Applications of Green's function theory to medium-mass nuclei

C. Barbieri


JAPAN-ITALY EFES Workshop, 6-8 September 2010
Future Challenges in Nuclear Structure

How to predict exotic isotopes?
How to extract information from measured reactions?

the nuclear spectral is function a valuable path

[Picture credit: Isotope Science Facility MSUCL-1345 ]
One-hole spectral function -- example

\[ S^{(h)} (p_m, E_m) = \sum_n |\langle \Psi^{A-1}_n | c_{\Psi_0} | \Psi^A \rangle|^2 \delta(E_m - (E^A_0 - E^{A-1}_n)) \]

\( \rightarrow \) distribution of momentum (\( p_m \)) and energies (\( E_m \))
One-body Green's function (or propagator) describes the motion of quasi-particles and holes:

\[ g_{\alpha\beta}(\omega) = \sum_n \frac{\langle \Psi_0^A | c^-_\alpha | \Psi_{n+1}^A \rangle \langle \Psi_{n+1}^A | c^+_\beta | \Psi_0^A \rangle}{\omega - (E_{n+1}^A - E_0^A) + i\eta} + \sum_k \frac{\langle \Psi_0^A | c^+_\beta | \Psi_k^A \rangle \langle \Psi_k^A | c^-_\alpha | \Psi_0^A \rangle}{\omega - (E_0^A - E_k^{A-1}) - i\eta} \]

...this contains all the structure information probed by nucleon transfer (spectral function):

\[ S_\alpha(\omega) = \frac{\mp 1}{\pi} \text{Im} \ g_{\alpha\alpha}(\omega) = \sum_n \left| \langle \Psi_{n+1}^A | c^-_\alpha | \Psi_0^A \rangle \right|^2 \delta(\omega \pm (E_0^A - E_{n+1}^A)) \]
Why many-body Green's functions??

**Theory Features:**

- Fully microscopic $\rightarrow$ “ab-initio” approach
- Linked diags. $\rightarrow$ **size extensivity**
- Hierarchy of equations—can improve systematically
- The computational cost **scales gently** with increasing $A$
- Suitable for parallel computing
- **Self-consistency**:
  - fulfillment of conservation laws
  - “no” reference state

**Links to Physics:**

- Closely related to **spectroscopy** $\leftrightarrow$ experiments
- “phonons” are the low-energy degrees of freedom $\leftrightarrow$ **phenomenological apps. possible**
- The self-energy is a nucleon-nucleus **optical potential** (see, e.g. DOM applications)

GFs are the **method of choice** for a **global picture** of nuclear dynamics

...and, yes, of course lots of information requires hard work...
Faddeev-RPA (FRPA) is a *many-body* method:
random phase approx. (RPA) for collective vibrations
Faddeev eqs. for particle-vibration coupling

- up to $A \approx 56$ (for now)
- $^{100-132}$Sn, $^{78}$Ni possible (parallelization)

Large bases & coupling to resonances do explain well
the quenching of spectroscopic factors

[Phys Rev. Lett. 103, 202502 (2009)]

[CB, M.Hjorth-Jensen, Phys.Rev.C79, 064313 (2009);
CB, Phys. Rev. Lett. 103, 202502 (2009)]
Particle vibration coupling is the main cause driving the distribution of particle strength.

Finite Systems (and nuclei) are \textit{special}, they require \textit{all types} of particle-vibration coupling:
- pairing effects, two-nucleon transfer
- collective motion, resonances, Gamow-Teller
- interference among them

- Use \textit{random phase approximation} (RPA) to get response functions of vibrations ($g_{\Pi}(\omega)$, $\Pi^{(ph)}(\omega)$)

- Use Faddeev’s equation to couple them

\textbf{Faddeev-RPA}

\begin{align*}
\text{Phys.Rev.C63, 034313 (2001)} \\
\text{Phys.Rev.C65, 064313 (2002)} \\
\text{Phys.Rev.A76, 052503 (2007)}
\end{align*}
Self-Consistent Green's Function Approach

pp/hh-RPA; two-nucleon transfer

\[ g^{\Pi}(\omega) \]

\[ \Pi^{(ph)}(\omega) \]

Faddeev-RPA

\[ S(r, \omega) \]

Dyson Eq.

ph-RPA; nuclear response function, giant/pygmy resonances, Gamow-Teller

Faddeev-RPA is a many-body method:

✓ random phase approx. (RPA) for collective vibrations
✓ Faddeev eqs. for particle-vibration coupling

optical potential

\[ [CB, Jennings, Nucl. Phys A758, 395c (2005)
Phy Rev. C72, 014613 (2005)] \]

single-particle motion

CB, Phys. Rev. Lett. 103, 202502 (2009)] \]

Middleton, CB, et al., arXiv:0907.1758, EPJA in print]

CB, Langanke et al., Phys Rev. C77, 024304 (2008)]
Self-consistent FRPA compares well with benchmark calculations on $^4$He

FRPA/sc0

$V_{\text{low-k}}$: -29.00(2)

self-consistency in the mean field only

FRPA/sc

$V_{\text{low-k}}$: $-29.2 \pm 0.15$

estimates from different approx. to self-consistency -- preliminary

Exact:

$-29.19(5)$ (Fadd.-Yak.)

