Electromagnetic response functions and electric dipole polarizability from coupled-cluster theory

JG|U

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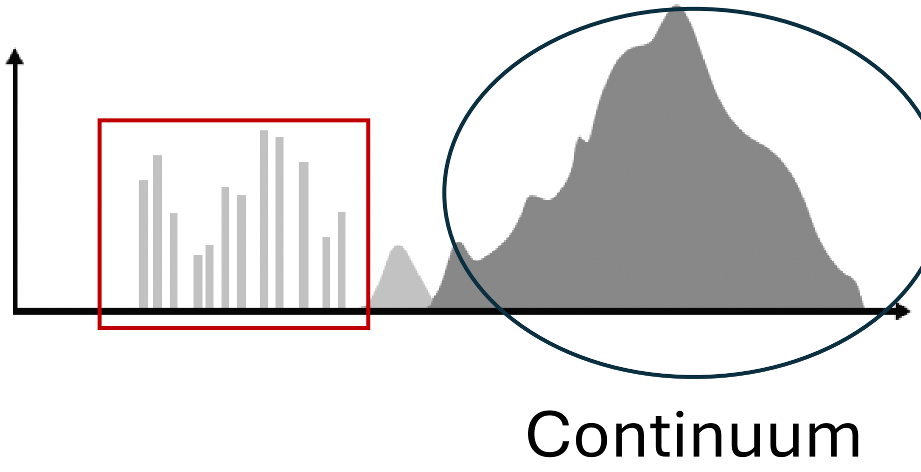
2025

Nuclear response functions

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

Θ: excitation operator



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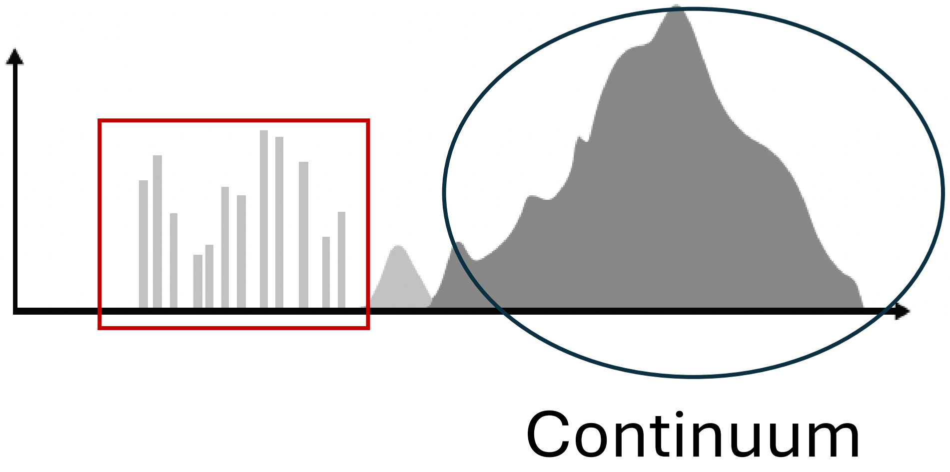


Θ: excitation operator

Electric dipole field $$\Theta = \sum_{i=1}^{Z} (\boldsymbol{r} - \boldsymbol{r}_{cm})_3$$

The response to the electric dipole is related to the photo-absorption cross section

$$\sigma_\gamma(\omega) = 4\pi^2 \alpha \omega R(\omega)$$

The equation of state of infinite nuclear matter

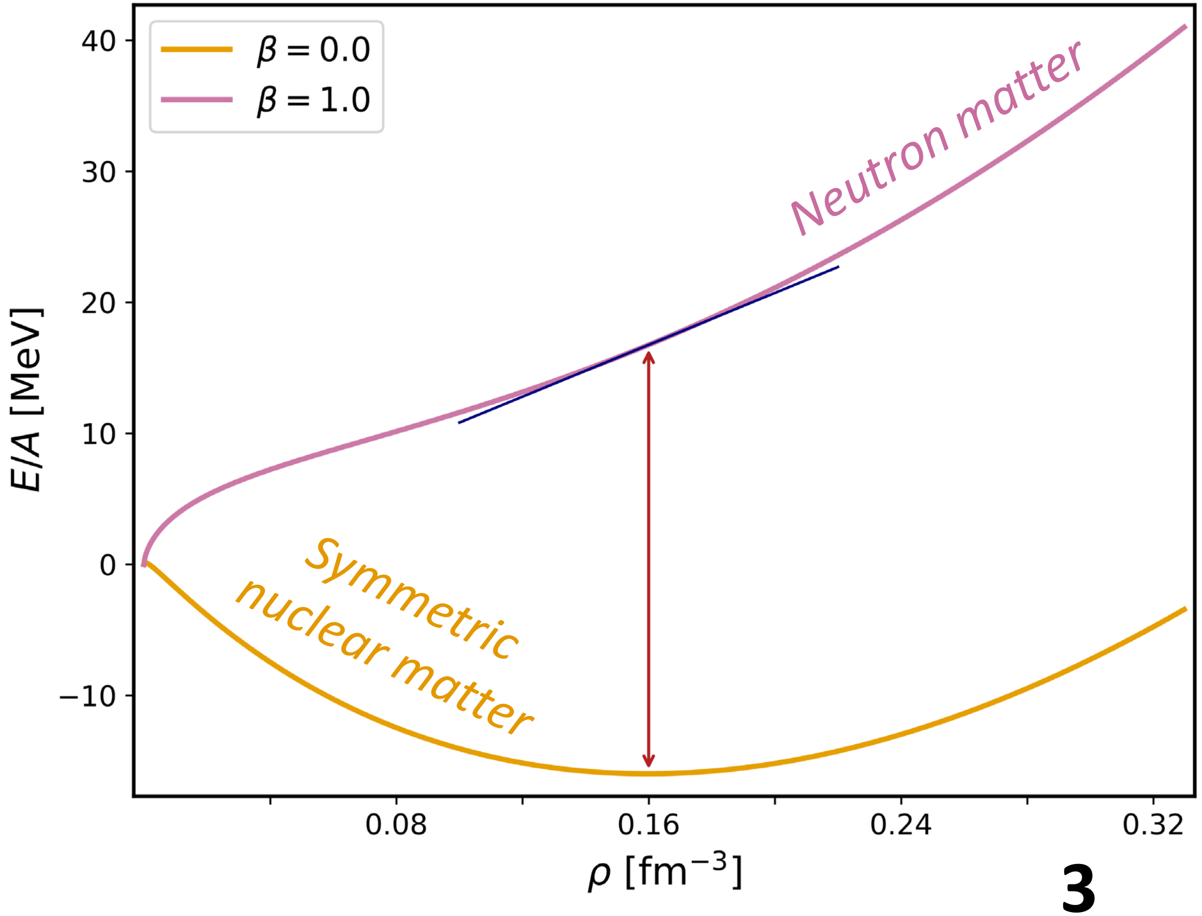
$$\frac{E}{A}(\rho,\beta) = \frac{E}{A}(\rho,0) + S(\rho)\beta^2 + O(\beta^4)$$

