

Electromagnetic observables from first principles

Sonia Bacca

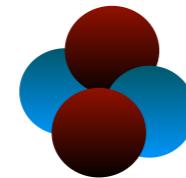
Johannes Gutenberg Universität Mainz

January 17th, 2023

Hirschgägg 2023: Effective field theories for nuclei and nuclear matter

Ab initio nuclear theory

- Start from neutrons and protons as building blocks
(centre of mass coordinates, spins, isospins)

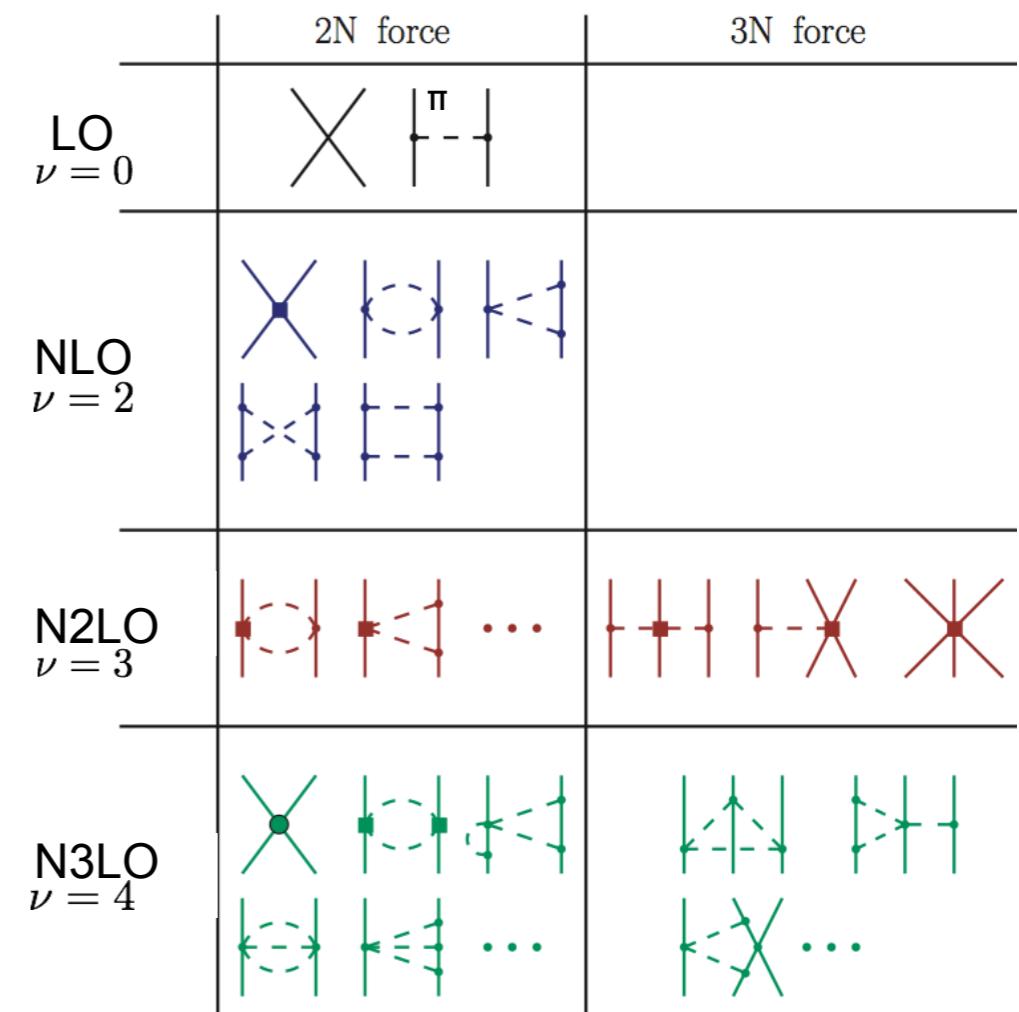


- Solve the non-relativistic quantum mechanical problem of A-interacting nucleons

$$H|\psi_i\rangle = E_i|\psi_i\rangle$$

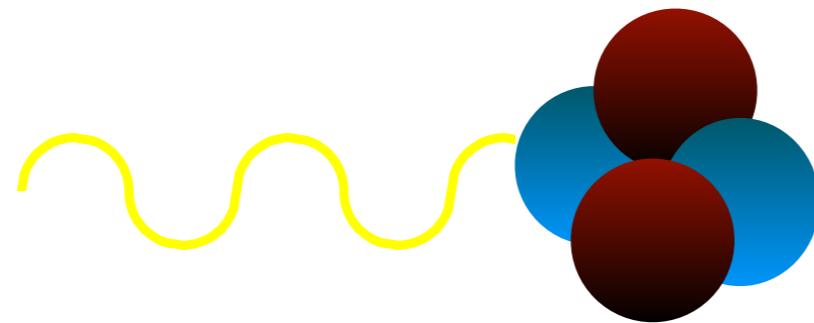
$$H = T + V_{NN}(\Lambda) + V_{3N}(\Lambda) + \dots$$

using interactions from chiral effective field theory



- Find numerical solutions with no approximations or controllable approximations

Coupling to the electromagnetic field



Cross
Section

$$\sigma_{ew} \sim R(\omega) = \sum_f \left| \langle \psi_f | \Theta | \psi_0 \rangle \right|^2 \delta(E_f - E_0 - \omega)$$



Em operator

The n $p \longleftrightarrow d \gamma$ reaction

B. Acharya and SB, Phys. Lett. B 827, 137011 (2022)



Dr. Bijaya Acharya

Semilocal NN forces up to 5th order from Reinert, Krebs, Epelbaum, Eur. Phys. J. A 54 (2018) 86
and fixed em operator: two-body + two-body (one-pion exchange level)

Uncertainty quantifications with tools developed by the Buqeye collaboration

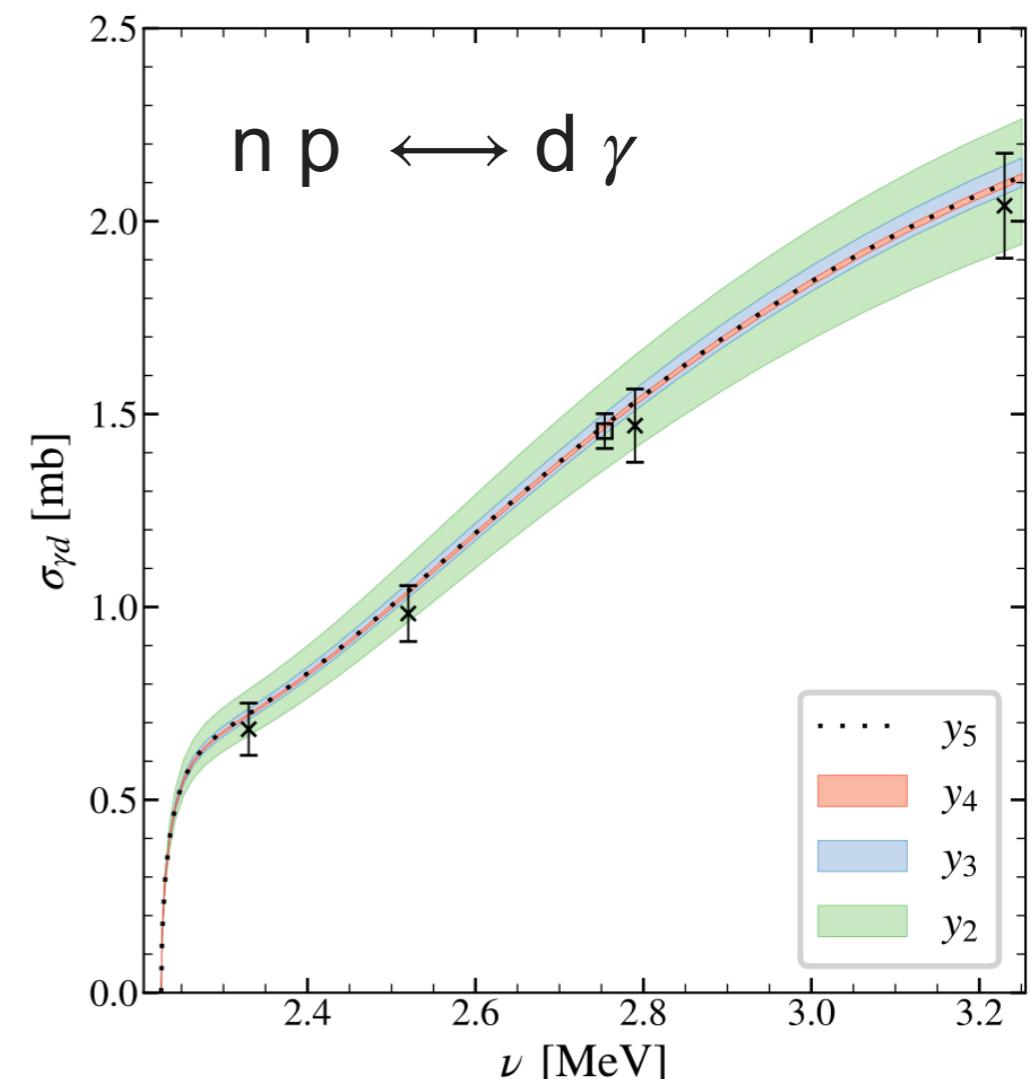
- Express observable as

$$y(\nu) = y_{ref}(\nu) \sum_{n=0}^{\infty} c_n(\nu) (Q/\Lambda)^n$$

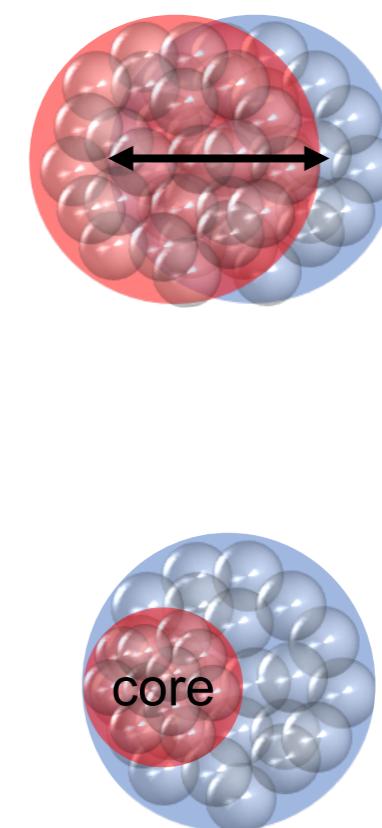
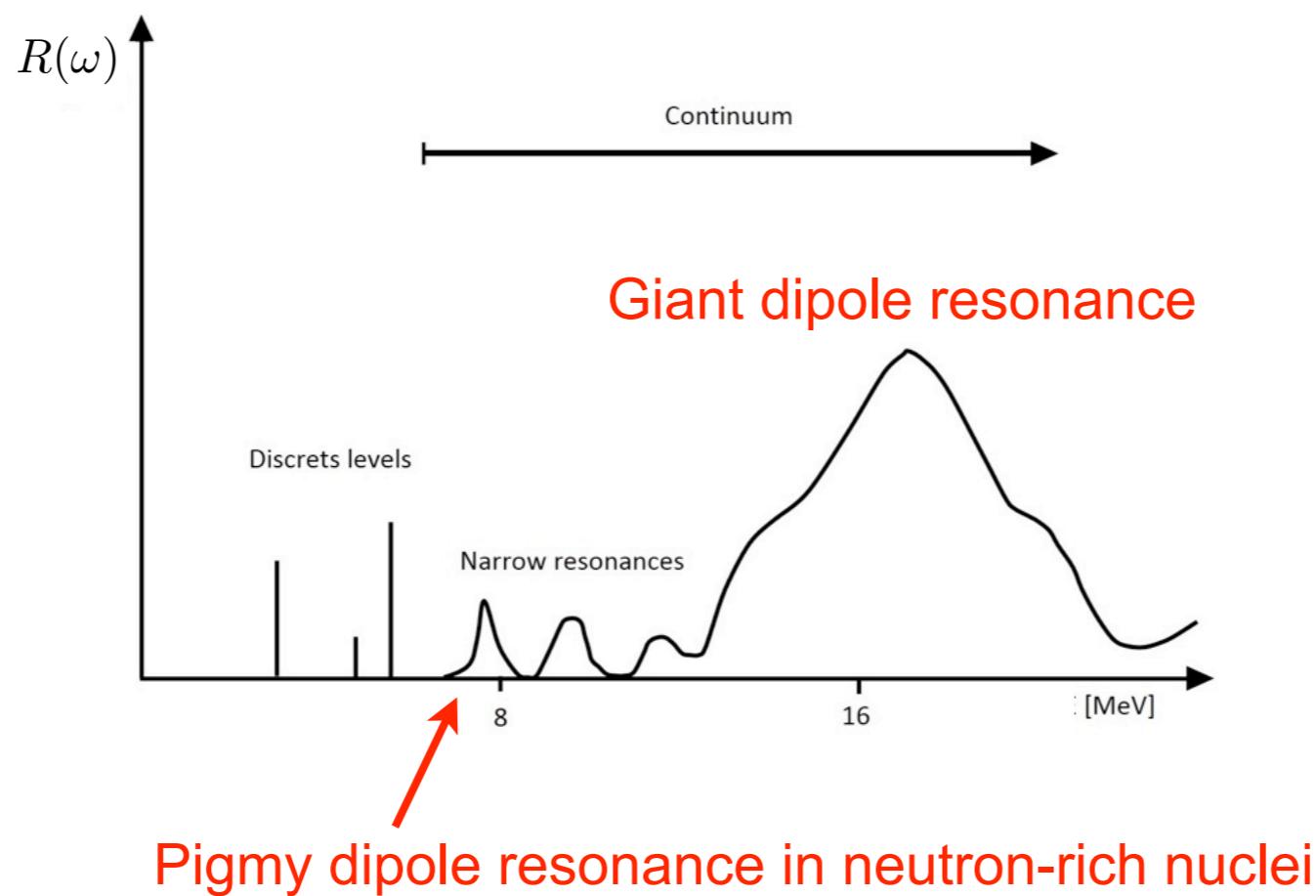
$$\delta y_k(\nu) = y_{ref}(\nu) \sum_{n=k+1}^{\infty} c_n(\nu) (Q/\Lambda)^n$$

- Calibrate a Gaussian process emulator using physics-based info on $c_n(\nu)$ as “prior”

- Calculate “Bayesian posterior” for $c_{n>k}(\nu)$, obtaining statistically interpretable truncation error, amounting to 0.2% at the highest order.



