Progress on coupled cluster calculations of electroweak nuclear properties

Sonia Bacca

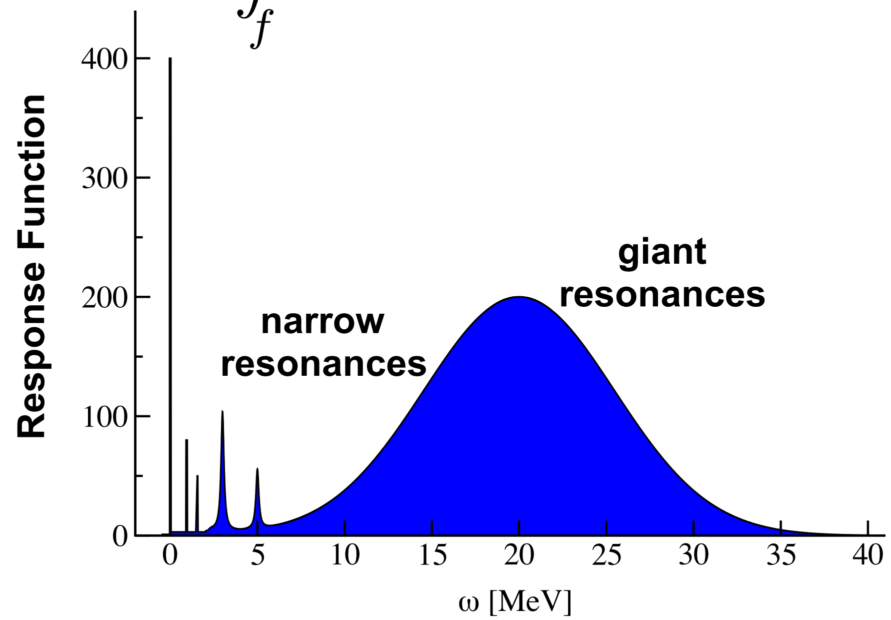
Johannes Gutenberg Universität Mainz

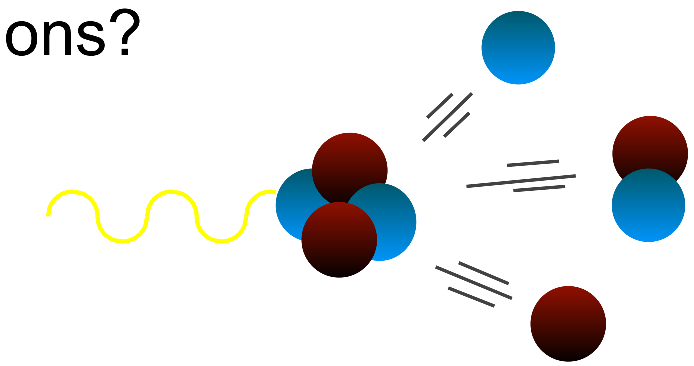
March 5th, 2020

Electroweak processes

- How does the nucleus respond to external electroweak excitations?

$$R(\omega, q) = \sum\!\!\!\!\!\!\int_f |\langle \Psi_f | \Theta(q) | \Psi_0 \rangle|^2 \delta(\omega - E_f + E_0)$$





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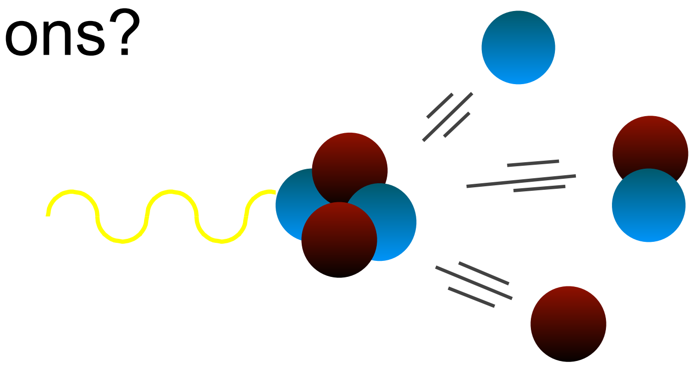

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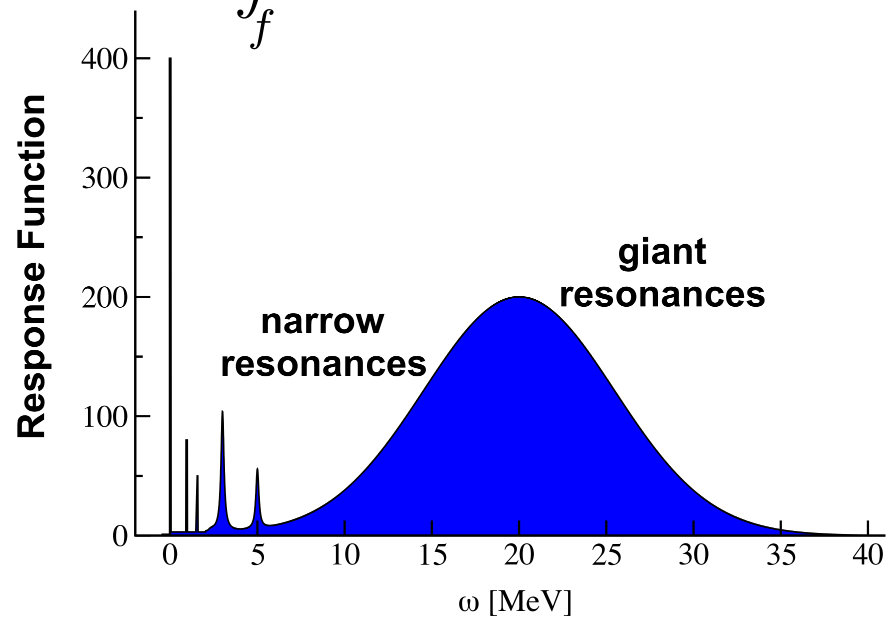

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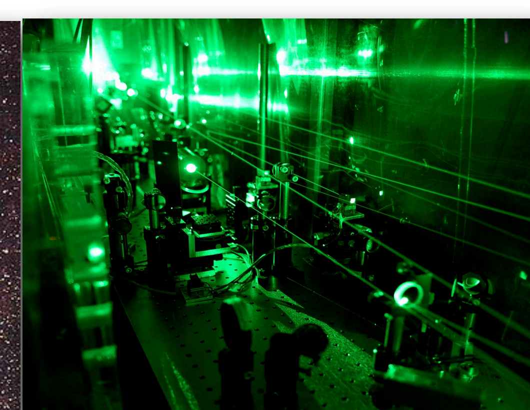
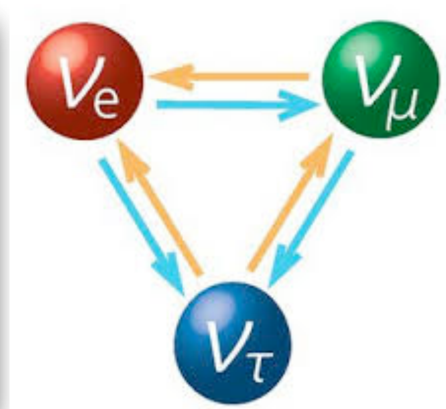
  - Astrophysics:
  - Atomic physics
  - Particle physics





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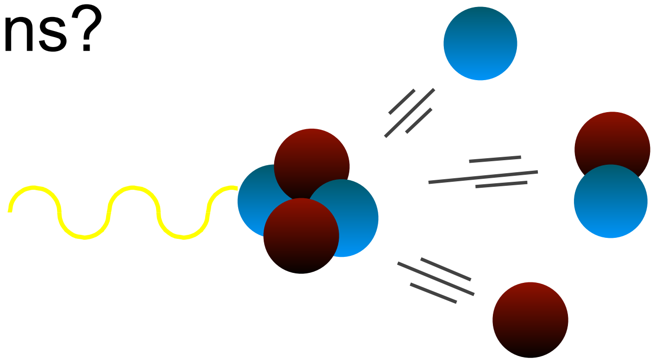

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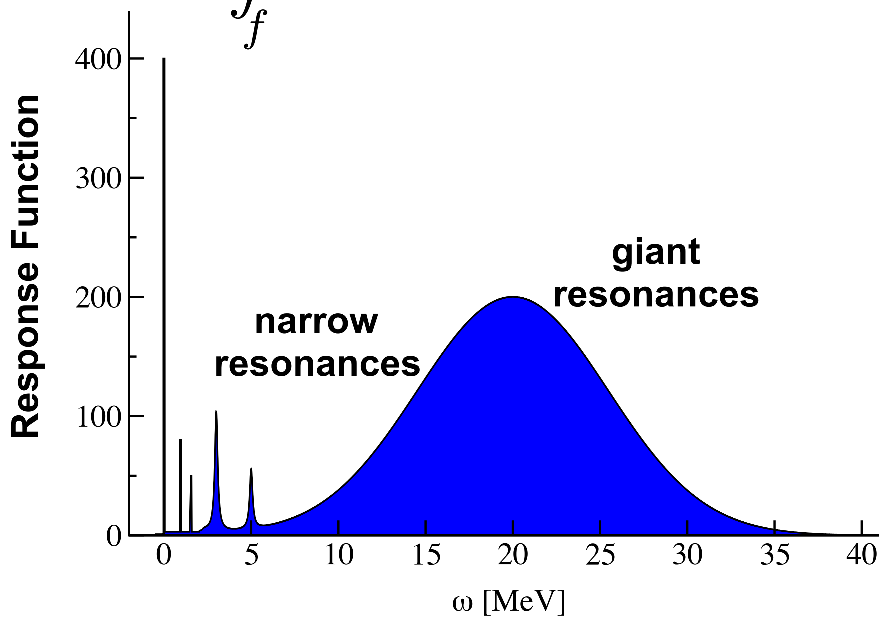

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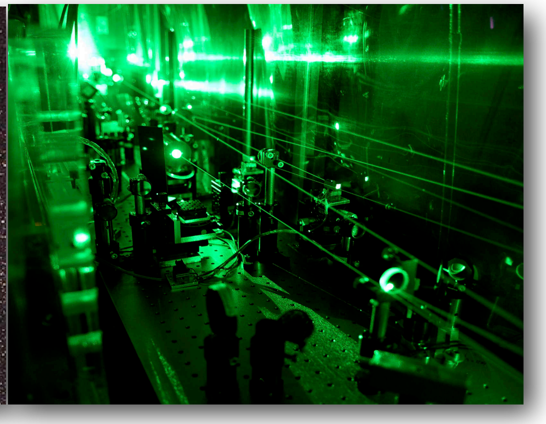

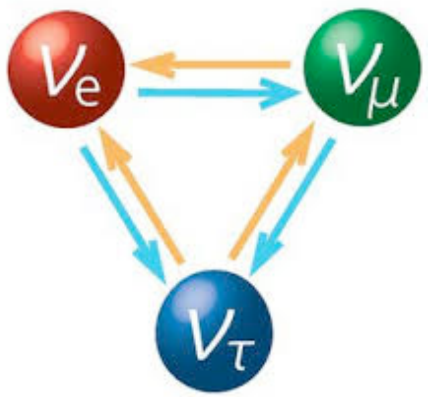

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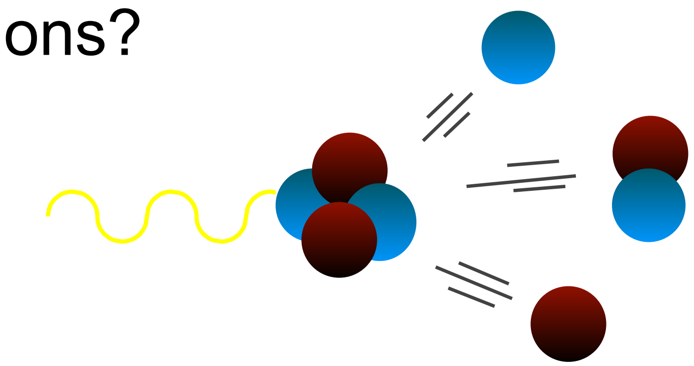

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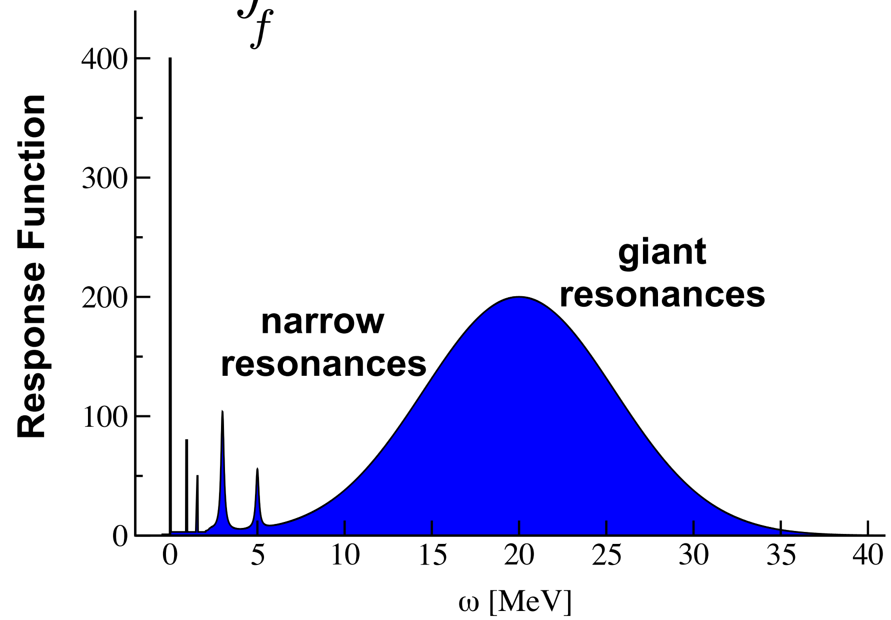

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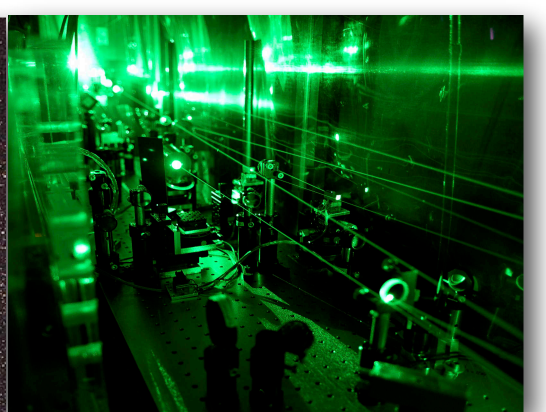
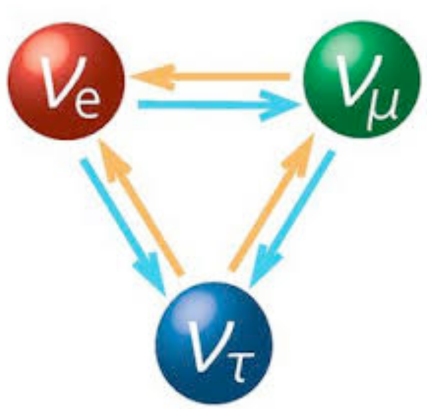
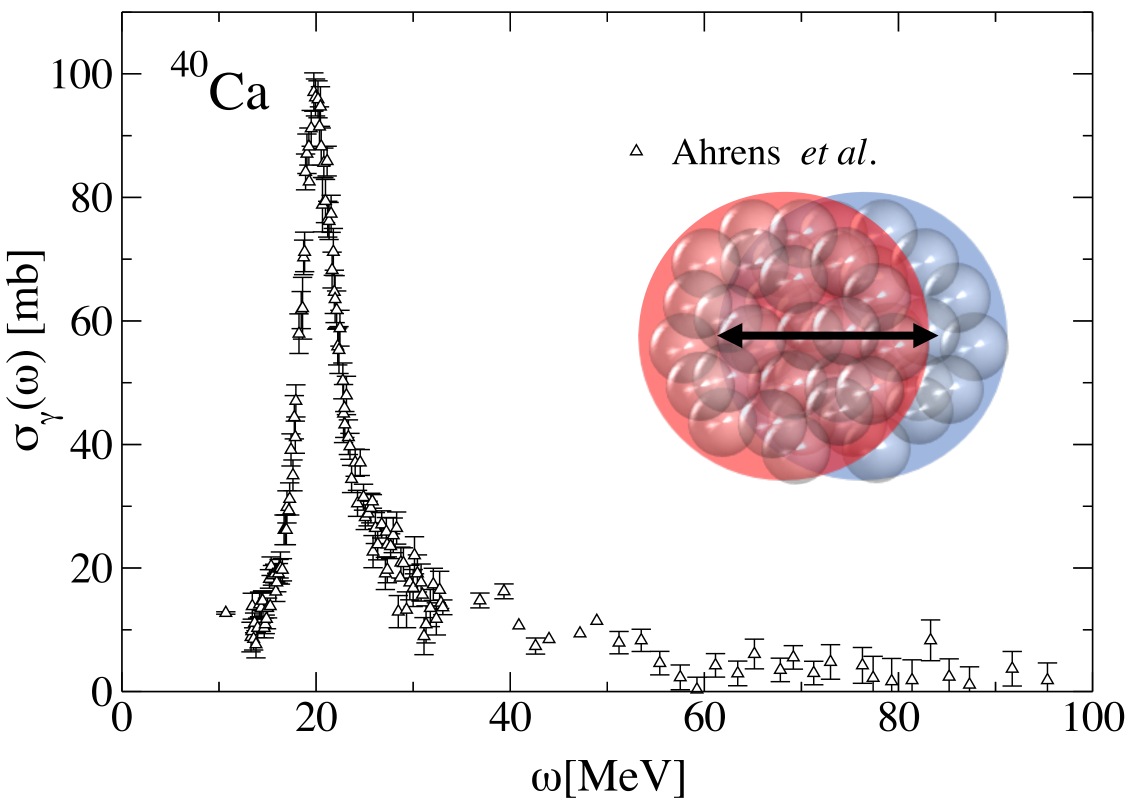