$$\rho = \rho_n + \rho_p$$

$$\beta = \frac{\rho_n - \rho_p}{\rho}$$

Symmetry energy

$$S(\rho) = J + \frac{\rho - \rho_0}{3\rho_0} L$$



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Symmetry energy

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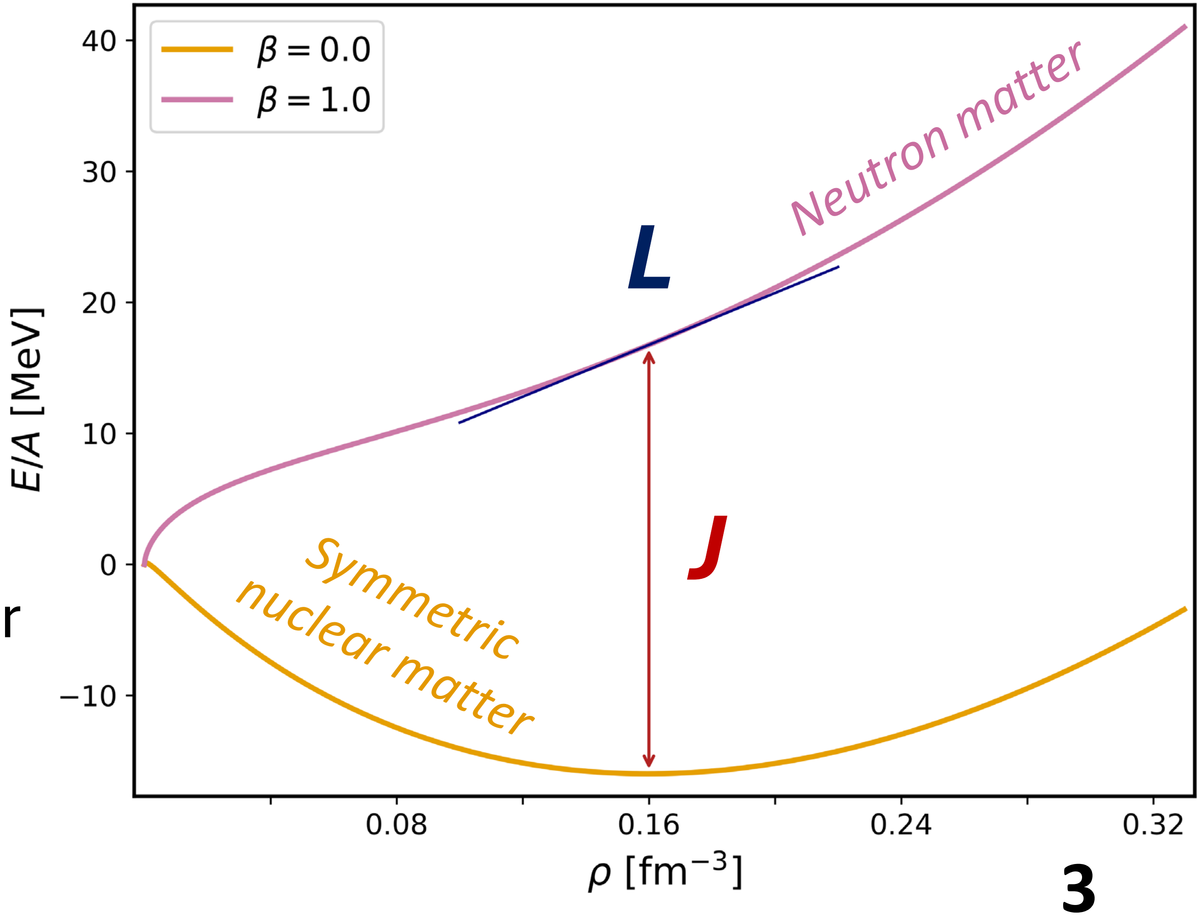
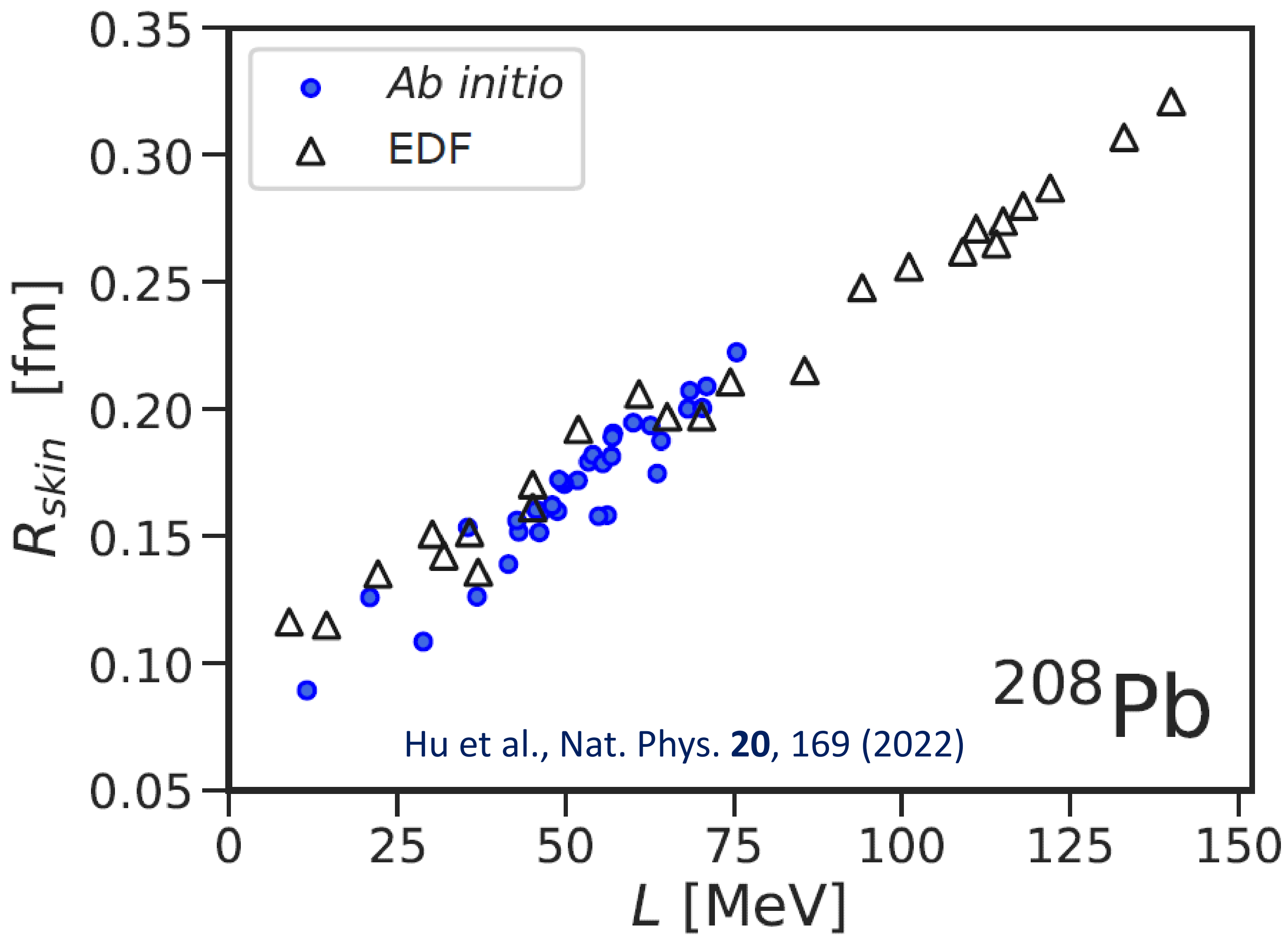
J: symmetry energy at saturation density

L: slope parameter



How do we constrain the slope *L*?

Exploit correlations with measurable nuclear properties



Neutron skins

$$R_{skin} = R_n - R_p$$

Well-defined trend, but difficult to measure neutron radii

The electric dipole polarizability

Electric dipole polarizability $$\alpha_D = 2\alpha \int d\omega \frac{R(\omega)}{\omega}$$

Neumann-Cosel et al.,
Front. Phys. **13**, 1629987 (2025)

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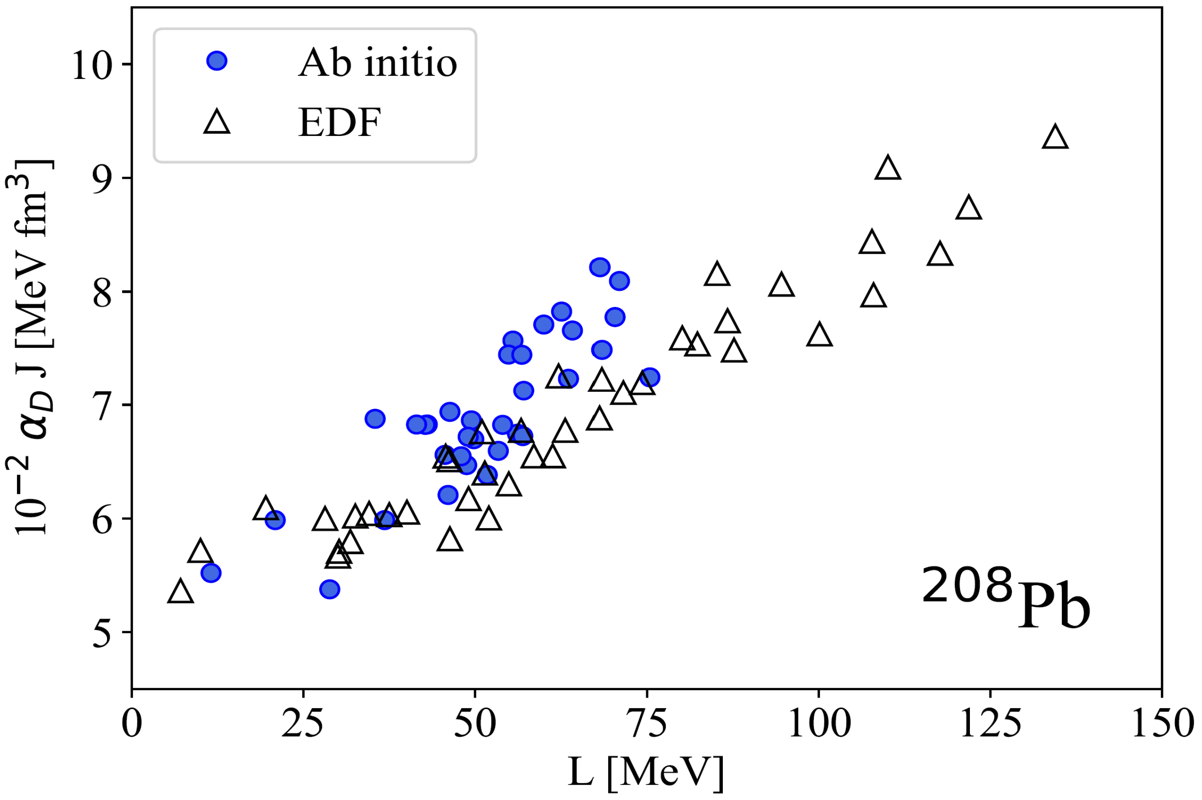
Courtesy: Francesca Bonaiti



