Nuclear structure and dynamics from coupled-cluster theory

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Challenges in effective field theory descriptions of nuclei
Hirschegg 2026

Outline

Structure and electromagnetic sum rules of open-shell nuclei

Bridging nuclear structure and reactions: the case of pion-nucleus scattering

Coupled-cluster theory

Coupled-cluster (CC) ground-state

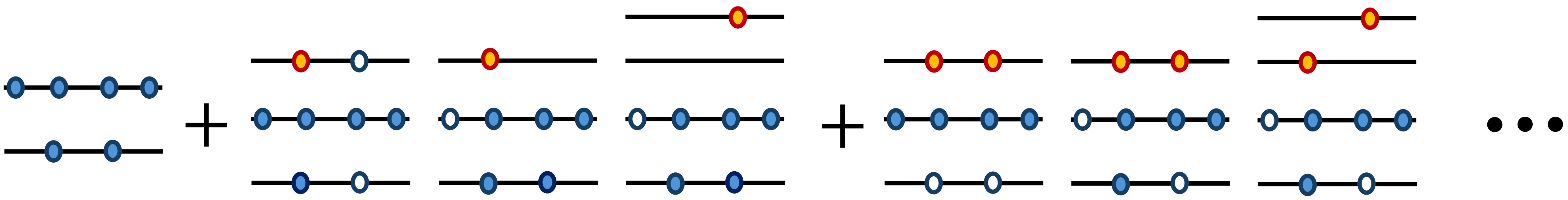
$$|\Psi_0\rangle = e^{T}\boxed{|\Phi_0\rangle}$$

$|\Phi_0\rangle$ Reference state

$$T \approx \overbrace{\underbrace{T_1 + T_2}_{\text{CCSD}} + T_3}^{\text{CCSDT-1: approximate triples}} + \cdots$$

n-particle n-hole amplitudes

$|\Psi_0\rangle =$



$|\Phi_0\rangle$ $1p1h$ excitations $2p2h$ excitations

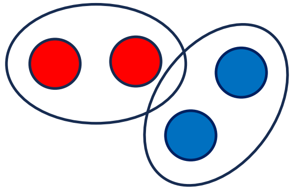
Hagen et al., Rep. Prog. Phys. **77**, 096302 (2014)

Structure of open-shell nuclei

Towards open-shell nuclei

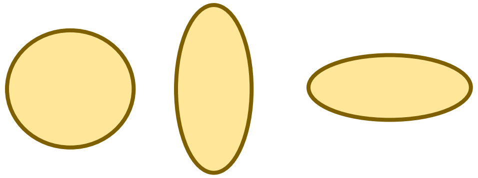
Symmetry-breaking approaches

Pairing



Bogoliubov CC

Deformation



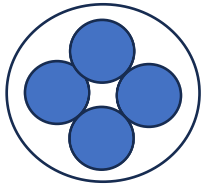
Deformed CC

Tichai et al., Phys. Lett. B **851**, 138571 (2024)

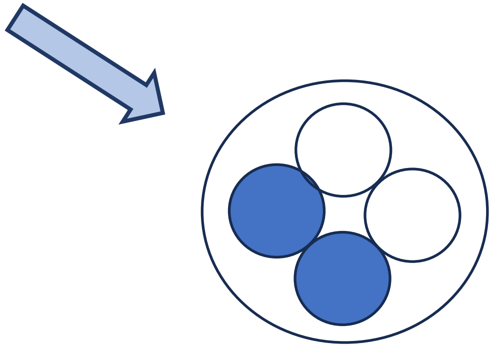
Hagen et al., Phys. Rev. C **105**, 064311 (2022)

Equations-of-motion

Closed-shell



$$|\Psi_0\rangle = e^{T}|\Phi_0\rangle$$

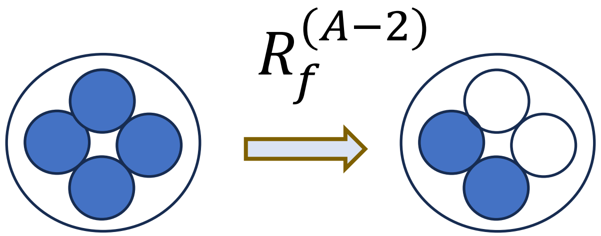


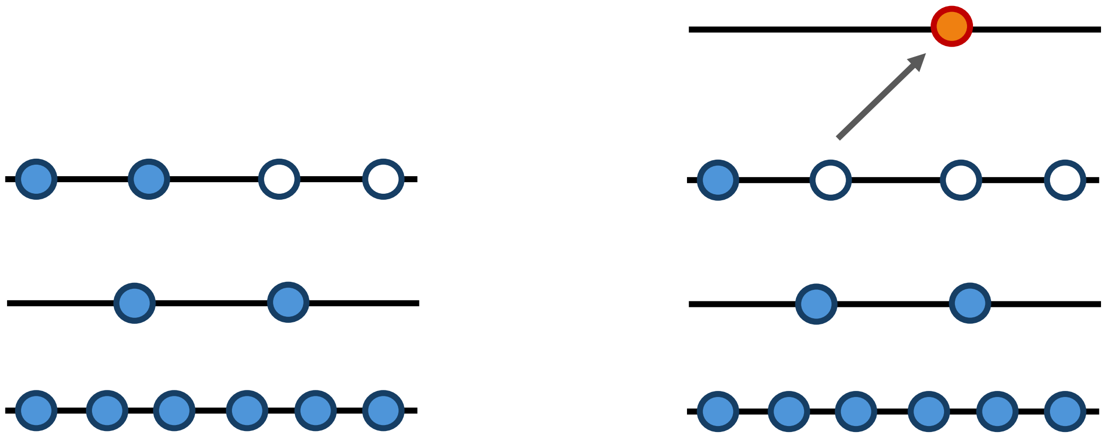
Two-particle-removed (2PR) nucleus

Excitation operator

$$|\Psi_f^{(A-2)}\rangle = R_f^{(A-2)}|\Psi_0\rangle$$

The two-particle-removed ansatz





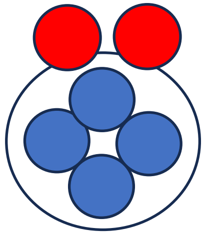
Two-hole

One-particle three-hole

$$R_f^{(A-2)} = \frac{1}{2}\sum_{ij} r_{ij} c_j c_i + \frac{1}{6}\sum_{ijka} r_{ijk}^{a}\, c_a^{\dagger} c_k c_j c_i$$

FM et al., Phys. Rev. C **112**, 014315 (2025)