Dipole Strength functions



$$\alpha_D = 2\alpha \int_{\omega_{th}}^{\infty} d\omega \frac{R(\omega)}{\omega}$$

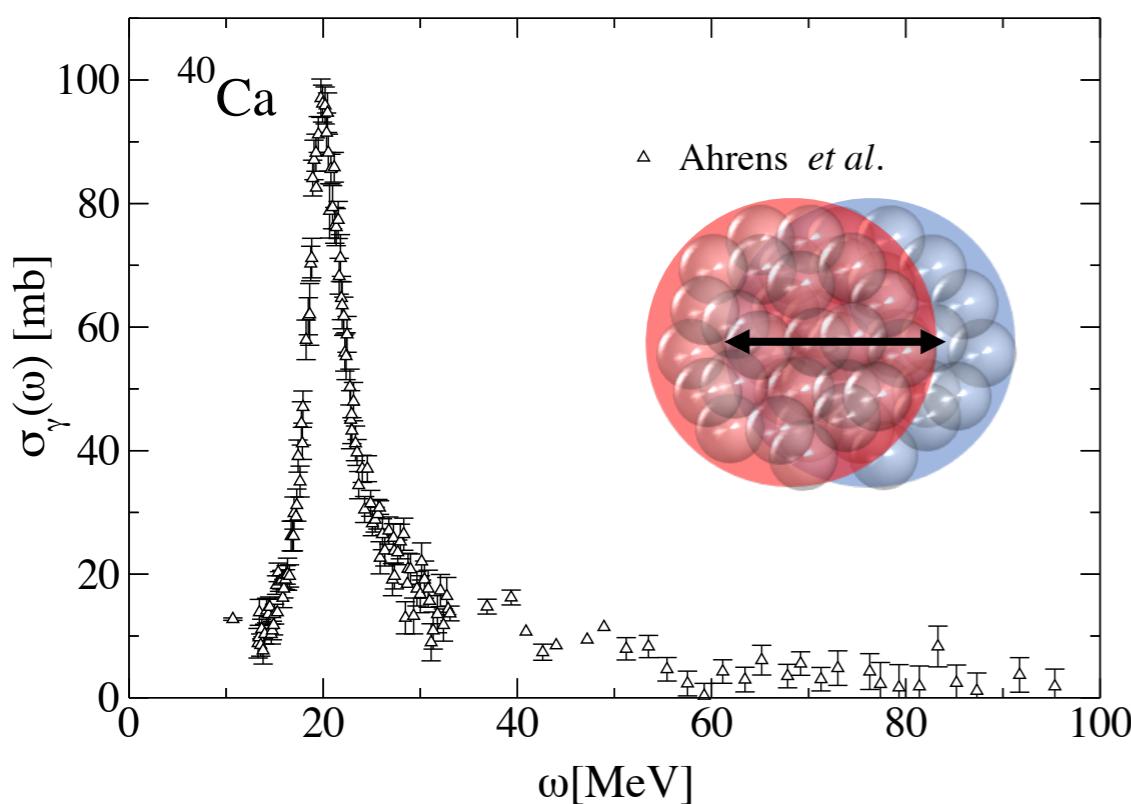
→ Low-energy part of strength dominates

Experimental extractions

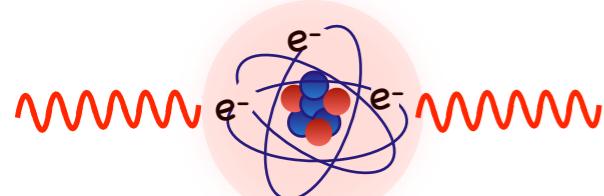
Stable Nuclei

We have data on ~180 stable nuclei

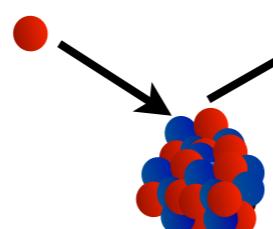
Giant dipole resonances



From photoabsorption experiments

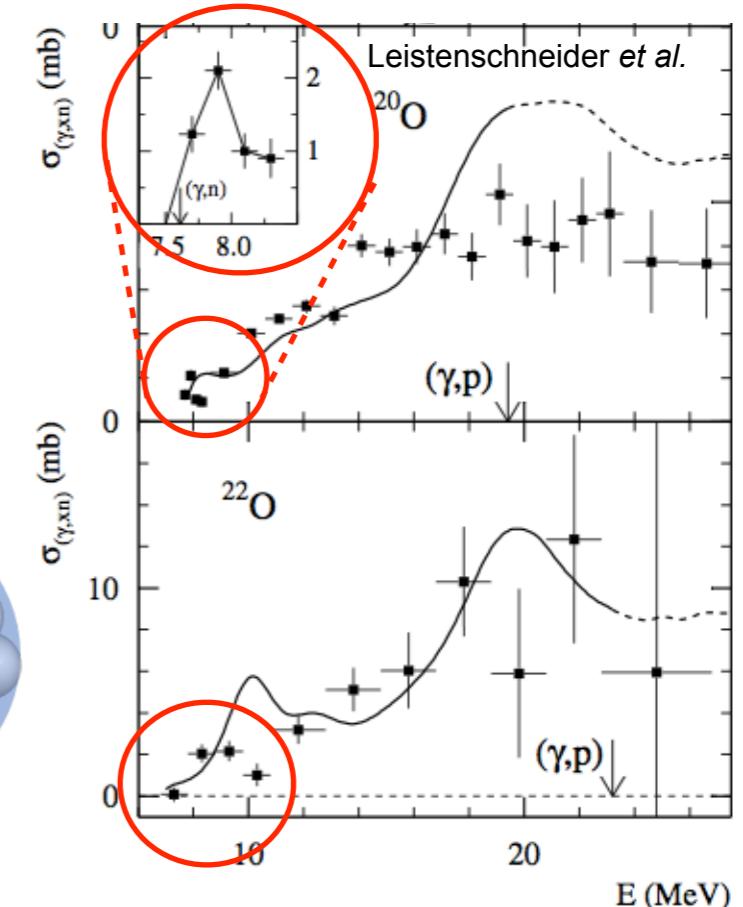


(p,p') experiments

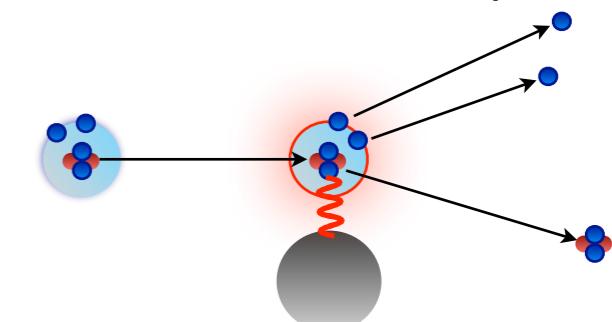


Unstable Nuclei

Fewer data, **pigmy dipole resonances**



From Coulomb excitation experiments

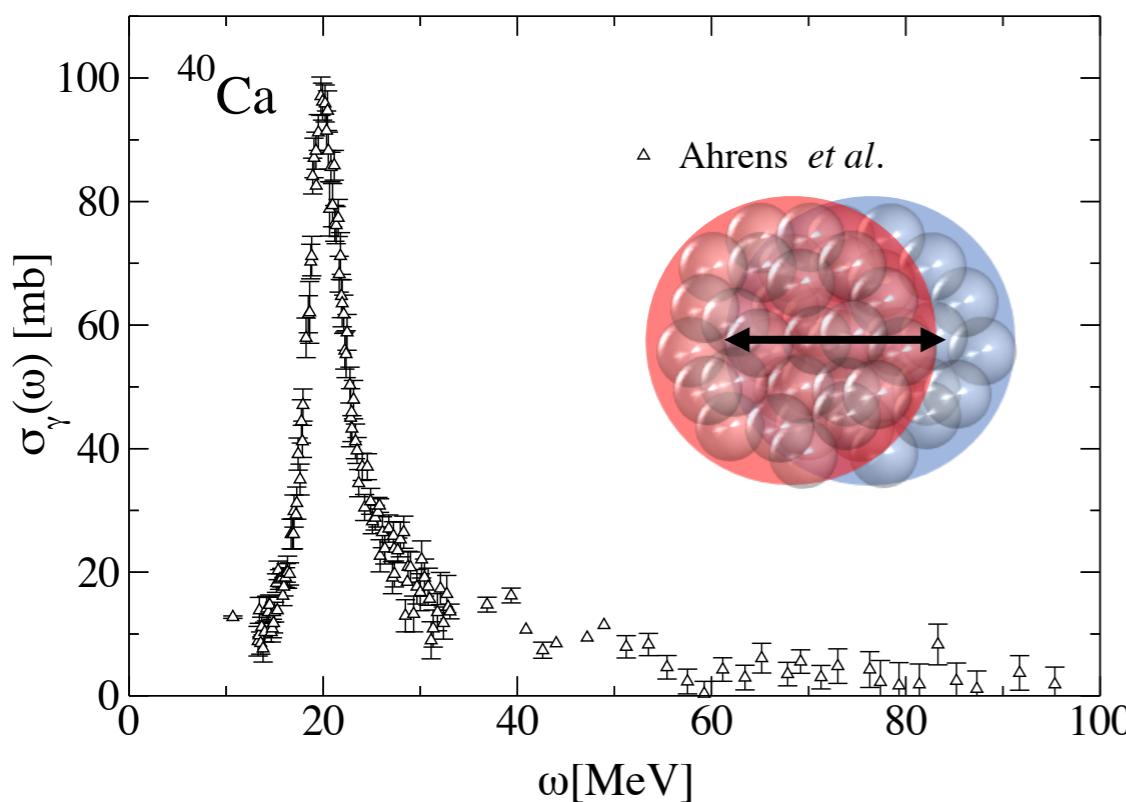


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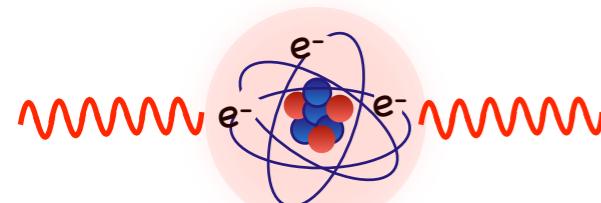
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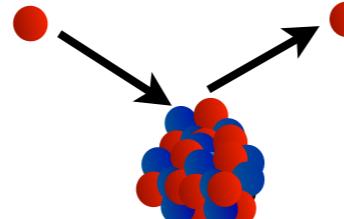
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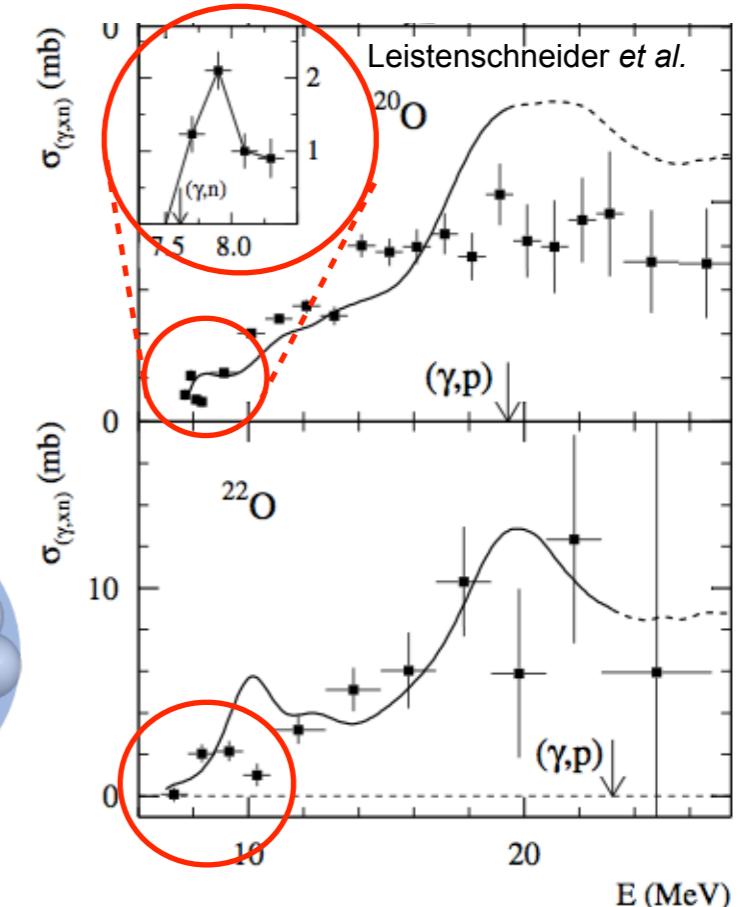
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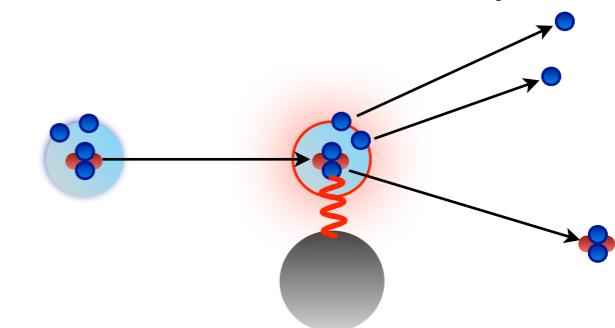
Do we see the emergence of collective motions from first principle calculations?

Unstable Nuclei

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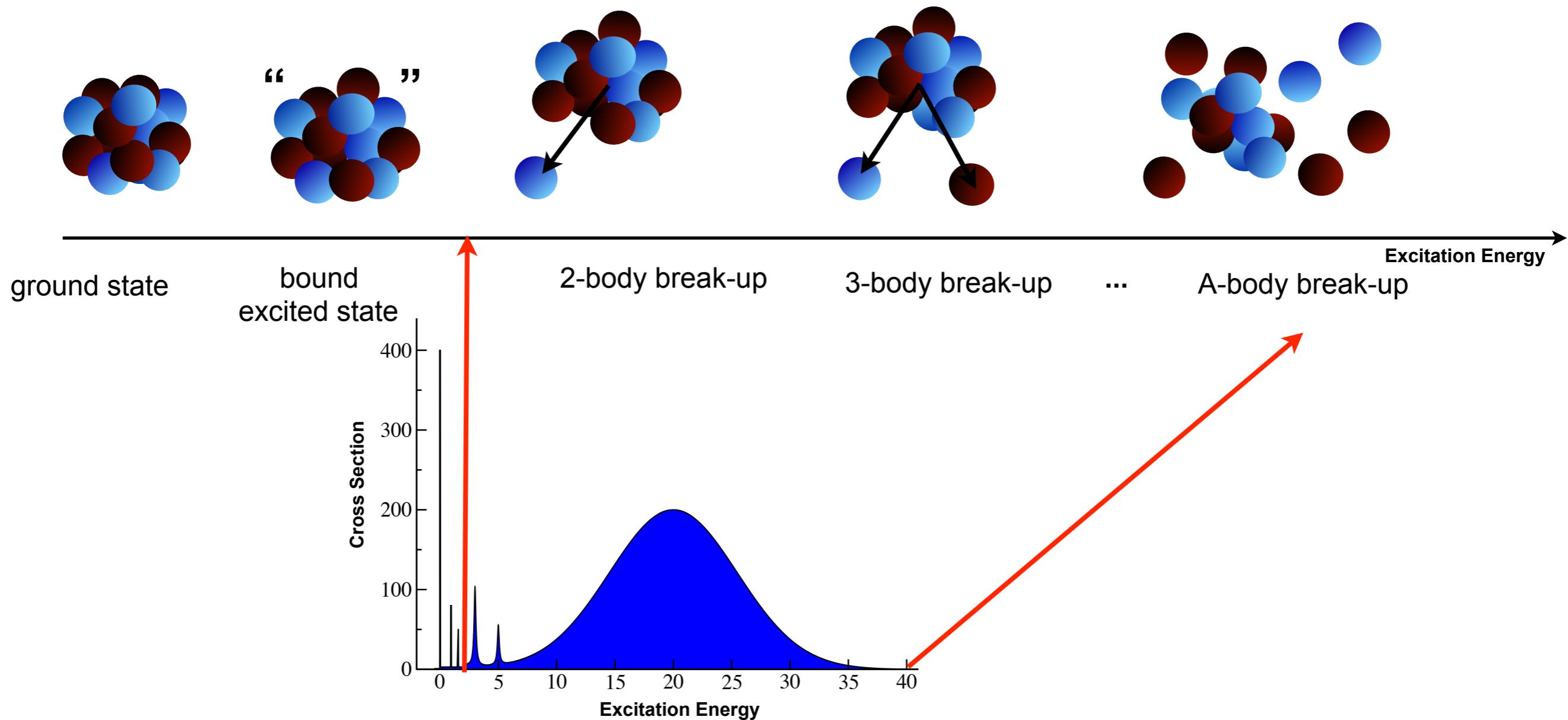
From Coulomb excitation experiments