Strong linear correlation between α_D and the slope of the symmetry energy L

Coupled-cluster theory

Coupled-cluster (CC) ground-state

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

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

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CCSDT-1: approximate triples

$$T \approx T_1 + T_2 + T_3 + \cdots$$

n-particle *n*-hole amplitudes

CCSD

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

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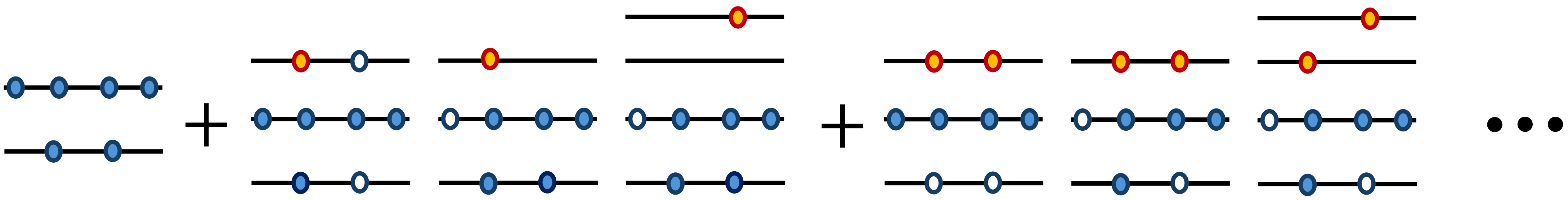
CCSD

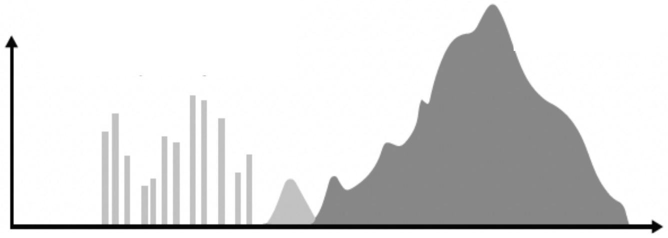
$|\Psi_0\rangle =$



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

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

The LIT-CC method



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

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)

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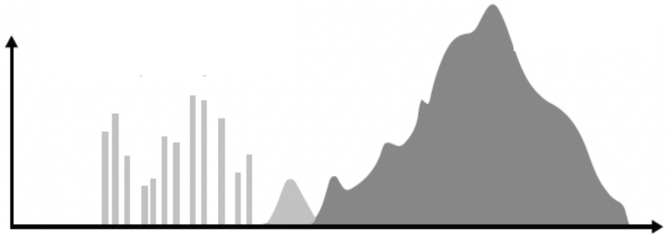

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- Sum rules of the response directly from $L(\sigma, \Gamma \to 0)$
- Inversion needed to find $R(\omega)$

The LIT-CC method

Pseudo-states from Schödinger eqs with source term

$$(\,\overline{H} - z)\left|\widetilde{\Psi}_R\right\rangle = \overline{\Theta}|\Phi_0\rangle \qquad z = \sigma + i\Gamma$$

Similarity-transformed operators

$$\overline{H} = e^{-T}\widehat{H}_N\, e^T$$
$$\overline{\Theta} = e^{-T}\widehat{\Theta}_N\, e^T$$

Correlations included through ground-state amplitudes *T*

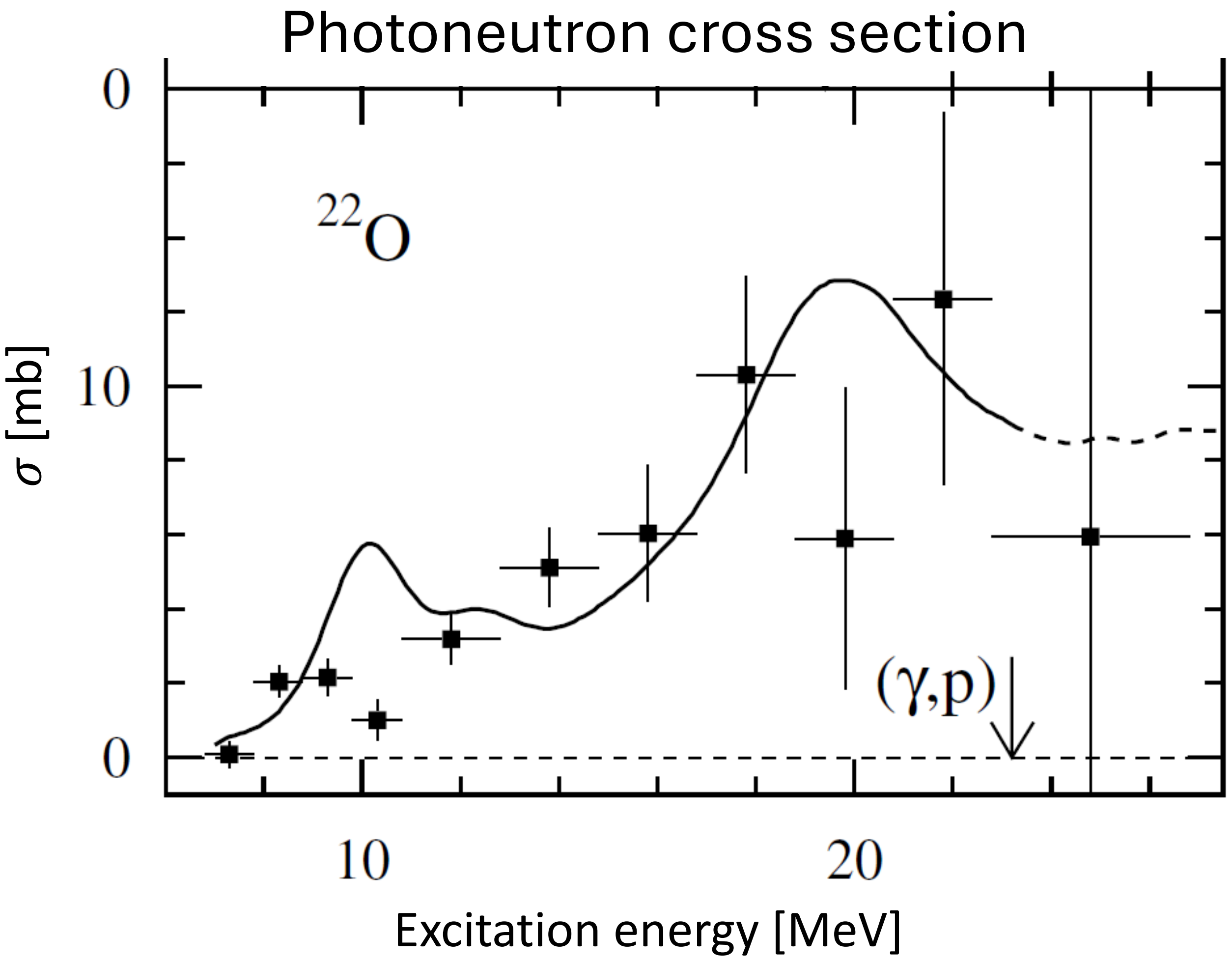
$\left|\widetilde{\Psi}_R\right\rangle$ obtained in the space of 2p2h configurations

Electric dipole response of ^{22}O from coupled-cluster theory

A study of ^{22}O

^{22}O is one of the few neutron-rich nuclei for which the dipole response has been measured

