Masses and spectroscopy of medium mass nuclei based on many-body perturbation theory

Javier Menéndez

Institut für Kernphysik, TU Darmstadt
ExtreMe Matter Institute (EMMI)

with Jason D. Holt, Achim Schwenk and Johannes Simonis

Three-body forces: from matter to nuclei
ECT* Trento, 8 May 2014
Medium-mass calculations: shell model

Chose as basis states that of the 3D Harmonic Oscillator

To keep the problem feasible, the configuration space is separated into:

- **Outer orbits:** orbits that are always empty
- **Valence space:** the space in which we explicitly solve the problem
- **Inner core:** orbits that are always filled

Solve in valence space: \[ H |\psi\rangle = E |\psi\rangle \rightarrow H_{\text{eff}} |\psi\rangle_{\text{eff}} = E |\psi\rangle_{\text{eff}} \]

where \( H_{\text{eff}} \) is obtained in many-body perturbation theory (MBPT) includes the effect of inner core and outer orbits.
Many Body Perturbation Theory

Better convergence of chiral forces after RG transformation

Valence-shell MBPT approach
Results: masses and spectroscopy
Status and needs

Many-body perturbation theory to third order: obtain effective Shell Model interaction in the valence space

Single Particle Energies
Two-Body Matrix Elements

Solve many-body problem with ISM codes ANTOINE/NATHAN
Diagonalize up to $10^{10}$ Slater determinants Caurier et al. RMP 77 (2005)

$$|\phi_\alpha\rangle = a_{i1}^+ a_{i2}^+ \ldots a_{iA}^+ |0\rangle$$
$$|\psi\rangle_{\text{eff}} = \sum_{\alpha} c_\alpha |\phi_\alpha\rangle$$
Chiral EFT NN+3N Forces

Systematic expansion: state-of-the-art chiral EFT forces

- **NN forces** included up to $N^3\text{LO}$
- **3N forces** included up to $N^2\text{LO}$

<table>
<thead>
<tr>
<th></th>
<th>2N force</th>
<th>3N force</th>
<th>4N force</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>LO</strong></td>
<td><img src="Diagram-1" alt="Diagram" /></td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>NLO</strong></td>
<td>![Diagram-2]</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td><strong>$N^2\text{LO}$</strong></td>
<td>![Diagram-3]</td>
<td>![Diagram-4]</td>
<td>—</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>$N^3\text{LO}$</strong></td>
<td>![Diagram-5]</td>
<td>![Diagram-6]</td>
<td>![Diagram-7]</td>
</tr>
</tbody>
</table>

Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Meißner...
Medium-mass nuclei

Javier Menéndez (TU Darmstadt)

Medium-mass nuclei based on MBPT
Uncertainties in MBPT valence-shell calculations

Sensitivity to initial Hamiltonian and low-energy couplings

Sensitivity due to the RG evolution:
Johannes Simonis talk

Treatment of 3N forces:
Normal-ordered 1b and 2b parts and residual 3N force

Convergence in the MBPT expansion:
Estimate order-by-order convergence, assess with non-perturbative methods

Convergence in intermediate-state excitations in MBPT

Convergence in size of valence space
Which orbitals can be treated perturbatively?
Valence-shell MBPT approach
Results: masses and spectroscopy
Status and needs

Many-body perturbation theory convergence

Order-by-order convergence in many-body perturbation theory
(NN forces evolved to $V_{\text{lowk}}$ interaction, empirical spe’s)

Associated uncertainty difficult to quantify, 3\textsuperscript{rd} order reasonable
Beyond third order very expensive: non-perturbative approaches
Convergence in term of intermediate states

Javier Menéndez (TU Darmstadt)
Medium-mass nuclei based on MBPT
Intermediate-state excitations convergence

Single-particle energies, most sensitive ingredient in calculation, convergence in terms of intermediate states (NN forces only)

Intermediate-state excitations seem to be under control
Valence-shell MBPT approach

Results: masses and spectroscopy

Status and needs

Benchmark to coupled-cluster

Benchmark against coupled-cluster calculations, same $V_{\text{lowk}}$ NN interaction, $\hbar \omega = 12$ MeV

Single-particle energies from coupled-cluster PA-EOM-CCSD energies in $^{41}\text{Ca}$