The continuum problem

$$R(\omega) = \sum_f \left| \langle \psi_f | \Theta | \psi_0 \rangle \right|^2 \delta(E_f - E_0 - \omega)$$

Depending on E_f , many channels may be involved



Integral Transforms

$$R(\omega) = \sum_f |\langle \psi_f | \Theta | \psi_0 \rangle|^2 \delta(E_f - E_0 - \omega)$$



Exact knowledge limited in
energy and mass number

Integral Transforms

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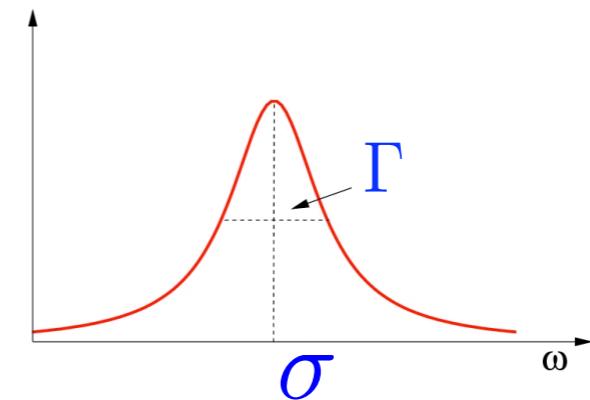


Exact knowledge limited in energy and mass number

Lorentz Integral Transform

Efros, et al., JPG.:
Nucl.Part.Phys. **34** (2007) R459

$$L(\sigma, \Gamma) = \frac{1}{\pi} \int d\omega \frac{R(\omega)}{(\omega - \sigma)^2 + \Gamma^2} = \langle \tilde{\psi} | \tilde{\psi} \rangle$$



$$(H - E_0 - \sigma + i\Gamma) | \tilde{\psi} \rangle = \Theta | \psi_0 \rangle$$

Reduce the continuum problem to a bound-state-like equation

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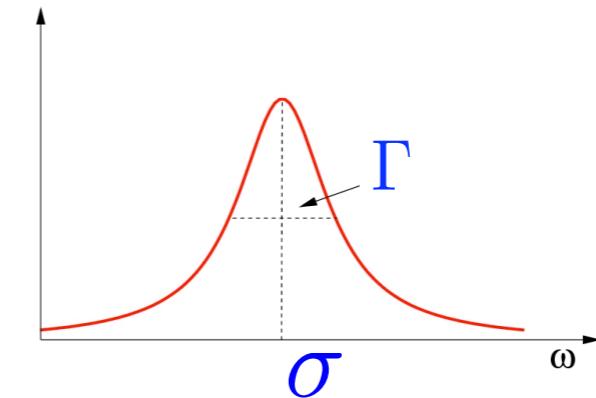
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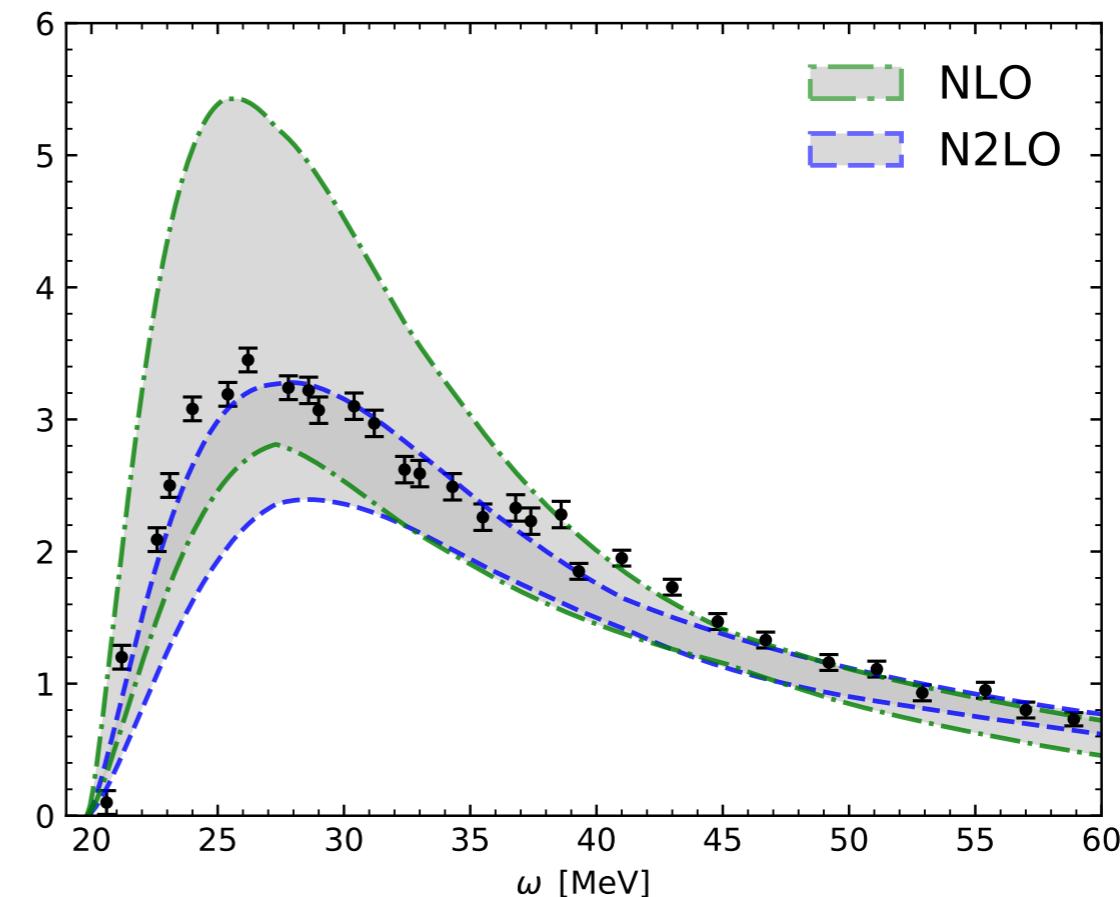
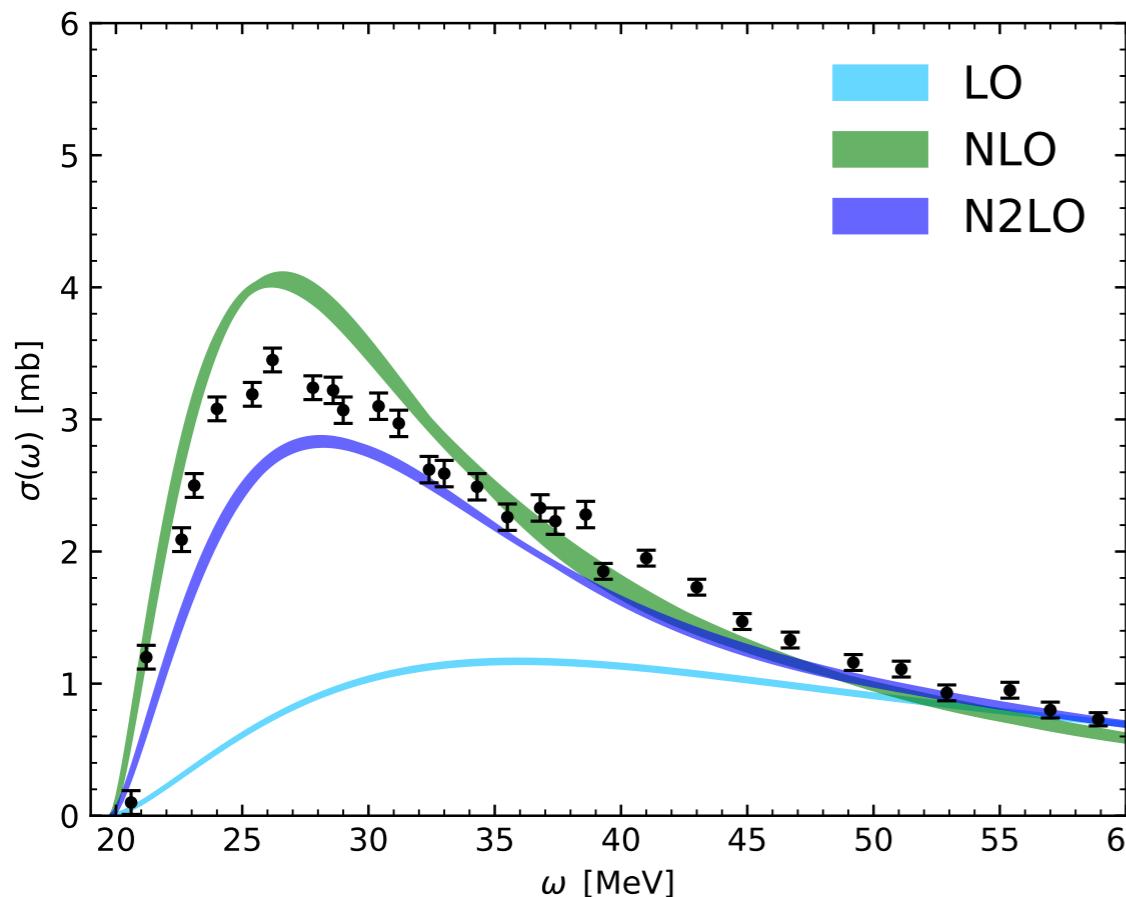
^4He Photo-absorption cross section

Acharya, SB, Bonaiti, Li Muli, J.E. Sobczyk, Front. Phys.10:1066035 (2023).

With local chiral potentials from Phys. Rev. C 90, 054323 and hyper-spherical harmonics



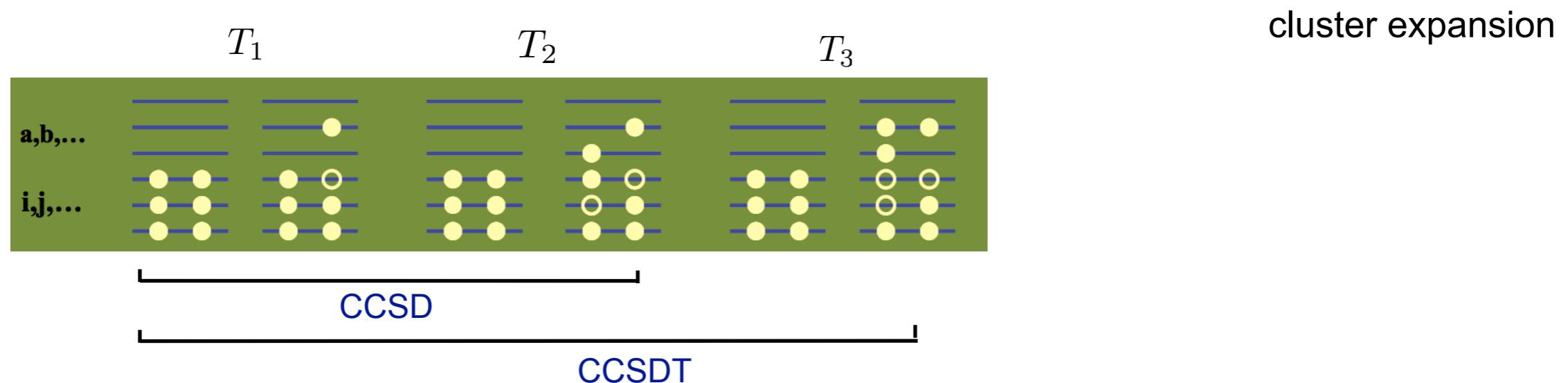
Simone Li Muli



$$\delta_{\mathcal{O}}^{\chi\text{EFT}} = \max \left\{ \left(\frac{Q}{\Lambda} \right)^{k+1} |\mathcal{O}_{\nu_0}|, \left(\frac{Q}{\Lambda} \right)^k |\mathcal{O}_{\nu_0+1} - \mathcal{O}_{\nu_0}|, \dots, \left(\frac{Q}{\Lambda} \right) |\mathcal{O}_{\nu_0+k} - \mathcal{O}_{\nu_0+k-1}| \right\}$$

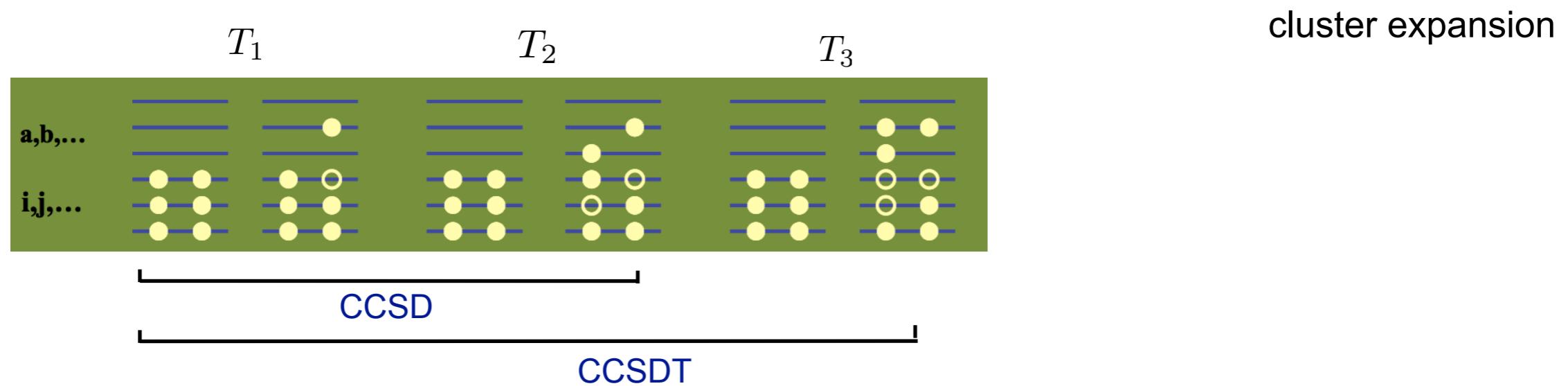
Coupled-cluster theory formulation

$$|\psi_0(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_A)\rangle = e^T |\phi_0(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_A)\rangle \quad T = \sum T_{(A)}$$