Some applications to nuclei...

- quenching of absolute spect. factors ($^{56}$Ni)
- optical potentials
- two nucleon correlations $^{16}$O(e,e'pn)
Single neutron levels around $^{16}\text{O}$ with FRPA

<table>
<thead>
<tr>
<th>Theory(MeV)</th>
<th>Exp.[MeV]</th>
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<tbody>
<tr>
<td>$E_{d3/2}-E_{d5/2}$</td>
<td>3.5</td>
</tr>
<tr>
<td>$E_{p1/2}-E_{p3/2}$</td>
<td>3.1</td>
</tr>
</tbody>
</table>

p-h gap:
- $E_{d3/2}-E_{p1/2}$: 16.5 - 16.6
- $E_{s1/2}-E_{p1/2}$: 12.2 - 12.4

- Particle-hole gap accurate with a G-matrix with $\omega$-dependence
- $p_{3/2}-p_{1/2}$ spin-orbit splitting agrees with $\approx 3.4\text{MeV}$ from variational Monte Carlo (VMC) [S. Pieper et al. Phys. Rev. Lett. 70 (93) 2541, using $AV_{14}$]
Particle-vibration coupling dominates the quenching of spectroscopic factors

Relative strength among fragments requires shell-model approach


<table>
<thead>
<tr>
<th></th>
<th>10 osc. shells</th>
<th>Exp. [30]</th>
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<tr>
<td></td>
<td>FRPA (SRC)</td>
<td>full FRPA</td>
<td>+ΔZα FRPA</td>
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<td></td>
<td>FRPA</td>
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<tr>
<td>57Ni:</td>
<td>v1p1/2</td>
<td>0.96</td>
<td>0.63</td>
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<tr>
<td></td>
<td>v0f5/2</td>
<td>0.95</td>
<td>0.59</td>
</tr>
<tr>
<td></td>
<td>v1p3/2</td>
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<td>0.65</td>
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<tr>
<td></td>
<td>v1p1/2</td>
<td>0.95</td>
<td>0.72</td>
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<tr>
<td>55Ni:</td>
<td>v0f7/2</td>
<td>0.95</td>
<td>0.72</td>
</tr>
<tr>
<td>57Cu:</td>
<td>π1p1/2</td>
<td>0.96</td>
<td>0.63</td>
</tr>
<tr>
<td></td>
<td>π0f3/2</td>
<td>0.96</td>
<td>0.60</td>
</tr>
<tr>
<td></td>
<td>π1p3/2</td>
<td>0.96</td>
<td>0.67</td>
</tr>
<tr>
<td></td>
<td>π0f7/2</td>
<td>0.95</td>
<td>0.73</td>
</tr>
<tr>
<td>55Co:</td>
<td>π0f7/2</td>
<td>0.95</td>
<td>0.73</td>
</tr>
</tbody>
</table>

[CB, Phys. Rev. Lett. 103, 202502 (2009)]
Asymmetry dependence: F-RPA estimate...

Explorative, FRPA calculations show only a slight dependence of spectroscopic factors on separation energies (asymmetry):

- in agreement with other calculations
- in disagreement with experimental analysis
- collective modes may not (yet) be fully realistic... (try Skyrme? phen. corr.?)

\[ \rightarrow \text{OPEN PUZZLE!!!} \]


\[ \text{Phys. Rev. C77, 044306 (2008)} \]
The dispersive optical model (DOM) also predicts a "weak" asymmetry dependence for spectroscopic factors.

[W.H.Dickhoff, communication]
Further away from $E_F$: elastic scattering...

