter-nucleon interactions (χEFT)
- Long-term goal: model-independent + uncertainties
- Current situation: proliferation of models

**Many-body approaches**

- Exact methods limited to light nuclei
- Expansion methods up to mass \( A \sim 100 \)
- Several complementary methods exist → **benchmarks**
Approximate/truncated methods capture correlations via an expansion in \textbf{ph excitations}.

- Reference states respects symmetries of $H$ → works well in closed-shell systems.

Open-shell nuclei are \textbf{(near-)degenerate} with respect to ph excitations.

A \textbf{symmetry-breaking} reference lifts the degeneracy.

<table>
<thead>
<tr>
<th>Pairing correlations</th>
<th>Quadrupole correlations</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Superfluidity</strong></td>
<td><strong>Deformation</strong></td>
</tr>
<tr>
<td><strong>Breaking of U(1)</strong></td>
<td><strong>Breaking of SU(2)</strong></td>
</tr>
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</table>

- **Singly** open-shells
- **Doubly** open-shells

![Graph showing the variation of $\Delta E/A$ with $N$ for Cr](image)
Set up

- Many-body approach: Self-Consistent Green’s Functions
  - Generalised to Gorkov scheme  [Somà, Duguet, Barbieri 2011]
  - G.s. properties of even-even $A$ + spectra of odd-even
  - Self-energy → Optical potential for $NA$ scattering

- Hamiltonians
  - $\textbf{NNLO}_{\text{sat}}$ (2015)  [Ekström $et$ $al.$ 2015]
Energy systematics: binding energies

- First objective: ab initio calculations as a **diagnostic tool** for the development of Hamiltonian
  - Novel Hamiltonians correct overbinding
  - 3rd-order yields needed correlations
  - Very reasonable agreement for S2n
  - N=20 gap still overestimated
Energy systematics: binding energies

- Total energies $E(N, Z)$

![Graph showing energy systematics for different isotopic chains]

- Several chains, not only semi-magic
- Trend w.r.t. experiment similar for all $Z$
Two-neutron separation energies $S_{2n}(N, Z) \equiv |E(N, Z)| - |E(N - 2, Z)|$

- High-order corrections ~ cancel out
- Overall good agreement with data
- N=20 gap overestimated
- Excellent reproduction for N>28
Energy systematics: gaps & magic numbers

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

![Graph showing neutron gaps and magic numbers over various elements.](image_url)
Three-point mass differences

\[ \Delta^{(3)}(N, Z) \equiv \frac{(-1)^N}{2} \left[ E(N-1, Z) - 2E(N, Z) + E(N+1, Z) \right] \]

- Magic peaks nicely visible
- Pairing too weak
- Dynamic contributions beyond second order?
- Interaction?
Charge radii & density distributions

○ NNLO\textsubscript{sat} successful for absolute $r\text{\textsubscript{ch}}$

○ Different behaviours for small $N$

○ All interactions struggle after $N=28$

○ Excellent reproduction of $\rho\text{\textsubscript{ch}}$
Charge radii & density distributions

- NNLO$_{\text{sat}}$ successful for absolute $r_{\text{ch}}$
- Different behaviours for small $N$
- Good agreement for differential $r_{\text{ch}}$
- Reproduction of $\rho_{\text{ch}}$ slightly deteriorates

(a) $\langle r_{\text{ch}}^2 \rangle^{1/2}$ [fm]
(b) $\Delta \langle r_{\text{ch}}^2 \rangle^{1/2}$ [fm]
One-nucleon addition/removal spectra

Reflects overestimation of N=20 gap

NN+3N(lnl) gives better splitting

Reflects good reproduction of N=28 gap

Different predictions for g.s. spin

NN+3N(lnl)  Exp.  NNLOsat
Quasi-free knockout cross sections

**Distorted-wave impulse approximation (DWIA)**

\[
\left( \frac{d\sigma}{d^3Q} \right)_{\text{DWIA}} = SF \times \left\langle \frac{d\sigma_{pN}}{d\Omega} \right\rangle \times \left\langle S_{pA} S_{p(A-1)} S_{N(A-1)} \Psi_N \right\rangle
\]

Spectroscopic factor  
NN cross section

Scattering matrices for effective d.o.f.  
(One-body overlaps + optical potentials)

<table>
<thead>
<tr>
<th>( \sigma ) [mb]</th>
<th>Exp.</th>
<th>GF</th>
<th>SM</th>
</tr>
</thead>
<tbody>
<tr>
<td>( ^{52}\text{Ca}(p,2p)^{51}\text{K} )</td>
<td>3/2(^+)</td>
<td>5.2(4)</td>
<td>3.56</td>
</tr>
<tr>
<td></td>
<td>1/2(^+)</td>
<td>1.7(2)</td>
<td>1.87</td>
</tr>
<tr>
<td>( ^{54}\text{Ca}(p,2p)^{53}\text{K} )</td>
<td>3/2(^+)</td>
<td>3.8(3)</td>
<td>3.25</td>
</tr>
<tr>
<td></td>
<td>1/2(^+)</td>
<td>1.5(2)</td>
<td>1.71</td>
</tr>
<tr>
<td>( ^{54}\text{Ca}(p,\text{pn})^{53}\text{Ca} )</td>
<td>1/2(^-)</td>
<td>15.9(17)</td>
<td>11.6</td>
</tr>
<tr>
<td></td>
<td>3/2(^-)</td>
<td>19.1(12)</td>
<td>17.0</td>
</tr>
</tbody>
</table>

[Sun et al., submitted, 2019 & Chen et al., submitted, 2019]
**Spectra of K isotopes**

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

**Laser spectroscopy COLAPS @ ISOLDE**

![Graph showing energy levels and transitions in K isotopes](image)

- Recent experiment confirms NN+3N(lnl) prediction for $^{51}$K and $^{53}$K

[Sun et al. submitted, 2019]
Electron and neutrino scattering

- Next-generation neutrino experiments (e.g. DUNE) make use of liquid-argon TPCs
- Modelling neutrino-$^{40}$Ar cross section crucial
- Impulse approximation → nuclear structure effects encoded in the spectral function

Motivated e-scattering experiments @JLAB
Electron and neutrino scattering

- Application to electron and neutrino scattering

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

- Small contribution from final-state interactions

- Approximation $^{40}\text{Ar}[n] \leftrightarrow ^{48}\text{Ti}[p]$ validated

- To be included next: 2B currents
Conclusions

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

Many-body approaches

- Complementary methods → benchmarks
- 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