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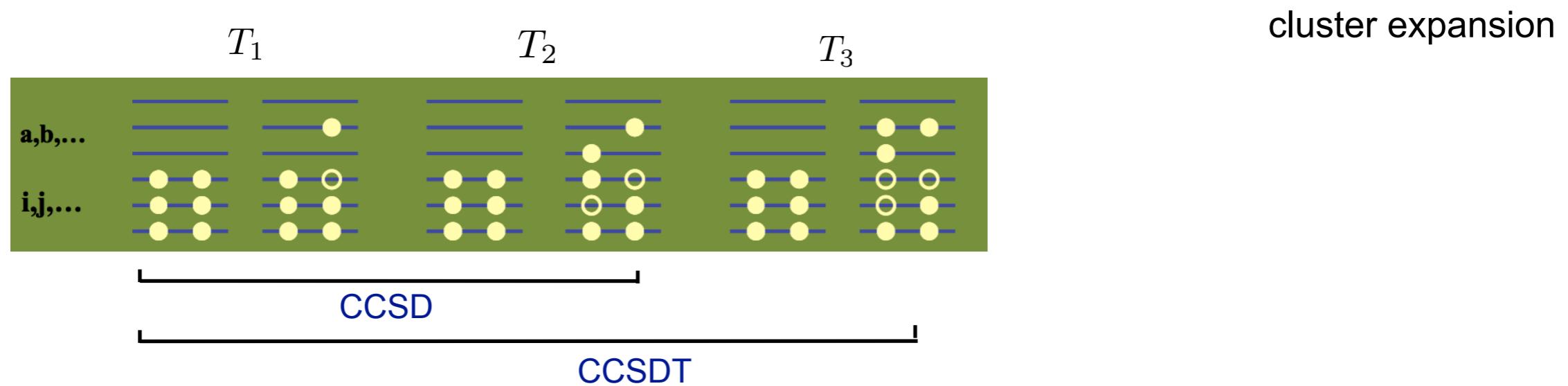


SB *et al.*, Phys. Rev. Lett. **111**, 122502 (2013)

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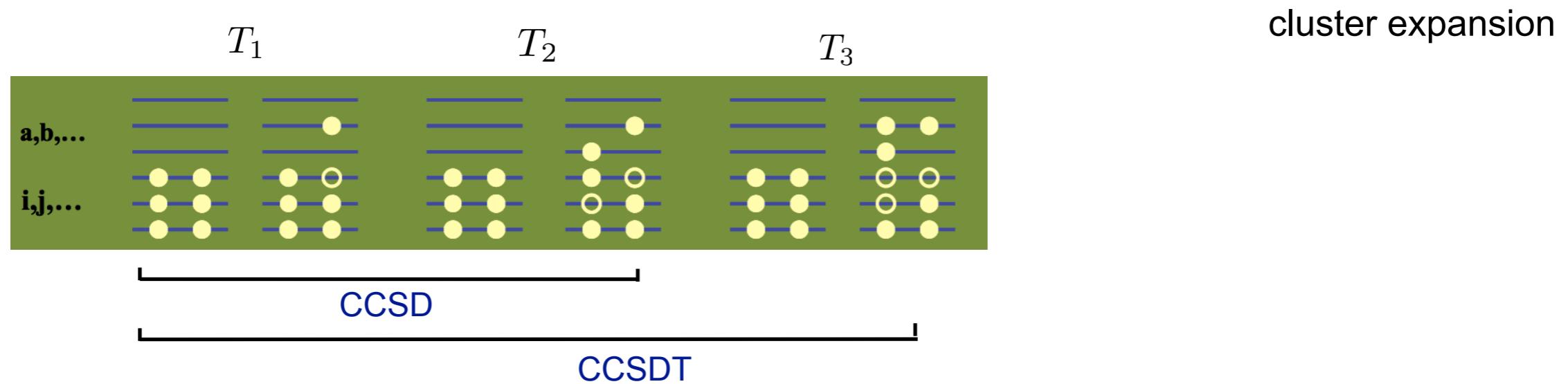
SB *et al.*, Phys. Rev. Lett. **111**, 122502 (2013)

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$$\left\{ \begin{array}{l} \bar{H} = e^{-T} H e^T \\ \bar{\Theta} = e^{-T} \Theta e^T \\ |\tilde{\Psi}_R\rangle = \hat{R} |\Phi_0\rangle \end{array} \right.$$

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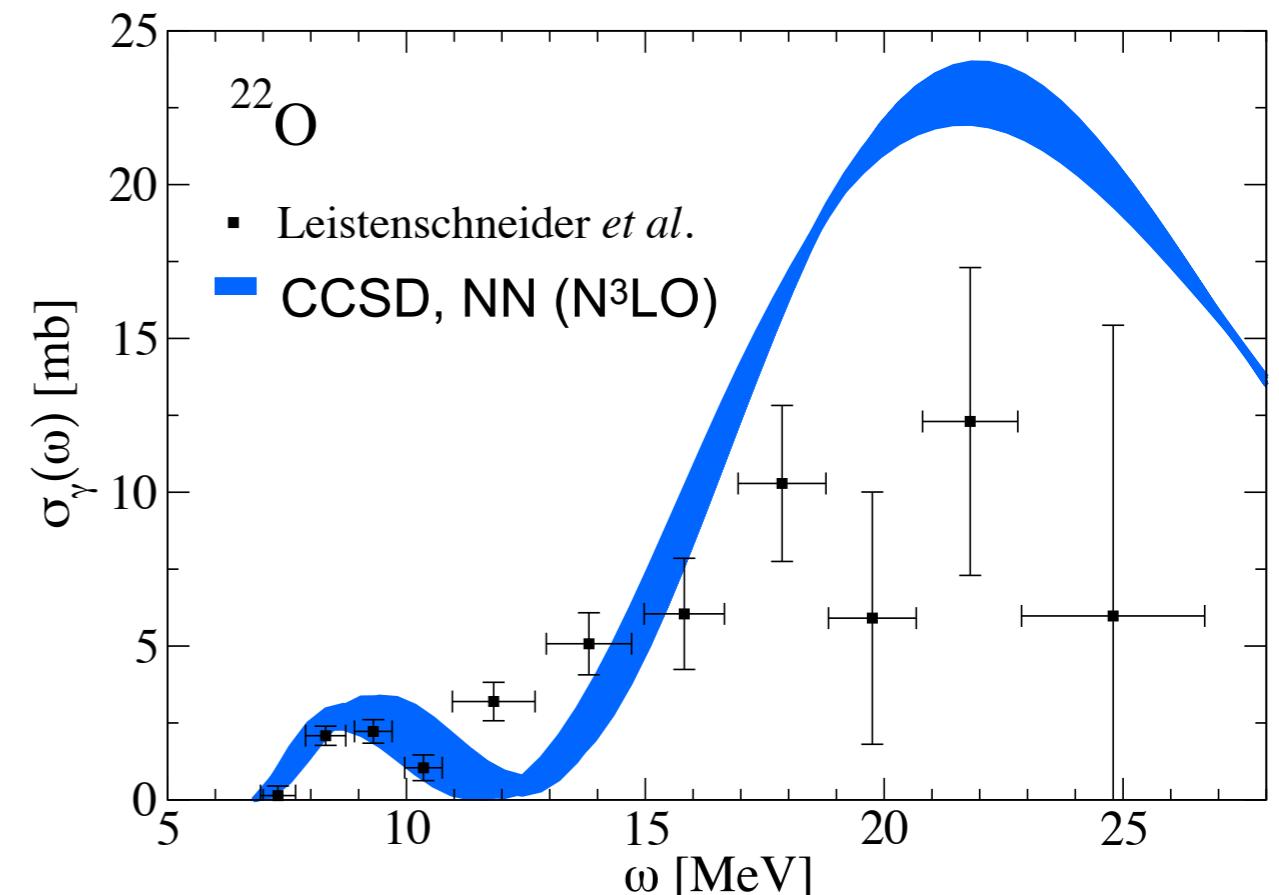
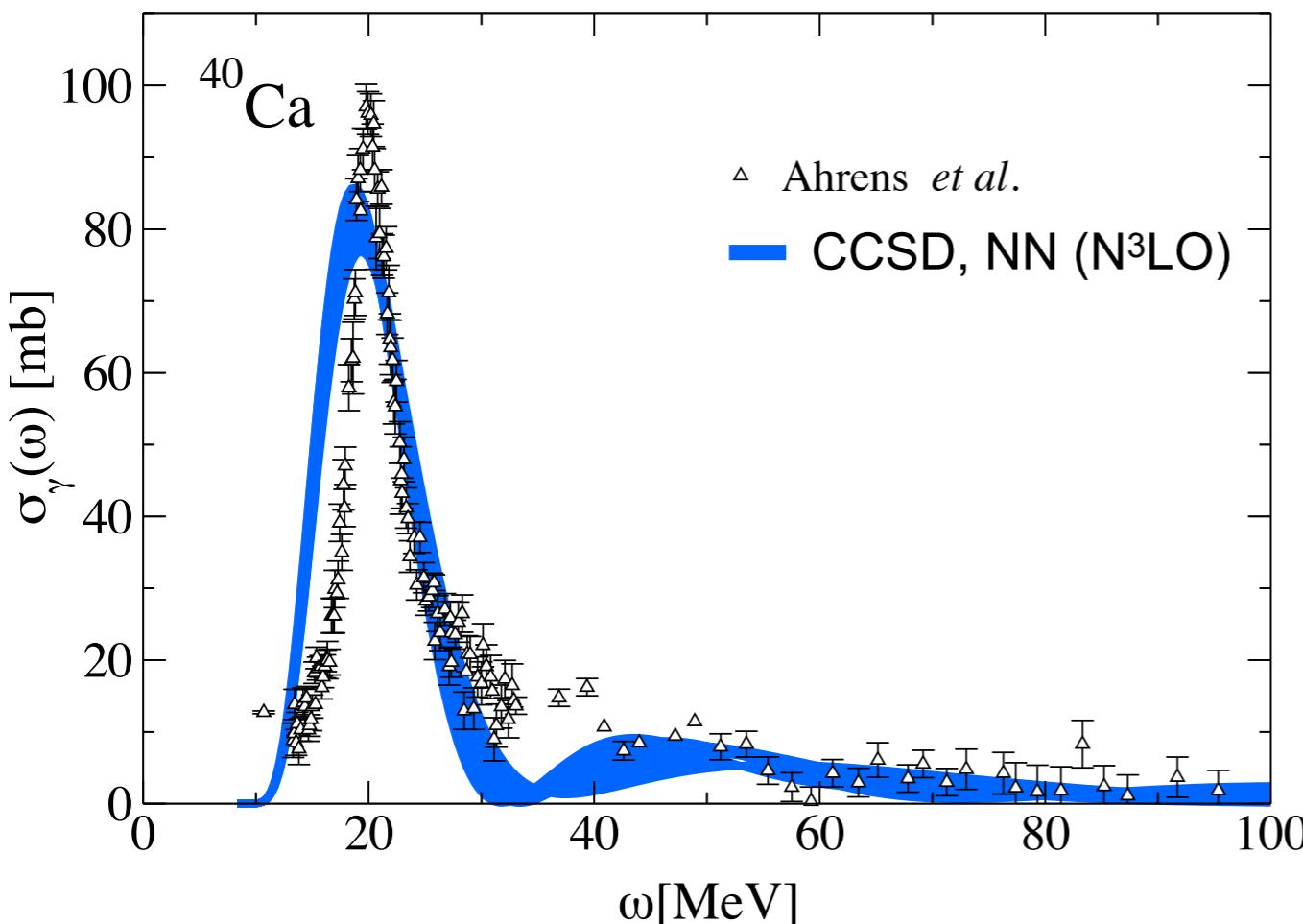
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$$\mathcal{R}(z) = r_0(z) + \sum_{ai} r_i^a(z) a_a^\dagger a_i + \frac{1}{4} \sum_{abij} r_{ij}^{ab}(z) a_a^\dagger a_b^\dagger a_j a_i + \dots$$

Benchmarked implementation at CCSD with hyperspherical harmonics obtaining a few % error

Addressing medium-mass nuclei

SB et al., PRC **90**, 064619 (2014)



See Sobczyk's talk for applications with 3NF and other em operators

Nuclear Equation of State (EOS)

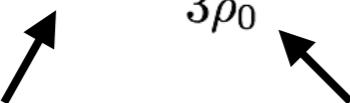
$$E(\rho, \delta) = E(\rho, 0) + S(\rho)\delta^2 + \mathcal{O}(\delta^4)$$

$$S(\rho) = S_0^- + \frac{L}{3\rho_0}(\rho - \rho_0) + \frac{K_{sym}}{18\rho_0^2}(\rho - \rho_0)^2 + \dots$$

Symmetry energy at saturation density

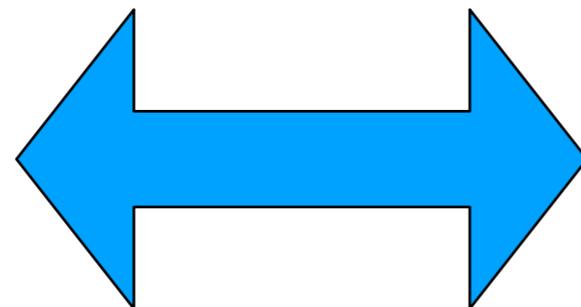
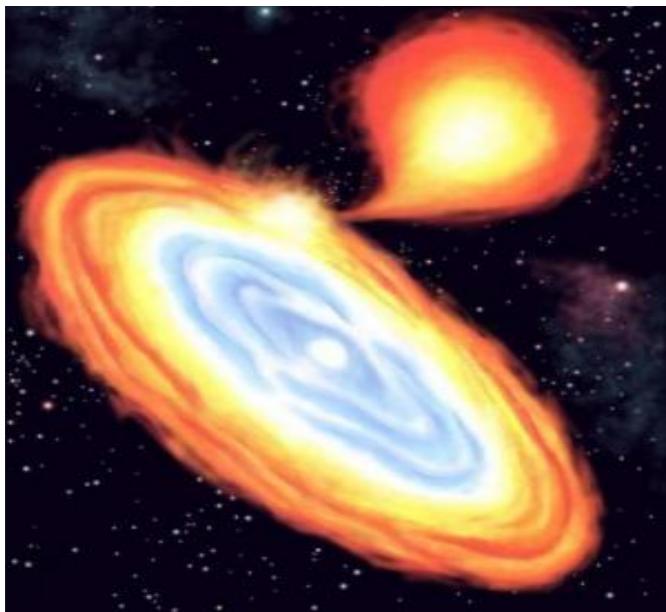
Slope parameter, related to pressure of pure neutron matter at saturation density

$$\rho = \rho_n + \rho_p, \quad \delta = \frac{\rho_n - \rho_p}{\rho_n + \rho_p}$$



Constraining the nuclear EOS is one of the fundamental goals of nuclear physics

Multi-messenger astrophysics



Laboratory measurements on finite nuclei

- Neutron-skin thickness
- Electric dipole polarizability

Sum Rules

$$m_n = \int_0^\infty d\omega \omega^n R(\omega) = \langle \Psi_0 | \hat{\Theta}^\dagger (\hat{H} - E_0)^n \hat{\Theta} | \Psi_0 \rangle$$