Nuclear self-energy:

$$\Sigma^*(r, r'; \varepsilon) = \Sigma_{\alpha\beta}^{HF} - \frac{1}{\pi} \int_{\varepsilon_T}^{\infty} dE' \frac{Im \Sigma^*(r, r'; E')}{\varepsilon - E' + i\eta}$$

$$+ \frac{1}{\pi} \int_{-\infty}^{\varepsilon_T} dE' \frac{Im \Sigma^*(r, r'; E')}{\varepsilon - E' - i\eta}$$

- it is proven to be a Feshbach's microscopic optical potential
- satisfies the dispersion relation (causality):
The dispersive optical model (DOM) is a parameterization of the self-energy based on theory. In particular it is made to satisfy the dispersion (i.e. parameterize ONLY $V_{HF}(r, E)$ and $W(r, E)$)!!

$$U(r, E) = V(r, E) + iW(r, E)$$

$$V(r, E) = V_{HF}(r, E) + \Delta V(r, E)$$

$$\Delta V(r, E) = \frac{1}{\pi} P \int W(r, E') \left( \frac{1}{E' - E} - \frac{1}{E' - E_F} \right) dE'$$

Recent developments: global model around the $^{40}$Ca chain (St.Louis):

Correlations in sp energies and strengths

Particle-vibration coupling dominates the quenching of spectroscopic factors

Relative strength among fragments requires shell-model approach

[see, e.g. Utsuno et al., AIP Conf. Proc. 1120, 81 (2009).
Tsang et al., Phys. Rev. Lett. 102, 062501 (2009)]

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<td></td>
</tr>
<tr>
<td>ν1p_{1/2}</td>
<td>0.96</td>
<td>0.63</td>
</tr>
<tr>
<td>ν0f_{3/2}</td>
<td>0.95</td>
<td>0.59</td>
</tr>
<tr>
<td>ν1p_{3/2}</td>
<td>0.95</td>
<td>0.65</td>
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<tr>
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[CB, Phys. Rev. Lett. 103, 202502 (2009)]
Correlations in sp energies and strengths

Single particle energies - driven by tensor + 3N force...
(see e.g. previous talk by T. Otsuka)

Quenching of spectral strength (spect. factor) - driven by coupling to collective modes...

• Role of tensor force??

• Collective, charge exchange effects??

Binding Energies of h_{11/2} & g_{7/2} States on Z=50

Correlations in sp energies and strengths
Microscopic Optical Potential from FRPA

- absorption away from $E_F$ is enhanced by the tensor force
- little effects from charge exchange (e.g. $p^{-48}Ca \leftrightarrow n^{-48}Sc$)

$$J_w: \text{integral over the imaginary opt. pot (overall absorption)}$$

- Full FRPA result (w/ av18)
- Charge-exchange d.o.f. suppressed
- Tensor force suppressed

S. Waldecker, CB, W. Dickhoff -- in preparation
• $^{16}\text{O}(e,e'pn)^{14}\text{N}$

• initial wave function from SCGF

• Pavia model for final state interactions

• $p_B \equiv q - p_1 - p_2$

• two orders of magnitude from long-range correlations.

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arXiv:1004.4568v1 [nucl-th]
Atoms and molecules...

- Ne as a test case
- Performance of FRPA for atoms and molecules
Spectral strength of Neon

Example of sole “ladder” or “ring” and full mixing

Fig. 4. (Color online) Spectral function for the $s$ states in Ne obtained with various self-energy approximations. From the top down: the second-order ($\Sigma^{(2)}$), the FRPA (ring), the FRPA (ladder), and the full FRPA self-energies. The strength is given relative to the Hartree-Fock occupation of each shell. Only fragments with strength larger than $Z > 0.005$ are shown.

Atom of Ne
(10 electrons problem)

Table IV. Energy (in a.u.) and strength (numbers in parentheses) of the main fragments in the spectral function of neon, generated by different self-energies. Results for the HF+continuum basis. Consecutive rows refer to (1) HF; (2) second-order self-energy; (3) $G_0W_0$ results from Ref. [14]; (4) FRPA self-energy with only $ph$ rings retained; (5) FRPA self-energy with only $pp$-$hh$ ladders retained; (6) complete FRPA self-energy. In all FRPA results the self-energy was corrected at third order through Eq. (8). The static self-energy was pure HF (no partial self-consistency). The experimental values are taken from Refs. [32,33].