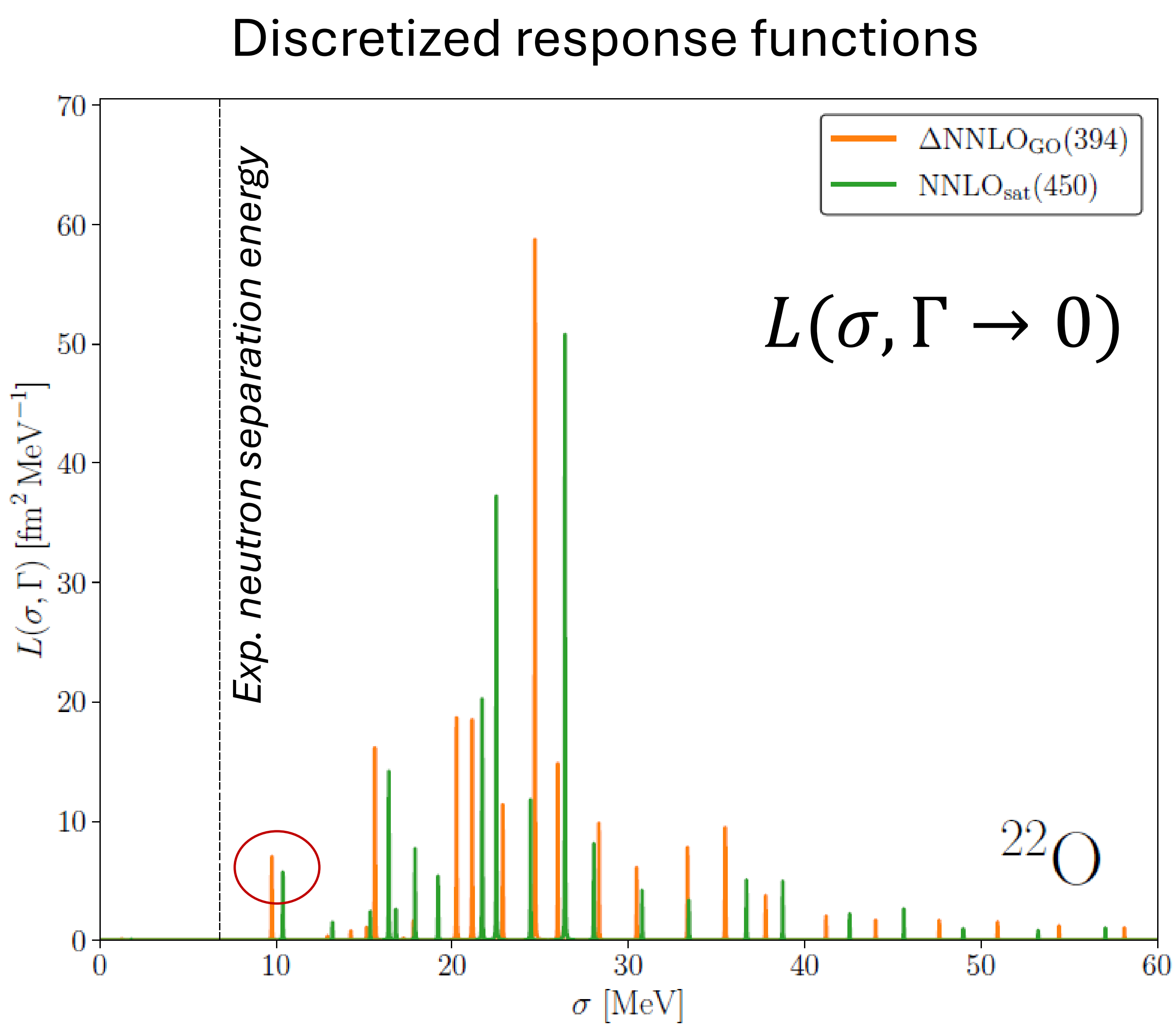
Leistenschneider et al., Phys. Rev. Lett. 86, 5442 (2001)



Photoneutron cross-section extracted from electromagnetic excitations cross-sections

Caveats: limited energy range, proton decay channel not resolved

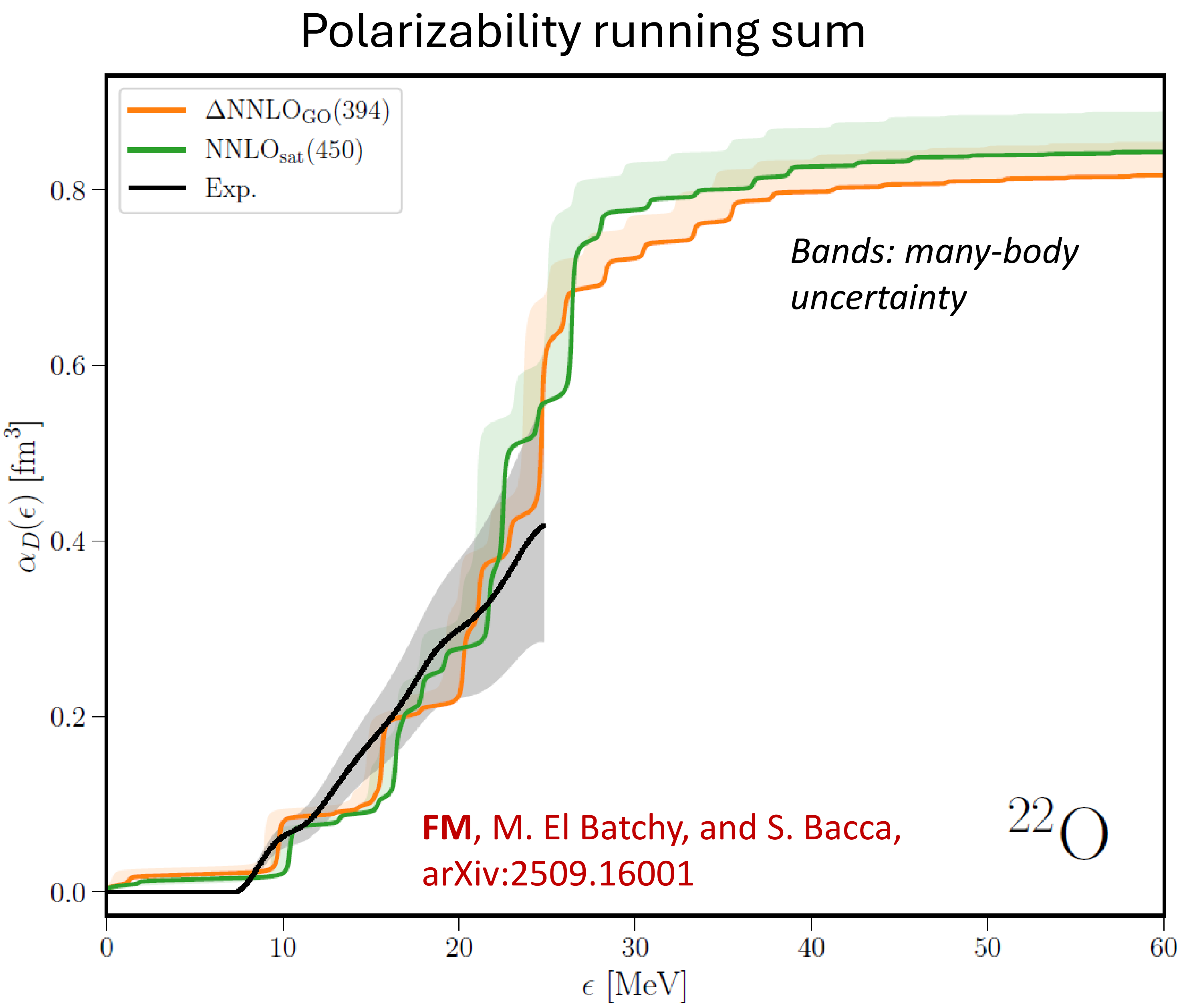
Theory predictions: the LIT



Calculations at the CCSDT-1 level

LIT-CC consistently predicts **low-lying strength** near the neutron threshold

The ^{22}O electric dipole polarizability



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

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

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

From the LIT to the response function

Problem: Determine the response function $\boldsymbol{R(\omega)}$ **from the LIT**

$$L(\sigma, \Gamma) \Longrightarrow R(\omega)$$

Ill-posed numerical inversion!

From the LIT to the response function

Problem: Determine the response function $\boldsymbol{R(\omega)}$ **from the LIT**

$$L(\sigma,\Gamma) \Longrightarrow R(\omega)$$ Ill-posed numerical inversion!