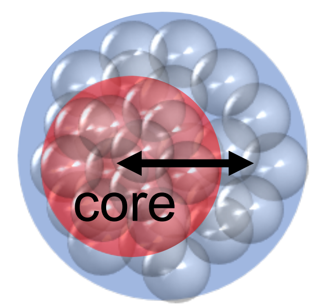


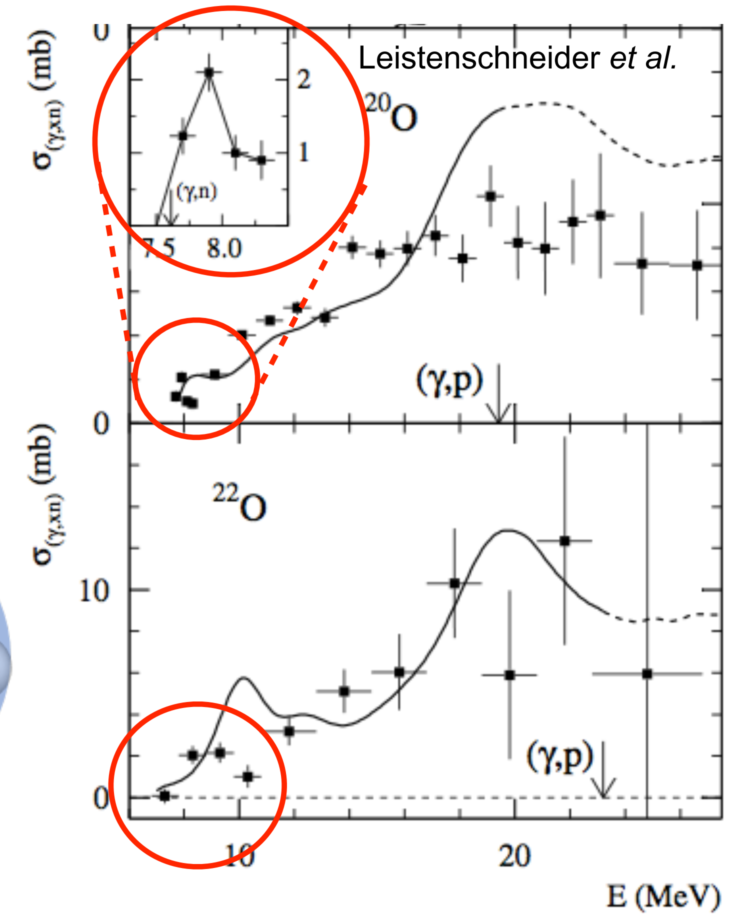
Electromagnetic sector

Unstable Nuclei

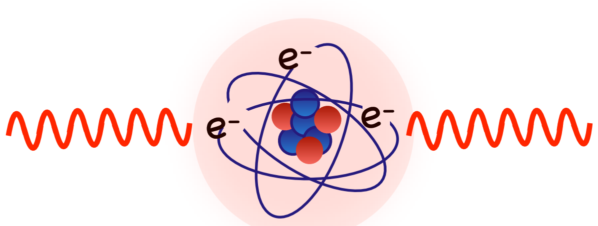
Stable Nuclei



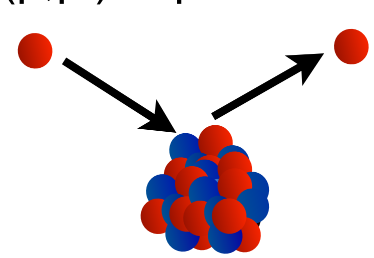




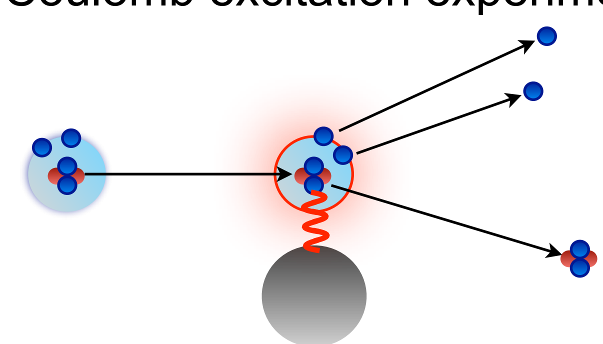
From photoabsorption experiments



(p,p') experiments



From Coulomb excitation experiments



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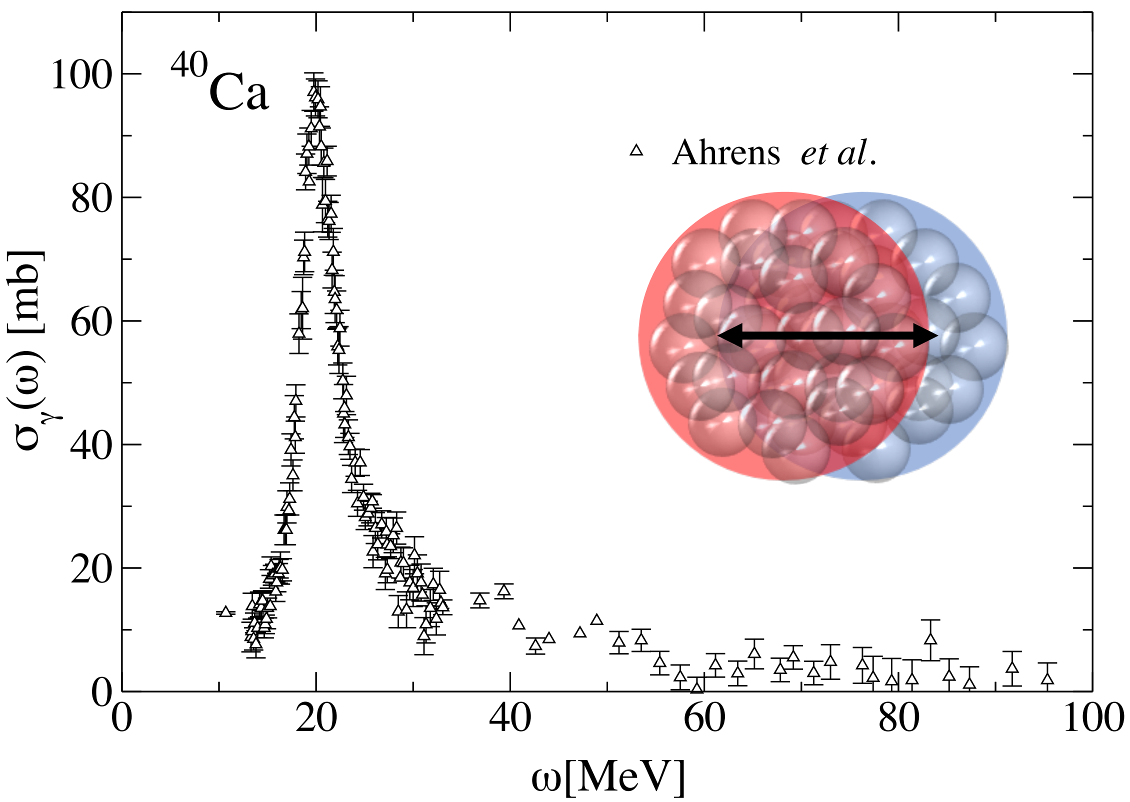

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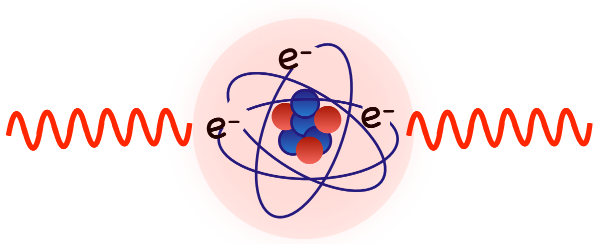

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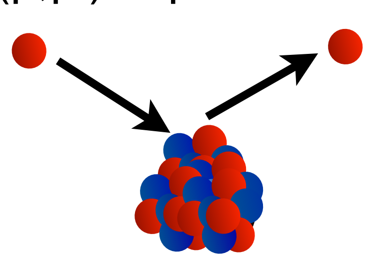

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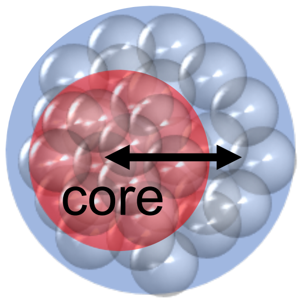

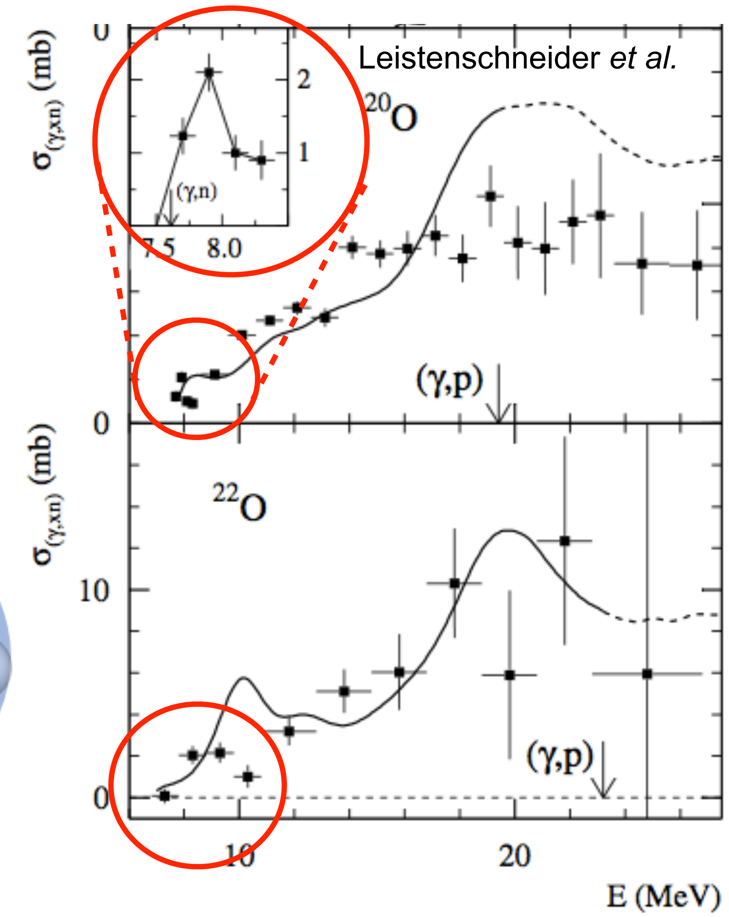

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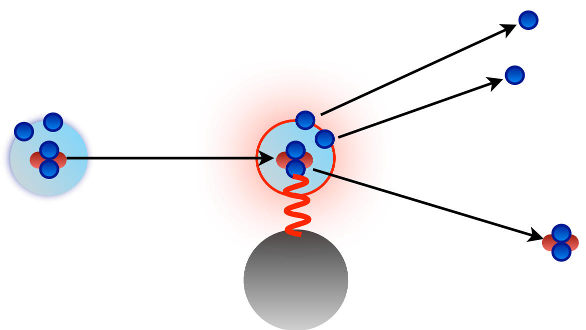
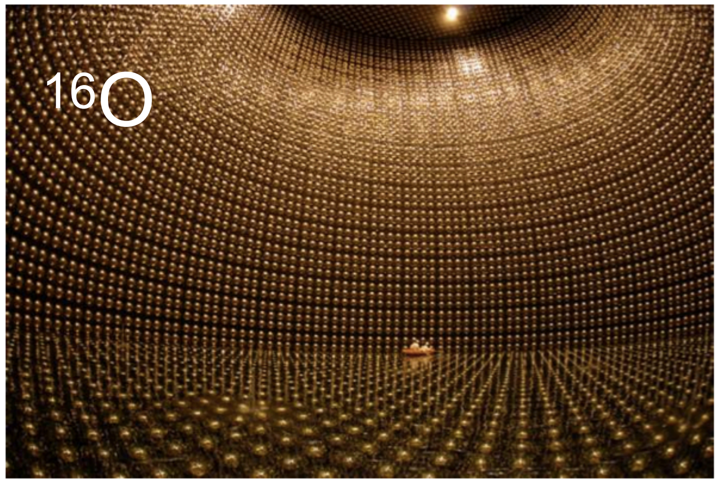


Are we able to explain these and new data from first principles?

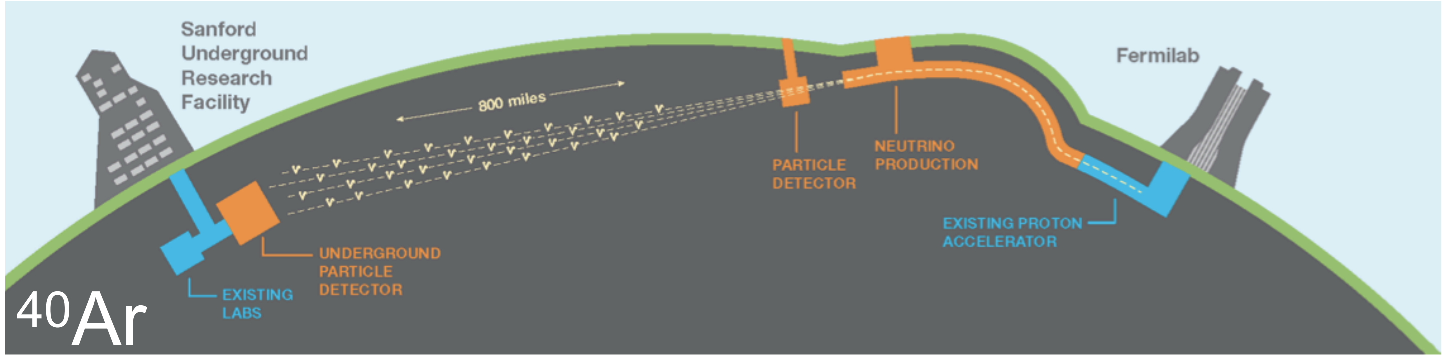
Electroweak sector

In neutrino experiments, detectors are made by complex nuclei



T2K

Short and Long-baseline neutrino experiments



DUNE

See Bijaya's talk tomorrow

Electroweak sector

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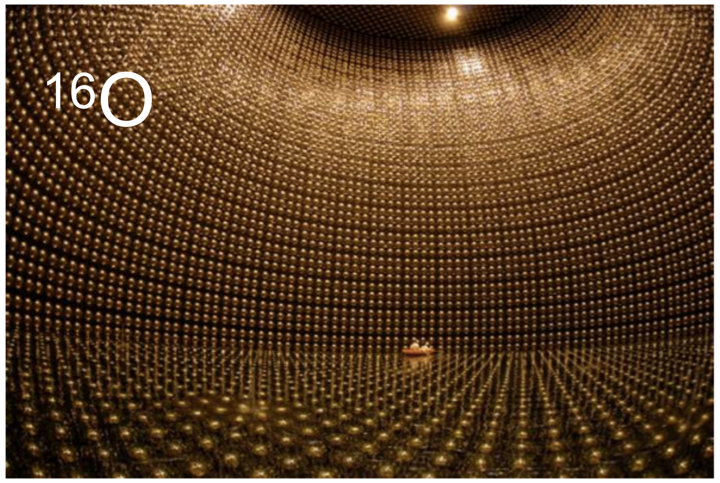

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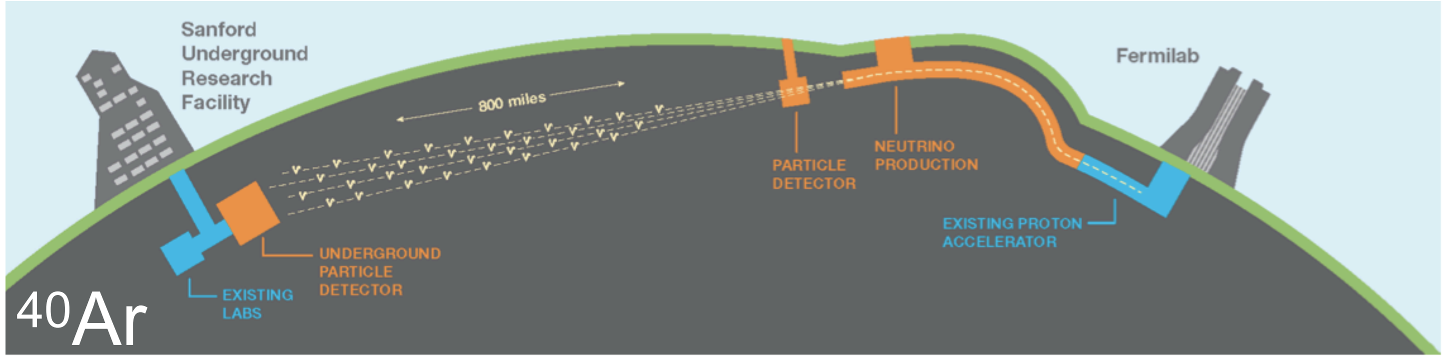


DUNE

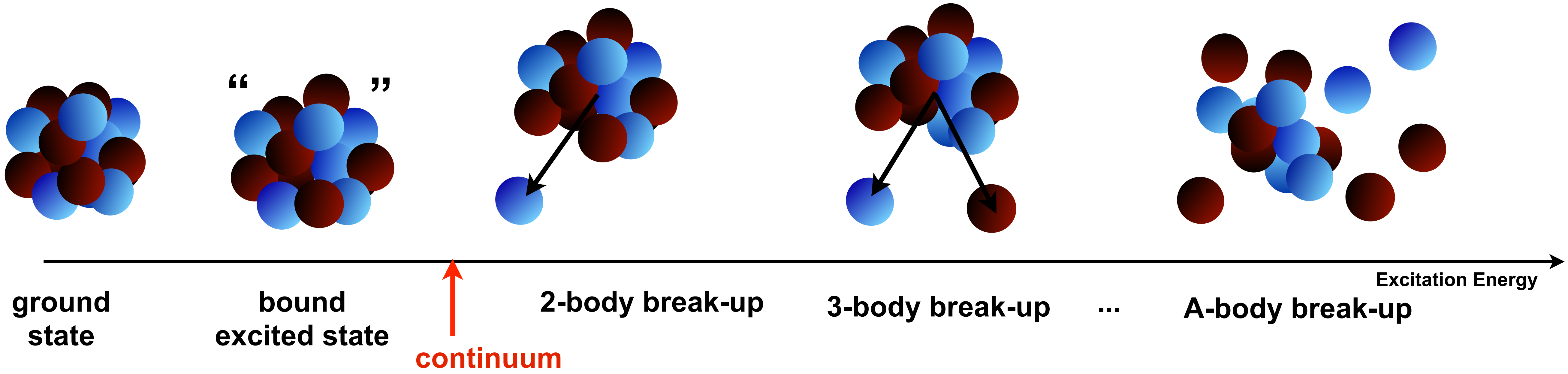
See Bijaya's talk tomorrow

Measuring the elusive neutrinos …

Various materials including, ^{40}Ar

Can ab-initio nuclear theory impact this field?