Agreement better than 5% in $pf$-shell nuclei: in heavier systems beyond-$pf$ orbitals start to be relevant in coupled-cluster calculations

Medium-mass nuclei based on MBPT
Normal-ordered 3N Forces

Treatment of 3N forces:

normal-ordered 2B: 2 valence, 1 core particle
⇒ Two-body Matrix Elements

normal-ordered 1B: 1 valence, 2 core particles
⇒ Single particle energies
Residual 3N Forces

In the most neutron-rich isotopes, 3N forces between 3 valence neutrons (suppressed by $N_{\text{valence}}/N_{\text{core}}$)

Evaluated perturbatively: $\langle \psi | V^{3N} | \psi \rangle$

Residual 3N small and repulsive Caesar, Simonis et al. PRC88 034313 (2013)
Towards uncertainty estimation

Sensitivity to resolution-scale dependence of RG-evolved nuclear forces: **Johannes Simonis talk**

Even though uncertainties in ground-state energies are relatively large, separation energies and excitation spectra significantly smaller.

Javier Menéndez (TU Darmstadt)  
Medium-mass nuclei based on MBPT
Ca masses

Ca isotopes: explore nuclear shell evolution $N = 20, 28, 32?, 34?$

Ca measured from $^{40}\text{Ca}$ core

$\hbar\omega = 11.48 \text{ MeV}$

$pf \ g_{9/2}$ valence space

3N forces repulsive contribution, chiral NN-only forces too attractive

Sensitivity to single particle energies

MBPT (calculated from NN+3N forces)

Empirical (from GXPF1 interaction)

Estimate of associated uncertainty
Precise (and accurate!) $^{51,52}\text{Ca} / ^{53,54}\text{Ca}$ masses at TRIUMF/ISOLDE

Excellent agreement with theoretical prediction

$S_{2n}$ evolution:
$^{52}\text{Ca}–^{54}\text{Ca}$ decrease similar to $^{48}\text{Ca}–^{50}\text{Ca}$ unambiguously establishes $N = 32$ shell closure

Gallant et al. PRL 109 032506 (2012)
Two-neutron separation energies

Compare to other theoretical calculations

Phenomenology
masses/gaps as input, differ markedly beyond $^{54}$Ca

Coupled-Cluster calculations
good agreement with adjusted 3N forces

Gallant et al. PRL 109 032506 (2012)
Shell closures and $2^+_1$ energies

$2^+_1$ energies characterize shell closures

Correct closure at $N = 28$ when 3N forces are included

Holt et al. JPG39 085111(2012)
Holt, JM, Schwenk,
JPG40 075105 (2013)

- 3N forces enhance closure at $N = 32$
- 3N forces reduce strong closure at $N = 34$ (1.7-2.2 MeV)
  Expt: 2.04 MeV, suggest $N = 34$ shell closure

O isotopes: masses and spectra

Chiral NN+3N forces give the correct picture for masses and spectra

Otsuka et al. PRL105 032501 (2010); Holt, JM, Schwenk EPJA49 39 (2013)
Proton-rich nuclei

Compare NN+3N theory to isobaric mass-multiplet formula (IMME)
\[ E(A, T, T_z) = E(A, T, -T_z) + 2b(A, T)T_z \]

Isospin-symmetry breaking terms predicted by chiral EFT
Coulomb included in calculations

Proton dripline not certain predicted at \(^{20}\text{Mg}\) or \(^{22}\text{Si}\):
\[ S_{2p} = -0.12 \text{ (Theory)} / +0.01 \text{ (IMME)} \]

Excitation spectra predicted: test in RIB facilities
Oxygen electromagnetic transitions

Electromagnetic transitions (decay lifetimes)

B(E2) transitions in $2^+_2$ states, $^{20}$O and $^{22}$O

Javier Menéndez (TU Darmstadt)

Medium-mass nuclei based on MBPT
Valence-shell MBPT approach
Results: masses and spectroscopy
Status and needs

Calcium B(E2) transition strengths

B(E2)s in reasonable agreement with experiment, spread over order of magnitude

Similar quality as phenomenological interactions, in particular very close to KB3G

$^{46}\text{Ca}$: $sd$ degrees of freedom?