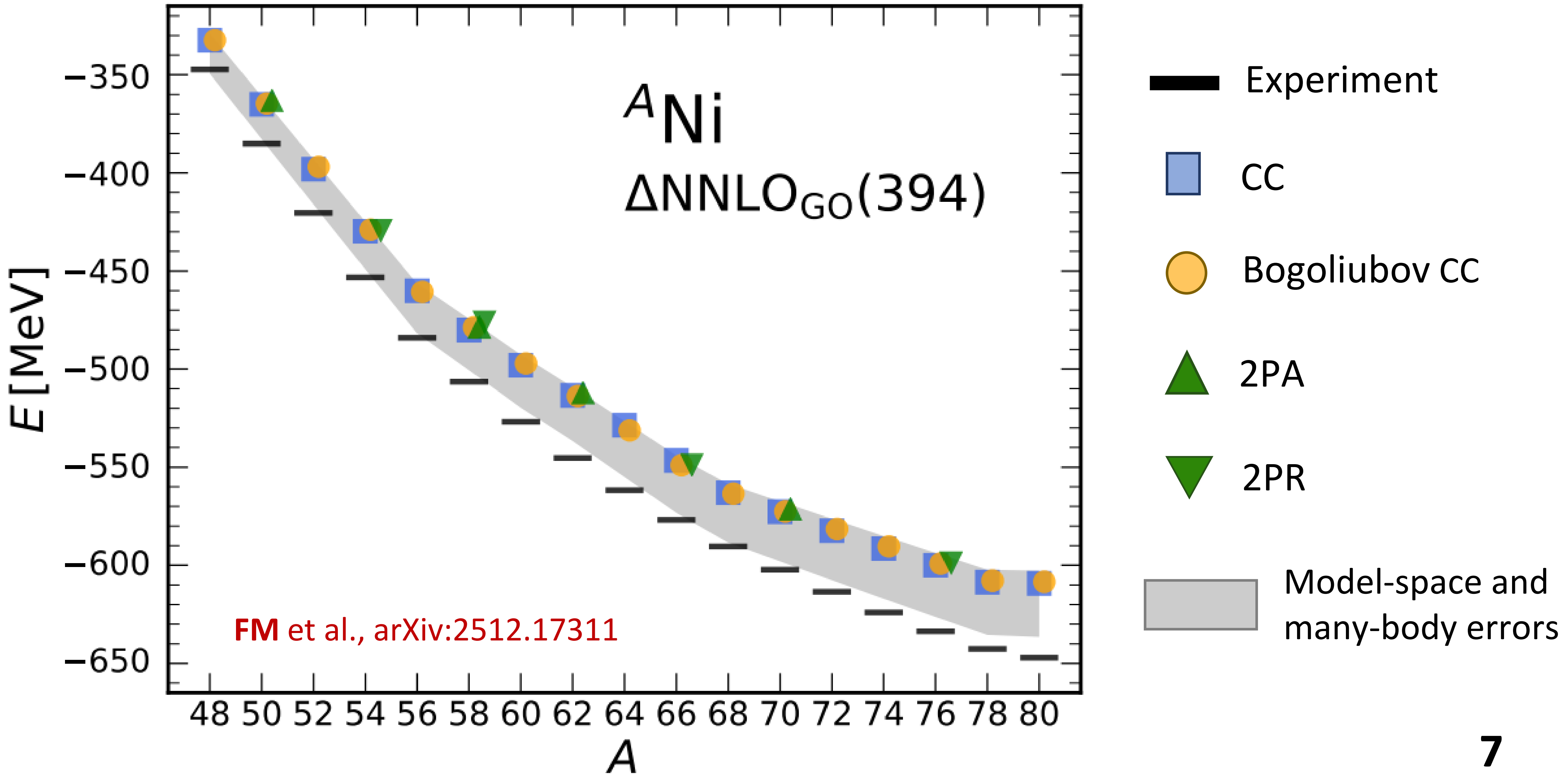
See also



Two-particle-attached (2PA)

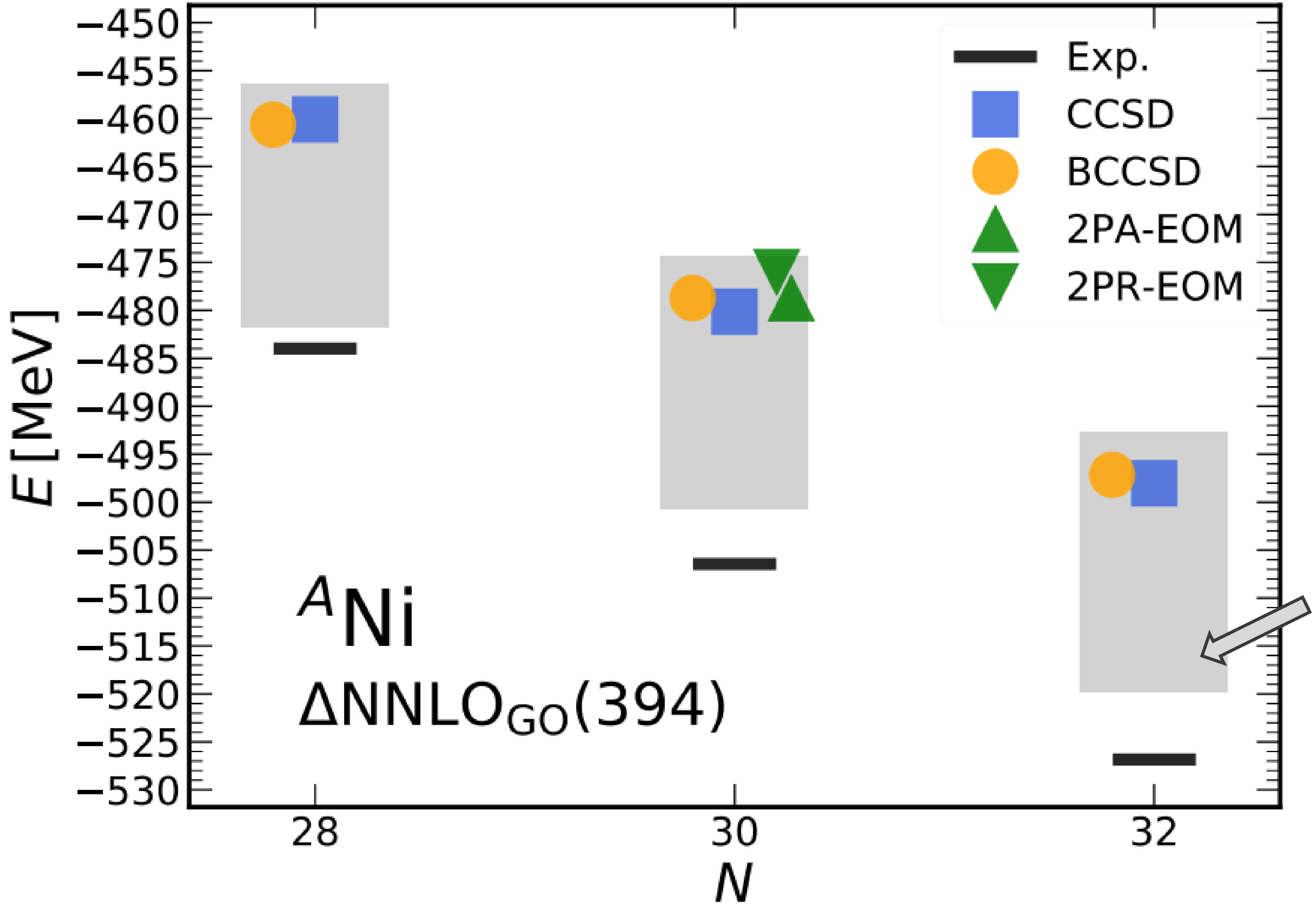
Jansen, Phys. Rev. C **88**, 024305 (2013)
Bonaiti et al., PRC **110**, 044306 (2024)

