Ab initio nuclear structure using coupled cluster

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In collaboration with:
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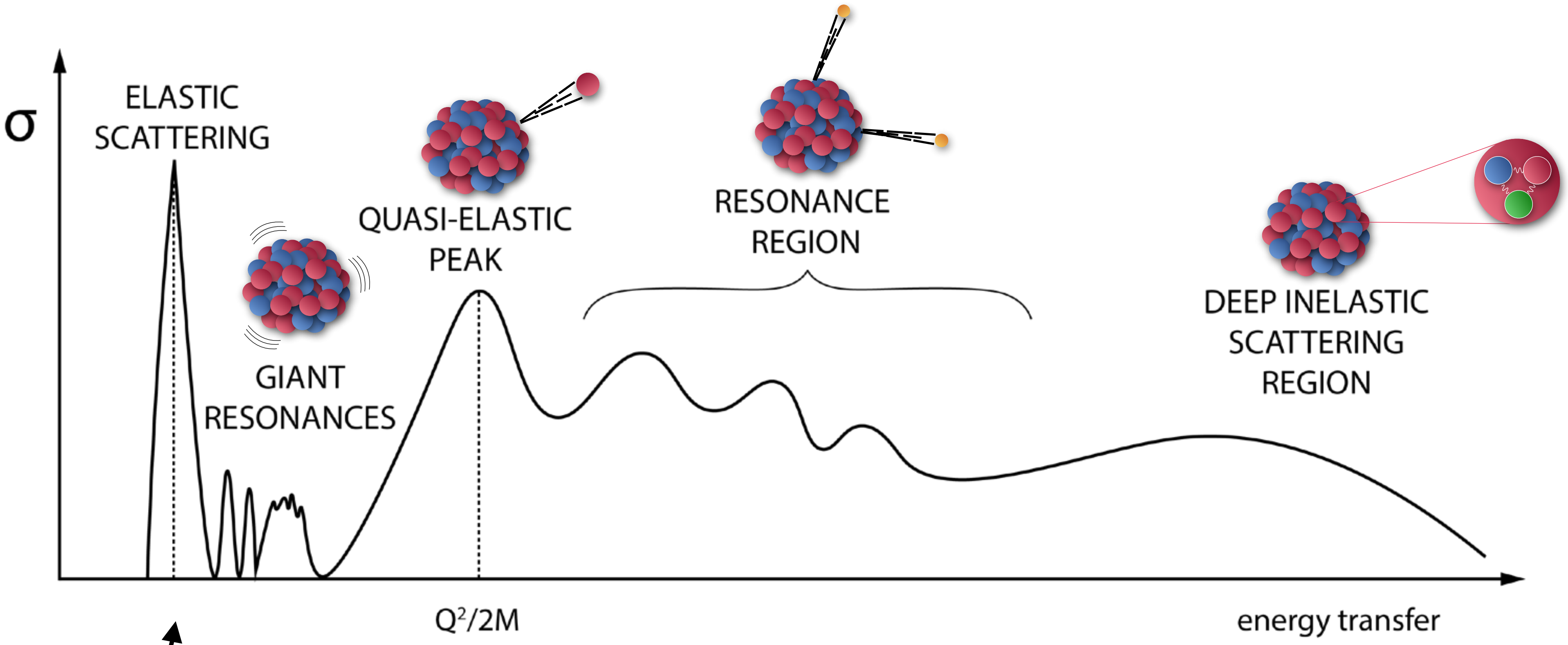
"Short-distance nuclear structure and pdfs" ECT*, 18/07/2023

Cluster of Excellence PRISMA+ Precision Physics, Fundamental Interactions and Structure of Matter
JG|U
Alexander von Humboldt Stiftung / Foundation
MARIE CURIE ACTIONS
This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 101026014

Motivation

Electro(weak) nuclear responses



Inelastic scattering

Elastic scattering: CEvNS (coherent elastic neutrino-nucleus scattering)