Ansatz: Basis expansion with hyperparameters α, β, ν

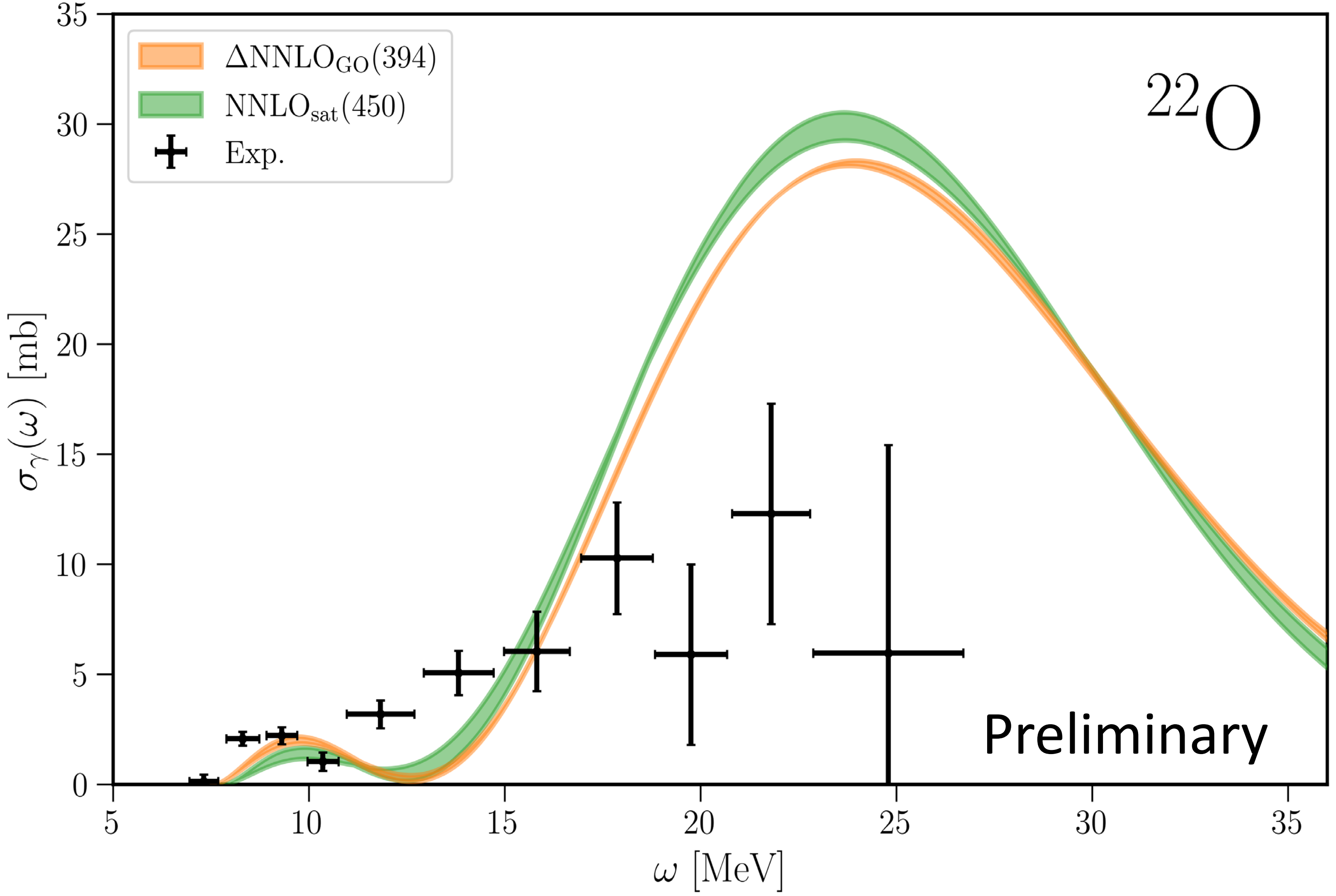
$$\tilde{R}(\omega) = \sum_{n=1}^{\nu} c_n f_n(\omega;\alpha,\beta) \qquad f_n(\omega;\alpha,\beta) = \omega^{\alpha} e^{-\frac{\omega}{n\beta}}$$

χ^2 minimization $$\chi^2 = \left| L(\sigma,\Gamma) - \tilde{L}(\sigma,\Gamma) \right|^2$$

Uncertainties on $R(\omega)$ from varying the number of basis states ν and width Γ

^{22}O cross sections

Credit: Miriam El Batchy



$$\sigma_\gamma(\omega) = 4\pi^2 \alpha \omega R(\omega)$$

Exp. photoneutron cross sections from [Phys. Rev. Lett. 86, 5442 (2001)]

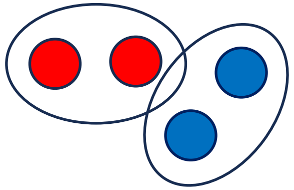
Cross sections with quantified **uncertainties** from the **inversion** of the LIT

Structure and electric dipole polarizability of open-shell nuclei

Towards open-shell nuclei

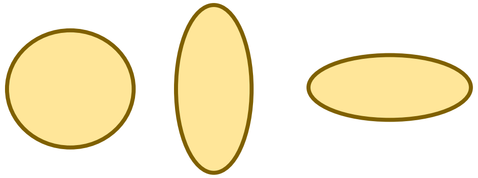
Symmetry-breaking approaches

Pairing



Bogoliubov CC

Deformation



Deformed CC

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

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

Towards open-shell nuclei

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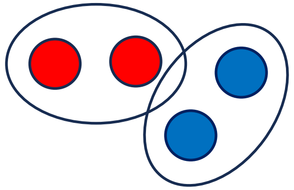

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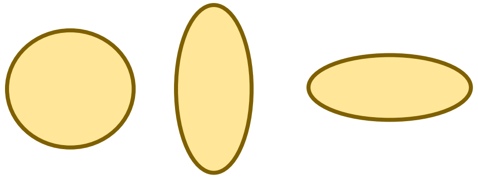

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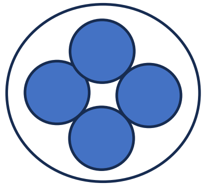
Equations-of-motion

Closed-shell



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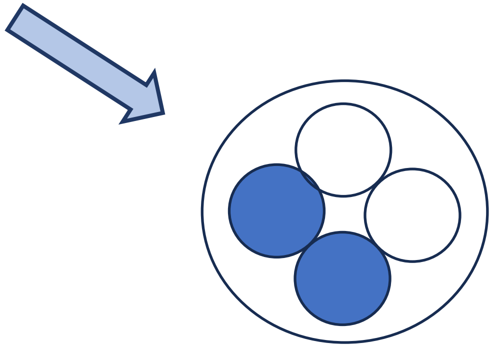

Two-particle-removed (2PR) nucleus

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

Towards open-shell nuclei

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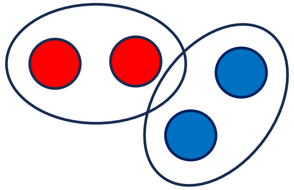

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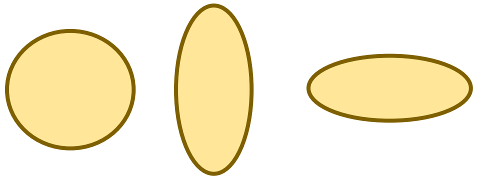

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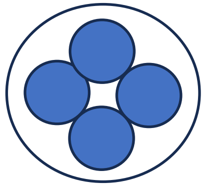

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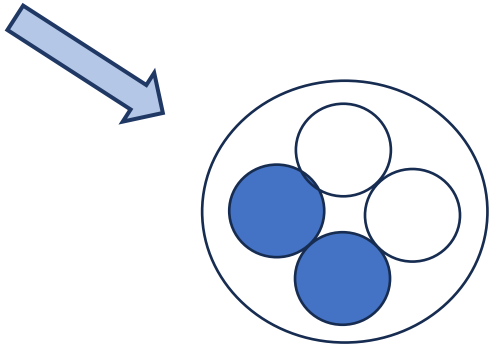
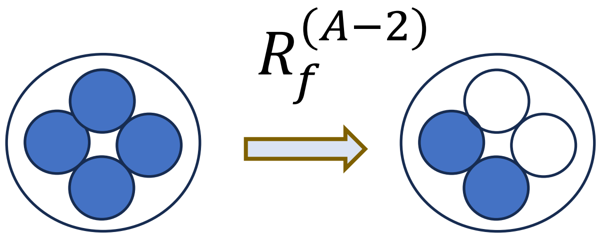