The **electric-dipole polarizability** is an inverse-energy weighted sum rule of the dipole response function

$$\alpha_D = 2 \alpha m_{-1} = 2 \alpha \langle \Psi_0 | \Theta^\dagger \frac{1}{(H - E_0)} \Theta | \Psi_0 \rangle$$

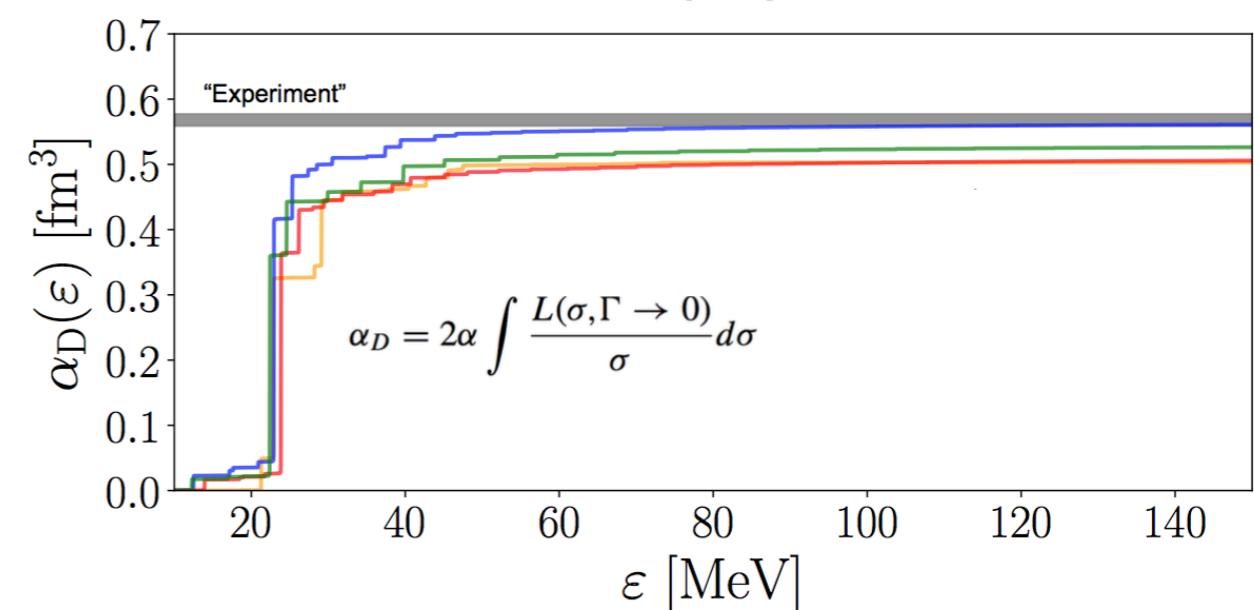
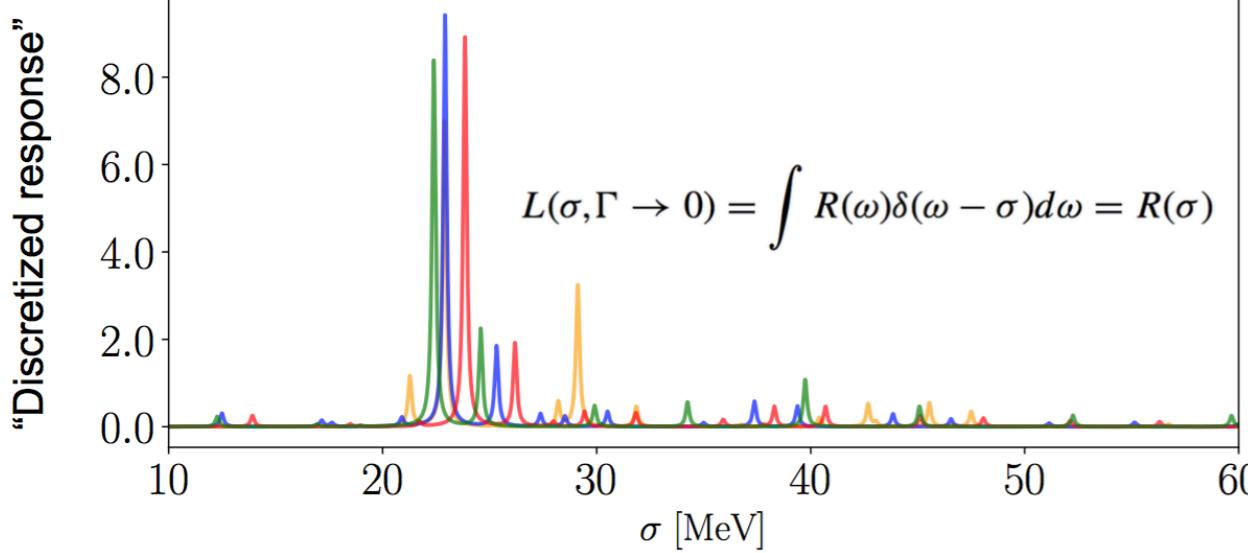
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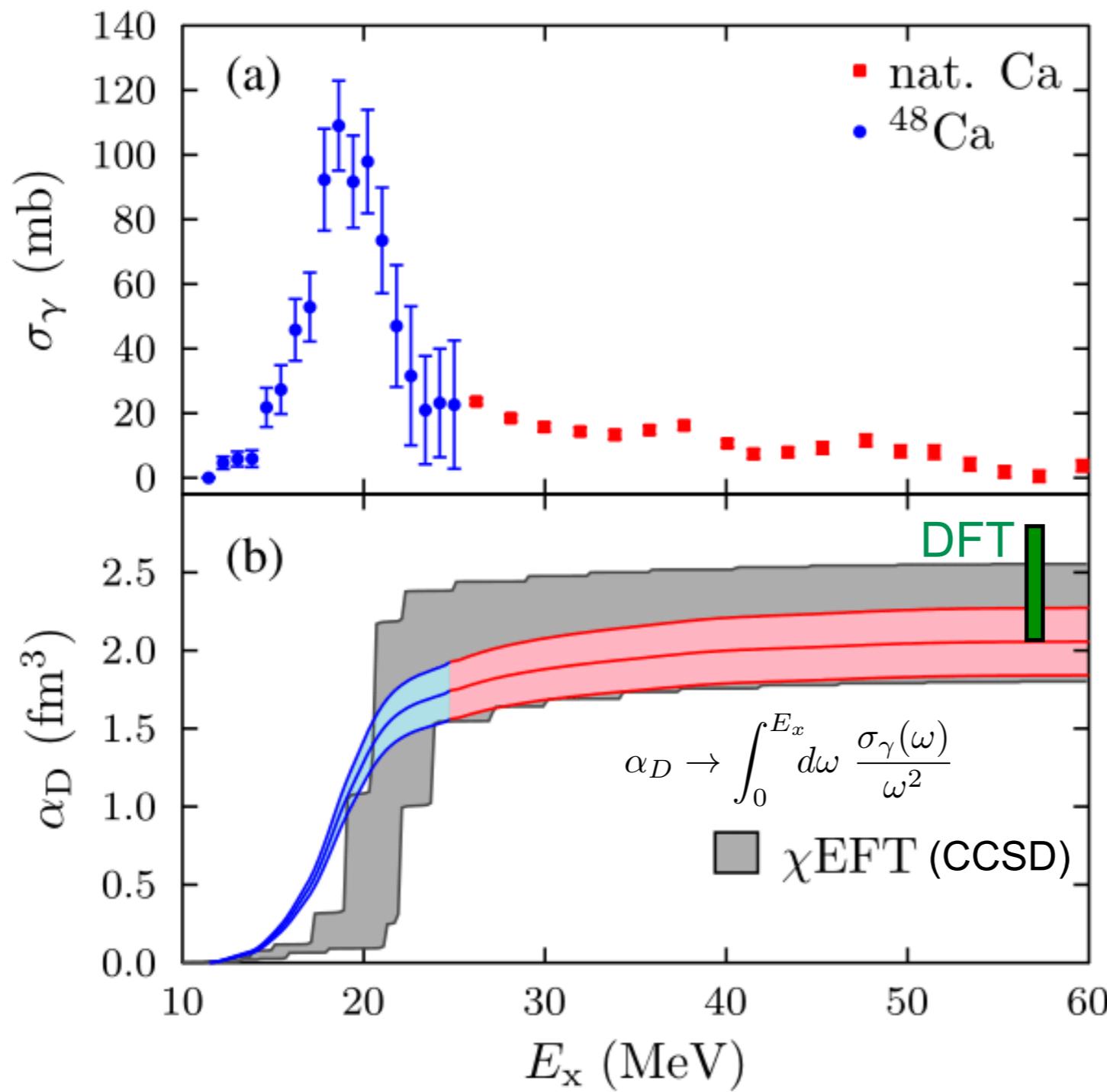
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Can be obtained from the Lorentz Integral Transform in the limit of $\Gamma \rightarrow 0$

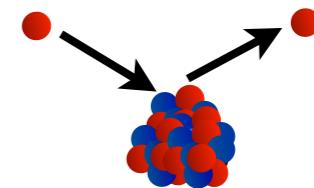


The ^{48}Ca nucleus

Birkhan, Miorelli, SB *et al.*, Phys. Rev. Lett. **118**, 252501 (2017)



RCPN (p,p') experiment



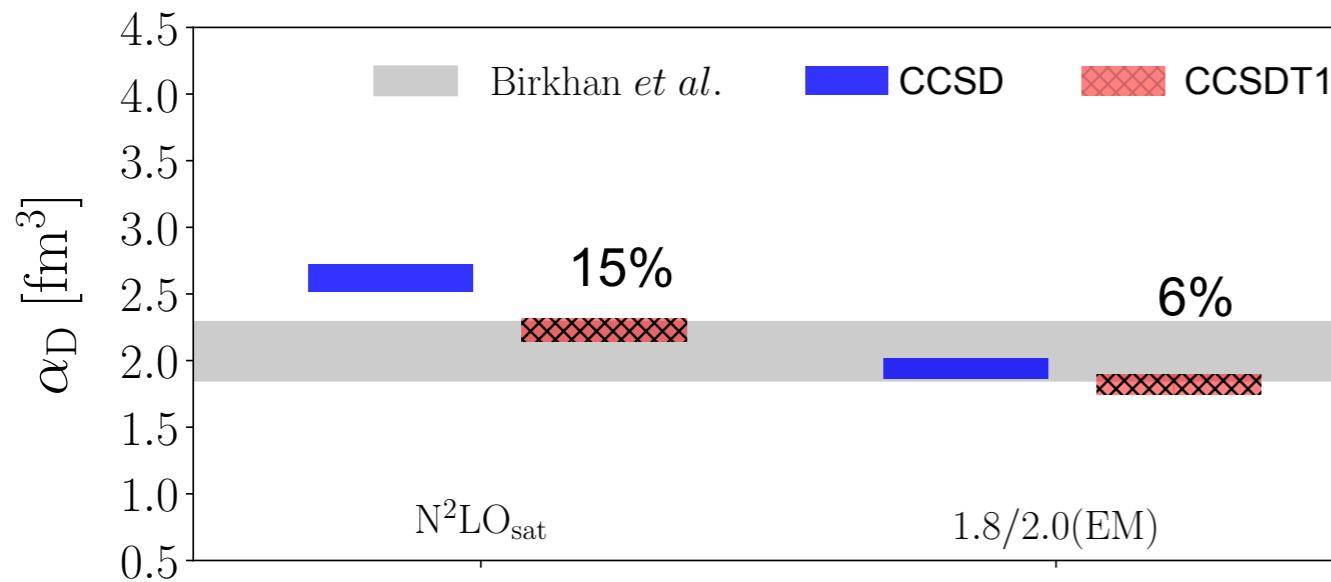
New constraint on the EOS

$$28.5 \leq S_0 \leq 33.3 \text{ MeV}$$

$$43.8 \leq L \leq 48.6 \text{ MeV}$$

Revisiting ^{48}Ca with 3p-3h

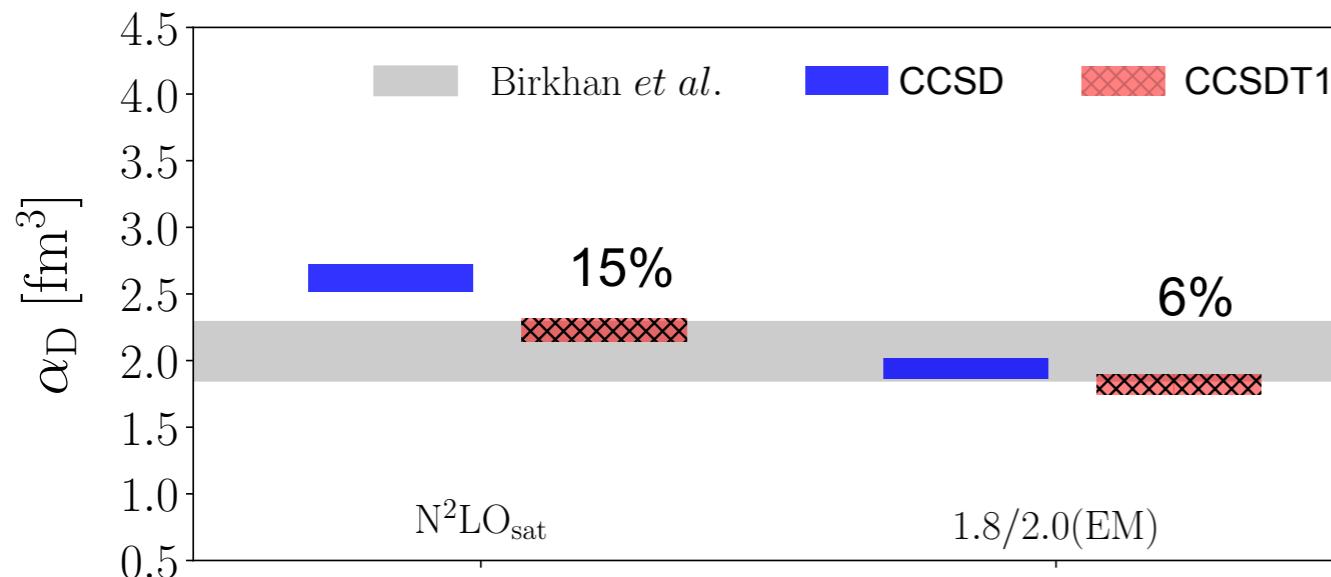
M. Miorelli, SB *et al.*, PRC 98, 014324 (2018)