e.g. Supernovae neutrinos

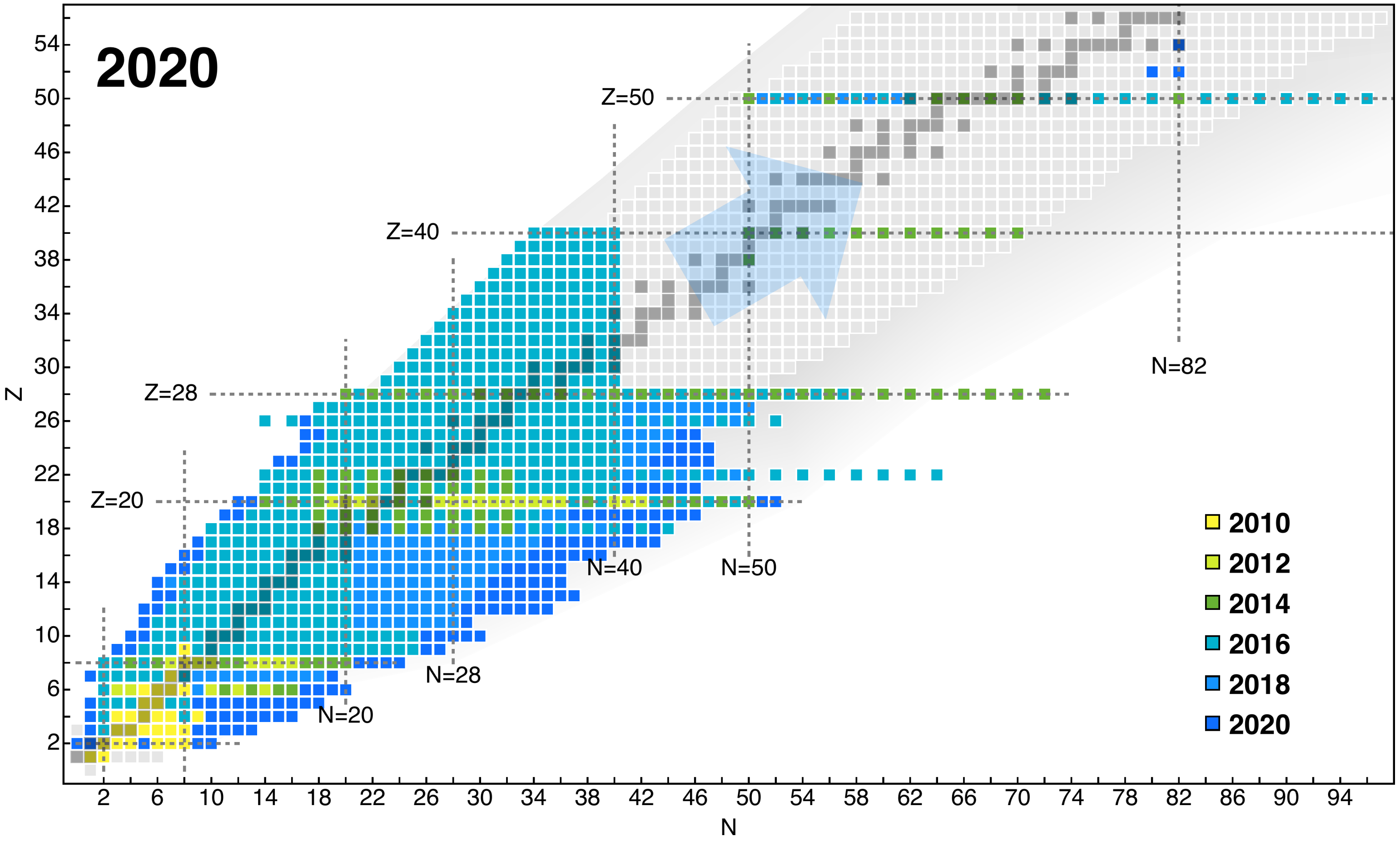
Long-baseline experiments (DUNE, HyperK)

An initio nuclear methods

$$\mathscr{H}\,|\Psi\rangle = E\,|\Psi\rangle$$

> *"we interpret the ab initio method to be a systematically improvable approach for quantitatively describing nuclei using the finest resolution scale possible while maximizing its predictive capabilities."*