Benchmark: the nickel chain



Focusing on ^{58}Ni

FM et al., arXiv:2512.17311

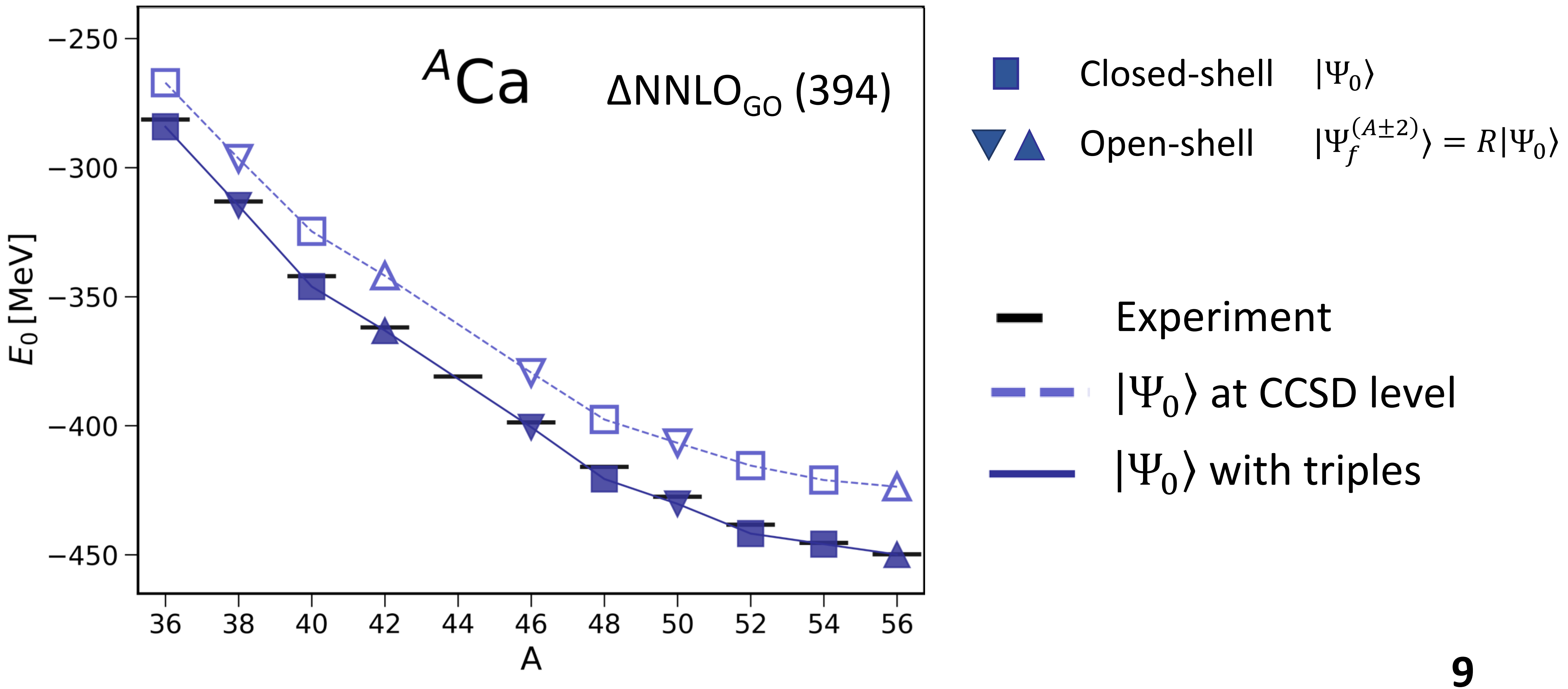


Excellent agreement between coupled-cluster variants

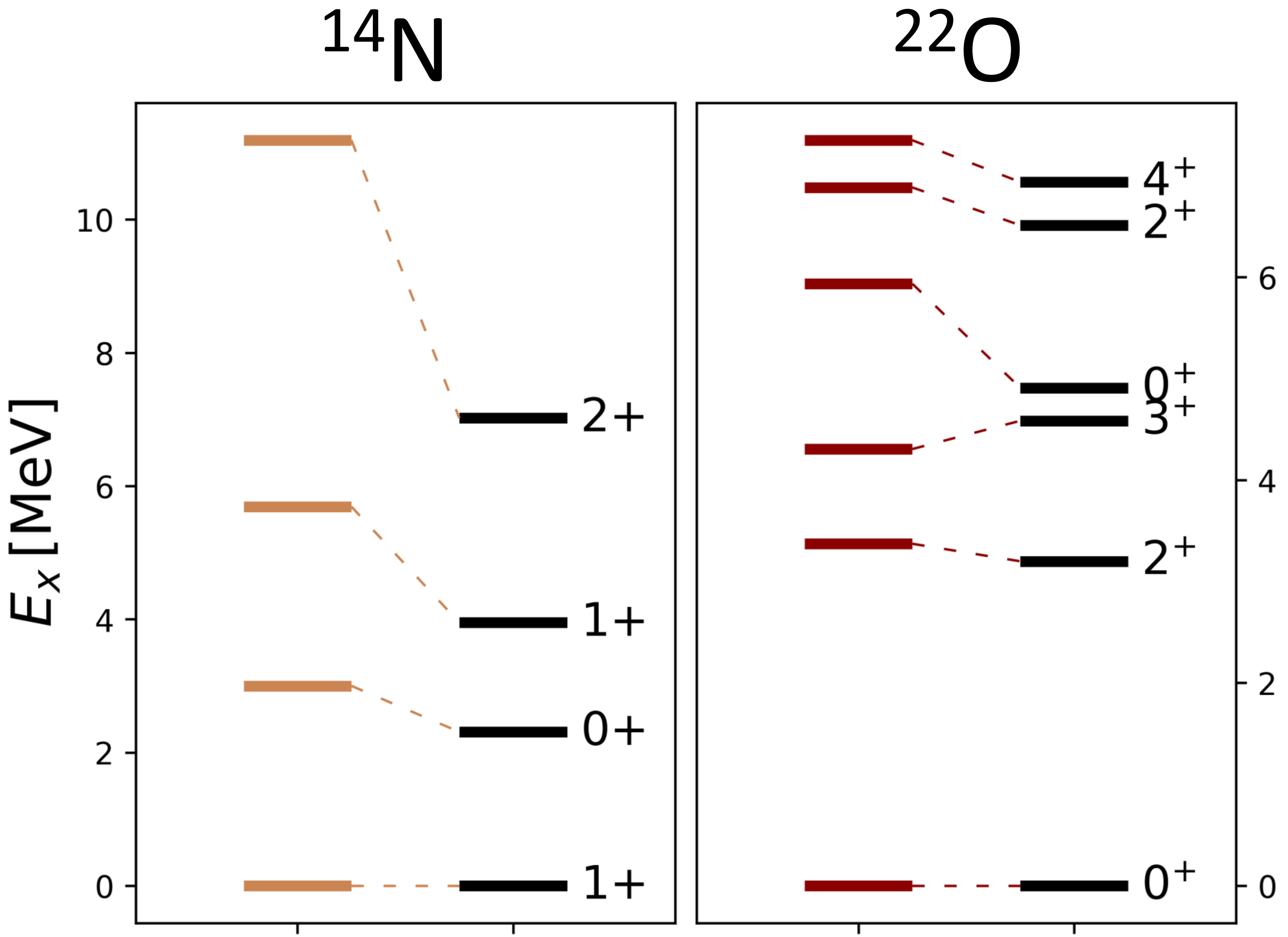
Main uncertainty: missing **triples** corrections