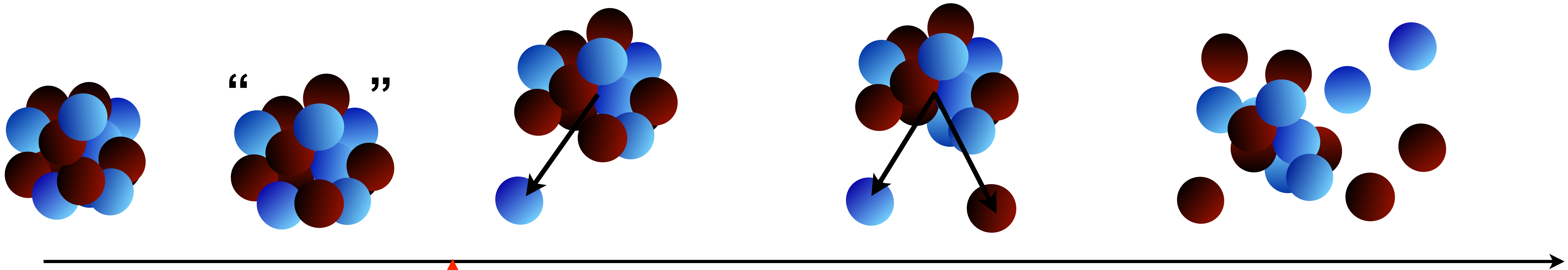
Continuum problem



$$R(\omega) \propto \left| \langle \Psi_f | \, \Theta \, | \Psi_0 \rangle \right|^2$$

Exact knowledge limited in energy and mass number

Continuum problem

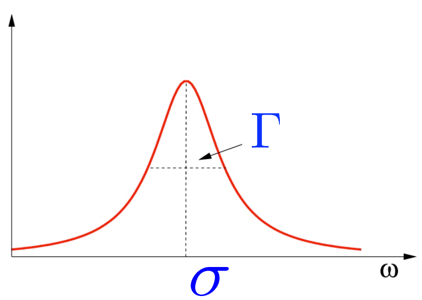


$$R(\omega) \propto \left| \langle \Psi_f | \, \Theta \, | \Psi_0 \rangle \right|^2 \quad \Longleftrightarrow \quad L(\sigma,\Gamma) = \frac{\Gamma}{\pi} \int d\omega \frac{R(\omega)}{(\omega-\sigma)^2+\Gamma^2} = \langle \tilde{\psi} | \tilde{\psi} \rangle$$

Exact knowledge limited in energy and mass number

Lorentz Integral Transform

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

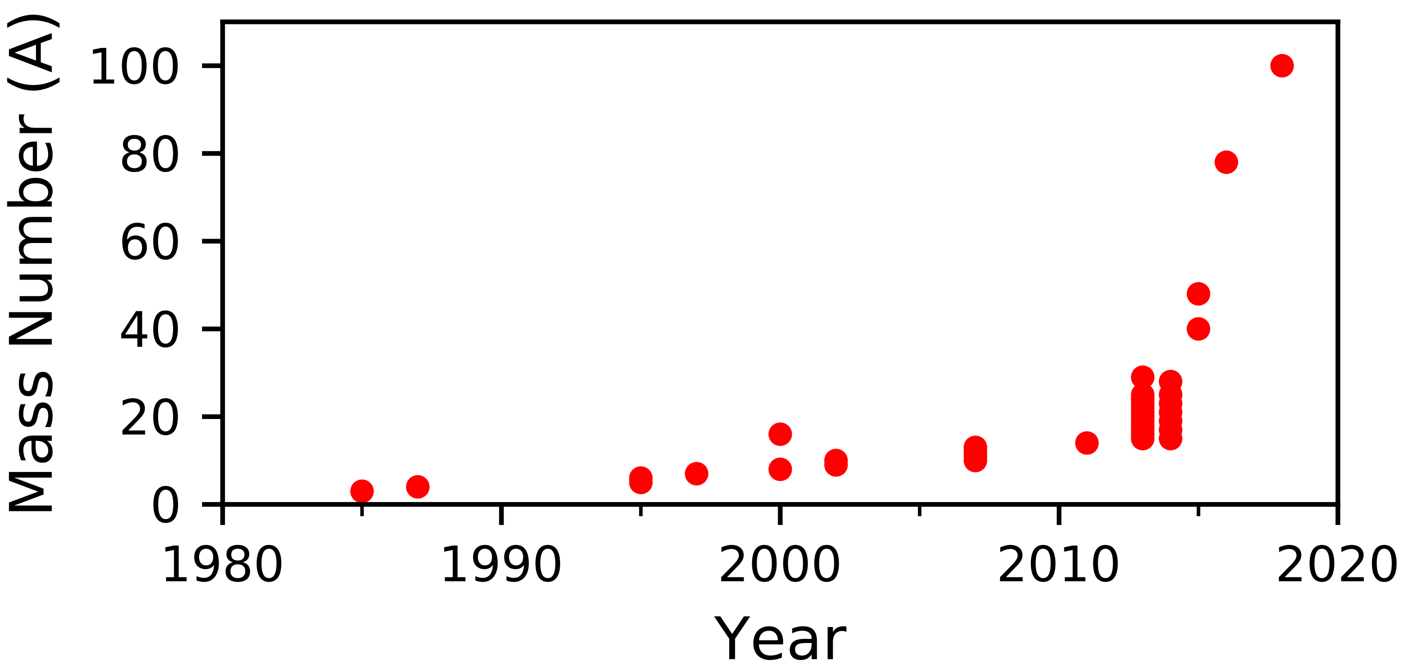


$$\Rightarrow \quad (H - E_0 - \sigma + i\Gamma) \, | \, \tilde{\psi} \rangle = \Theta \, | \, \psi_0 \rangle$$

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

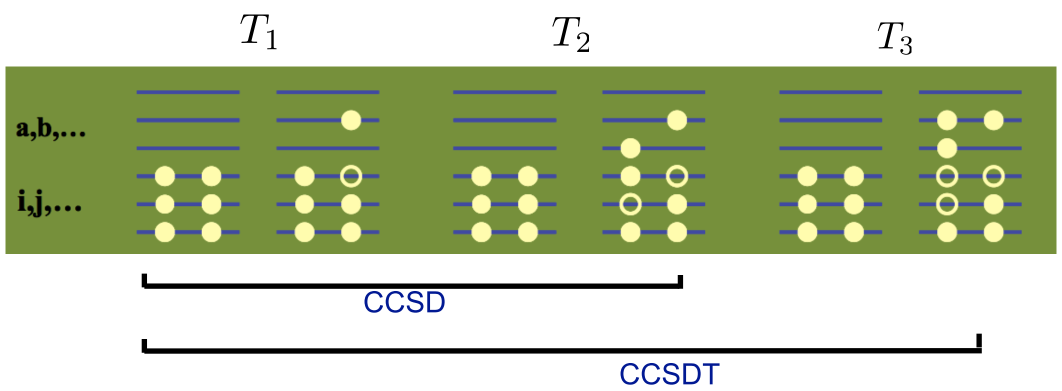
Coupled-cluster theory formulation

In collaboration with ORNL group



$$|\psi_0(\vec{r}_1, \vec{r}_2, ..., \vec{r}_A)\rangle = e^T |\phi_0(\vec{r}_1, \vec{r}_2, ..., \vec{r}_A)\rangle$$

$$T = \sum T_{(A)}$$ cluster expansion



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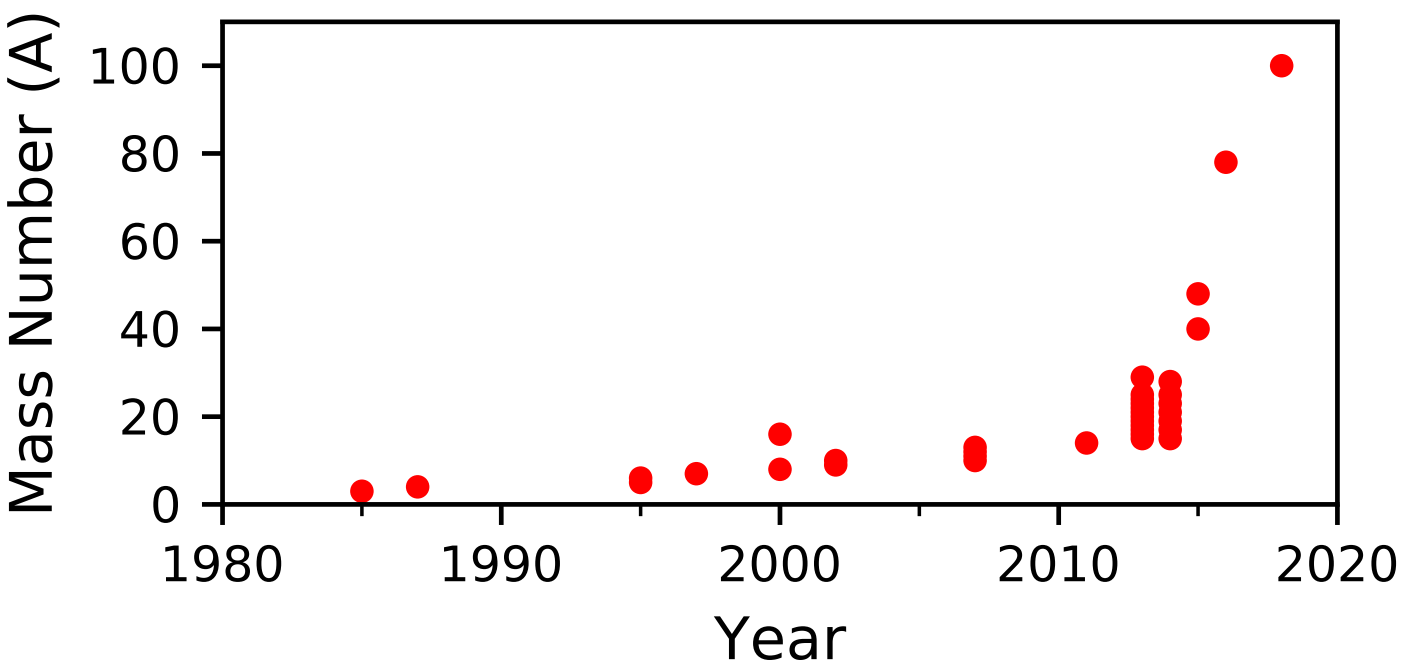

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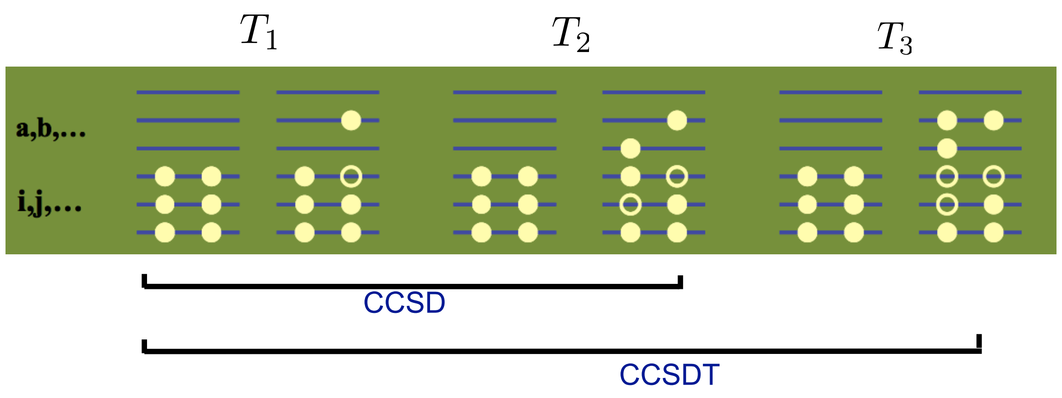

SB *et al.*, Phys. Rev. Lett. **111**, 122502 (2013)

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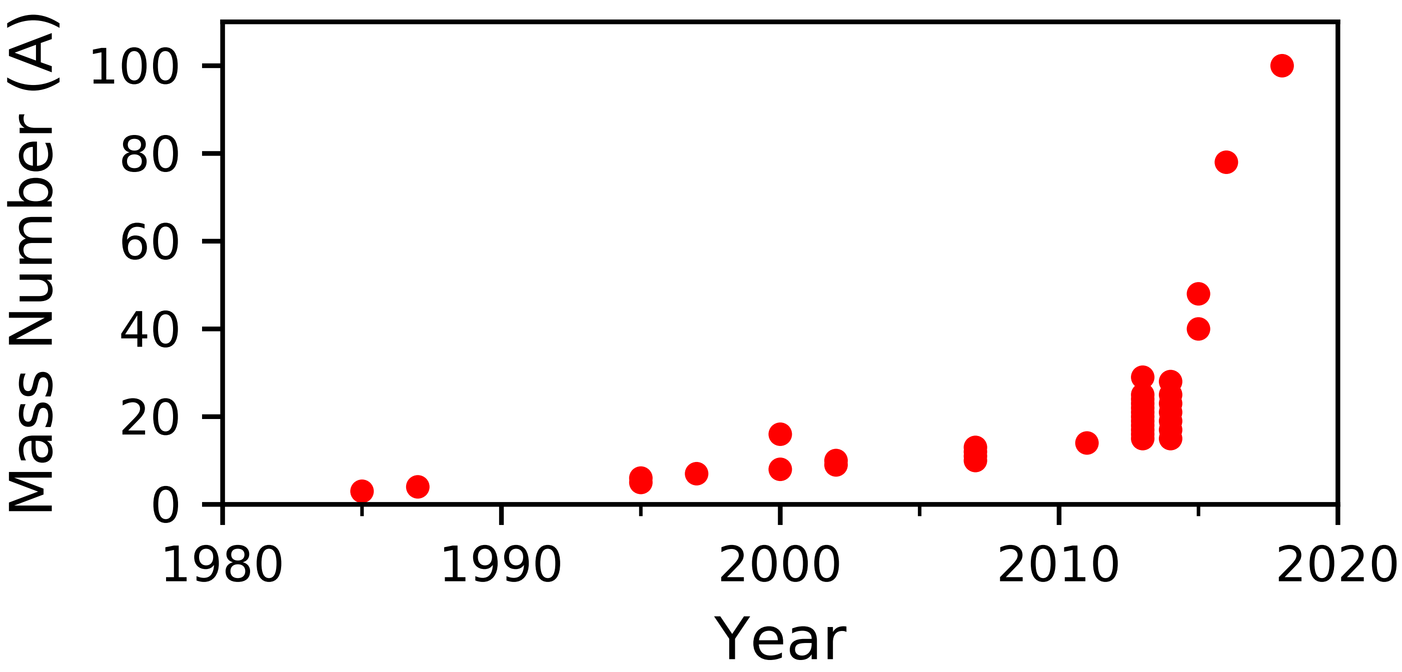

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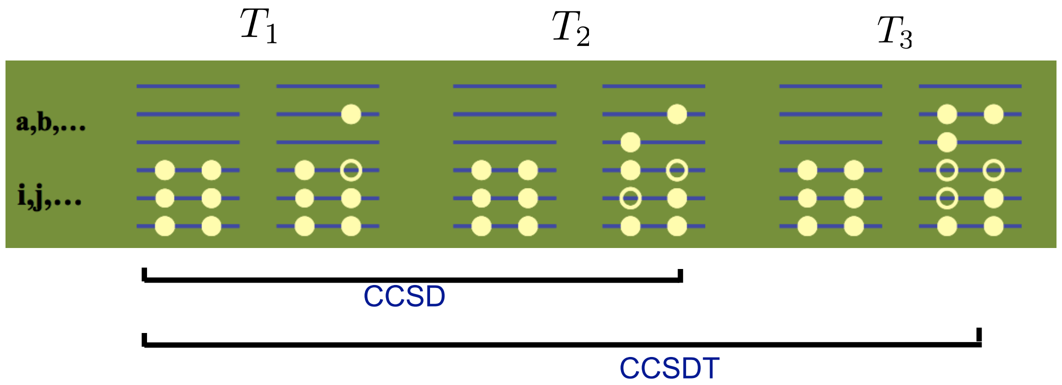