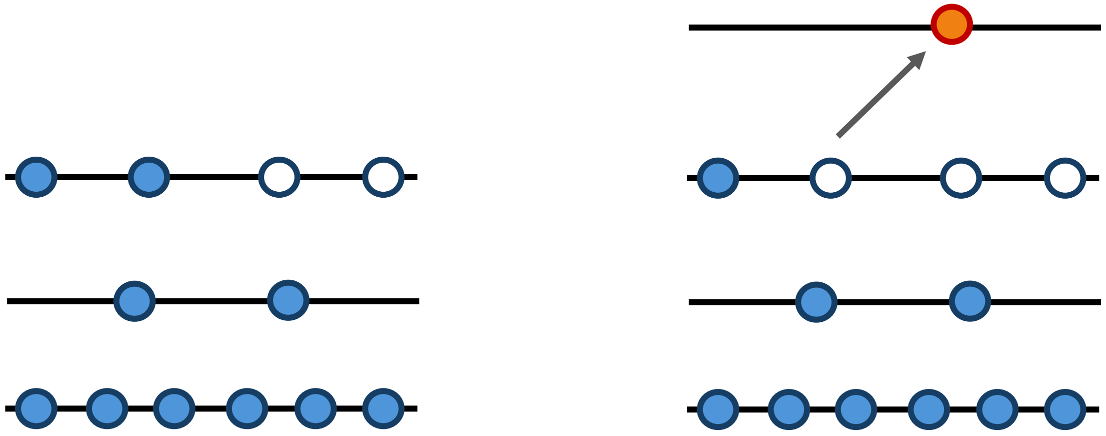
Two-particle-removed (2PR) nucleus

Excitation operator

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

The two-particle-removed ansatz





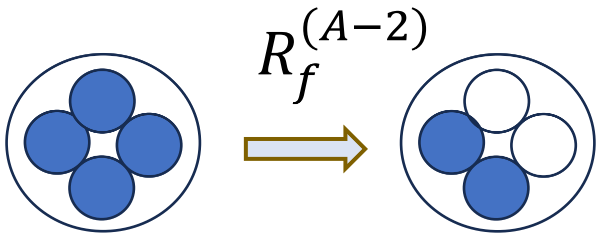
Two-hole

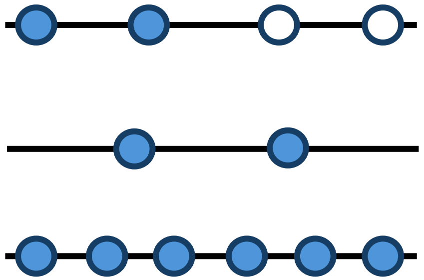
One-particle three-hole

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

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

The two-particle-removed ansatz





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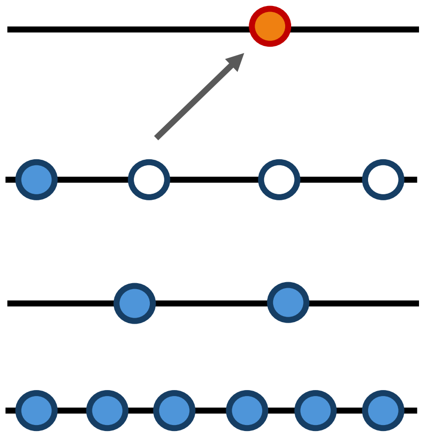

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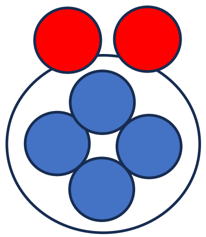
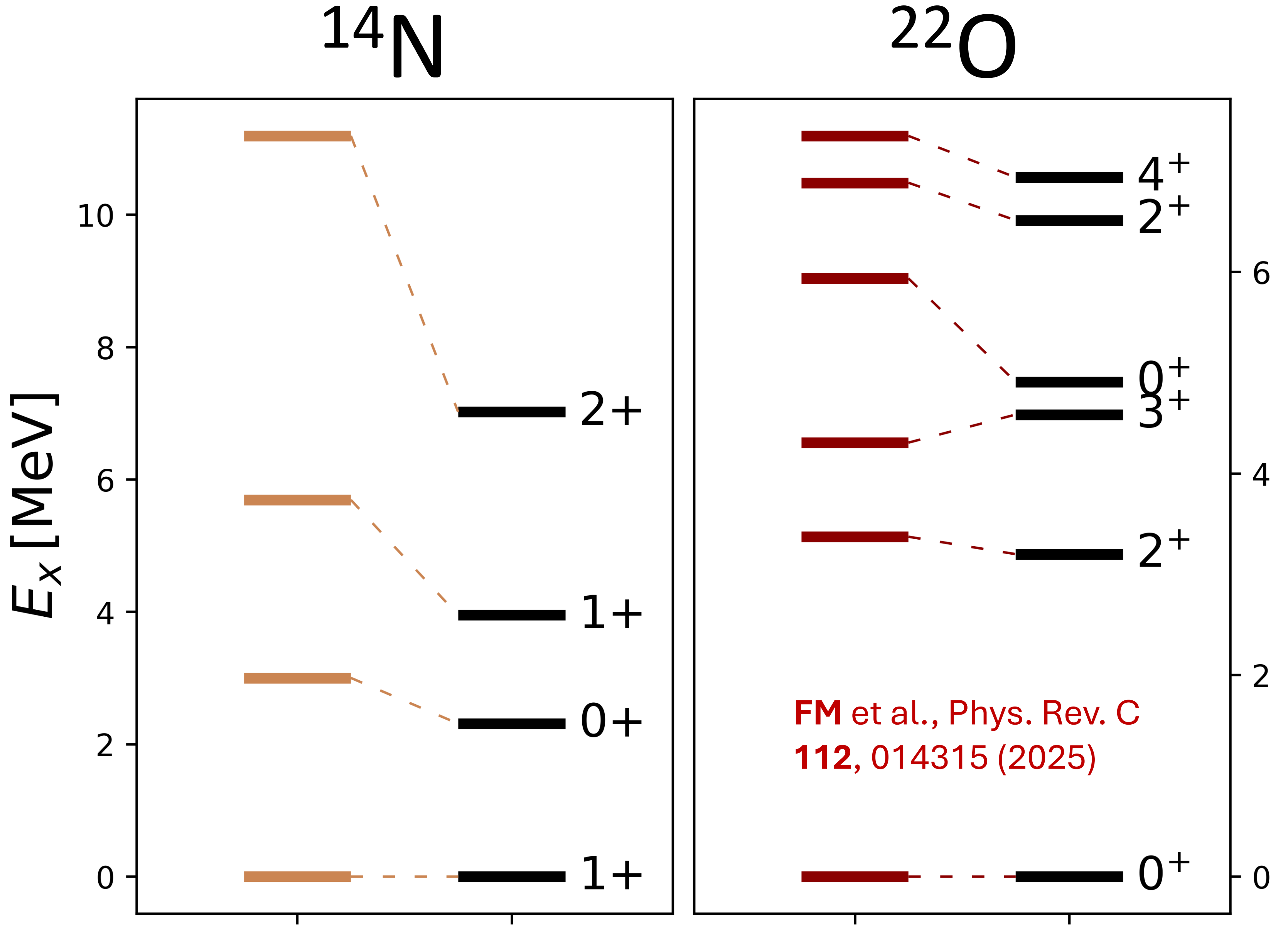
See also

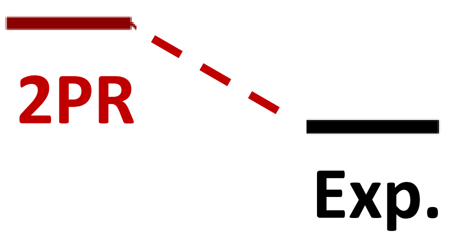


Two-particle-attached (2PA)