Triples corrections

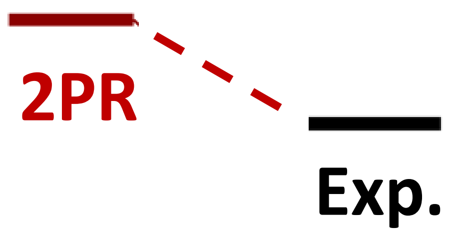
FM et al., Phys. Rev. C **112**, 014315 (2025)



Low-lying spectra



FM et al., Phys. Rev. C **112**, 014315 (2025)



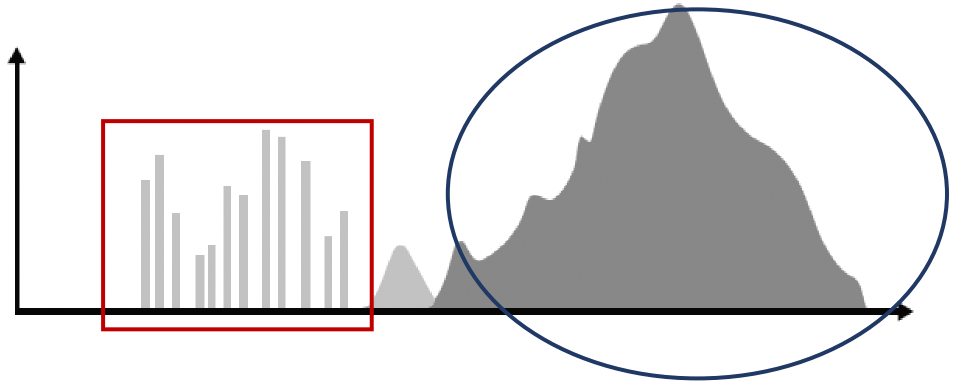
2PR with the ΔNNLO$_{GO}$ (394) interaction describes well several **excited states**

Electric dipole polarizability of open-shell nuclei

The Lorentz integral transform method

$$R(\omega) = \sum_f \left|\langle \Psi_f \boxed{|\Theta|} \Psi_0 \rangle\right|^2 \delta(E_f - E_0 - \omega)$$

Θ: excitation operator



Lorentz integral transform (LIT)

$$L(\sigma, \Gamma) = \frac{\Gamma}{\pi} \int d\omega \frac{R(\omega)}{(\omega - \sigma)^2 + \Gamma^2} = \frac{\Gamma}{\pi} \langle \widetilde{\Psi}_L | \widetilde{\Psi}_R \rangle$$

Bound pseudo-state $|\widetilde{\Psi}_R\rangle$

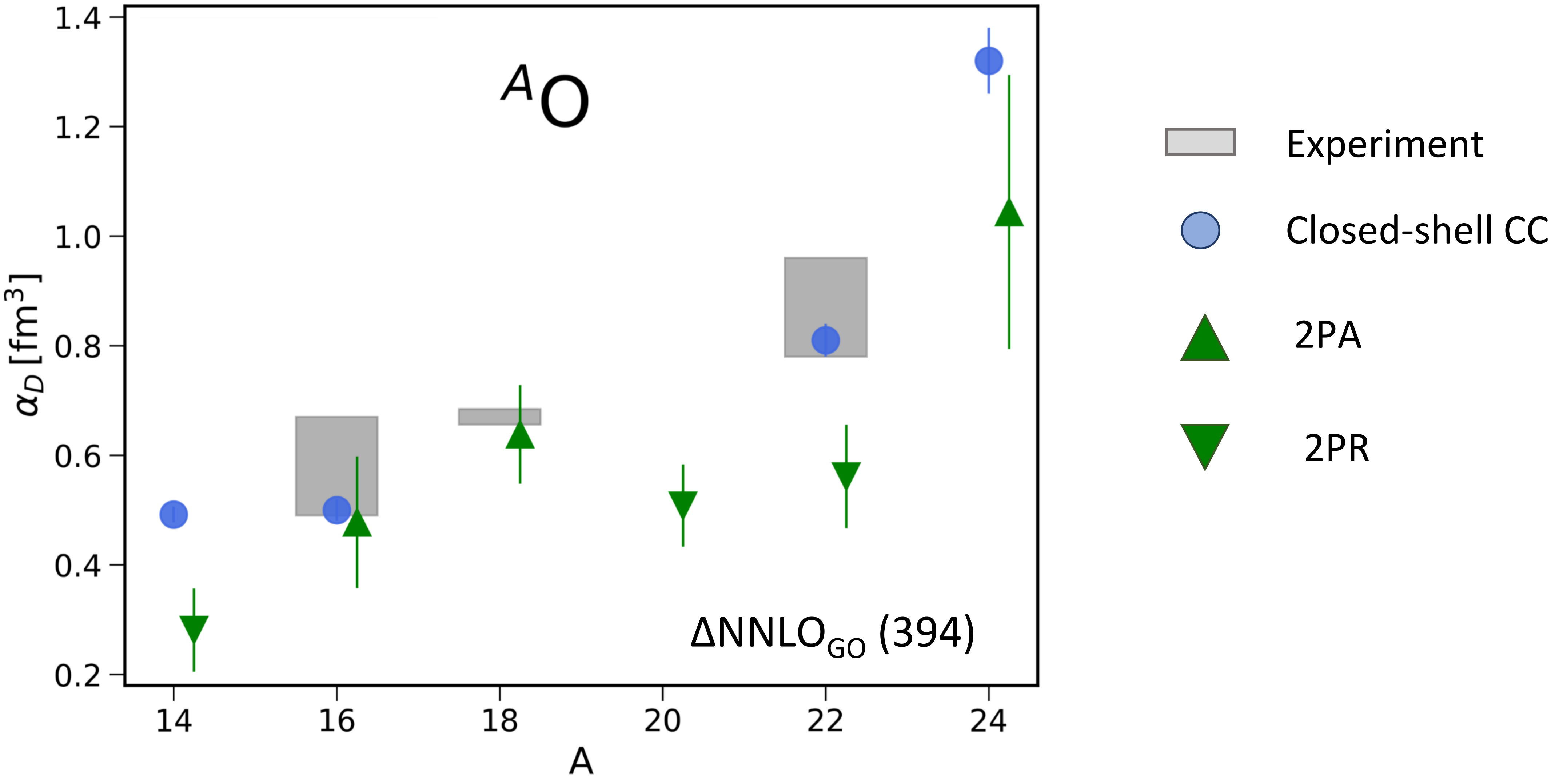
Bacca et al, Phys. Rev. Lett. **111**, 122502 (2013)