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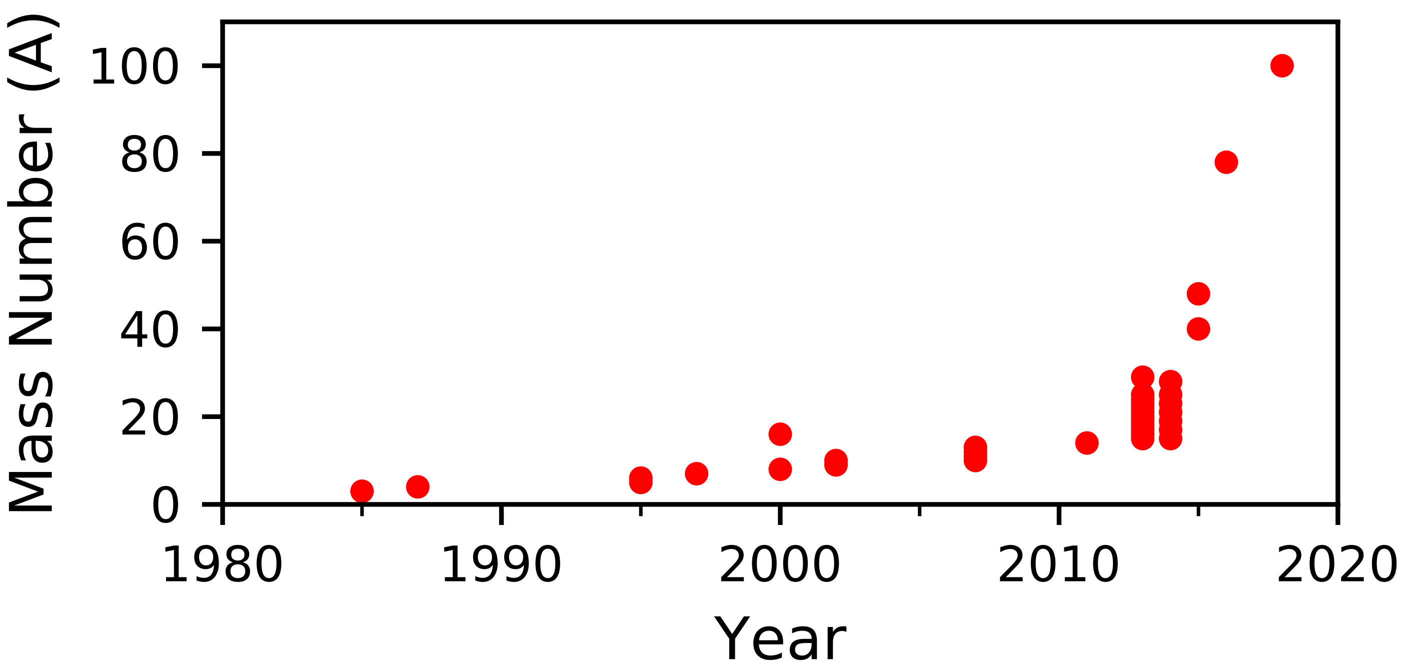

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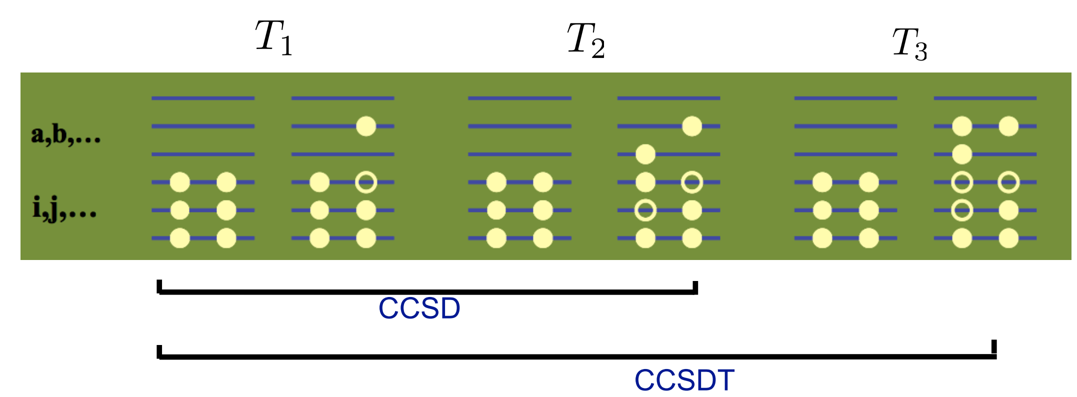

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Results with implementation at CCSD level

$$T = T_1 + T_2$$

$$R = R_0 + R_1 + R_2$$

Coupled-cluster theory formulation

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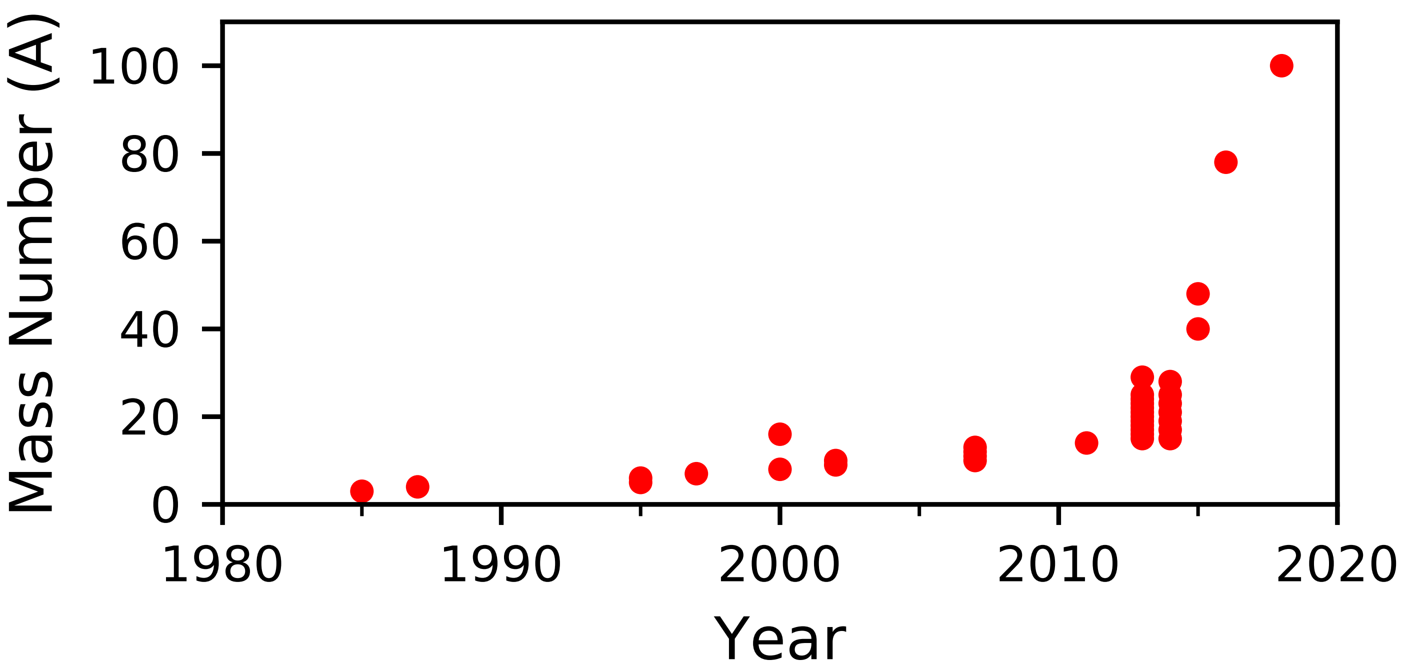

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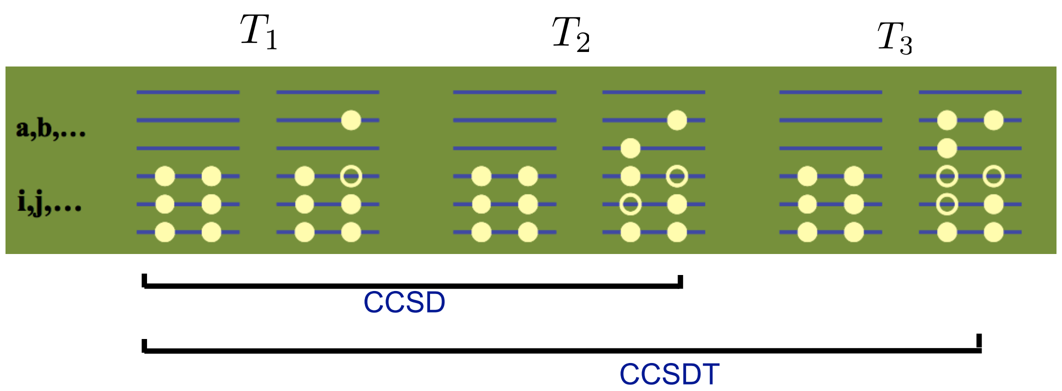

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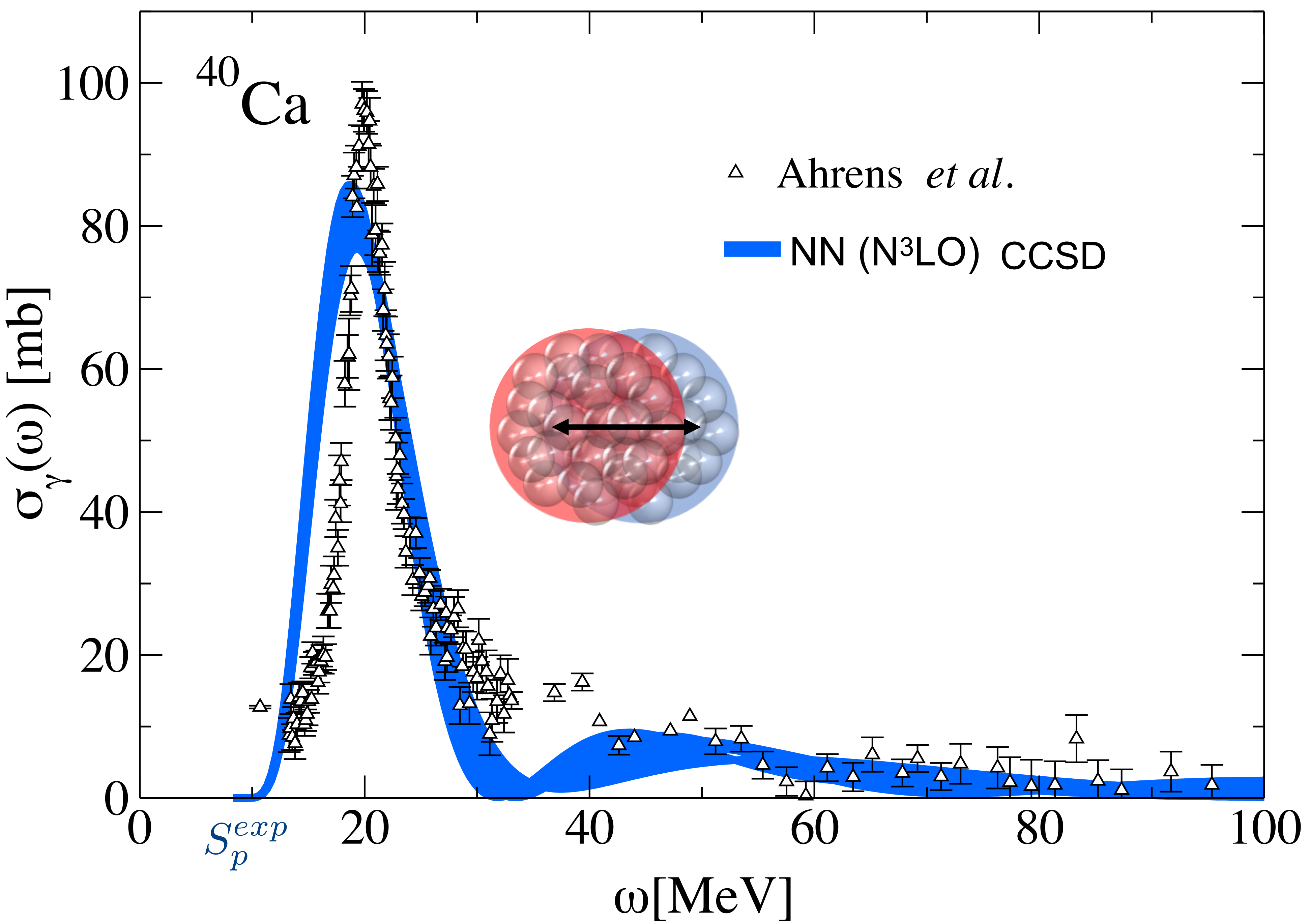
and triples as well

Addressing medium-mass nuclei

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



Electric dipole polarizability

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

Can be calculated:

(1) by integrating the strength obtained from LIT inversion

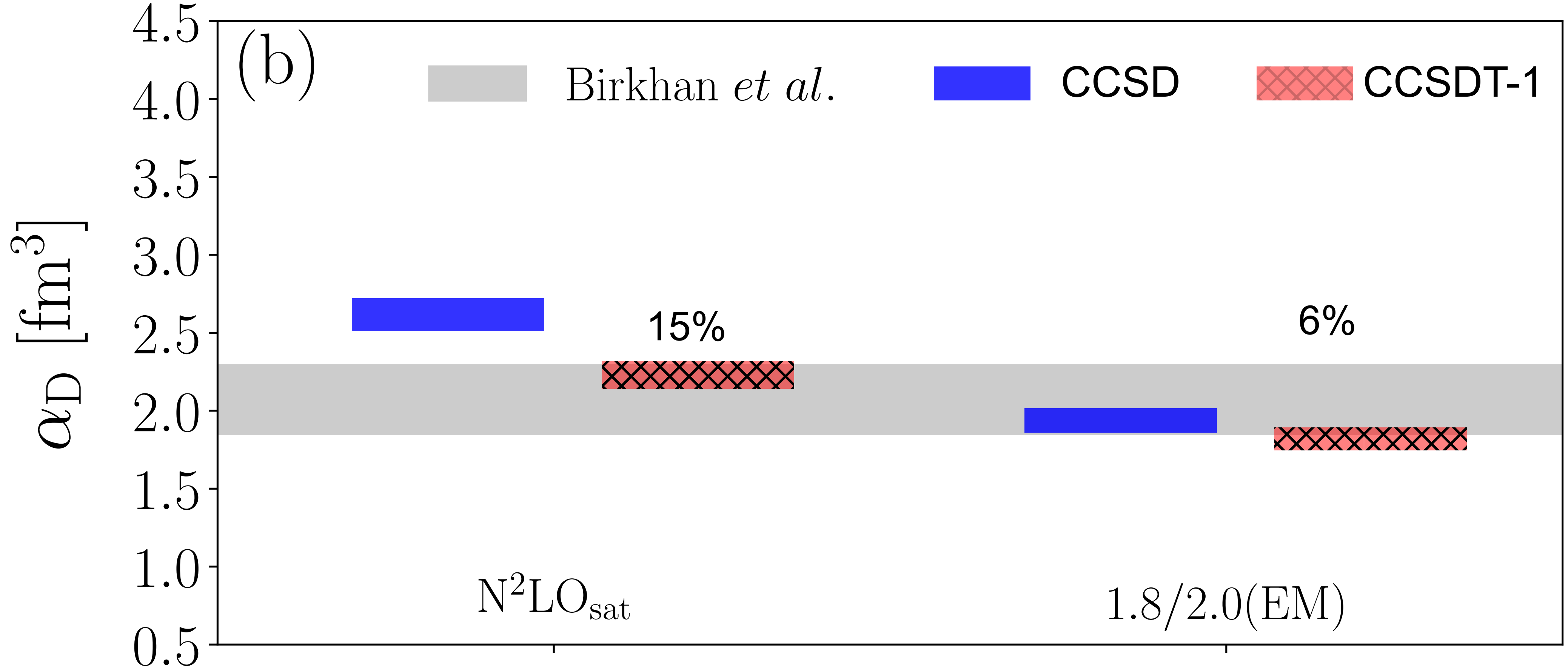
(2) Directly from the Lanczos coefficients (not going via the inversion)

Phys. Rev. C **94,** 034317 (2017)

$$\alpha_D \rightarrow \left\{ \frac{1}{(a_0+\sigma) - \frac{b_0^2}{(a_1+\sigma) - \frac{b_1^2}{(a_2+\sigma) - \cdots}}} \right\}$$

^{48}Ca electric dipole polarizability

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



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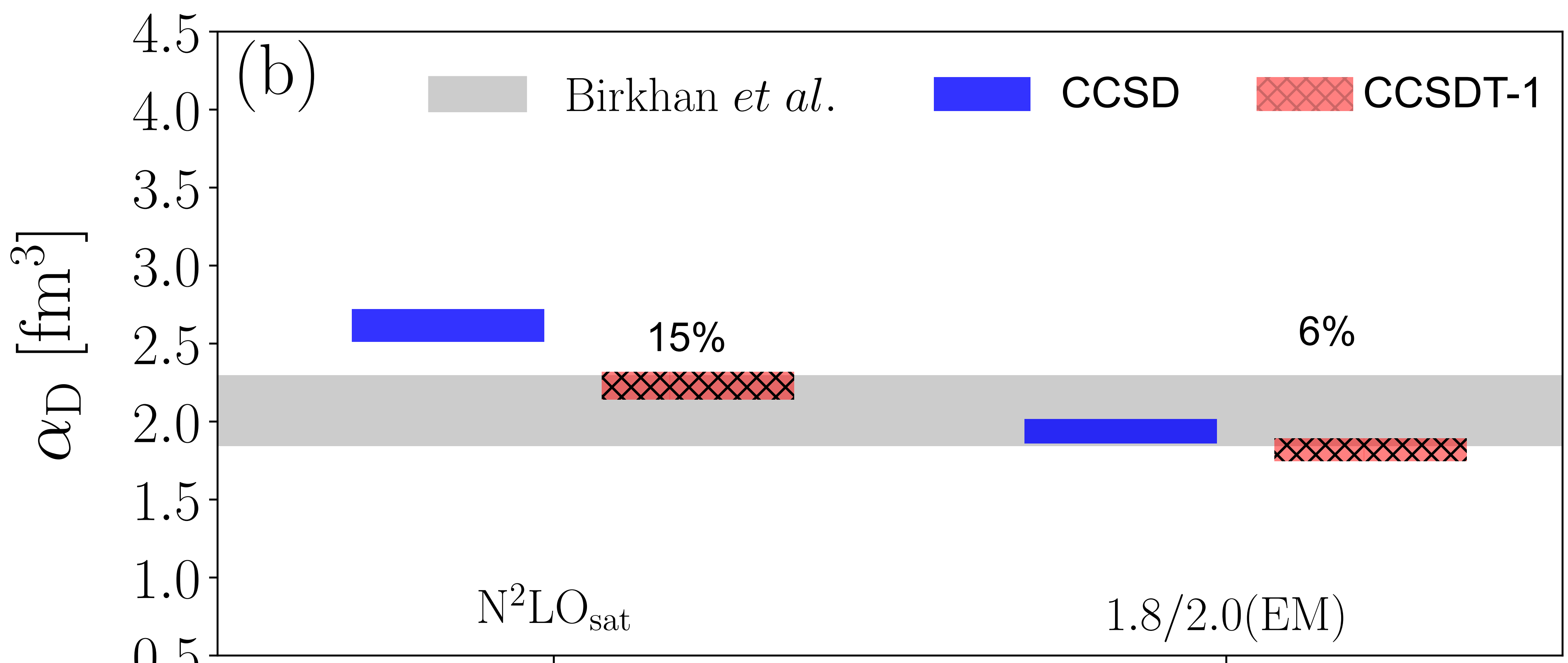
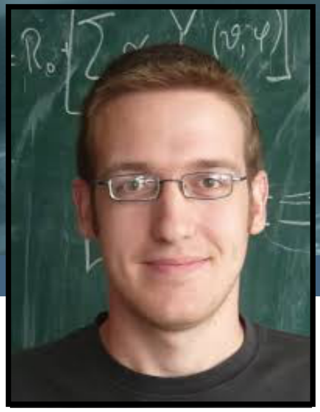