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

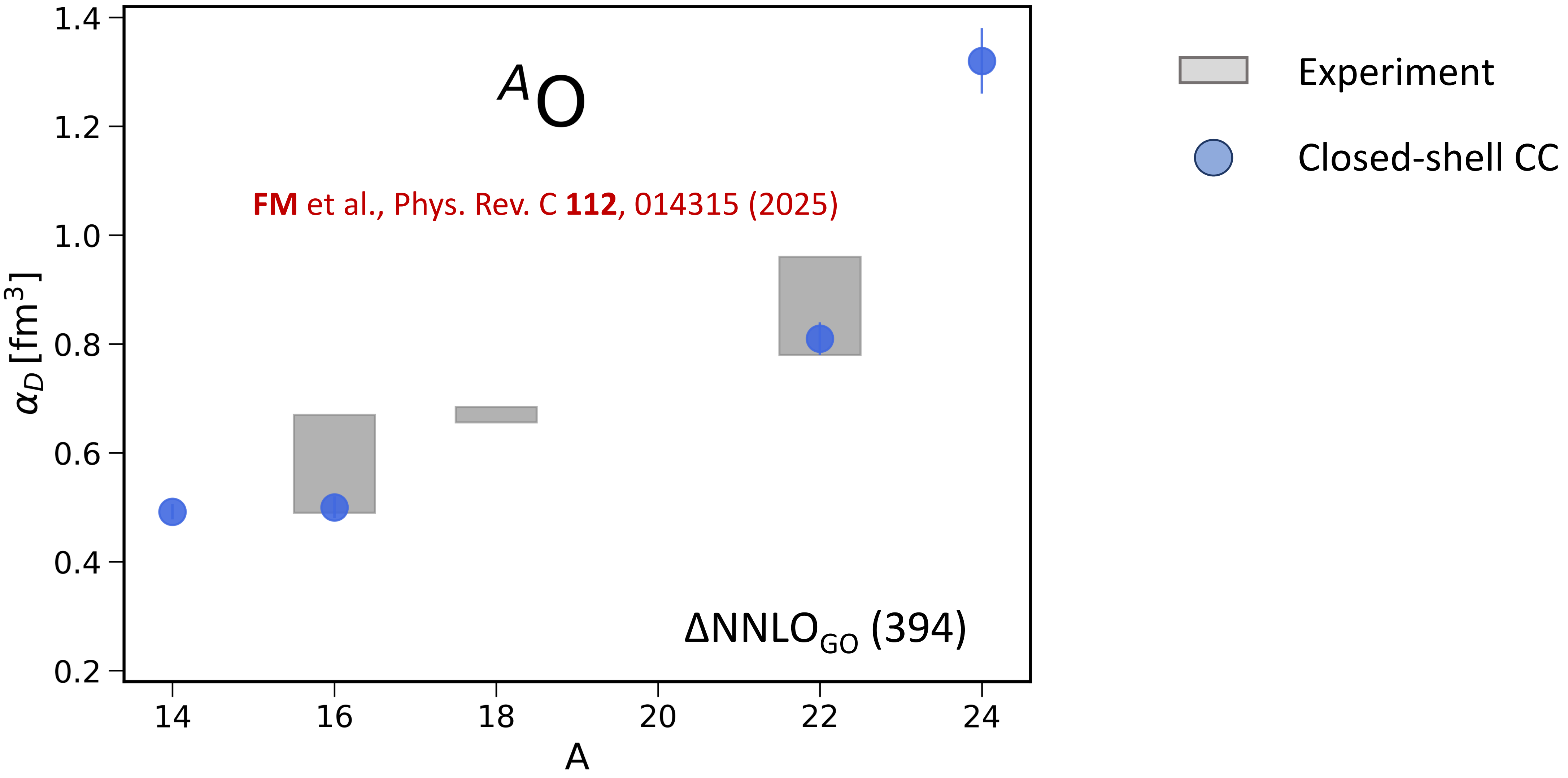
Low-lying spectra





2PR with the $\Delta NNLO_{GO}$ (394) interaction describes well several **excited states**

Electric dipole polarizability in O isotopes



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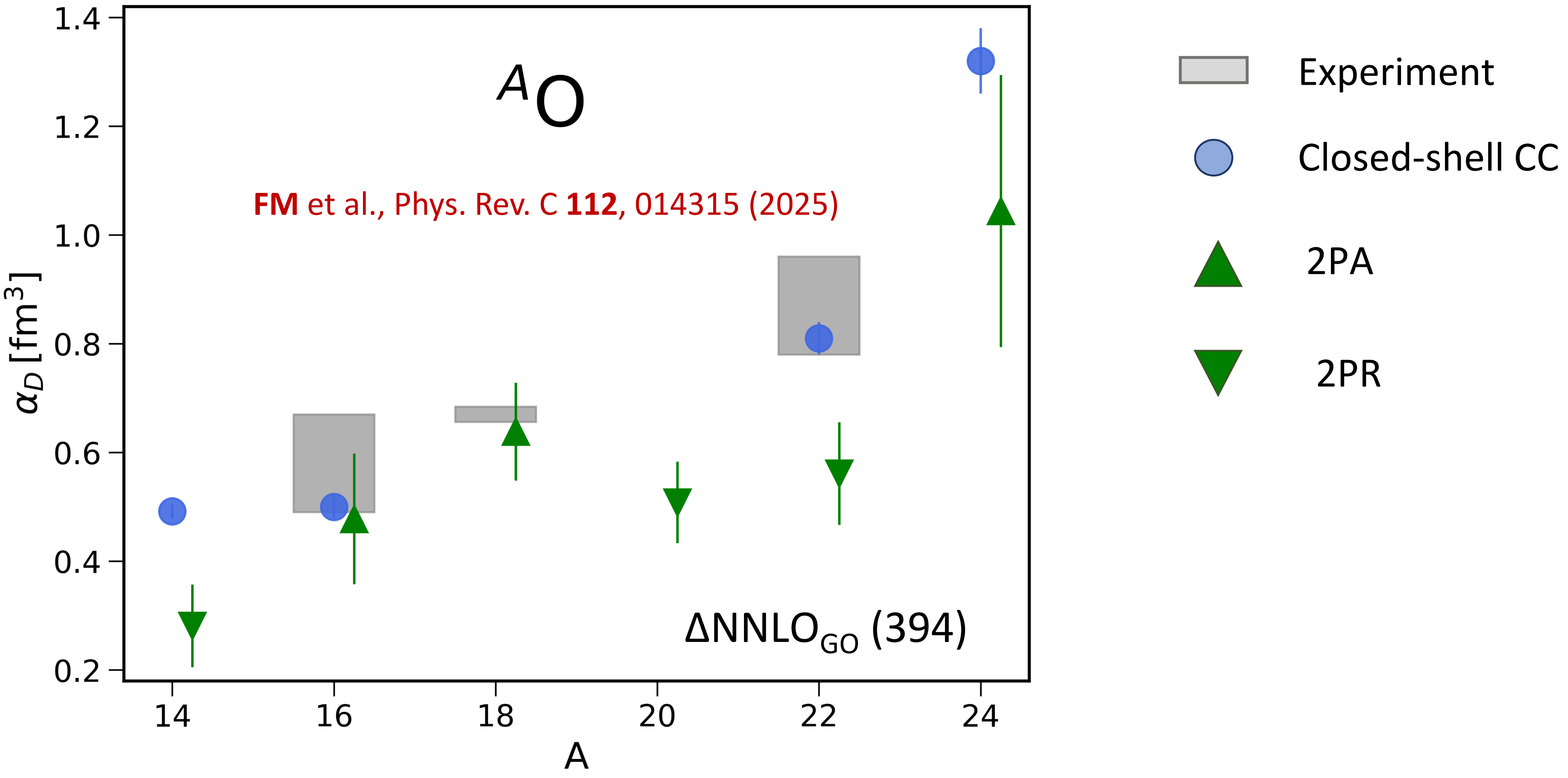
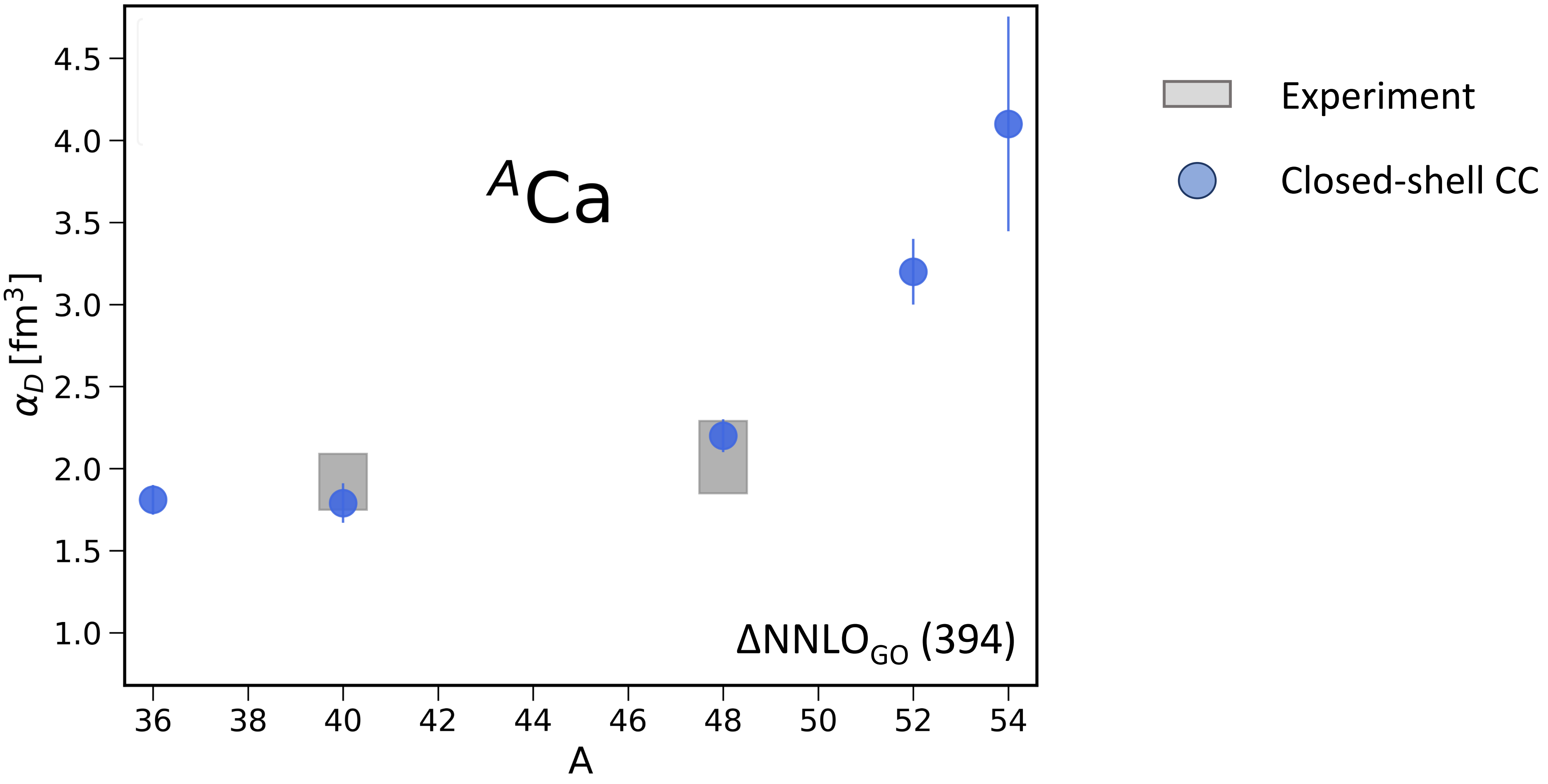