Sum rules of the response directly from $L(\sigma, \Gamma \rightarrow 0)$

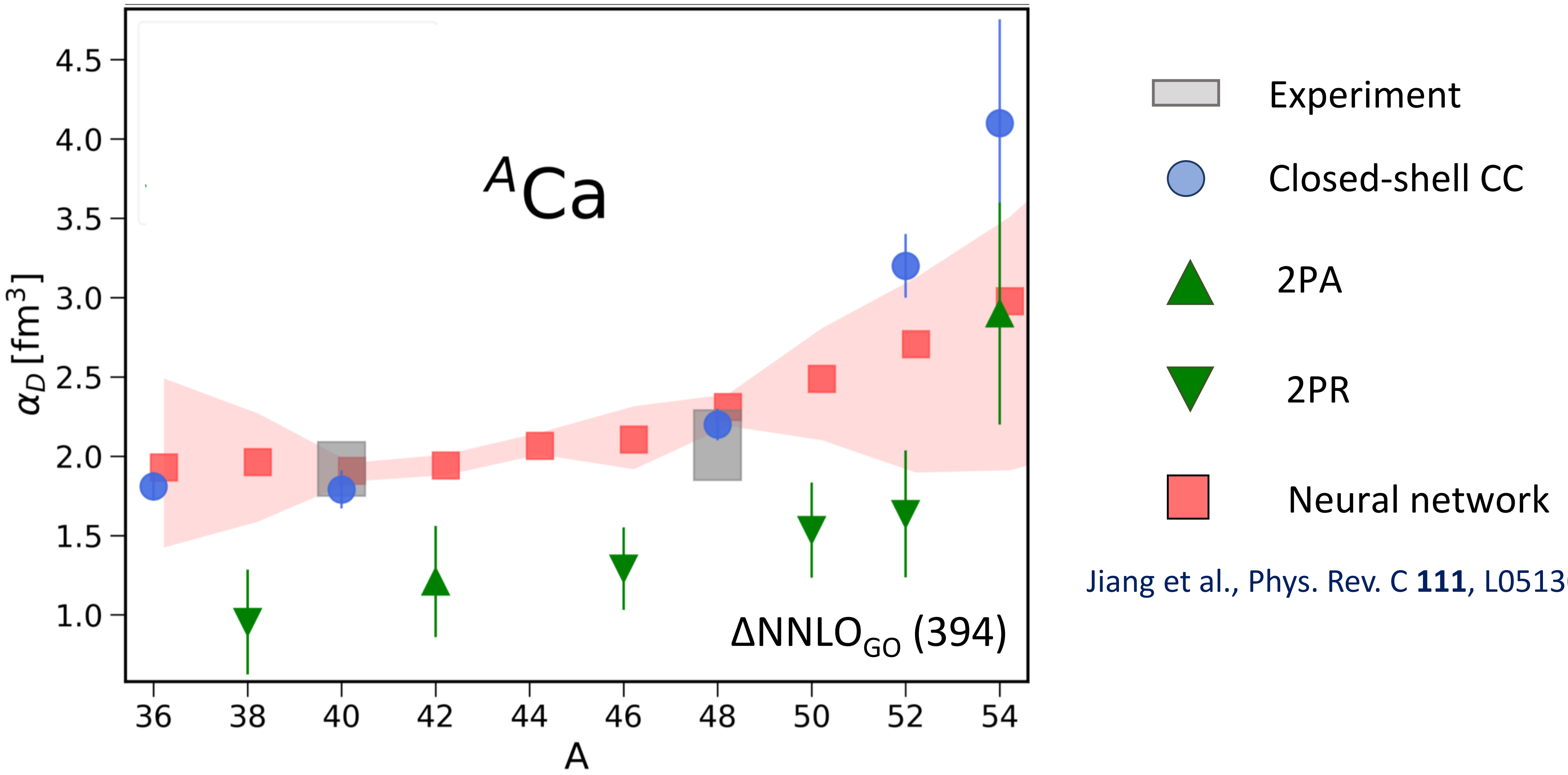
Inversion needed to find $R(\omega)$

Electric dipole polarizability in O isotopes

FM et al., Phys. Rev. C **112**, 014315 (2025)



Electric dipole polarizability in Ca isotopes

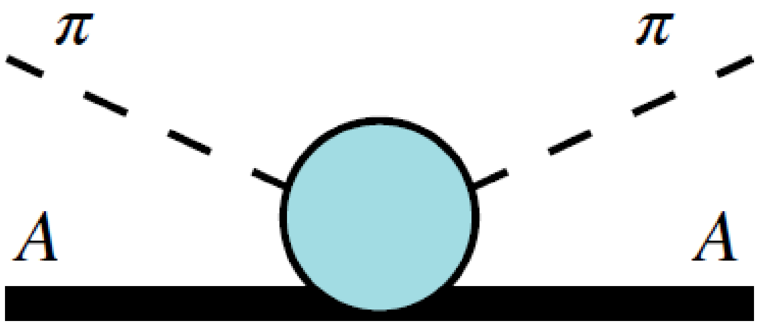


Jiang et al., Phys. Rev. C **111**, L051308 (2025)

Bridging structure and reactions:
Pion-nucleus elastic scattering

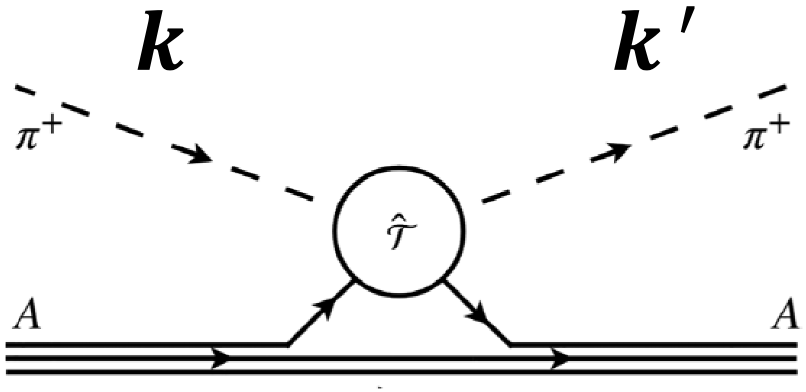
Motivation

Goal: understanding pion-nucleus elastic scattering using advanced nuclear **reaction** models combined with *ab initio* description of the **structure** of the target



V. Tsaran**, FM** et al., Phys. Rev. C **112**, 034608 (2025)

Leading-order scattering potential



$\boldsymbol{q} = \boldsymbol{k}' - \boldsymbol{k}$

$$V^{[1]}(\boldsymbol{k}', \boldsymbol{k}) = \mathscr{W}(\boldsymbol{k}', \boldsymbol{k})\mathrm{Tr}[\hat{f}(\boldsymbol{k}', \boldsymbol{k})\rho(\boldsymbol{q})]$$