Higher order correlations are important

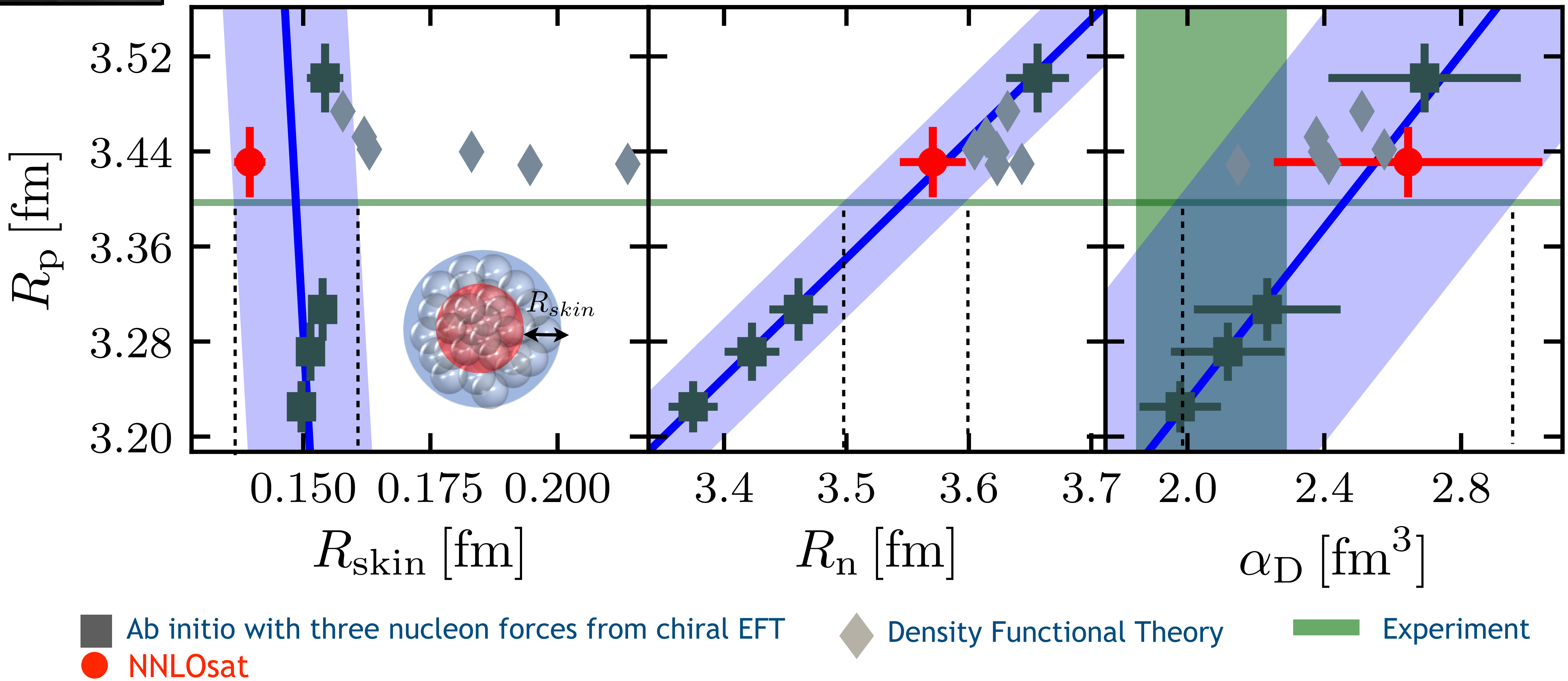
They improve the comparison with experiment



Revisiting ^{48}Ca

Similar to Nature Physics **12**, 186 (2016)

Coupled-cluster theory - CCSD

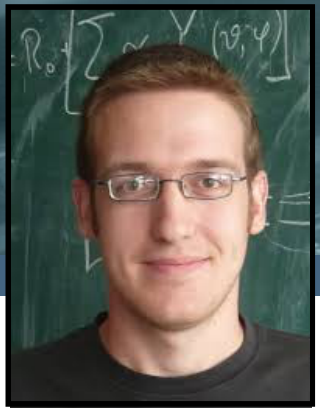


Ab-initio constraints:

$$0.12 \leq R_{\rm skin} \leq 0.15 \text{ fm}$$

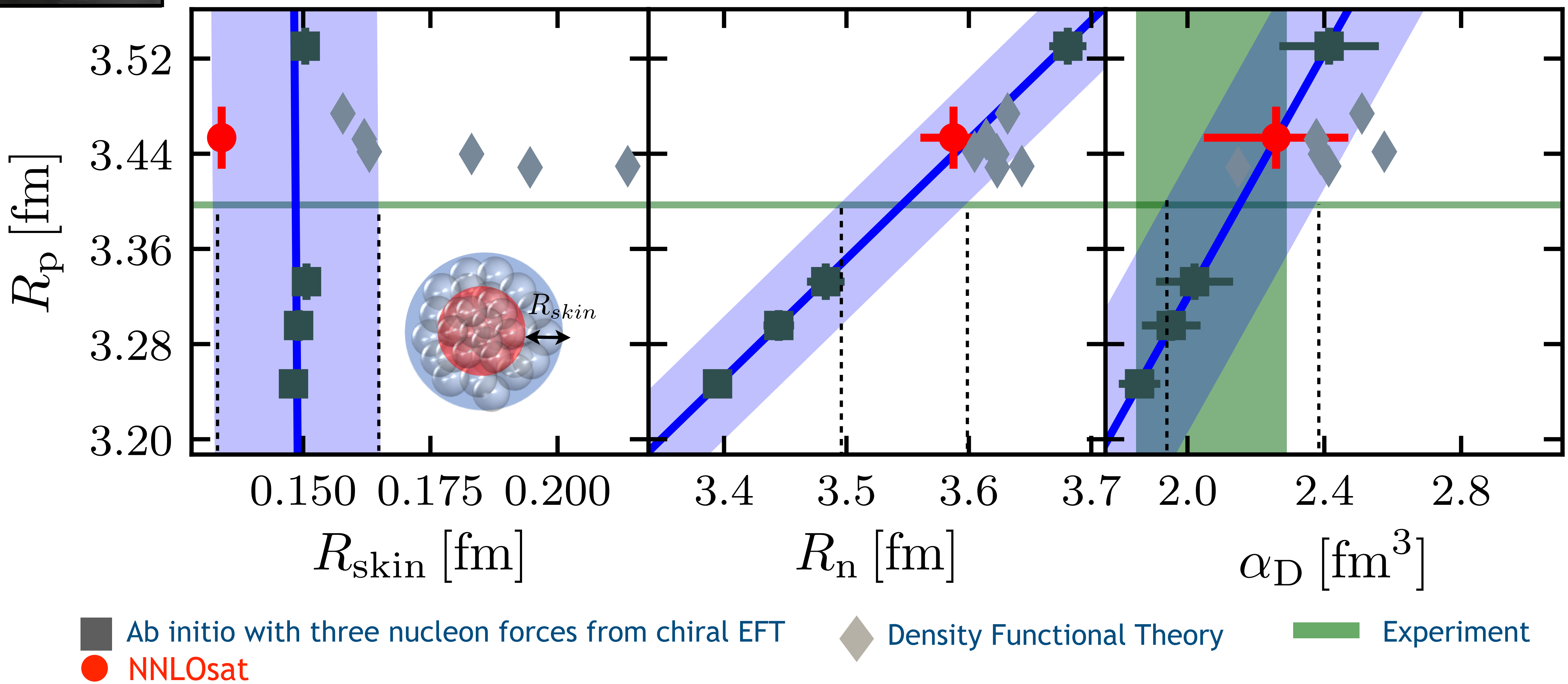
$$2.19 \leq \alpha_D \leq 2.60 \text{ fm}^3$$

Revisiting ^{48}Ca



Simonis, Bacca, Hagen, Eur. Phys. J. A 55, 241 (2019)

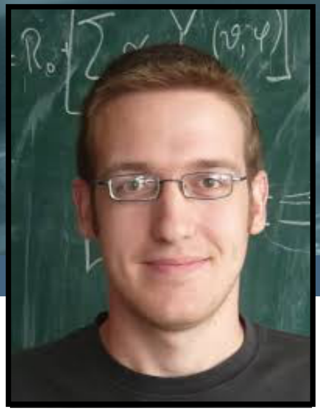
Coupled-cluster theory - CCSD-T1



Ab-initio constraints:

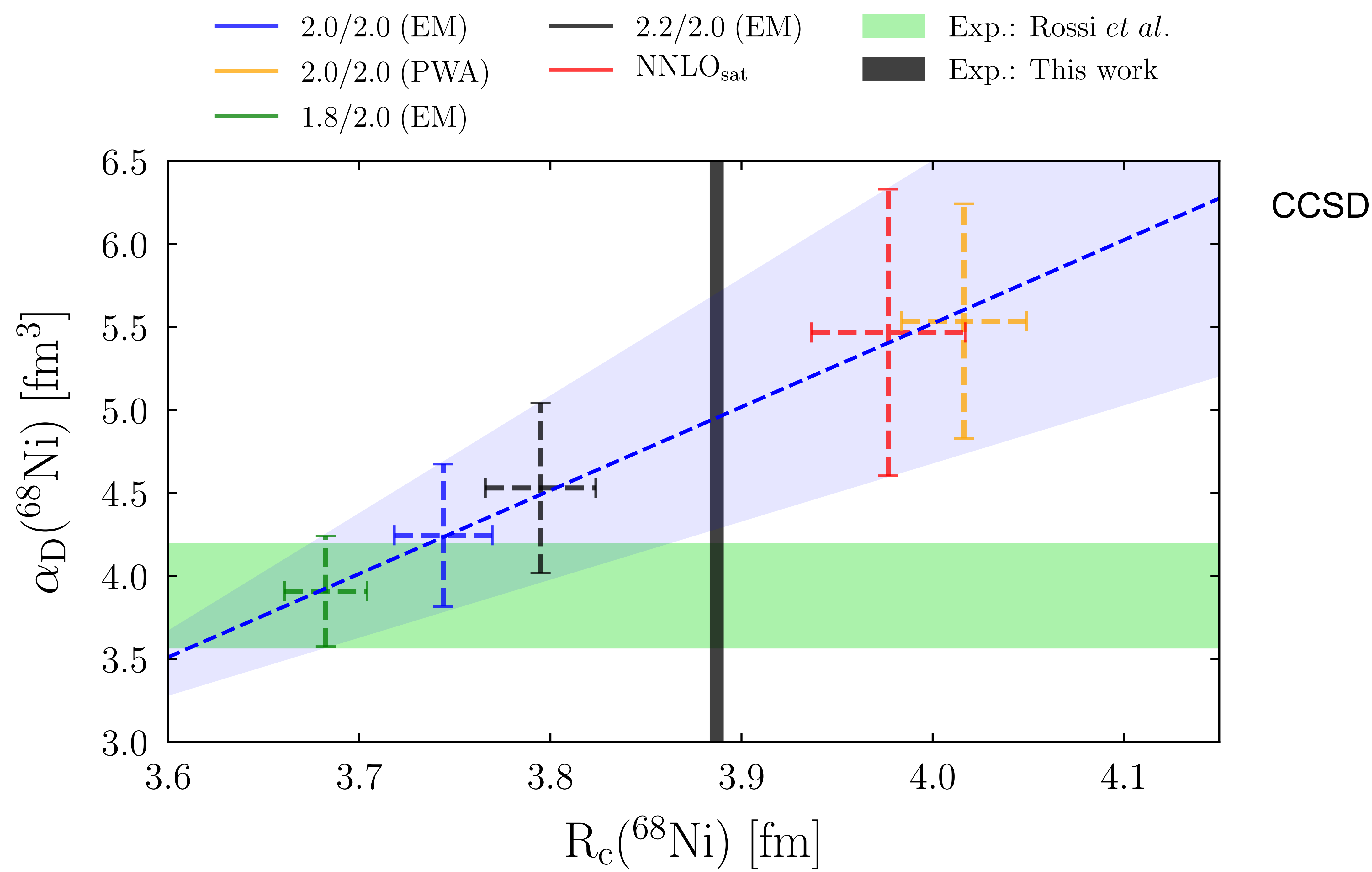
$$0.13 \leq R_{\rm skin} \leq 0.16 \text{ fm}$$

$$1.92 \leq \alpha_D \leq 2.38 \text{ fm}^3$$

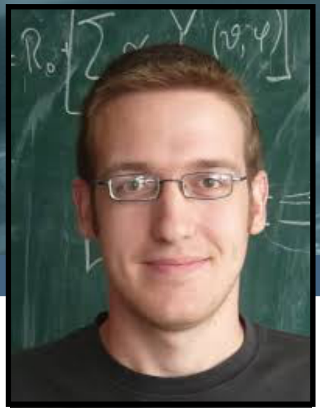


^{68}Ni from first principles

Kaufmann, Simonis, et al., (2020) submitted



NNLOsat $\alpha_D = 3.60\ \mathrm{fm}^3$ F. Raimondi and C. Barbieri, Phys. Rev. C **99**, 054327 (2019)



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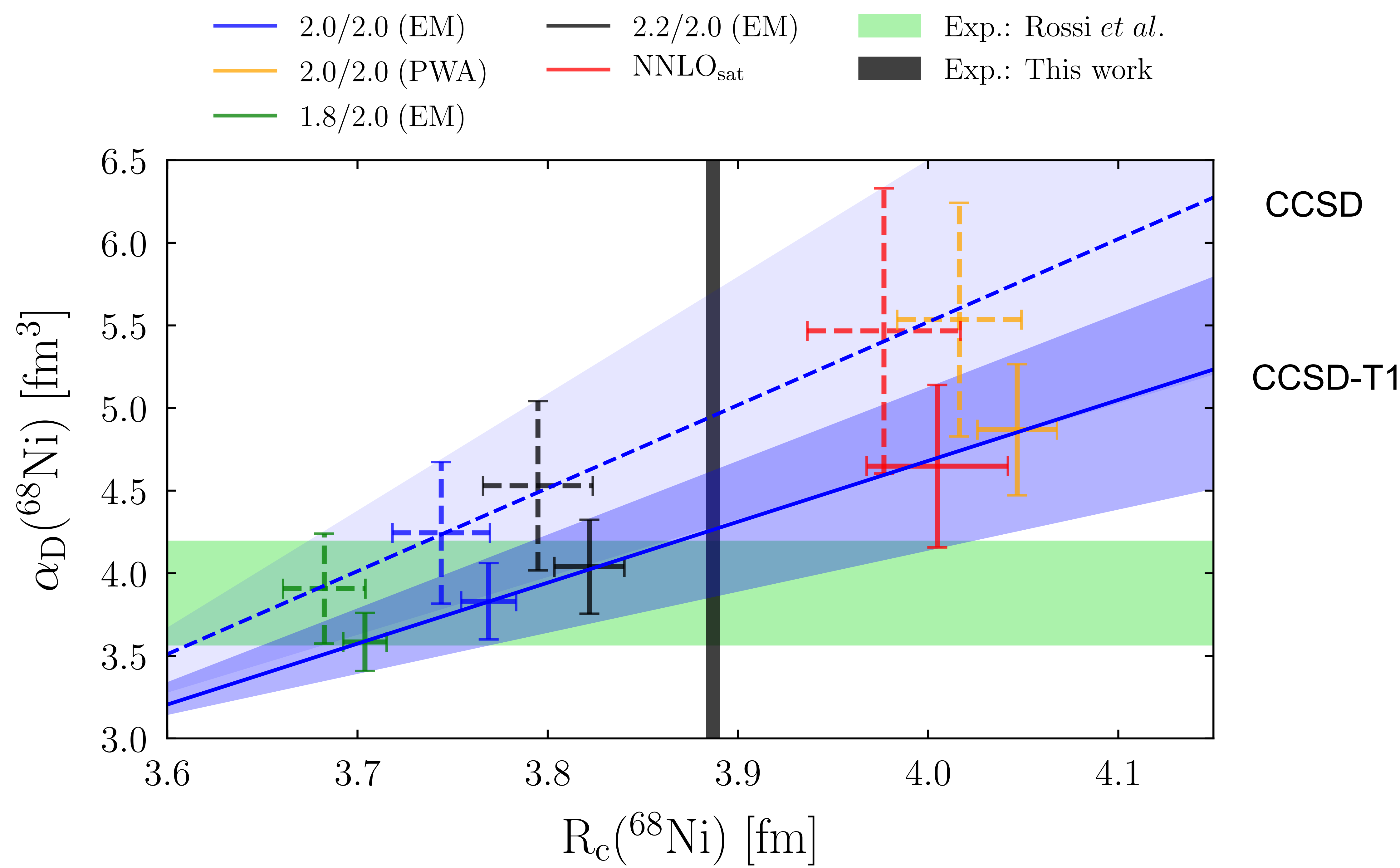

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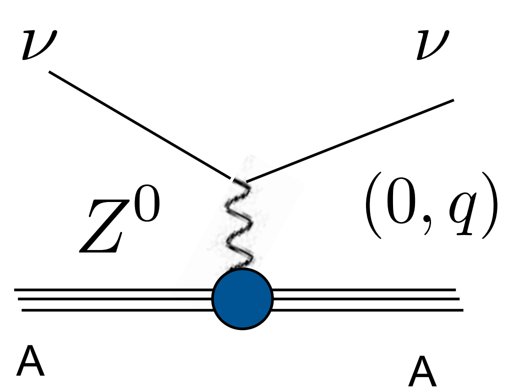
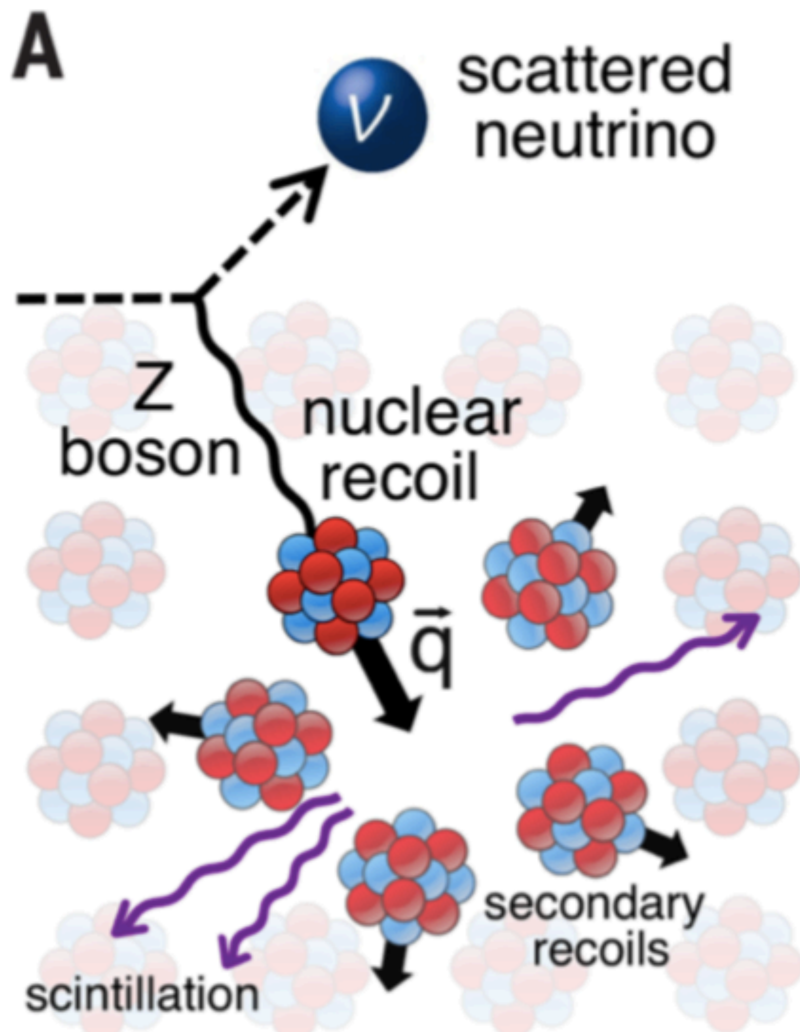
Coherent elastic neutrino scattering

CEvNS



The neutrino exchanges a Z-boson with the nucleus, that recoils as a whole (no internal excitation).