3p-3h correlations are important and improve the comparison with experiment

Revisiting ^{48}Ca with 3p-3h

M. Miorelli, SB *et al.*, PRC 98, 014324 (2018)



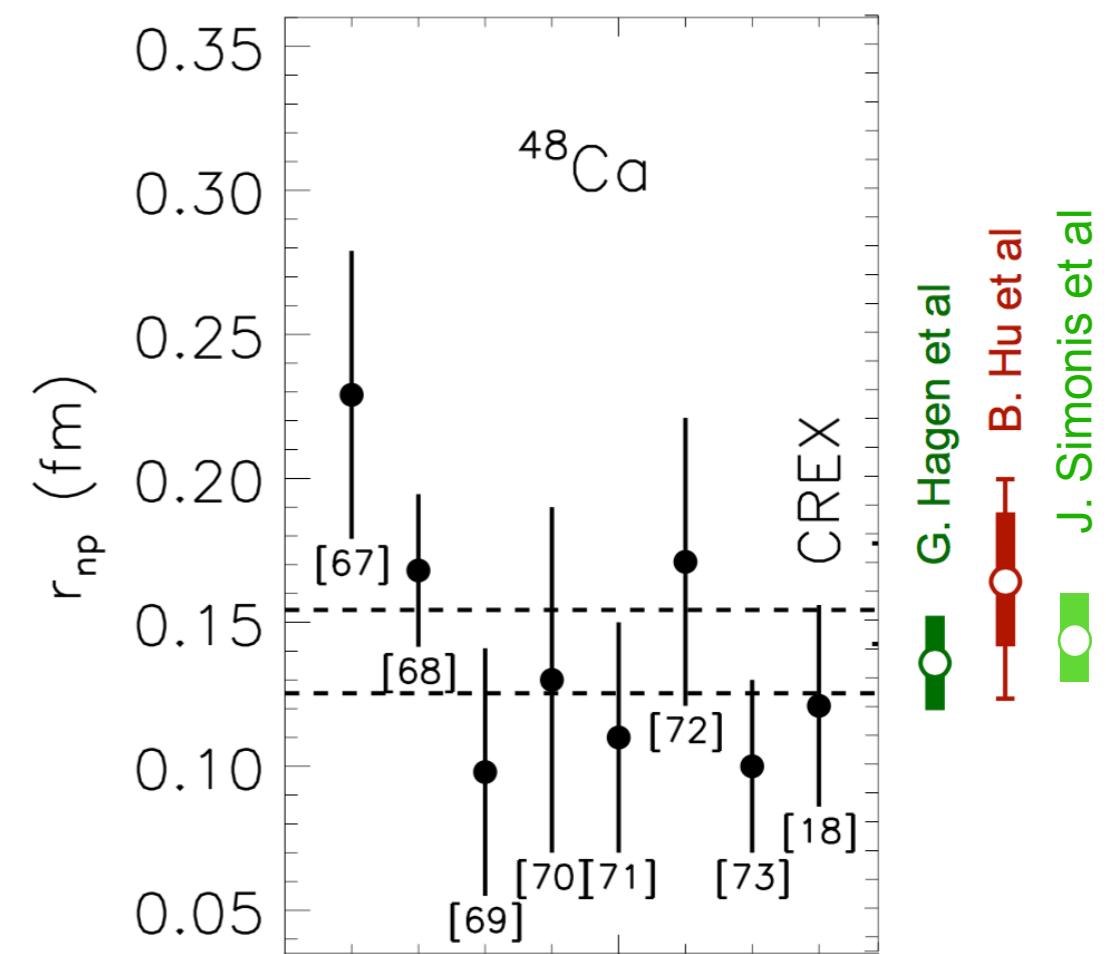
3p-3h correlations are important and improve the comparison with experiment

Simonis, Bacca, Hagen, EPJA 55, 241 (2019)

CCSD-T1 $0.13 \leq R_{\text{skin}} \leq 0.16 \text{ fm}$
 $1.92 \leq \alpha_D \leq 2.38 \text{ fm}^3$

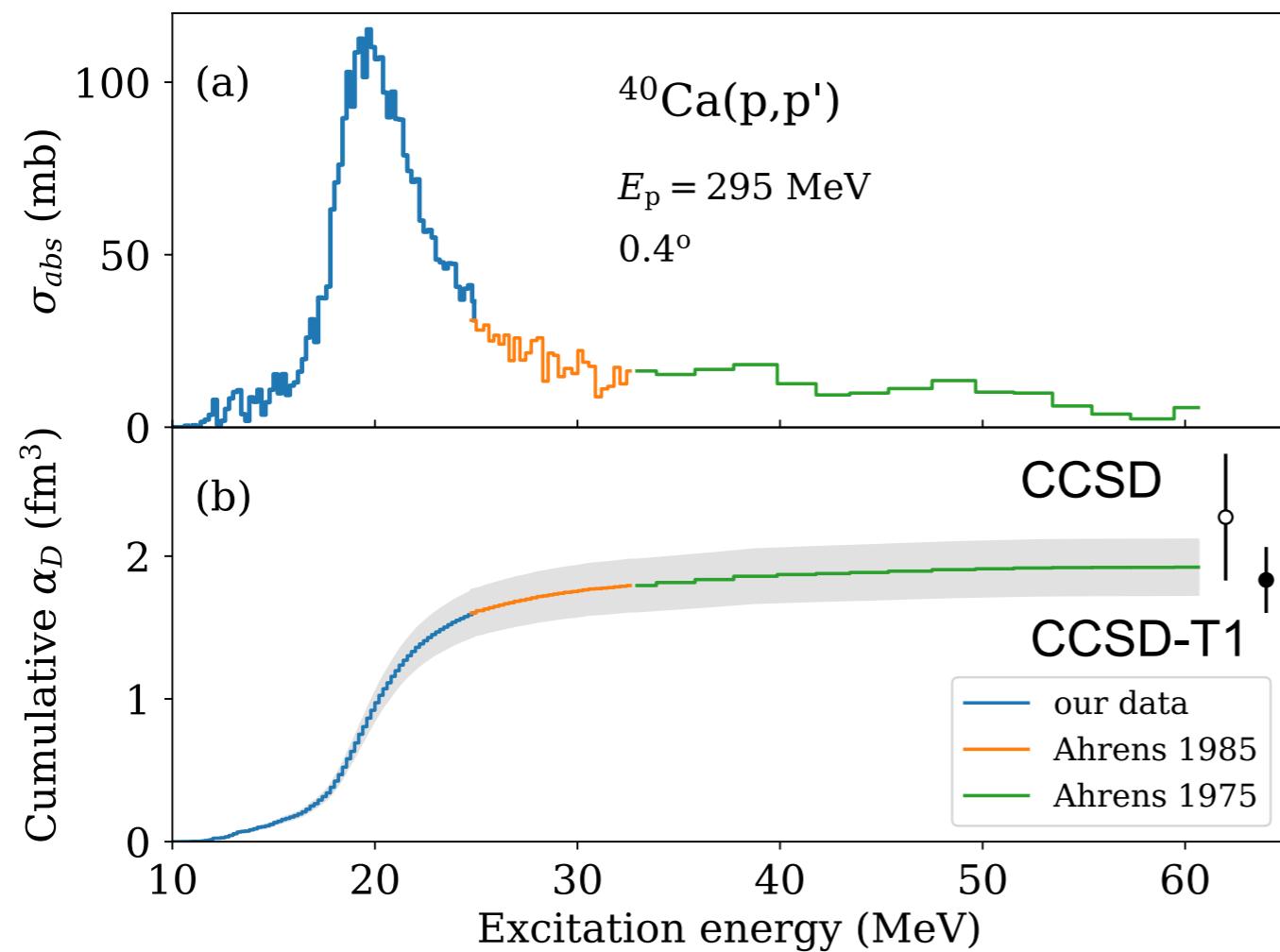
See C. Forssen's talk

Lattimer (2023)



The ^{40}Ca nucleus

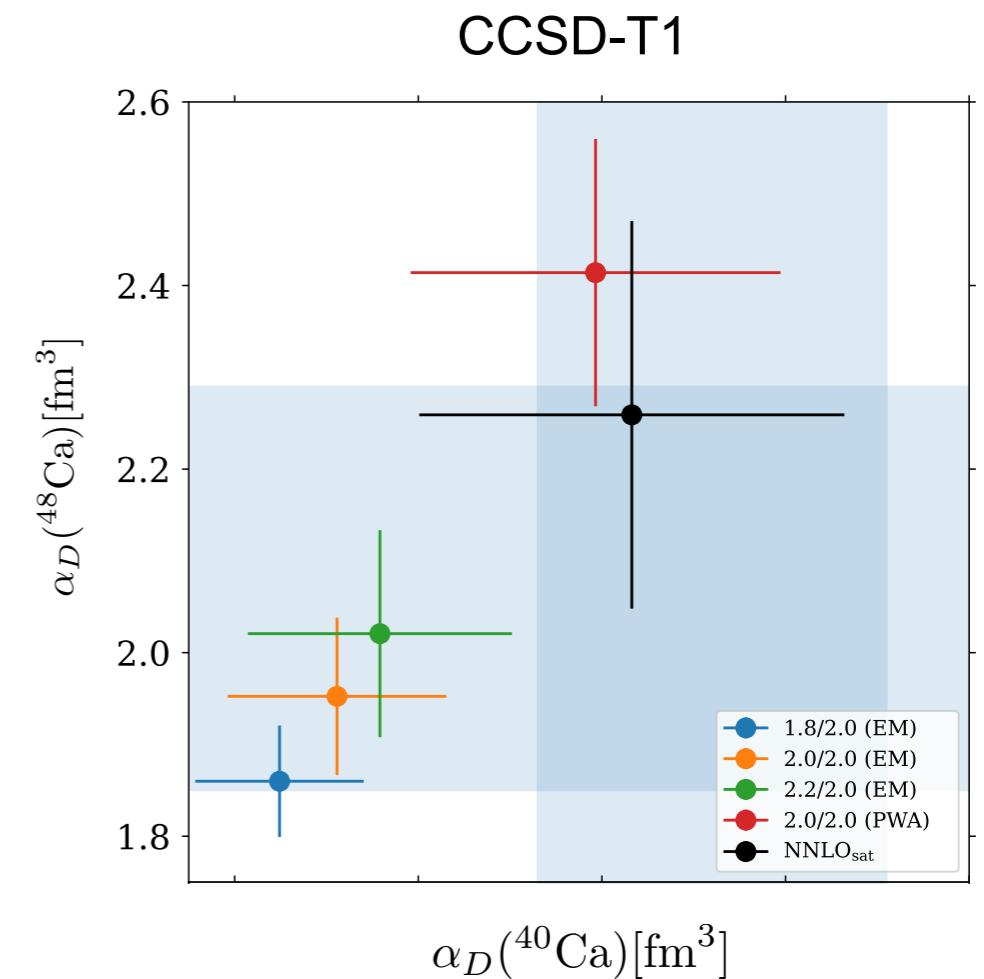
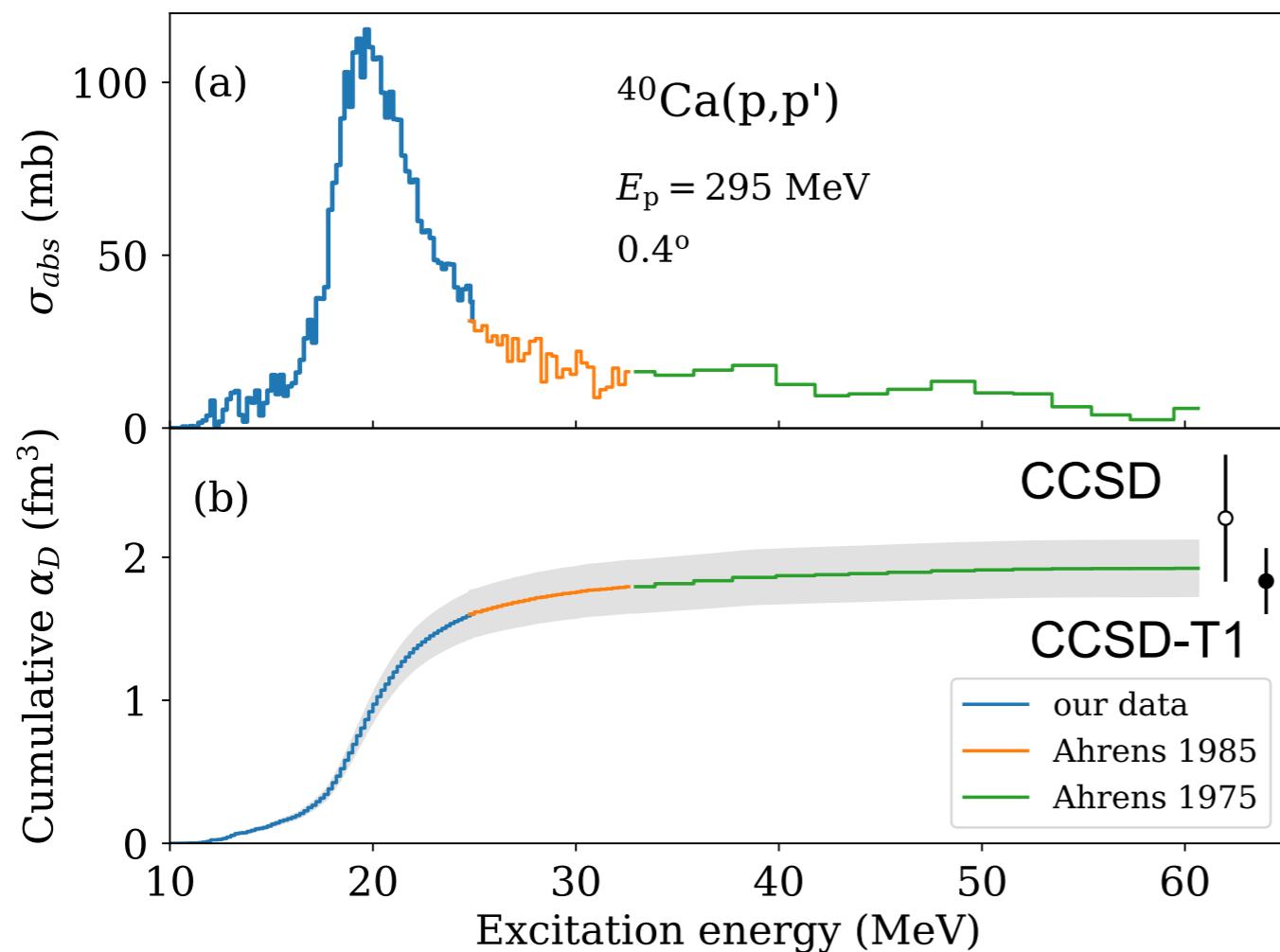
Fearick, von Neumann-Cosel, SB et al, in preparation (2023)



- Constraints on symmetry energy:
 $S_0 = 27 - 33 \text{ MeV}$ $L = 41 - 49 \text{ MeV}$

The ^{40}Ca nucleus

Fearick, von Neumann-Cosel, SB et al, in preparation (2023)