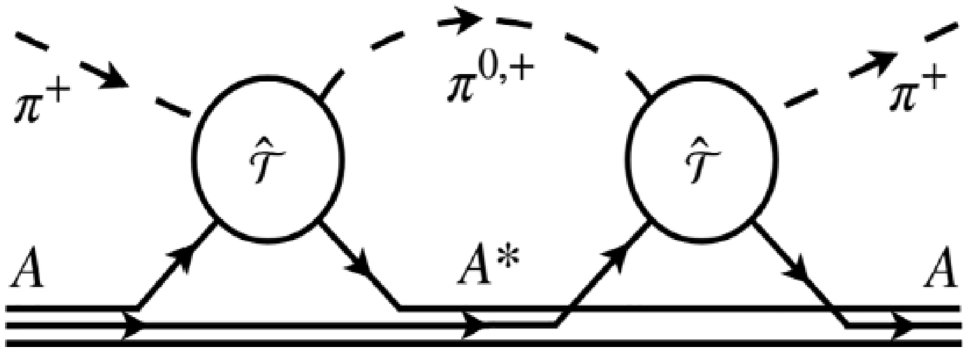
$\hat{f}$: In-medium pion-nucleon amplitude (fit to ^{12}C)

Tsaran et al., Phys. Rev. C **108**, 044608 (2023)

$\rho(\boldsymbol{q})$: One-nucleon form factors ⇨ Both proton and neutron form factors needed!

Second-order scattering potential

$$V^{[2]}$$

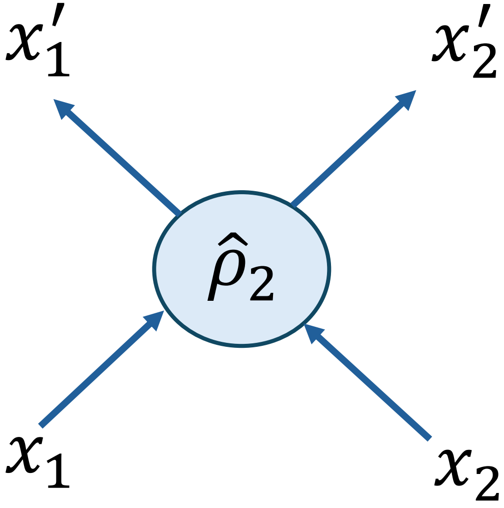


Pion re-scattering on nuclear excited states

Two-body density matrix

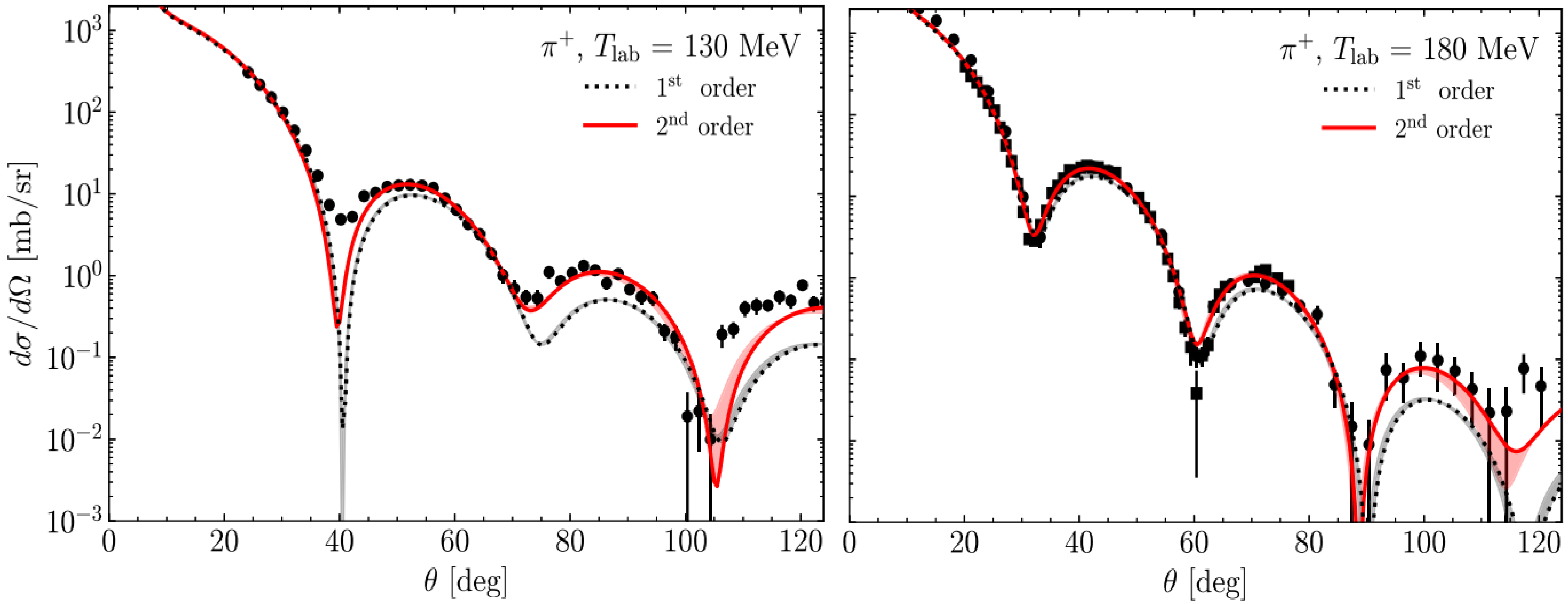
$$\hat{\rho}_2(x_1' x_2'; x_1 x_2) = \hat{\psi}^+(x_1')\,\hat{\psi}^+(x_2')\hat{\psi}(x_2)\hat{\psi}(x_1)$$