<table>
<thead>
<tr>
<th></th>
<th>1s</th>
<th>2s</th>
<th>2p</th>
</tr>
</thead>
<tbody>
<tr>
<td>HF</td>
<td>-32.77 (1.00)</td>
<td>-1.931 (1.00)</td>
<td>-0.850 (1.00)</td>
</tr>
<tr>
<td>$\Sigma^{(2)}$</td>
<td>-31.84 (0.74)</td>
<td>-1.736 (0.88)</td>
<td>-0.747 (0.91)</td>
</tr>
<tr>
<td>$G_0W_0$</td>
<td>-31.14 (0.85)</td>
<td>-1.774 (0.91)</td>
<td>-0.801 (0.94)</td>
</tr>
<tr>
<td>FRPA (ring)</td>
<td>-31.82 (0.73)</td>
<td>-1.636 (0.56)</td>
<td>-0.730 (0.80)</td>
</tr>
<tr>
<td>FRPA (ladder)</td>
<td>-32.04 (0.87)</td>
<td>-1.802 (0.95)</td>
<td>-0.781 (0.96)</td>
</tr>
<tr>
<td>FRPA</td>
<td>-32.10 (0.81)</td>
<td>-1.792 (0.91)</td>
<td>-0.799 (0.94)</td>
</tr>
<tr>
<td>Expt.</td>
<td>-31.70</td>
<td>-1.782 (0.85)</td>
<td>-0.793 (0.92)</td>
</tr>
</tbody>
</table>

**Spectral strength of Neon**

**Momentum distribution:**

![Graph showing momentum distribution for Ne with peaks labeled 1s, 2s, 2p, and 1/r.](image)

[C.B., Van Neck, AIP Conf.Proc.1120, 104 ('09)]

**FIGURE 2.** Hole spectral function (right) and momentum distribution (left) of the Ne atom. The dotted, dashed and dot-dashed lines are the contributions coming from the main 2p, 2s and 1s quasi-hole peaks seen on the right side.
## Accuracy of FRPA for atoms

### Binding energy

<table>
<thead>
<tr>
<th></th>
<th>Hartree-Fock</th>
<th>FTDAc</th>
<th>FRPAc</th>
<th>CCSD</th>
<th>Experiment</th>
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<tbody>
<tr>
<td>He</td>
<td>-2.8617 (+42.0)</td>
<td>-2.9028 (+0.9)</td>
<td>-2.9029 (+0.8)</td>
<td>-2.9039 (-0.2)</td>
<td>-2.9037</td>
</tr>
<tr>
<td>Be²⁺</td>
<td>-13.6117 (+43.9)</td>
<td>-13.6559 (-0.3)</td>
<td>-13.6559 (-0.3)</td>
<td>-13.6561 (-0.5)</td>
<td>-13.6556</td>
</tr>
<tr>
<td>Be</td>
<td>-14.5731 (+94.3)</td>
<td>-14.6438 (+23.6)</td>
<td>-14.6436 (+23.8)</td>
<td>-14.6522 (+15.2)</td>
<td>-14.6674</td>
</tr>
<tr>
<td>Ne</td>
<td>-128.5505 (+387.8)</td>
<td>-128.9343 (+4.0)</td>
<td>-128.9381 (+2.0)</td>
<td>-128.9353 (+3.0)</td>
<td>-128.9383</td>
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<tr>
<td>Mg²⁺</td>
<td>-198.837 (+444)</td>
<td>-199.226 (-5)</td>
<td>-199.228 (-7)</td>
<td>-199.225 (-4)</td>
<td>-199.221</td>
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<tr>
<td>Mg</td>
<td>-199.616 (+438)</td>
<td>-200.048 (+6)</td>
<td>-200.052 (+2)</td>
<td>-200.050 (+4)</td>
<td>-200.054</td>
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<tr>
<td>Ar</td>
<td>-526.820 (+724)</td>
<td>-527.543 (+1)</td>
<td>-527.548 (-4)</td>
<td>-527.536 (+8)</td>
<td>-527.544</td>
</tr>
</tbody>
</table>

\[ \sigma_{rms} \text{ [mH]} \]