This is valid for neutrino energies up to 50 MeV



Experimental signature: tiny energy deposited by nuclear recoils in the target material

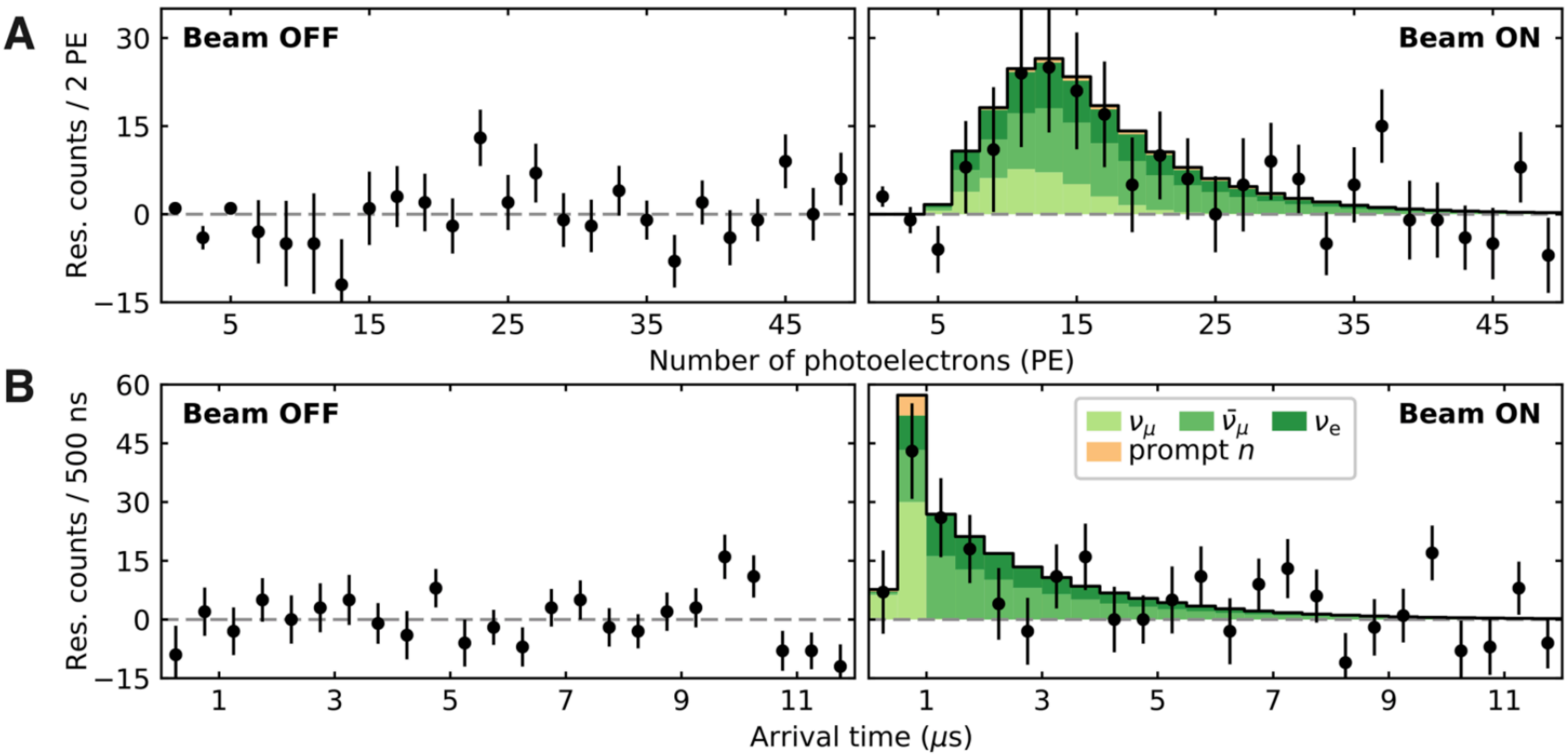
COHERENT@SNS-ORNL

Science

REPORTS

Cite as: D. Akimov *et al.*, *Science* 10.1126/science.aao0990 (2017).

Observation of coherent elastic neutrino-nucleus scattering



CEvNS cross section

$$\frac{d\sigma}{dT} = \frac{G_F^2}{4\pi} Q_W^2 M \left(1 - \frac{MT}{2E_\nu^2}\right) F_W^2(Q^2)$$

Weak form factor

$$F_W(Q) = \frac{1}{Q_W} \int d^3r \, \frac{\sin Qr}{Qr} \left[\rho_n(r) - (1 - 4\sin^2\theta_W)\rho_p(r)\right]$$

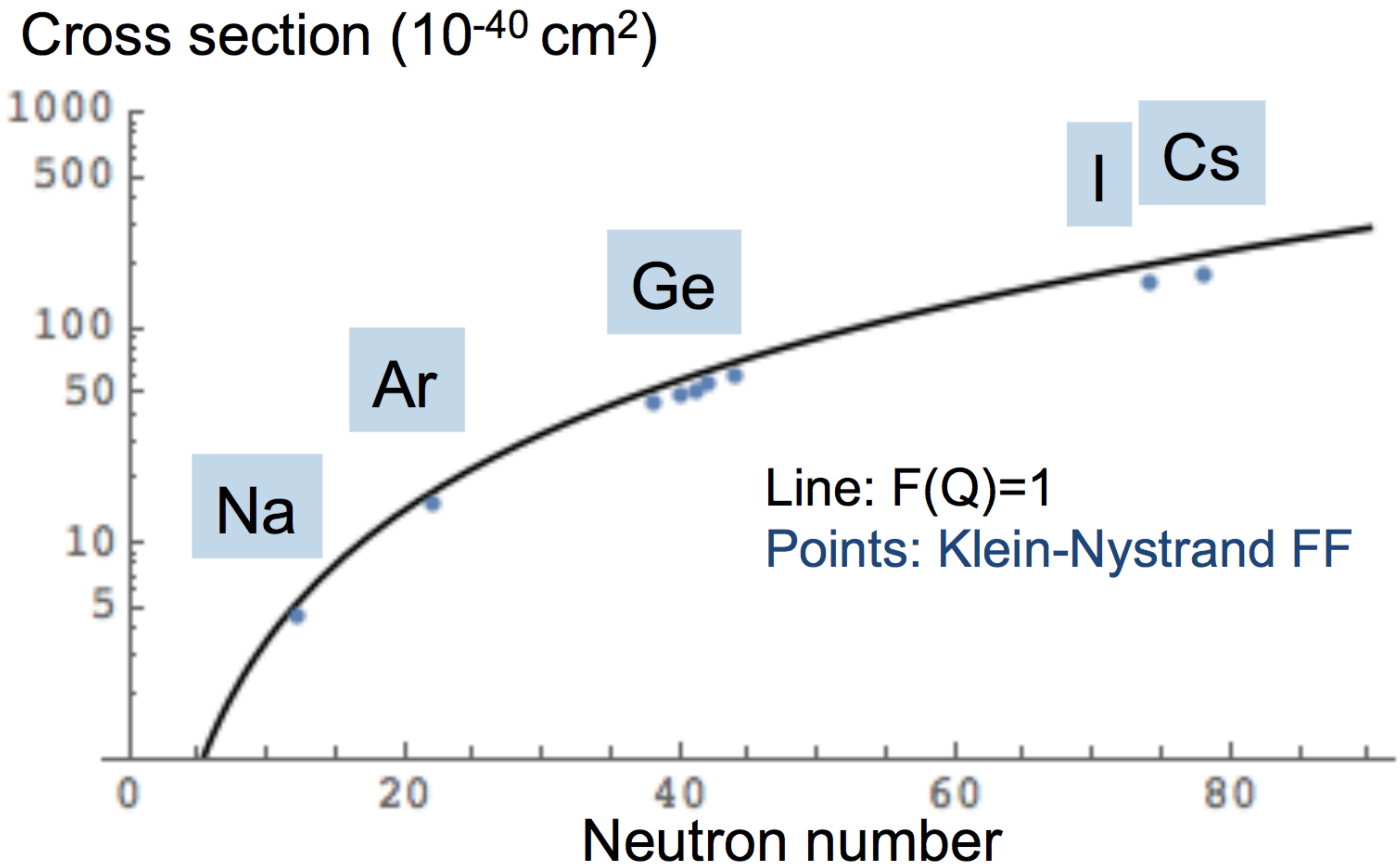
$$Q_W \equiv N - Z(1 - 4\sin^2\theta_W) \implies \frac{d\sigma}{dT} \propto N^2$$

$\sin^2\theta_W$ → 0.231

$$QR < 1 \implies Q_{\max} = \frac{1}{1.2(40)^{1/3}} = 0.24\,\text{fm}^{-1} \approx 50\,\text{MeV}$$

Nuclear structure information needed: elastic weak form factor

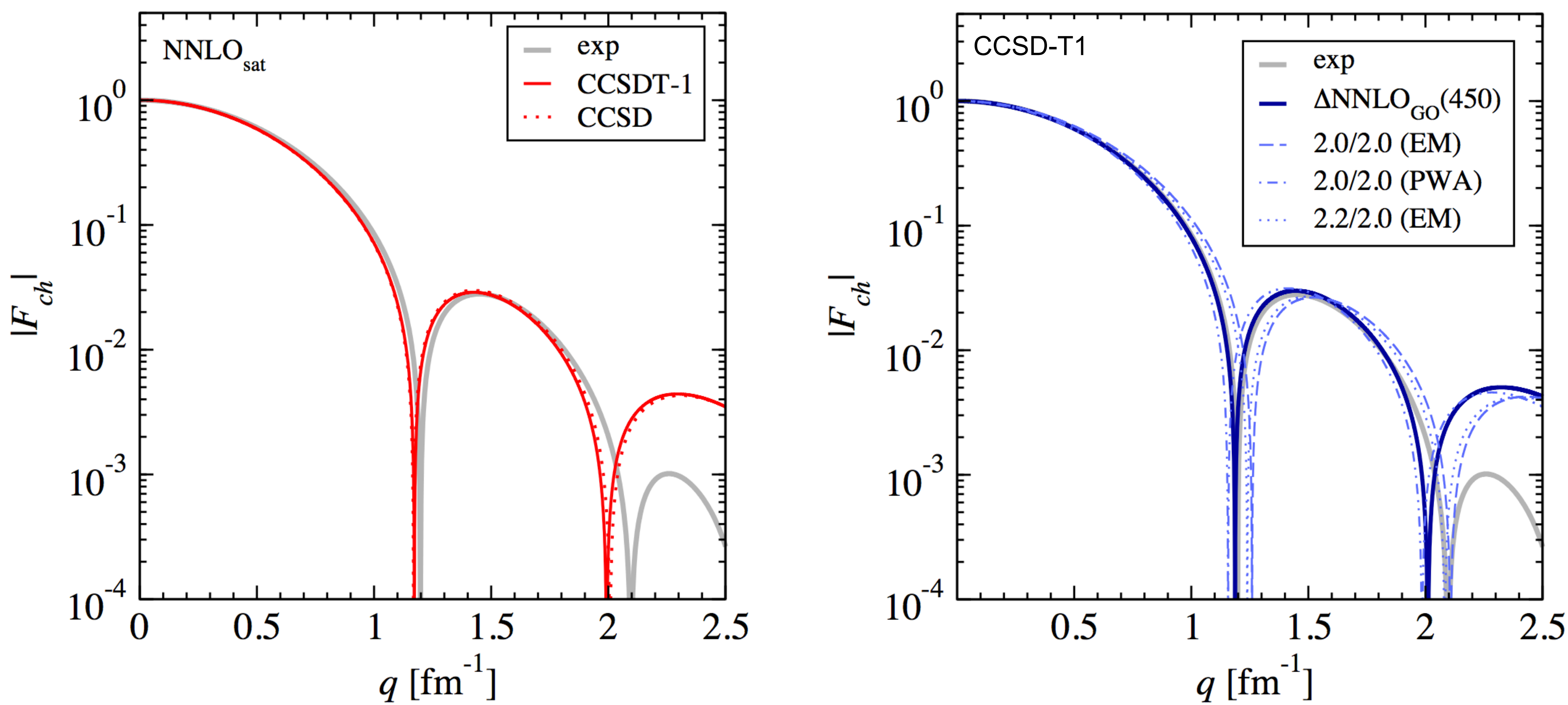
CEvNS cross section



From K. Scholberg

^{40}Ar Charge Form Factor

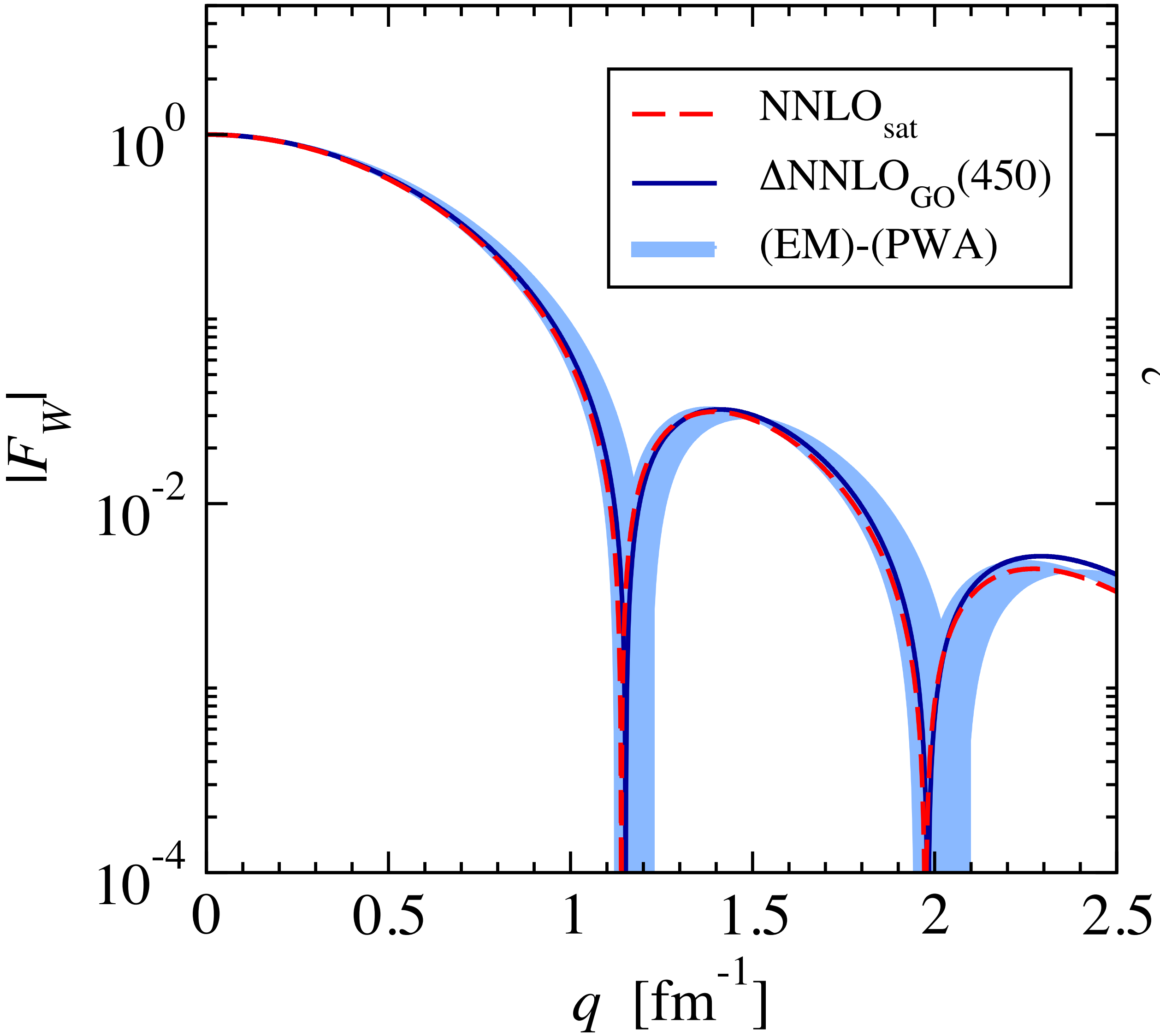
C. Payne et al., Phys. Rev. C 100, 061304(R) (2019)