$$x = (\boldsymbol{r}, \tau, \sigma)$$



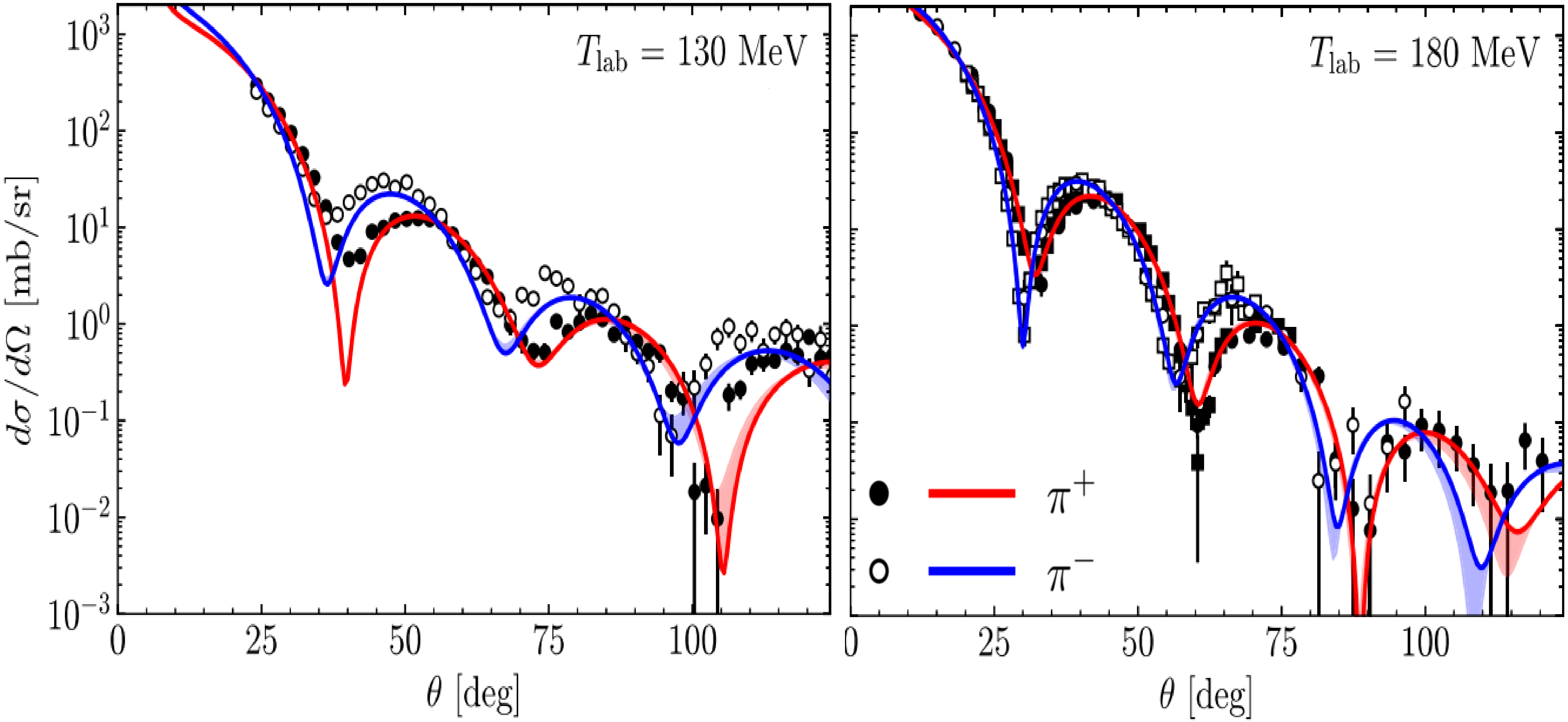
Impact of the second-order potential

π^+-^{48}Ca elastic cross sections



Second-order corrections improve the agreement with experimental cross sections

Pion-nucleus cross sections



Good description of the experimental cross-sections
with controlled nuclear-structure uncertainties

Conclusions and perspectives

- We have extended coupled-cluster theory to the ground state, excited states and electric dipole polarizability of open-shell nuclei close to magicity
- We have combined scattering theory with nuclear structure to describe pion-nucleus scattering
- Future developments: response of odd nuclei, response functions with theory uncertainties …

Registrations are open!

Many-body Theory:
Nuclear Physics Meets Quantum Chemistry

Aug 24th – Sep 4th 2026

Mainz Institute for Theoretical Physics

Organizers:

Francesco Marino (JGU Mainz)
Alexander Tichai (TU Darmstadt)
Sonia Bacca (JGU Mainz)
Jürgen Gauss (JGU Mainz)

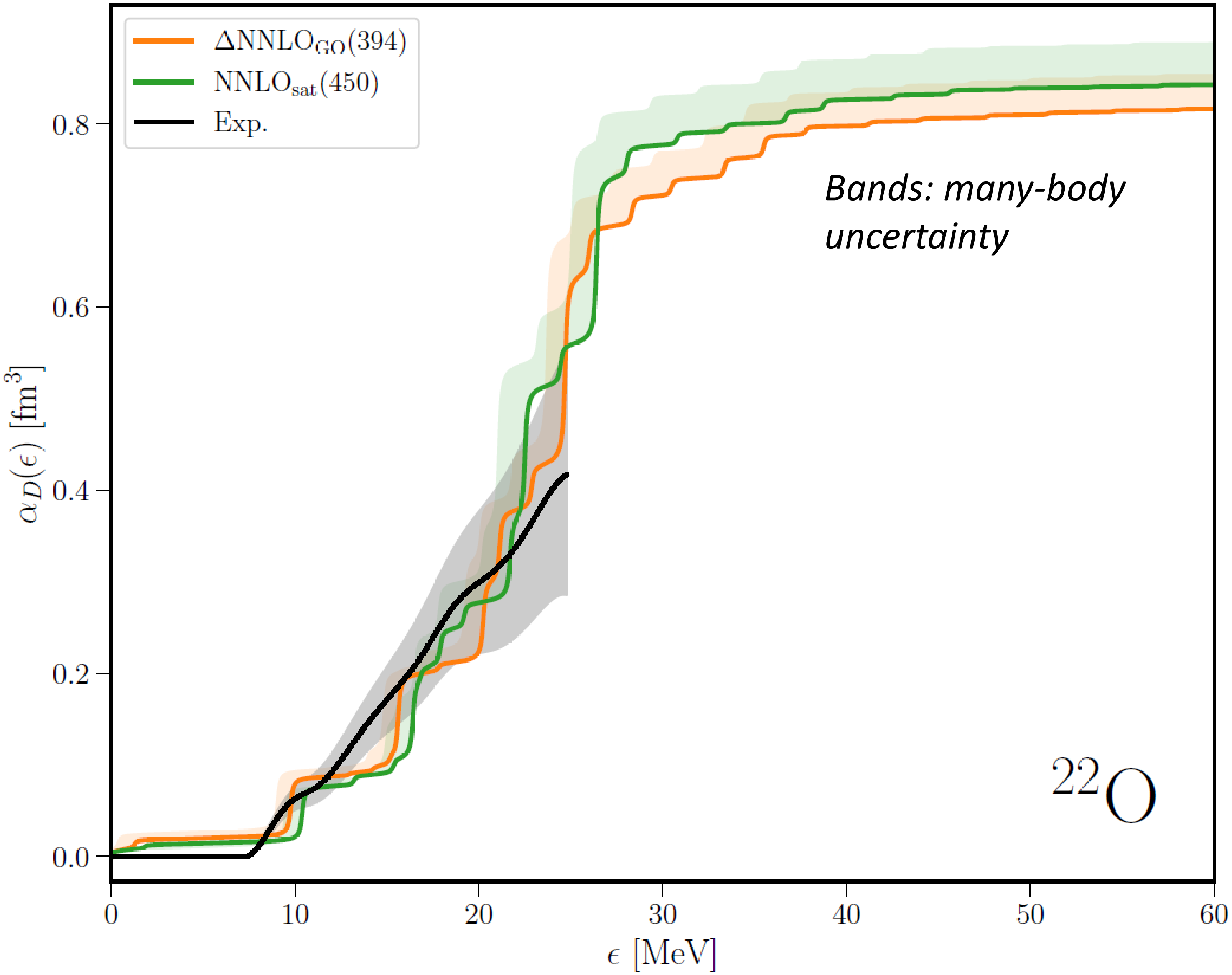
Thank you for your attention!