Electric dipole polarizability in Ca isotopes



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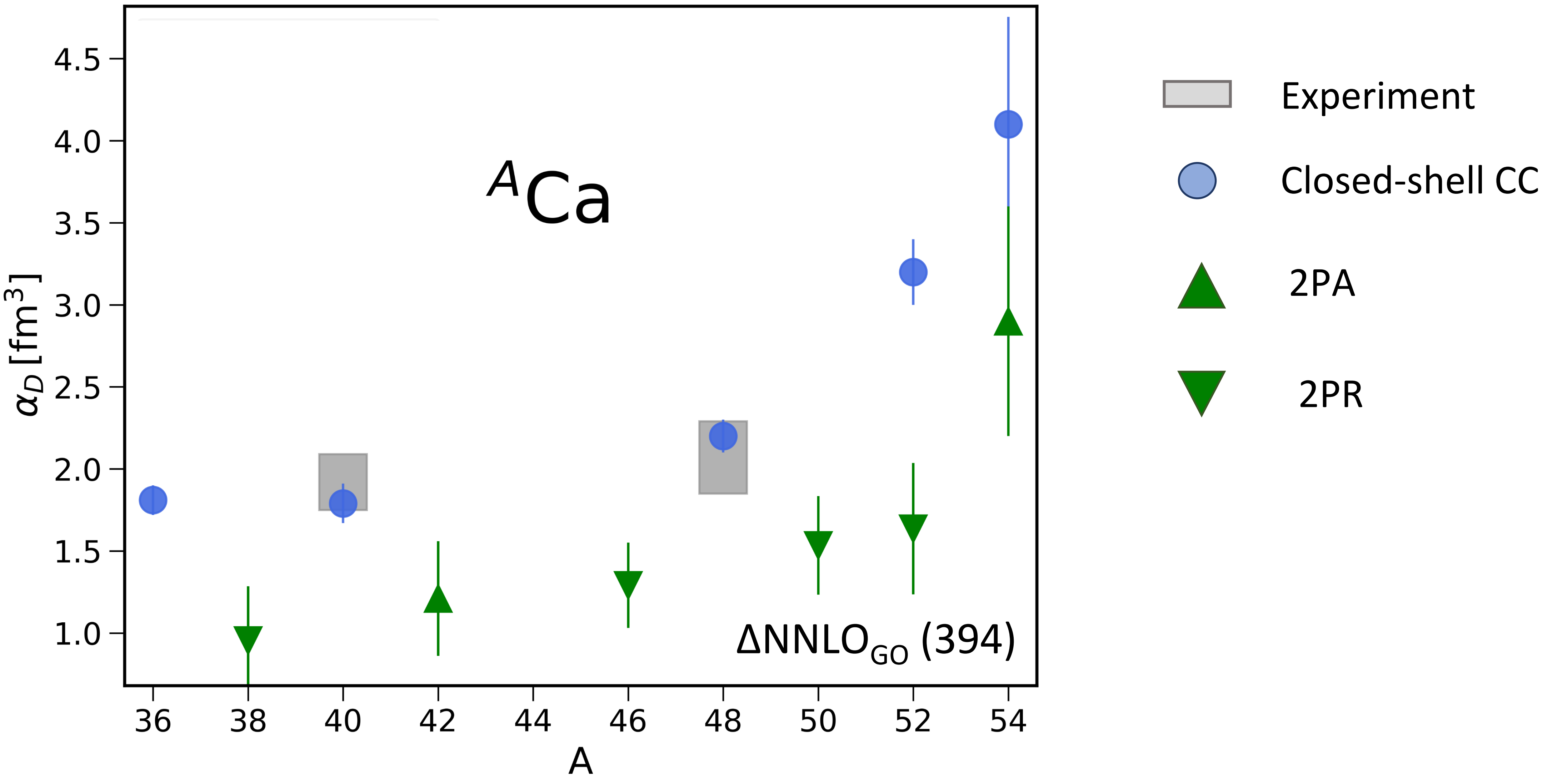

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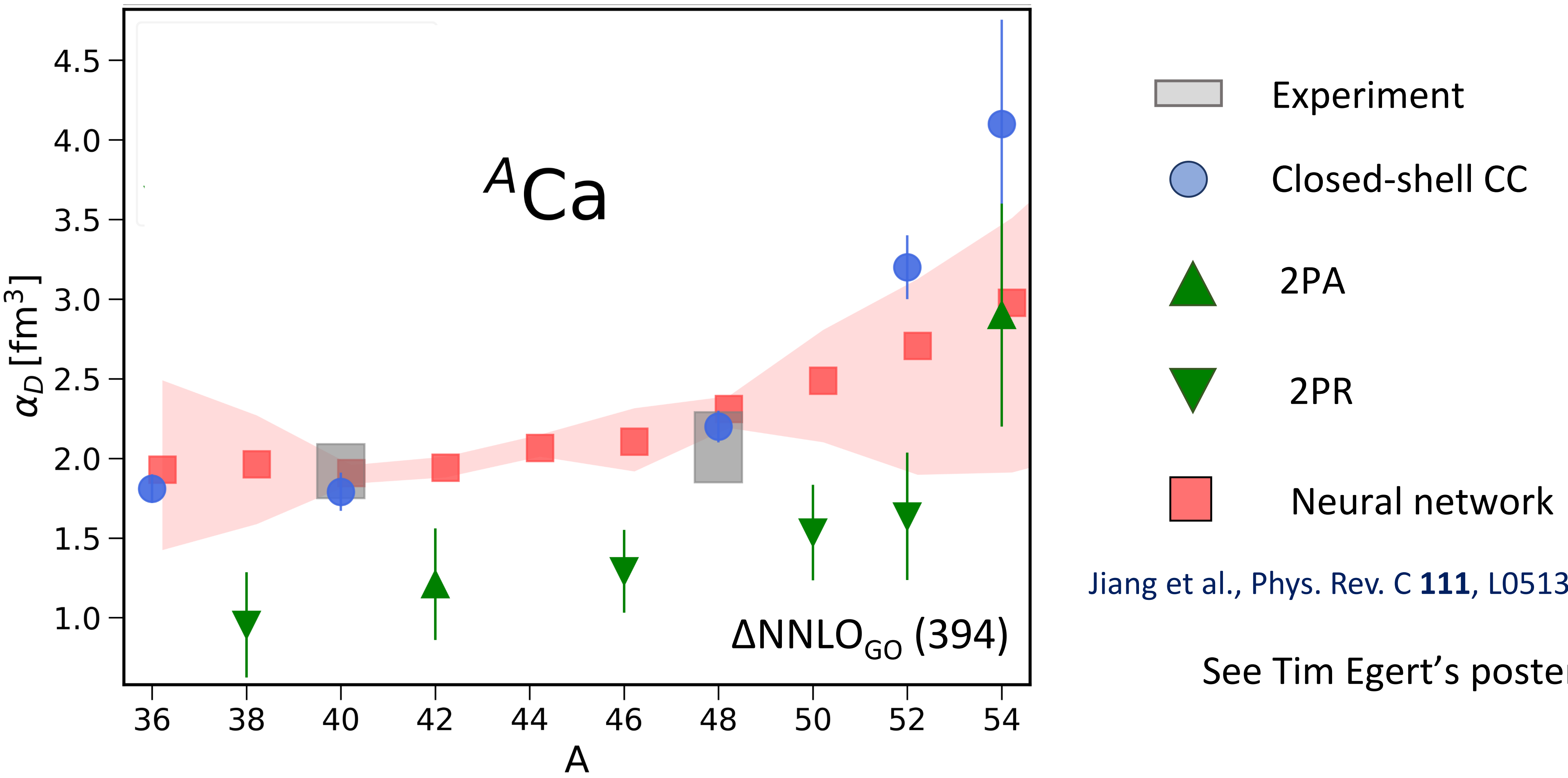

Jiang et al., Phys. Rev. C **111**, L051308 (2025)

See Tim Egert's poster

Conclusions and perspectives

- We have applied coupled-cluster to the dipole response and electric dipole polarizability of the neutron-rich O22 isotope

- We have extended the method to the ground state, excited states and electric dipole polarizability of open-shell nuclei close to magicity

- Future developments: response of odd nuclei, response functions with theory uncertainties …

Stay tuned!

Many-body Theory:
Nuclear Physics Meets Quantum Chemistry

Aug 24th – Sep 4th 2026

Mainz Institute for Theoretical Physics

Organizers:
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Alexander Tichai (TU Darmstadt)
Sonia Bacca (JGU Mainz)
Jürgen Gauss (JGU Mainz)