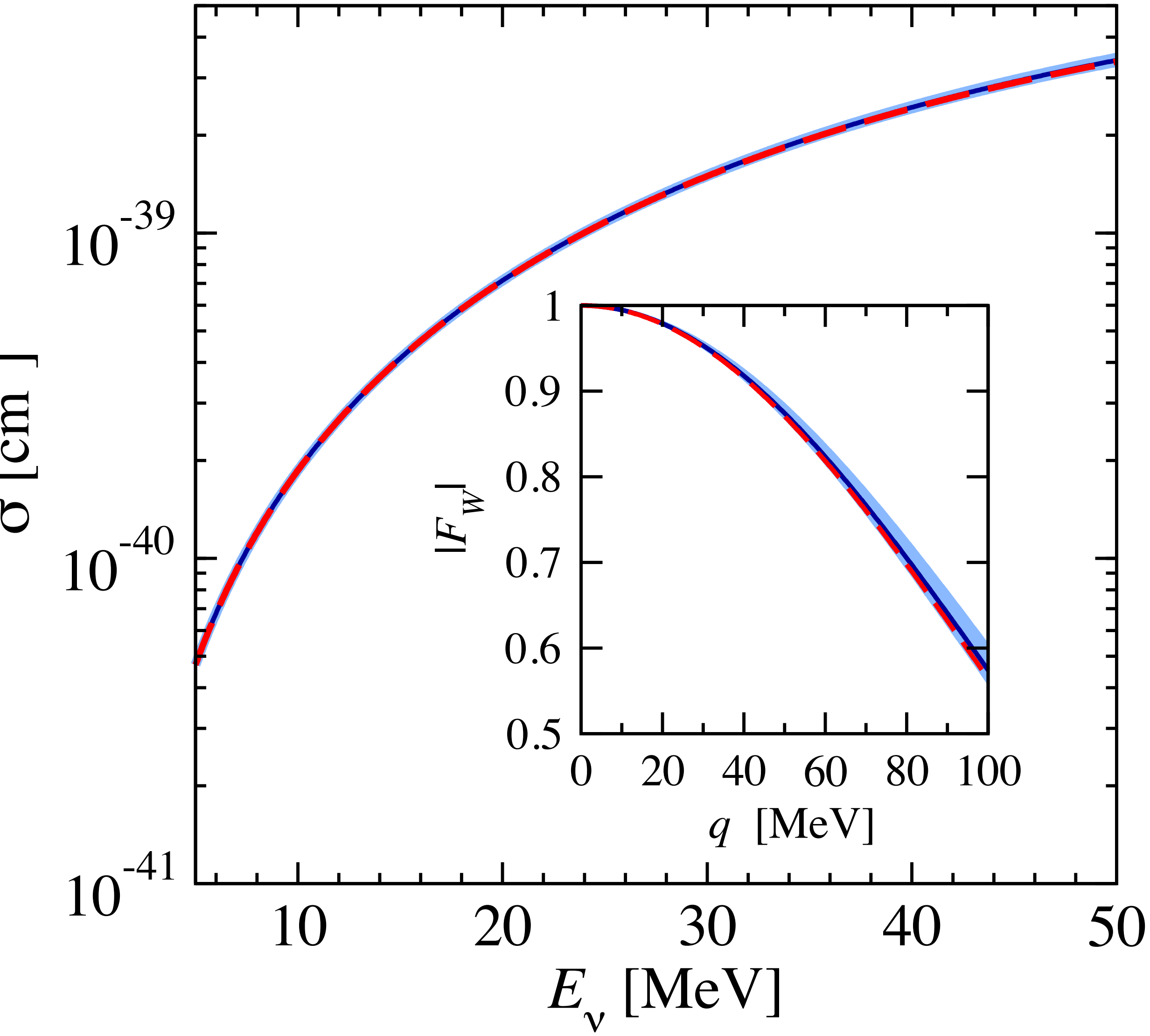


exp: in Mainz, Ottermann et. al., Nucl. Phys. A **379**, 396 (1982)

^{40}Ar Weak Form Factor

C. Payne et al., Phys. Rev. C 100, 061304(R) (2019)





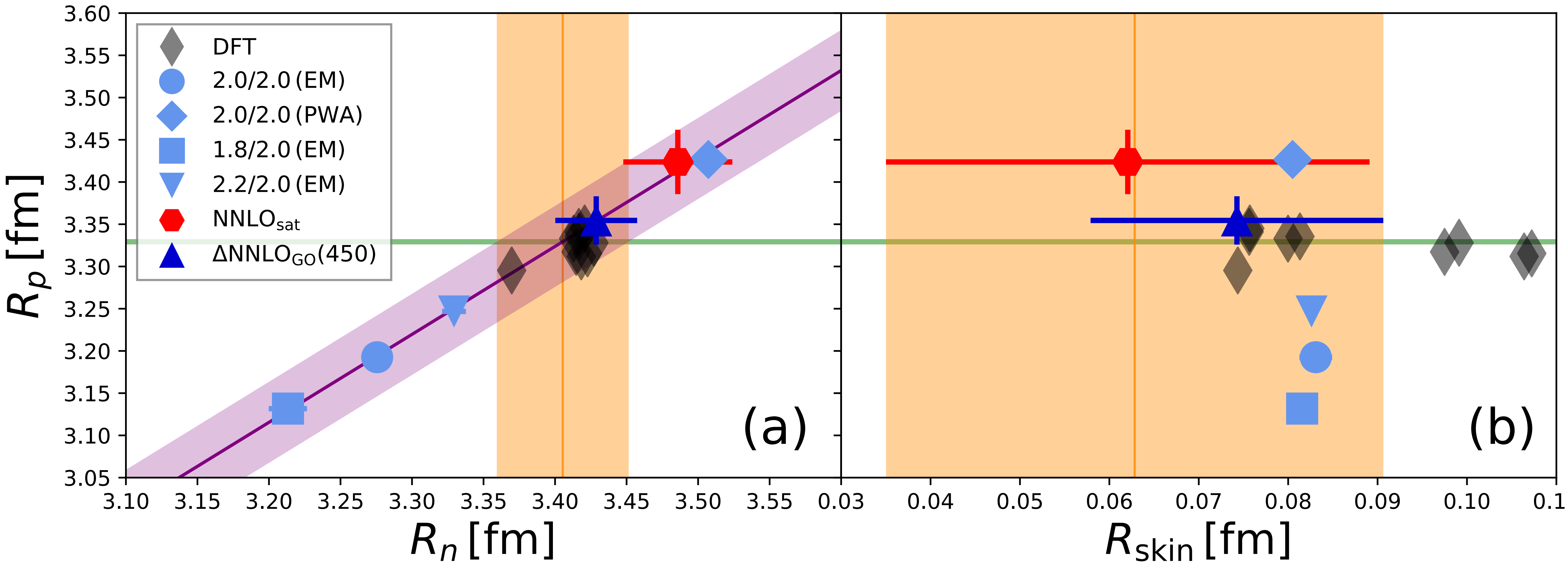
Not much Hamiltonian dependence is seen at low q.
Confirmed by DFT (Phys. Rev. C 100, 054301 (2019)) and RPA calculations (arXiv:2001.04684).

^{40}Ar neutron radius and skin-thickness

C. Payne et al., Phys. Rev. C 100, 061304(R) (2019)

Perhaps R_n and R_{skin} can be extracted from coherent elastic neutrino scattering

Amanik and McLaughlin, J. Phys. G: Nucl. Part. Phys. **36** 015105 (2009)
Cadeddu et al., Phys. Rev. Lett. **120**, 072501 (2018)



DFT from N. Schunk, private communication, **HFB9, SKI3, SKM*, SKO, SKX, SLY4, SLY5, UNEDF0, UNEDF1**

Outlook

- Triples corrections cannot be neglected in computing dipole polarizabilty
- CEvNS is not sensitive to details of the nuclear interactions

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Thanks to all my collaborators

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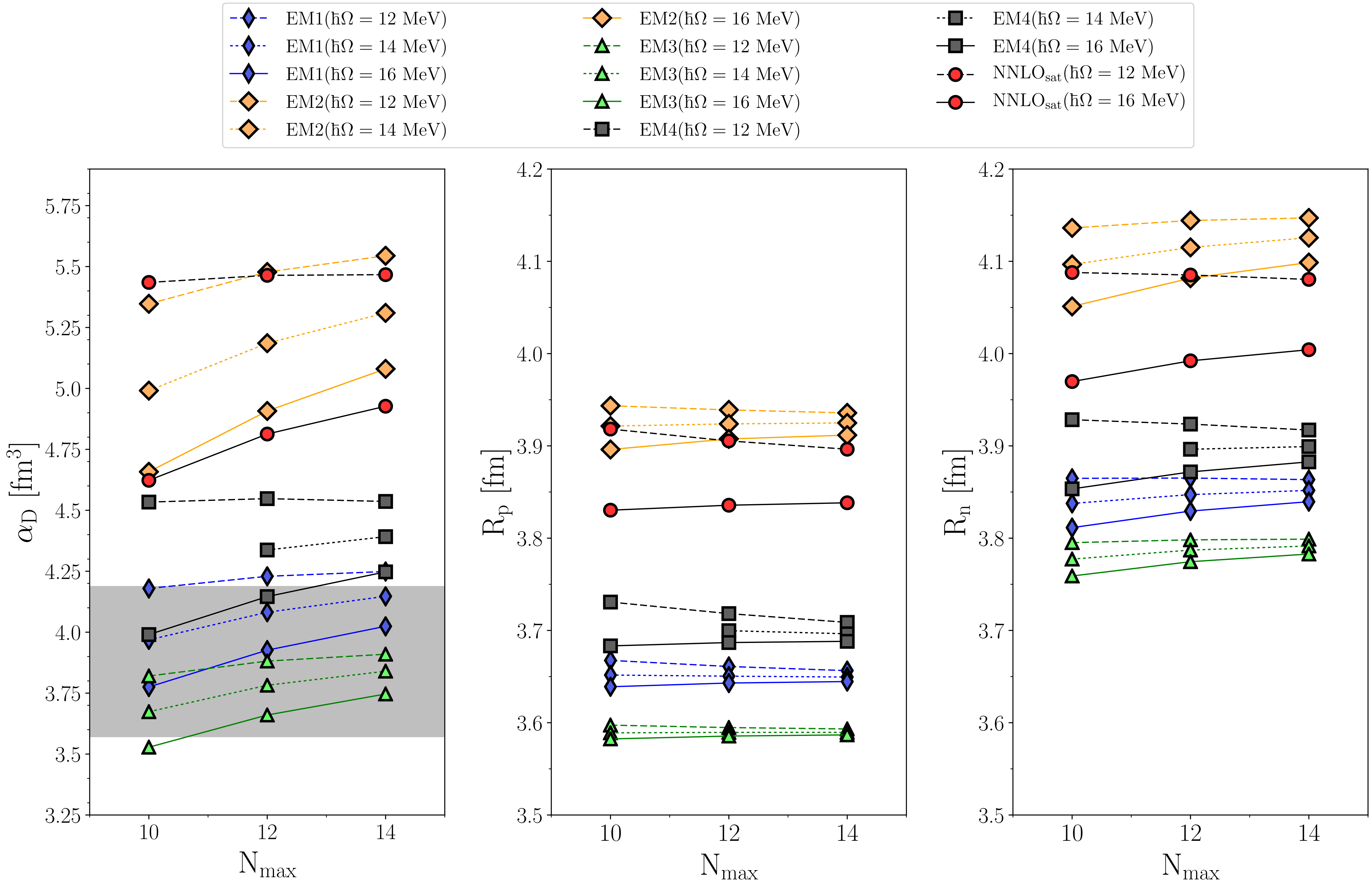
Thanks for your attention!

^{68}Ni convergence

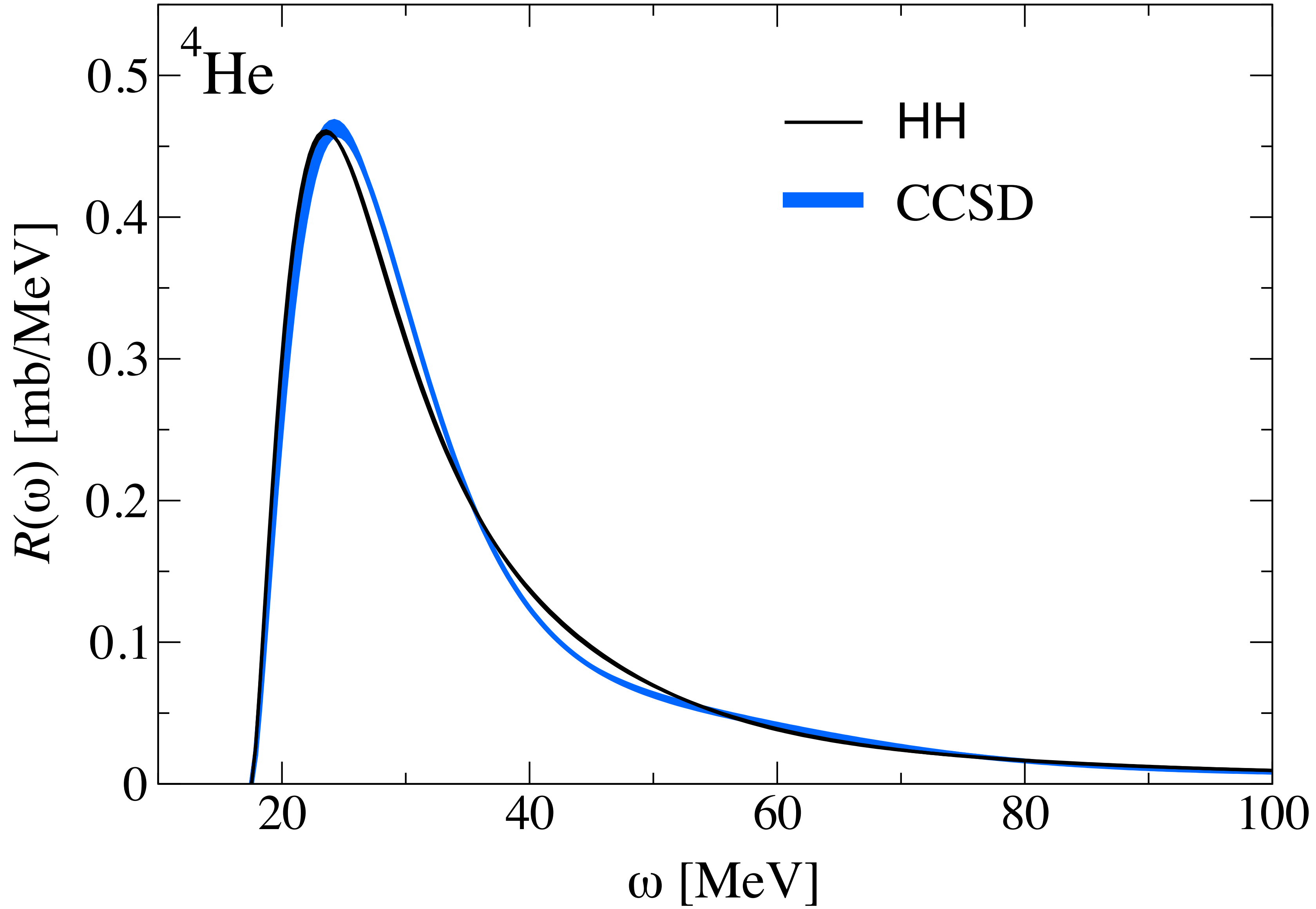


Validation in ^{4}He

Dipole response function

Comparison of CCSD with exact hyperspherical harmonics with NN forces at N^3LO

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



^{48}Ca electric dipole polarizability

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

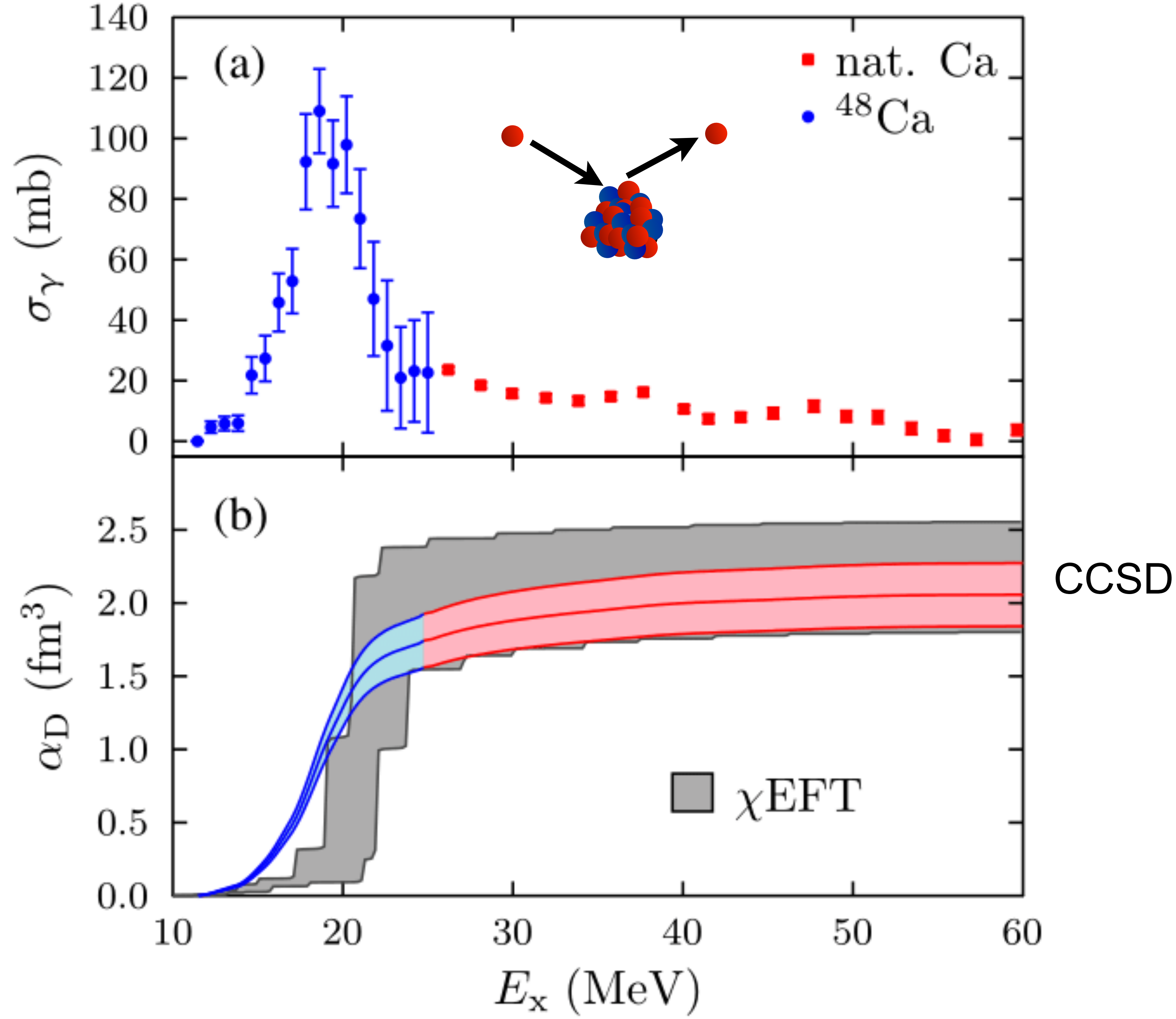
$$\alpha_D = 2\alpha \int_{\omega_{ex}}^{\infty} d\omega \frac{R(\omega)}{\omega}$$