Collaborators

Bruxelles:	Pepijn Demol
CEA Saclay:	Thomas Duguet
Darmstadt:	Alexander Tichai
Knoxville:	Thomas Papenbrock
Mainz:	Sonia Bacca, Miriam El Batchy, Viacheslav Tsaran, Marc Vanderhaeghen
Oak Ridge:	Francesca Bonaiti , Gaute Hagen, Gustav Jansen

The ^{22}O electric dipole polarizability

Polarizability running sum



$$\alpha_D(\epsilon) = 2\alpha\hbar c \int_0^{\epsilon} d\sigma \frac{L(\sigma, \Gamma')}{\sigma}$$

$\Gamma' = 10^{-4}$ MeV

Good agreement between theory and experiment (up to 25 MeV)

FM, M. El Batchy, and S. Bacca, EPJ WoC 342, 01019 (2025)

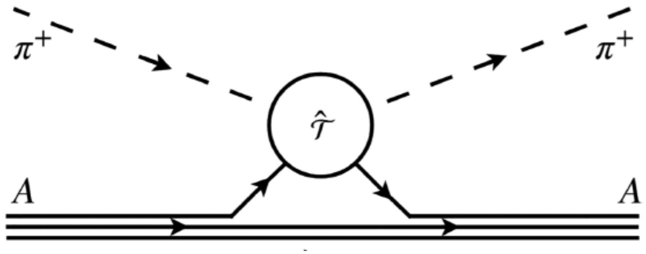
A primer on (multiple) scattering theory

$$F(\boldsymbol{k}', \boldsymbol{k}) = V(\boldsymbol{k}', \boldsymbol{k}) - \frac{A-1}{A} \int \frac{\mathrm{d}\boldsymbol{k}''}{2\pi^2} \frac{V(\boldsymbol{k}', \boldsymbol{k}'')F(\boldsymbol{k}'', \boldsymbol{k})}{k_0^2 - k''^2 + i\varepsilon}$$

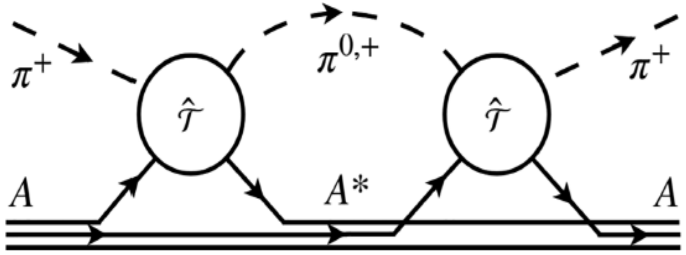
F: Elastic scattering amplitude

V: Pion-nucleus scattering potential

$$V(\boldsymbol{k}', \boldsymbol{k}) \approx V^{[1]}(\boldsymbol{k}', \boldsymbol{k}) + V^{[2]}(\boldsymbol{k}', \boldsymbol{k})$$



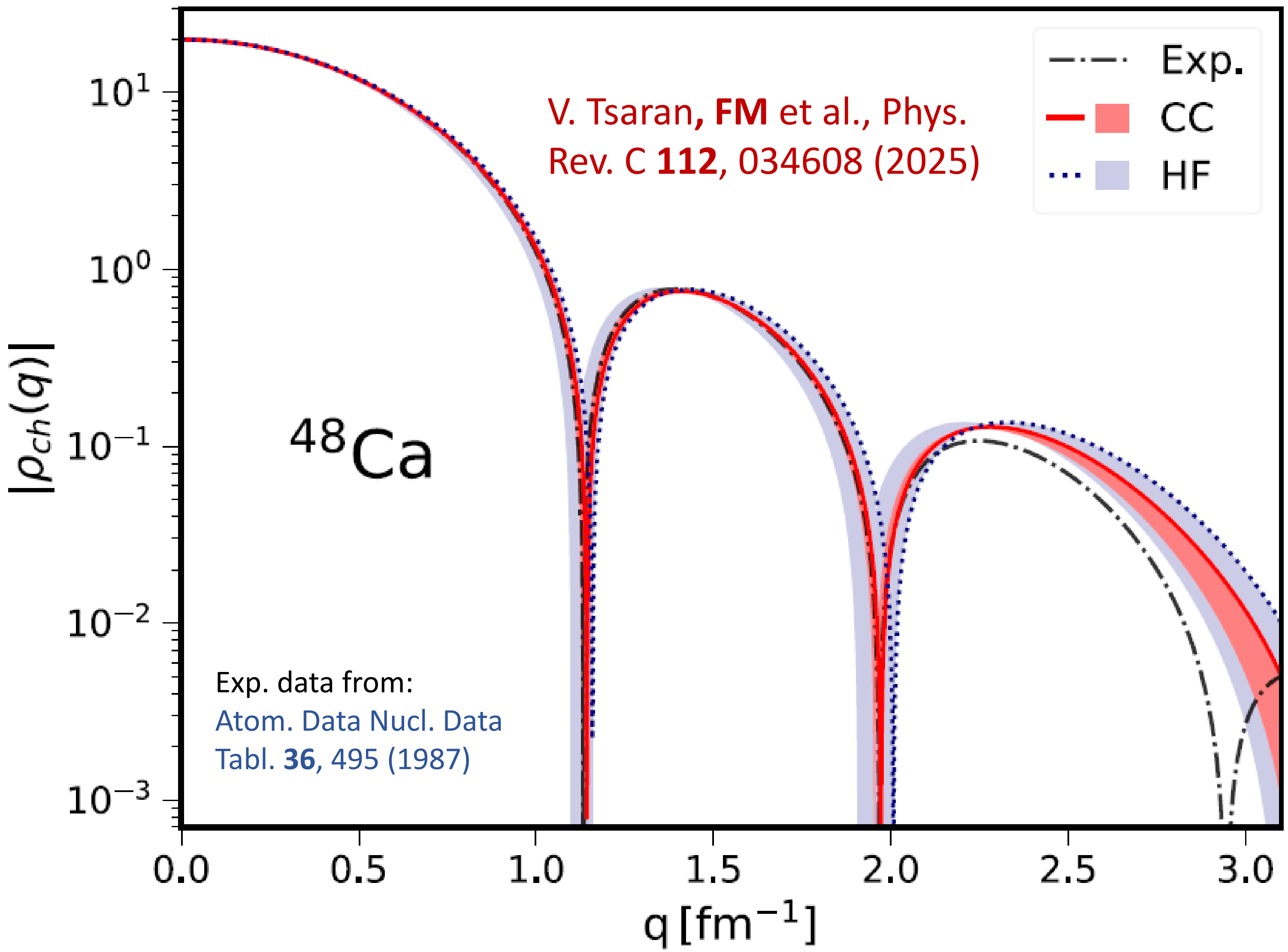
$V^{[1]}$



$V^{[2]}$

Validating the nuclear structure

^{48}Ca charge form factor



Coupled-cluster – CCSDT-1

Hartree-Fock

Mild interaction dependence (shaded band)

Excellent agreement up to the second minimum

The two-body density

Approximate $\hat{\rho}_2$ on the **Hartree-Fock** wave function $|\Phi_0\rangle$

$$\langle\Phi_0|\hat{\rho}_2(x_1'x_2';x_1x_2)|\Phi_0\rangle = \rho(x_1',x_1)\rho(x_1',x_1) - \rho(x_1',x_2)\rho(x_2',x_1)$$

⇨ Need just one-body density $\rho(x',x) = \langle\Phi_0\big|\hat{\psi}^+(x')\hat{\psi}(x)\big|\Phi_0\rangle$

V. Tsaran, **FM** et al., Phys. Rev. C **112**, 034608 (2025)