|     | 392 | 9.5 (3.6) | 9.5 (3.4) | 6.9 (4.2) |

# Accuracy of FRPA for atoms

## Binding energy

<table>
<thead>
<tr>
<th></th>
<th>Hartree-Fock</th>
<th>(2^{\text{nd}}) orderc</th>
<th>FTDAc/ADC(3)c</th>
<th>FRPAc</th>
<th>Experiment [51, 52]</th>
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<tbody>
<tr>
<td>He:</td>
<td></td>
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<tr>
<td>1s</td>
<td>0.918 (+14)</td>
<td>0.9012 (-2.5)</td>
<td>0.9025 (-1.2)</td>
<td>0.9008 (-2.9)</td>
<td>0.9037</td>
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<tr>
<td>Be(^{2+}):</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1s</td>
<td>5.6672 (+116)</td>
<td>5.6542 (-1.4)</td>
<td>5.6554 (-0.2)</td>
<td>5.6551 (-0.5)</td>
<td>5.6556</td>
</tr>
<tr>
<td>2s</td>
<td>0.3093 (-34)</td>
<td>0.3187 (-23.9)</td>
<td>0.3237 (-18.9)</td>
<td>0.3224 (-20.2)</td>
<td>0.3426</td>
</tr>
<tr>
<td>1s</td>
<td>4.733 (+200)</td>
<td>4.5892 (+56)</td>
<td>4.5439 (+11)</td>
<td>4.5405 (+8)</td>
<td>4.533</td>
</tr>
<tr>
<td>Ne:</td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>2p</td>
<td>0.852 (+57)</td>
<td>0.752 (-41)</td>
<td>0.8101 (+17)</td>
<td>0.8037 (+11)</td>
<td>0.793</td>
</tr>
<tr>
<td>1s</td>
<td>1.931 (+149)</td>
<td>1.750 (-39)</td>
<td>1.8057 (+24)</td>
<td>1.7967 (+15)</td>
<td>1.782</td>
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<td>Mg(^{2+}):</td>
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<tr>
<td>2p</td>
<td>3.0068 (+56.9)</td>
<td>2.9217 (-28.2)</td>
<td>2.9572 (+7.3)</td>
<td>2.9537 (+3.8)</td>
<td>2.9499</td>
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<tr>
<td>1s</td>
<td>4.4827</td>
<td>4.3283</td>
<td>4.3632</td>
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<tr>
<td>Mg:</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>3s</td>
<td>0.253 (-28)</td>
<td>0.267 (-14)</td>
<td>0.272 (-9)</td>
<td>0.280 (-1)</td>
<td>0.281</td>
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<tr>
<td>2p</td>
<td>2.282 (+162)</td>
<td>2.117 (-3)</td>
<td>2.141 (+21)</td>
<td>2.137 (+17)</td>
<td>2.12</td>
</tr>
<tr>
<td>Ar:</td>
<td></td>
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<td></td>
</tr>
<tr>
<td>3p</td>
<td>0.591 (+12)</td>
<td>0.563 (-16)</td>
<td>0.581 (+2)</td>
<td>0.579 (+0)</td>
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<tr>
<td>3s</td>
<td>1.277 (+202)</td>
<td>1.111 (+36)</td>
<td>1.087 (+12)</td>
<td>1.065 (-10)</td>
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<tr>
<td>3s</td>
<td>1.840</td>
<td>1.578</td>
<td>1.544</td>
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\(\sigma_{\text{rms}}\) [mH]

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<td>81.4</td>
<td>29.3</td>
<td>13.7</td>
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# Accuracy of FRPA for atoms

## Diatomic molecules

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<td><strong>N₂</strong></td>
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<tr>
<td>$E₀$</td>
<td>−109.258</td>
<td>−109.272</td>
<td>−109.276</td>
<td>−</td>
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<tr>
<td>$r₀$</td>
<td>1.104</td>
<td>1.106</td>
<td>1.119</td>
<td>1.098</td>
</tr>
<tr>
<td>I</td>
<td>0.565</td>
<td>0.544</td>
<td>0.602&lt;sup&gt;a&lt;/sup&gt;</td>
<td>0.573</td>
</tr>
<tr>
<td><strong>BF</strong></td>
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<tr>
<td>$E₀$</td>
<td>−124.365</td>
<td>−124.368</td>
<td>−124.380</td>
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<td>$r₀$</td>
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<td>1.295</td>
<td>1.267</td>
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<tr>
<td>I</td>
<td>0.395</td>
<td>0.402</td>
<td>0.406</td>
<td>−</td>
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<tr>
<td><strong>CO</strong></td>
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<tr>
<td>$E₀$</td>
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<td>−113.048</td>
<td>−113.055</td>
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<tr>
<td>I</td>
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<td>0.494</td>
<td>0.550&lt;sup&gt;a&lt;/sup&gt;</td>
<td>0.515</td>
</tr>
</tbody>
</table>

<sup>a</sup> Only up to CCE

[Degroote, Van Neck, CB, to be submitted]
Future Directions

- **Nuclear structure studies:**
  - Calculations of main chains (O, Ca, Ni...) to address:
    - quenching of spectroscopic factors vs. N/Z
    - origin shell closures and driplines location
    - SHELL MODEL's basis states, interactions and charges
    - properties of global optical potentials

- "Ab-initio" & tech. advances:
  - parallelization (\(\rightarrow^{100}\text{Sn},^{78}\text{Ni}\))
  - inclusion of 3NF
  - extension to Gorkov-formalism (Somà, Duguet):
    - open-shell nuclei
    - structure of next generation EDF

Thank you for your attention!!