Can be calculated:

(1) by integrating the strength obtained from LIT inversion

(2) Directly from the Lanczos coefficients (not going via the inversion)
Phys. Rev. C **94,** 034317 (2017)

$$\alpha_D \to \left\{ \frac{1}{(a_0+\sigma) - \frac{b_0^2}{(a_1+\sigma)-\frac{b_1^2}{(a_2+\sigma)-\cdots}}} \right\}$$



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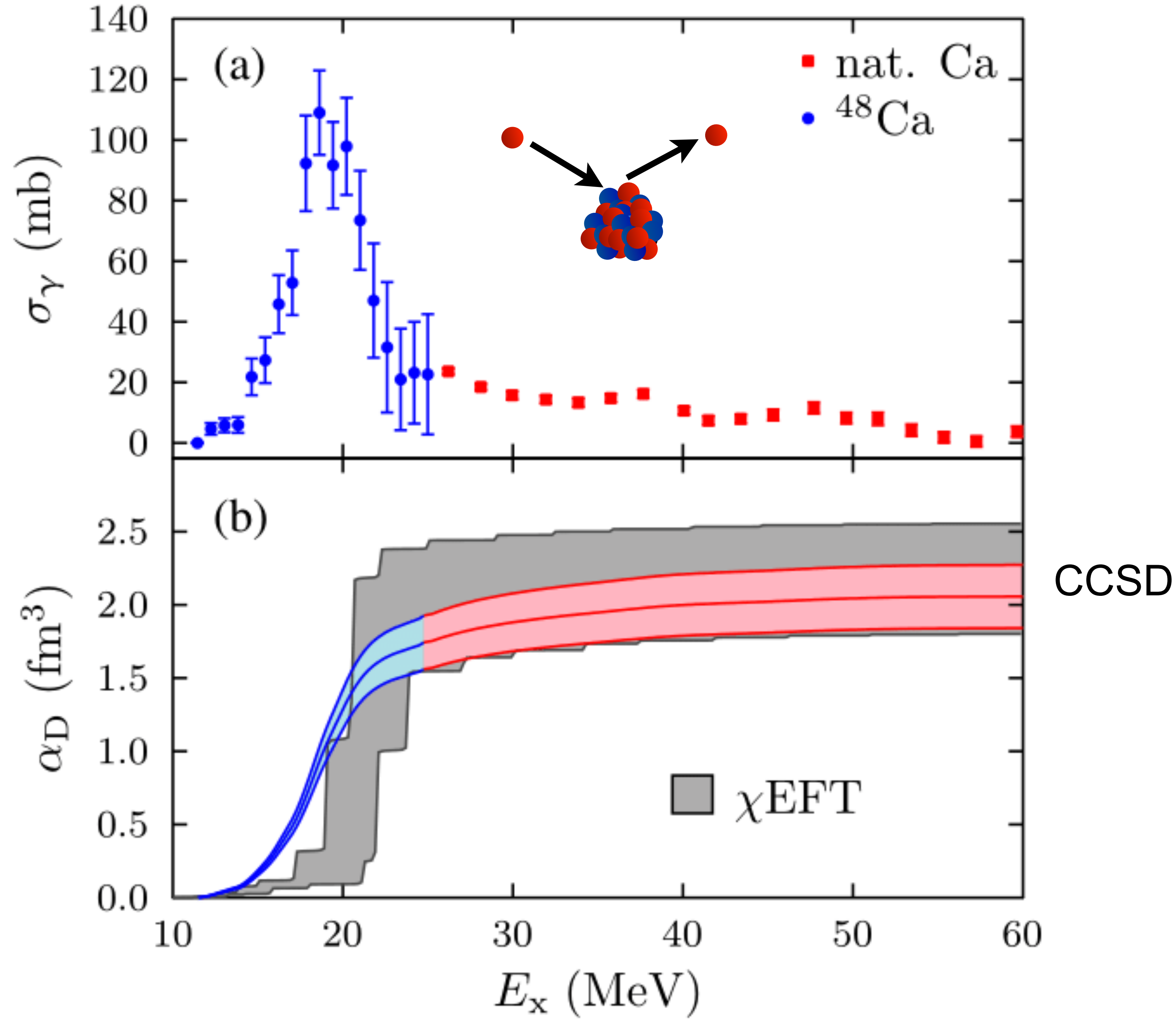


Theory tends to overestimate experiment

Can we improve the theoretical prediction?

^{68}Ni from first principles

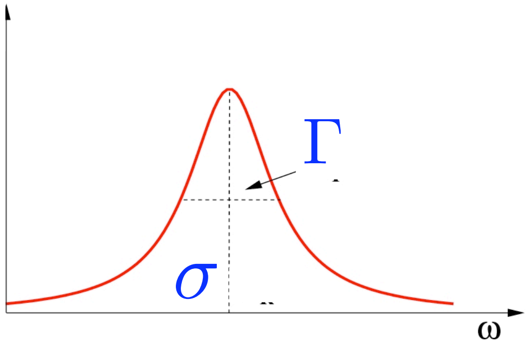
Hamiltonian	α_D	R_p	R_n	R_{skin}	R_c
1.8/2.0 (EM)	3.58(18)	3.62(1)	3.82(1)	0.201(1)	3.70(1)
2.0/2.0 (EM)	3.83(23)	3.69(2)	3.89(2)	0.202(3)	3.77(1)
2.2/2.0 (EM)	4.04(28)	3.74(2)	3.94(2)	0.203(4)	3.82(2)
2.0/2.0 (PWA)	4.87(40)	3.97(2)	4.17(3)	0.204(8)	4.05(2)
NNLO_{sat}	4.65(49)	3.93(4)	4.11(5)	0.183(8)	4.00(4)

NNLOsat $\alpha_D = 3.60\ \text{fm}^3$ F. Raimondi and C. Barbieri, Phys. Rev. C **99**, 054327 (2019)

The Lorentz Integral Transform

Reduce the continuum problem to a bound-state problem

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



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

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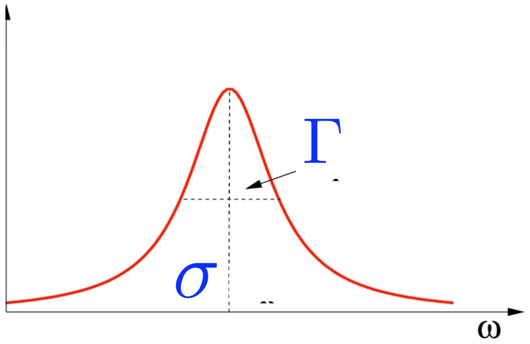

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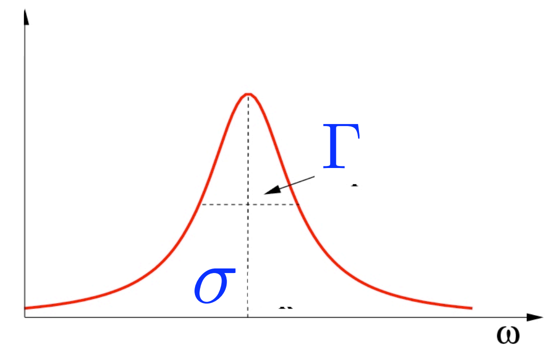

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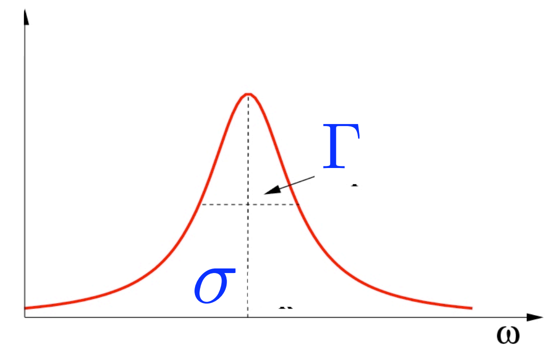

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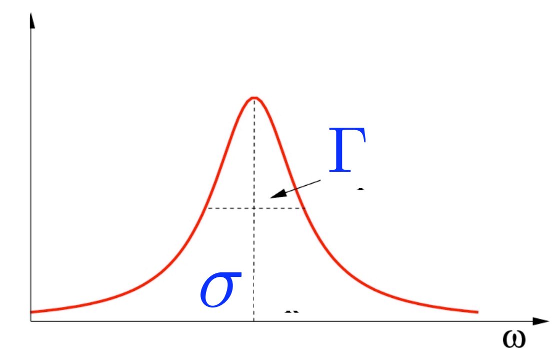

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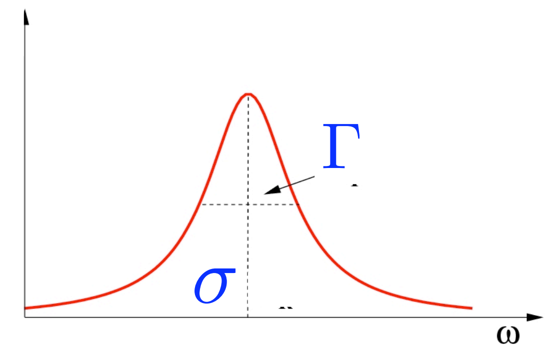

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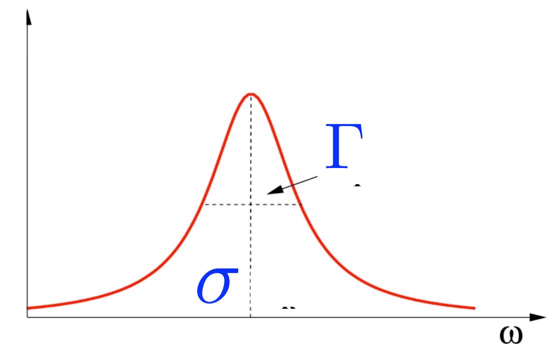

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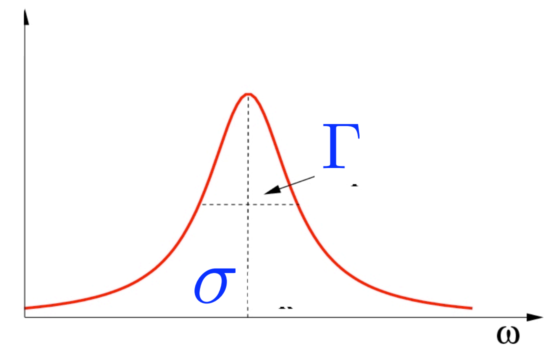

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$$\frac{1}{H - E_0 - \sigma + i\Gamma} \Theta | \psi_0 \rangle = | \tilde{\psi} \rangle$$

Inversion of the LIT

The inversion is performed numerically with a regularization procedure needed for the solution of an ill-posed problem

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

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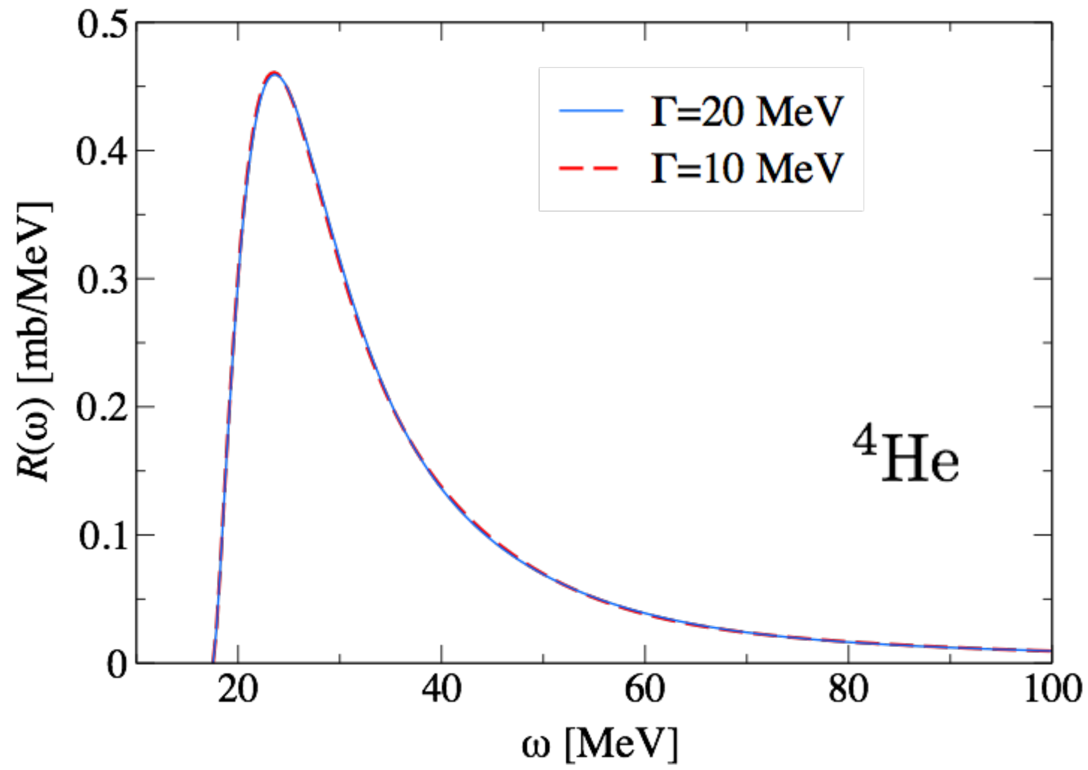
Least square fit of the coefficients c_i to reconstruct the response function



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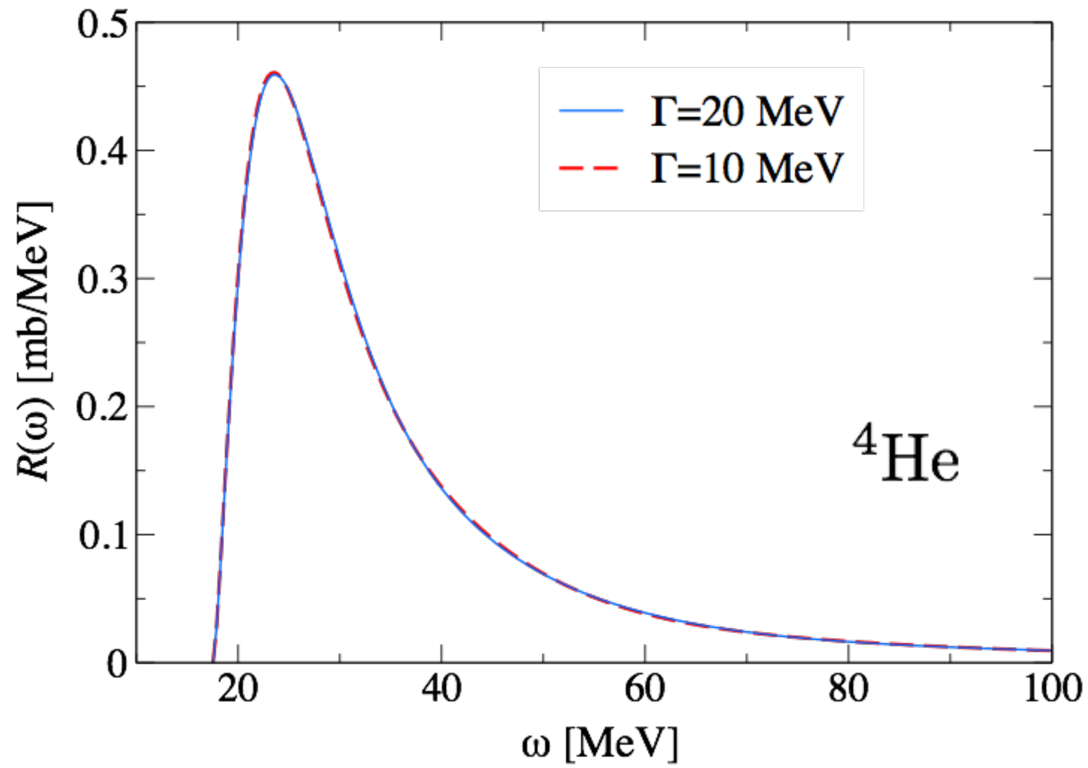

Message: using bound-states techniques to calculate the LIT is correct and inversions are stable If the LIT is calculated precisely enough