Phenomenological effective charges

\begin{align*}
^{46}\text{Ca}: 2^+ & \rightarrow 0^+ \quad \text{KB3G}\, \text{or GXPF1A}\, \text{or NN + 3N (MBPT)} \\
^{46}\text{Ca}: 4^+ & \rightarrow 2^+ \quad \text{Raman et al. (2001)} \\
^{46}\text{Ca}: 6^+ & \rightarrow 4^+ \quad \text{Montanari et al. (2012)}
\end{align*}
B(M1) Transition in $^{48}\text{Ca}$

B(M1) strength in $^{48}\text{Ca}$ too fragmented in $pf$ space

Phenomenological calculations reproduce experimental concentration

In the extended $pf_{9/2}$ space NN forces also fragmented strength

NN+3N calculation in $pf_{9/2}$ very good agreement with experiment

Phenomenological effective g-factors
Good agreement with ground-states, spectroscopy and electromagnetic transitions but with effective charges and g-factors

- **Shell-model calculation** in limited valence space: Appropriate effective operators to be obtained perturbatively or non-perturbatively
- **Operators are not complete**: Need of two-body currents well known from light nuclei

Pastore et al. PRC87 035503 (2013)
## Chiral 2b currents

### Chiral EFT: nuclear forces and electroweak currents

<table>
<thead>
<tr>
<th></th>
<th>2N force</th>
<th>3N force</th>
<th>4N force</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>LO</strong></td>
<td><img src="image1" alt="Diagram" /></td>
<td><img src="image2" alt="Diagram" /></td>
<td><img src="image3" alt="Diagram" /></td>
</tr>
<tr>
<td><strong>NLO</strong></td>
<td><img src="image4" alt="Diagram" /></td>
<td><img src="image5" alt="Diagram" /></td>
<td><img src="image6" alt="Diagram" /></td>
</tr>
<tr>
<td><strong>N^2LO</strong></td>
<td><img src="image7" alt="Diagram" /></td>
<td><img src="image8" alt="Diagram" /></td>
<td><img src="image9" alt="Diagram" /></td>
</tr>
<tr>
<td><strong>N^3LO</strong></td>
<td><img src="image10" alt="Diagram" /></td>
<td><img src="image11" alt="Diagram" /></td>
<td><img src="image12" alt="Diagram" /></td>
</tr>
</tbody>
</table>

Weinberg, van Kolck, Kaplan, Savage, Epelbaum, Kaiser, Meißner...

---

Park et al.

Short-range couplings fit to experiment once

Javier Menéndez (TU Darmstadt)  
Medium-mass nuclei based on MBPT
2b currents and Gamow-Teller quenching

2b currents at $p = 0$: GT decays, $2\nu\beta\beta$ decay

\[ J_{n,2b}^{\text{eff}} = -\frac{g_A \rho}{f_\pi^2} \tau_n^{-} \sigma_n \left[ I(\rho, P) \left( \frac{1}{3} (2c_4 - c_3) + \frac{1}{6m_N} \right) \right], \]

General density range
$\rho = 0.10 \ldots 0.12 \text{ fm}^{-3}$

Couplings $c_3, c_4$ from NN potentials
Entem et al. PRC68 041001(2003)
Epelbaum et al. NPA747 362(2005)
$\delta c_3 = -\delta c_4 \approx 1 \text{ GeV}^{-1}$

JM, Gazit, Schwenk PRL107 062501 (2011)
Nuclear matrix elements for $0\nu\beta\beta$ decay

Order $Q^0 + Q^2$ similar to phenomenological currents
JM, Poves, Caurier, Nowacki
NPA818 139 (2009)

Order $Q^3$ 2b currents reduce NMEs $\sim 15\% - 40\%$

Momentum-transfer dependence predicted

Similarly, vector currents for electromagnetic transitions

Valence-shell MBPT approach
Results: masses and spectroscopy
Status and needs

Medium-mass nuclei based on MBPT
3N forces: status and needs

Status

- Valence-shell calculations of ground-state properties, spectroscopy and electromagnetic transitions so far selected isotopes but extend to *sd* and *pf* shell nuclei
- One particular NN+3N interaction
- Towards and estimation of theoretical uncertainties

Needs

- 3N (and 4N) matrix elements at N^3LO
- Order-by-order fits to test chiral EFT convergence
- Delta-full NN and 3N matrix elements
- Test different NN+3N interactions
- Consistent matrix elements for chiral axial and vector currents