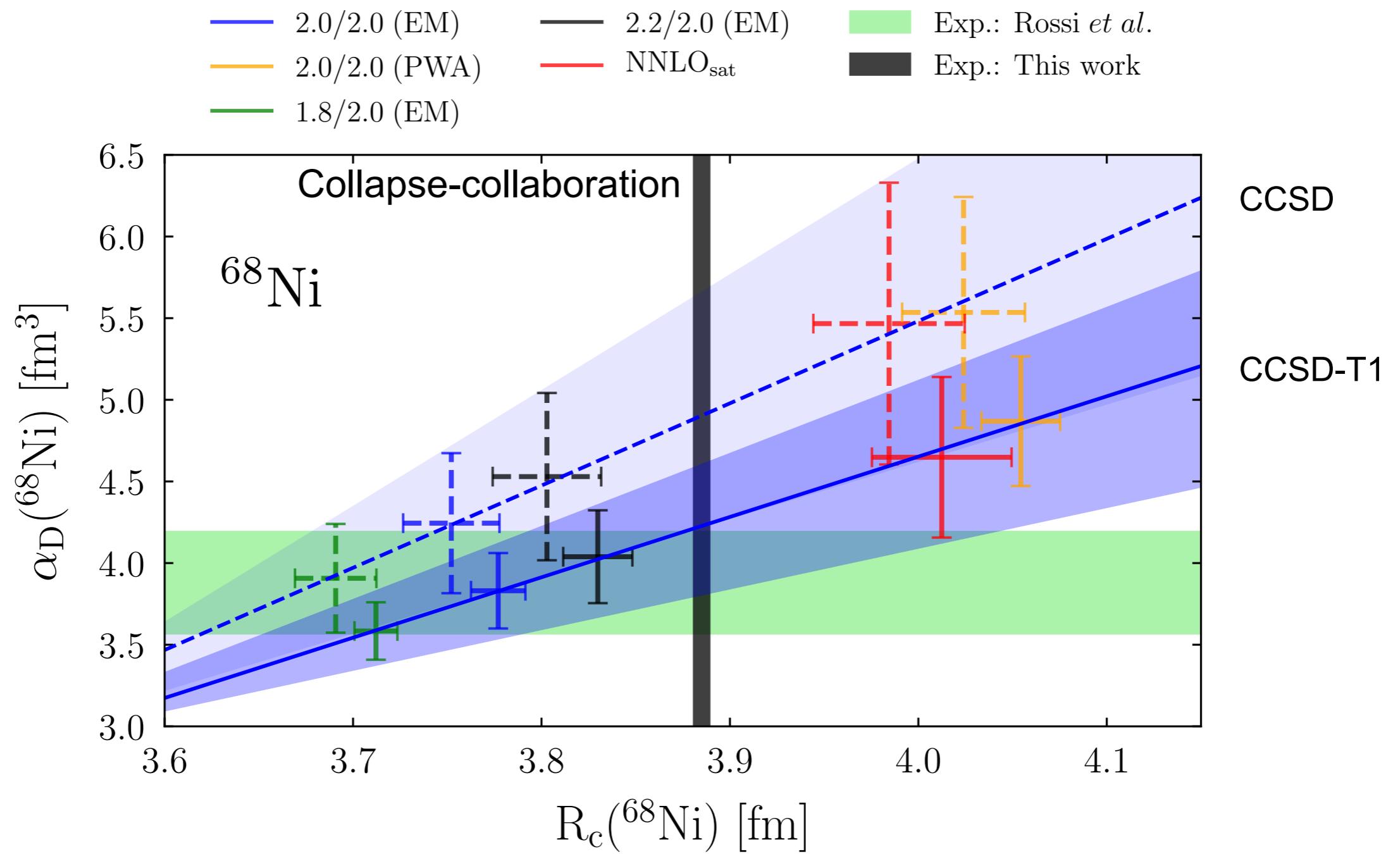


- Constraints on symmetry energy:
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- N2LO_{sat} well in agreement with experiment in mass range $A = 40-48$

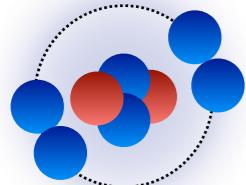
The ^{68}Ni nucleus

S.Kaufmann, J. Simonis, SB *et al.*, PRL 104 (2020) 132505



Halo nuclei

^8He



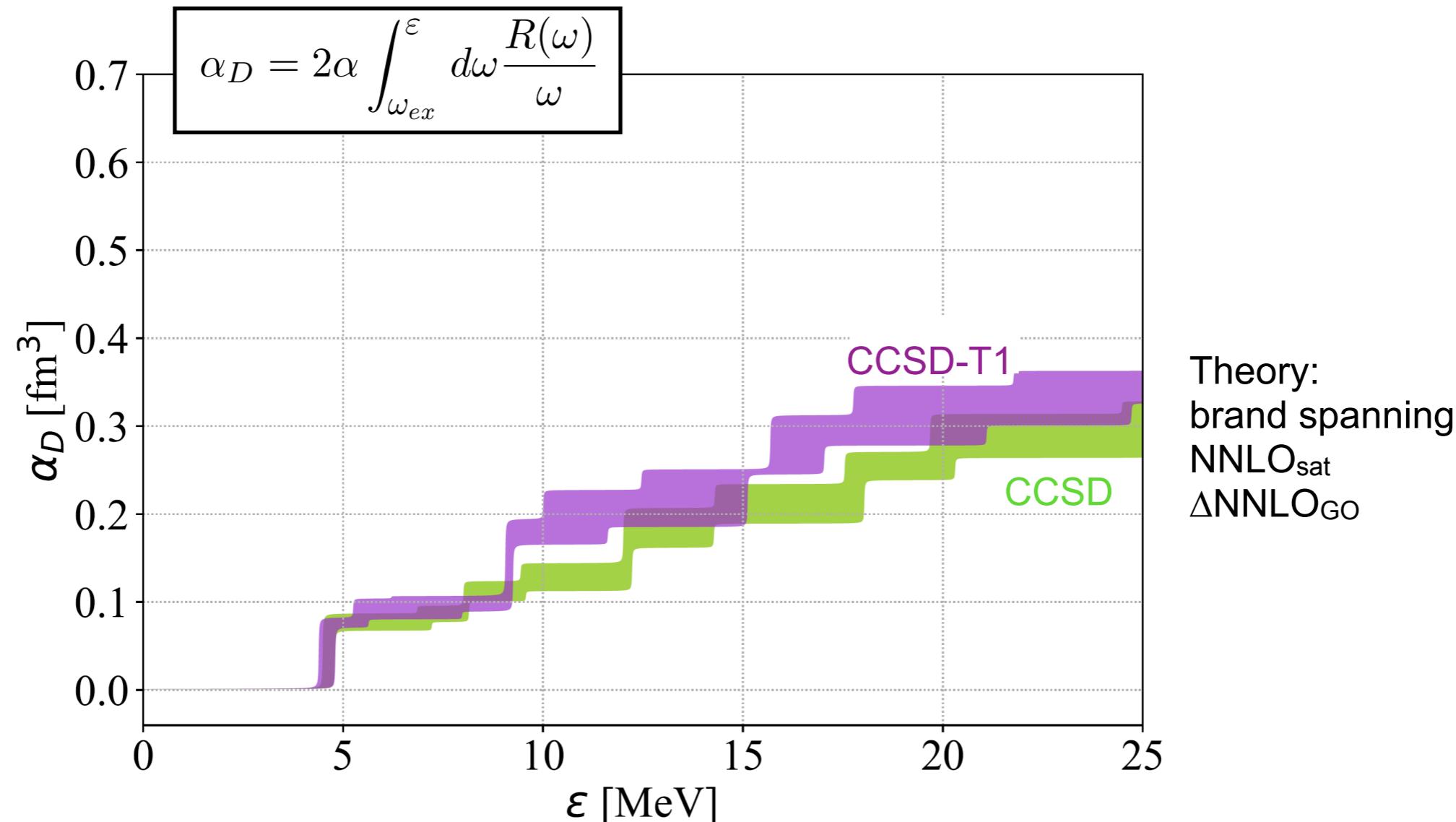
Halo nucleus

Electric dipole polarizability

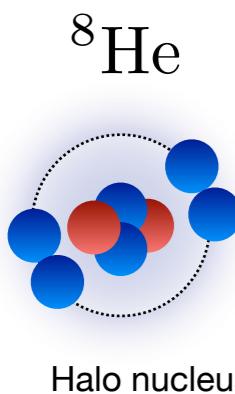
F. Bonaiti, SB, G.Hagen, PRC 105, 034313 (2022)



Francesca Bonaiti



Halo nuclei



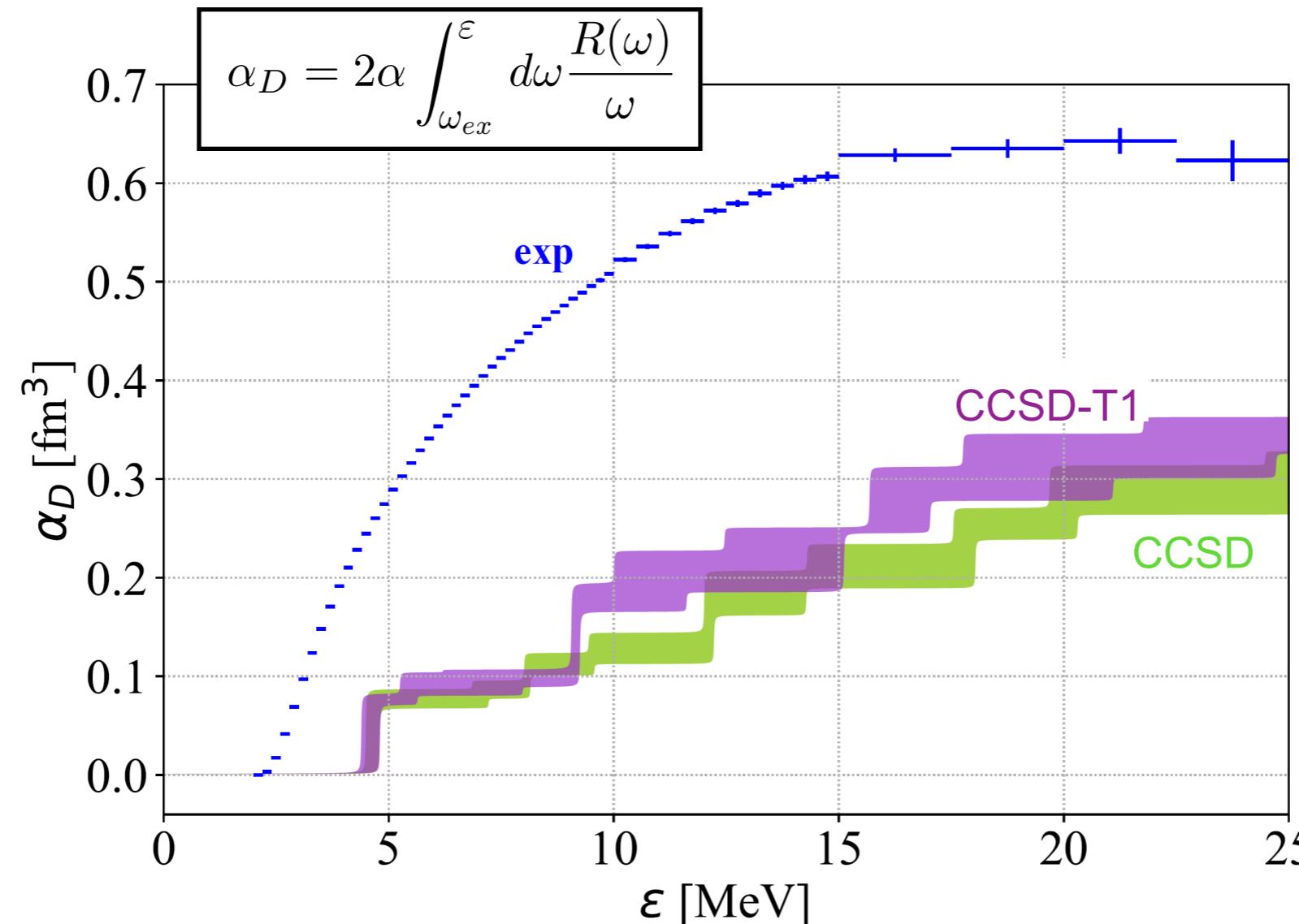
Electric dipole polarizability

F. Bonaiti, SB, G.Hagen, PRC 105, 034313 (2022)

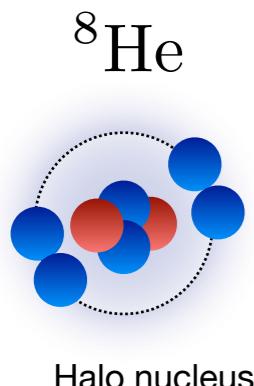


Francesca Bonaiti

Halo nucleus



Halo nuclei

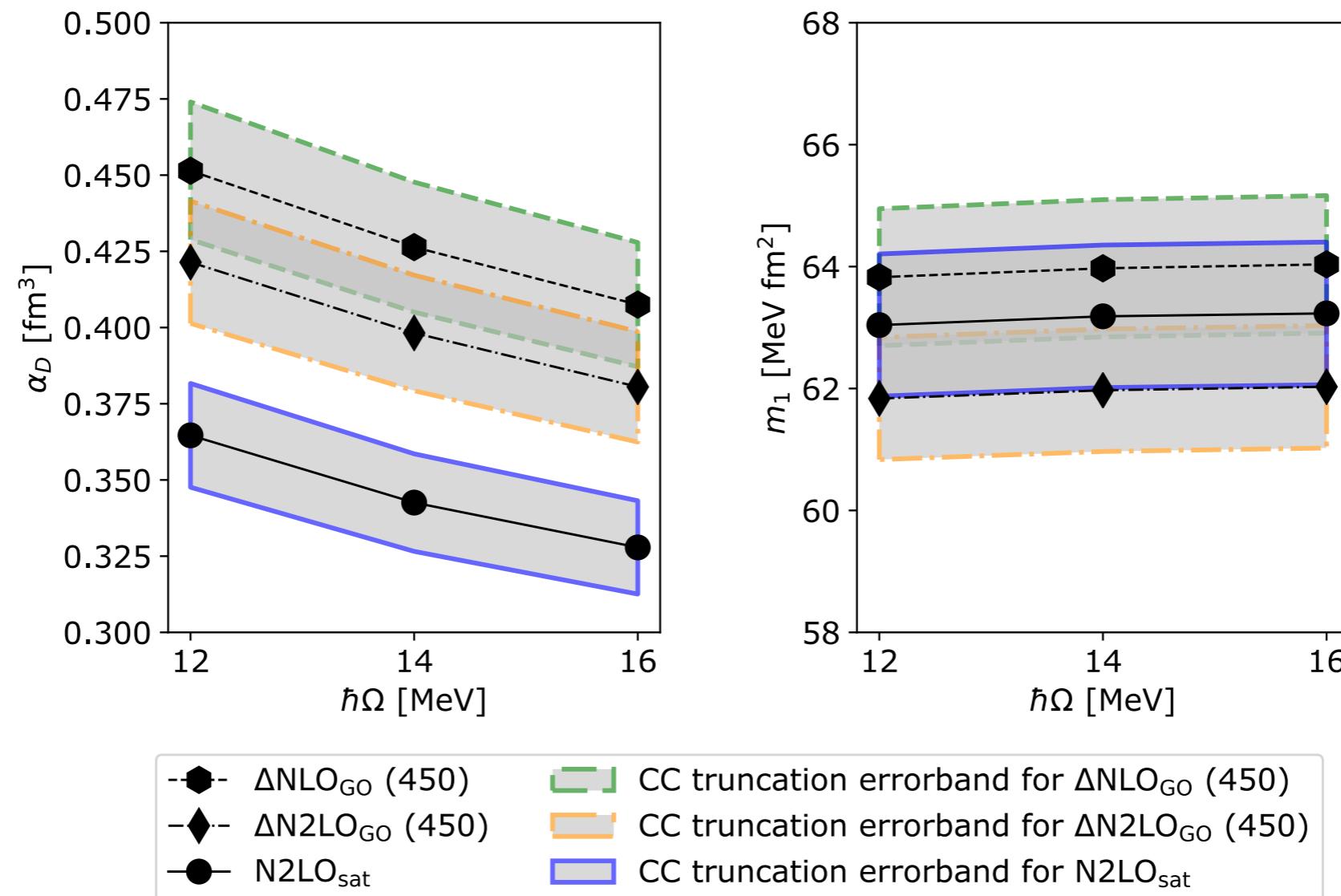


Electric dipole polarizability



Francesca Bonaiti

Acharya, SB, Bonaiti, Li Muli, Front.in Phys. 10:1066035 (2023)



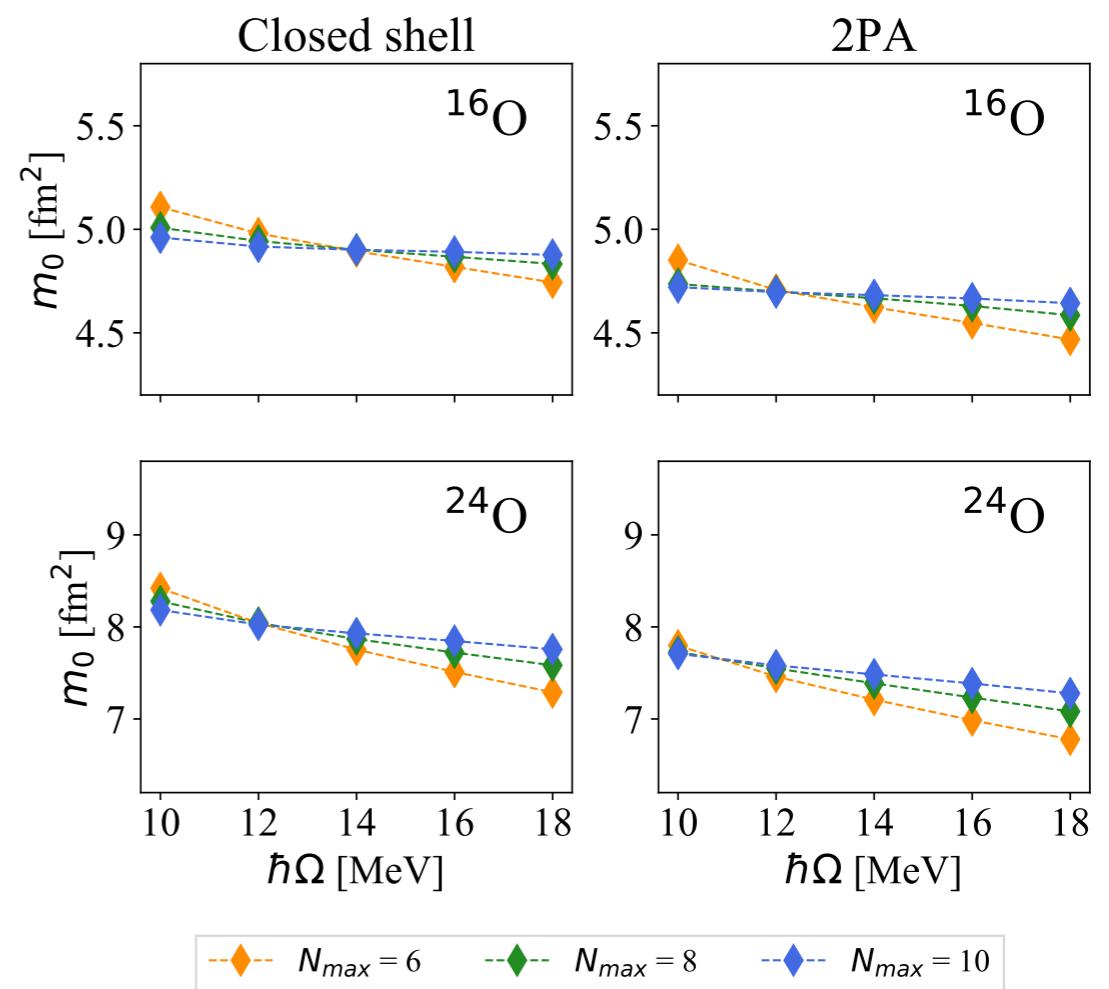
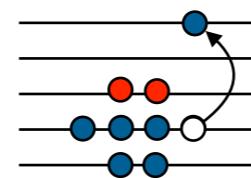
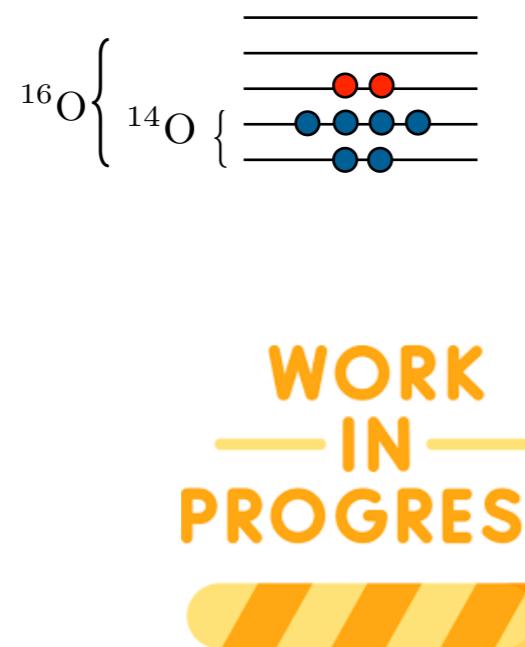
What's next

- Two-particle attached technique (lead by F. Bonaiti)



Francesca Bonaiti

$$\mathcal{R}(z)|\Phi_0\rangle = \left(\frac{1}{2} \sum_{ab} r^{ab}(z) a_a^\dagger a_b^\dagger + \frac{1}{6} \sum_{abci} r_i^{abc}(z) a_a^\dagger a_b^\dagger a_c^\dagger a_i + \dots \right) |\Phi_0\rangle$$



- Develop two-particle removed (^{14}N), one-particle removed (^{39}K) techniques

Conclusions

- Remarkable progress in first principle calculations of electromagnetic properties and more work is ahead of us

Thanks to all my collaborators:

**B. Acharya, F. Bonaiti, S. Li Muli, W. Jiang, J.E.Sobczyk,
G. Hagen, G. Jansen, T. Papenbrock, J. Simonis, A. Schwenk et al.**

Conclusions

- Remarkable progress in first principle calculations of electromagnetic properties and more work is ahead of us

Thanks to all my collaborators:

**B. Acharya, F. Bonaiti, S. Li Muli, W. Jiang, J.E.Sobczyk,
G. Hagen, G. Jansen, T. Papenbrock, J. Simonis, A. Schwenk et al.**

Thanks for your attention!



Backup

Inversion of the LIT

The inversion is performed numerically with a regularization procedure (ill-posed problem)

Ansatz

$$R(\omega) = \sum_i^{I_{\max}} c_i \chi_i(\omega, \alpha) \rightarrow L(\sigma, \Gamma) = \sum_i^{I_{\max}} c_i \mathcal{L}[\chi_i(\omega, \alpha)]$$

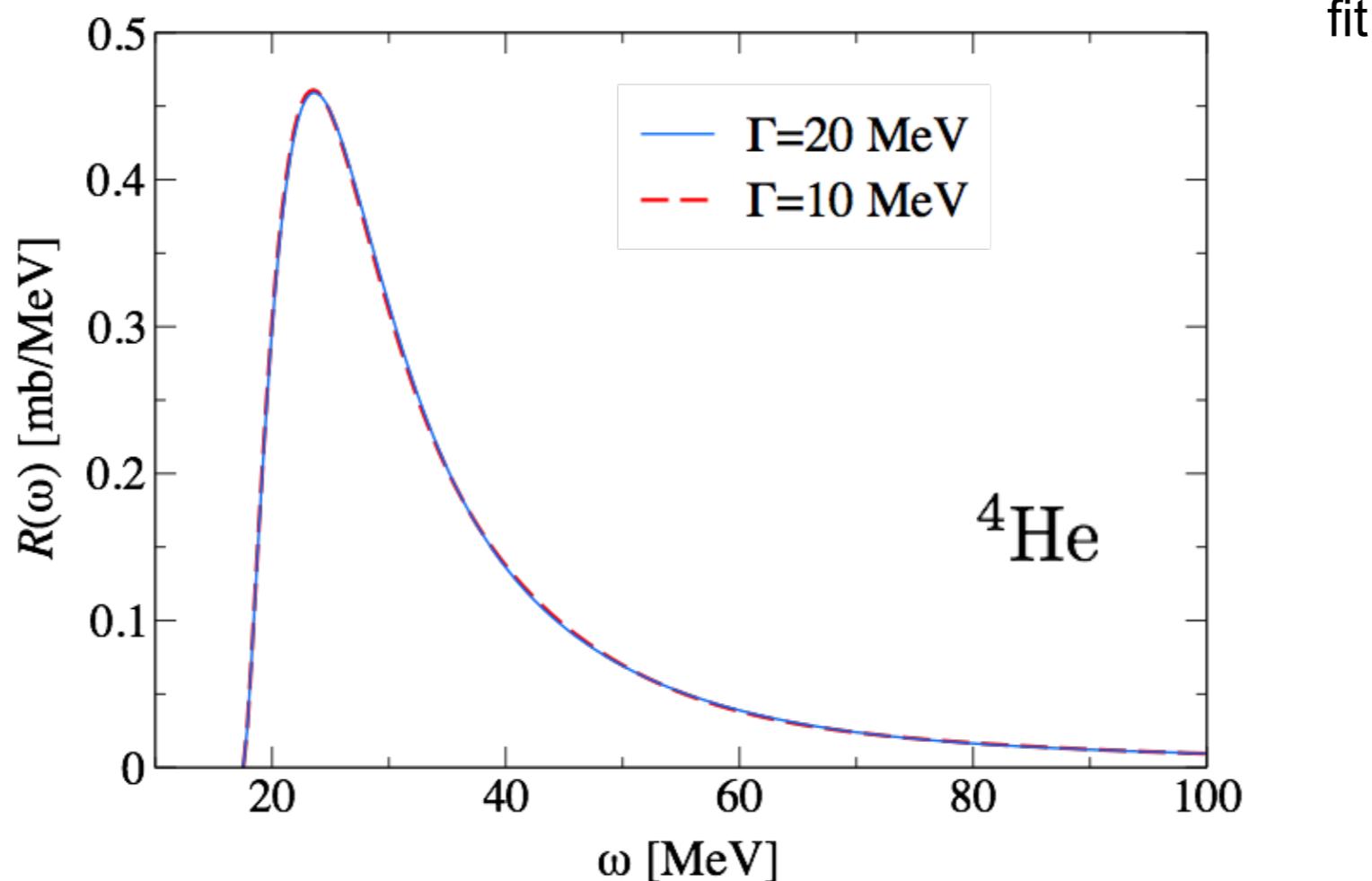
↑
fit

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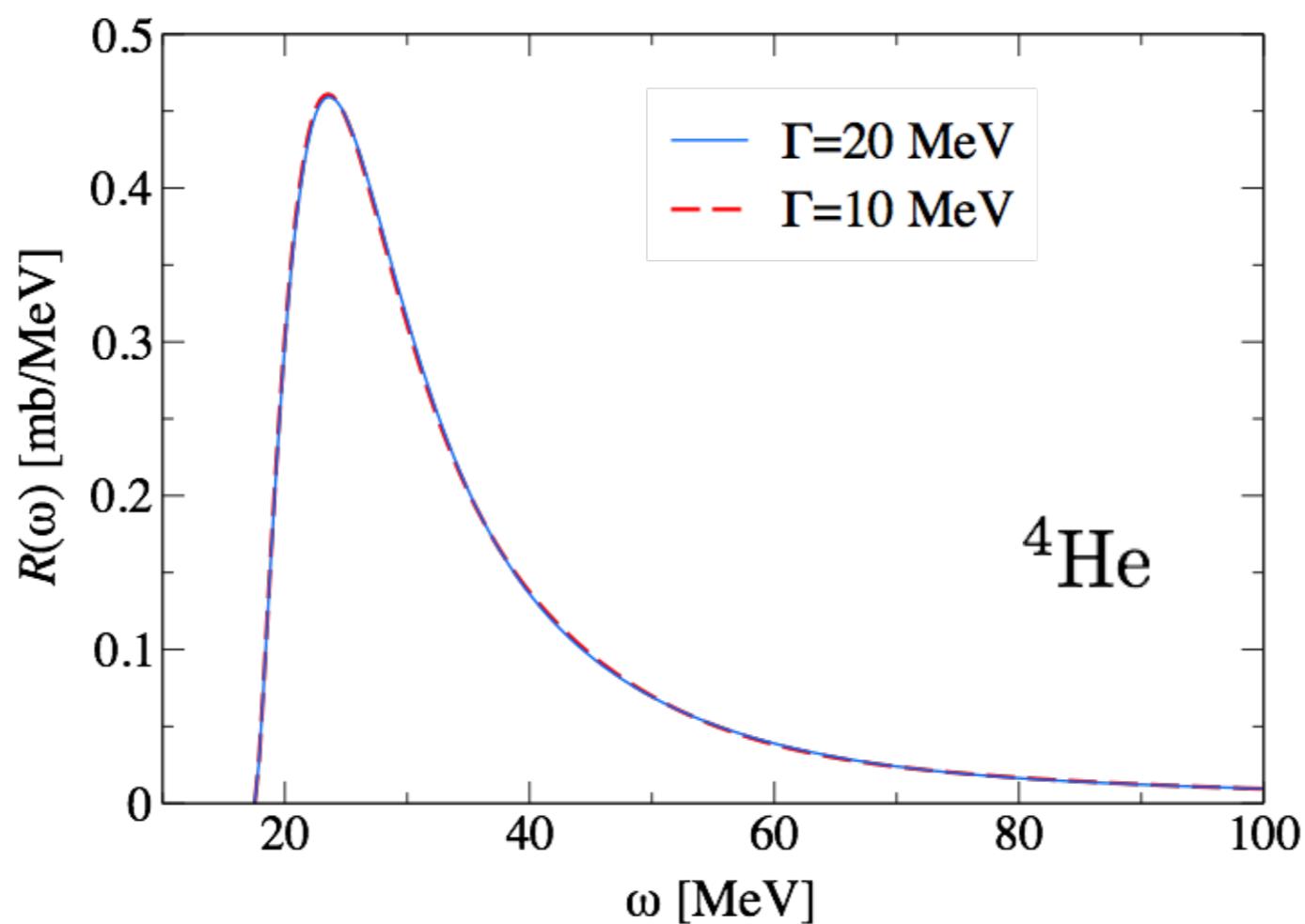
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↑
fit



Message: Inversions are stable if the LIT is calculated precisely enough

Validation in ${}^4\text{He}$

Dipole response function

Comparison of CCSD with exact hyperspherical harmonics with NN forces at N³LO

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