A. Ekström et al, *Front. Phys.*11 (2023) 29094

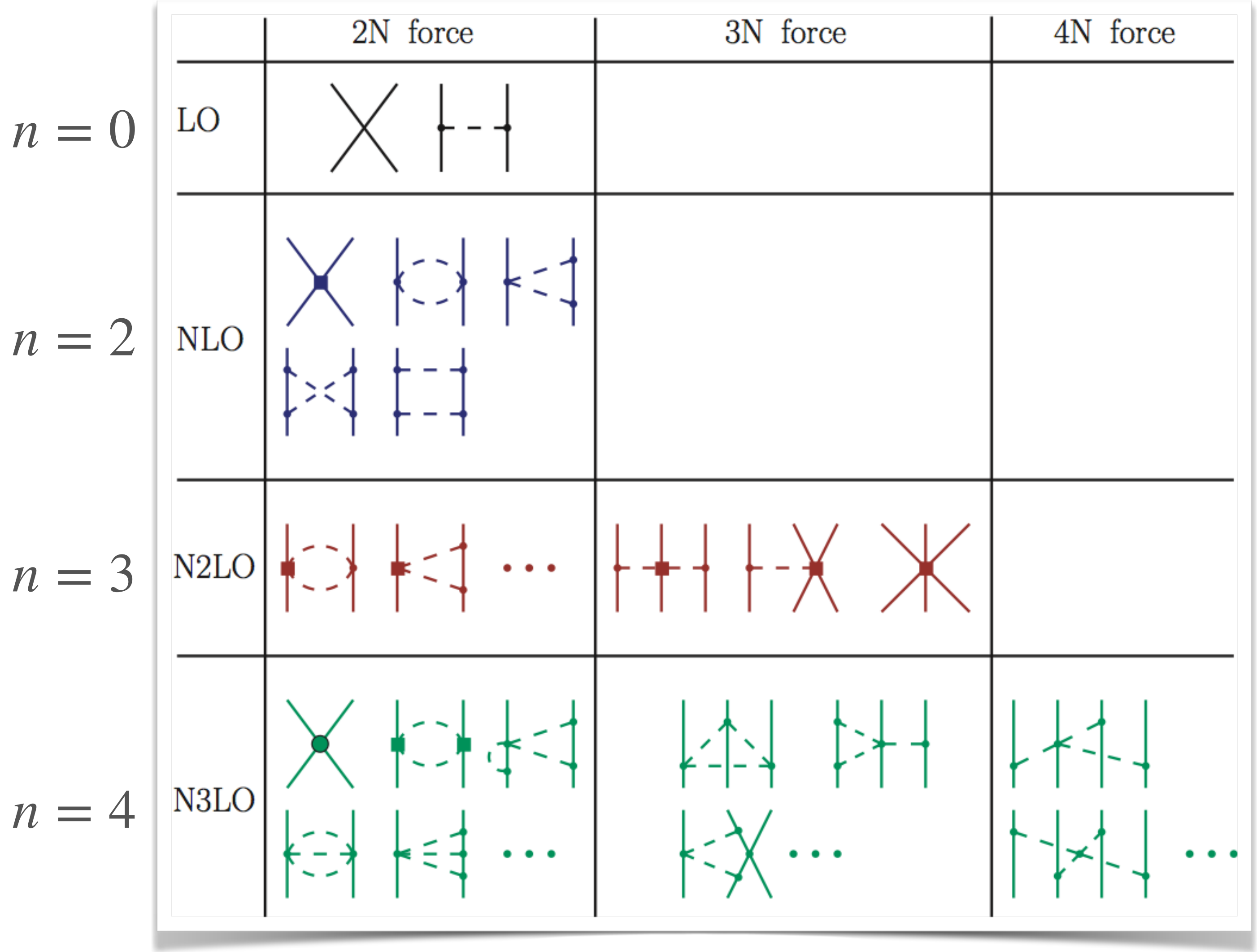


H. Hergert, *Front.in Phys.* 8 (2020) 379

- ➡ Developments on the side of many body methods (IMSRG, CC, SCGF, QMC, etc.)
- ➡ Developments of chiral nuclear forces (->faster convergence)

Nuclear hamiltonian

$$\mathscr{H} = \sum_{i} \frac{p_i^2}{2m} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk} + \dots$$



✓ Chiral Hamiltonians exploiting chiral symmetry (QCD); π, N, (Δ) degrees of freedom

✓ counting scheme in $\left(\frac{Q}{\Lambda}\right)^n$

✓ low energy constants (LEC) fit to data

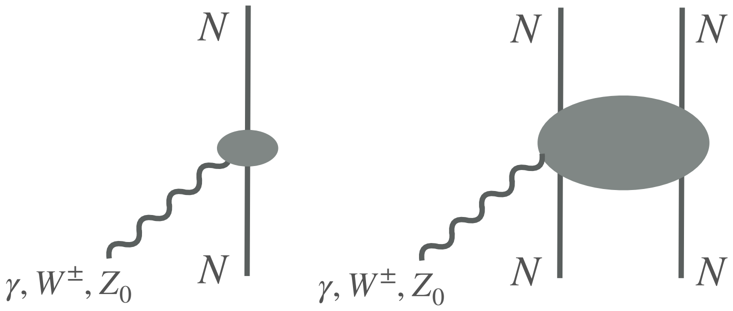
✓ uncertainty assessment

Chiral potentials: NNLO$_{\mathrm{sat}}$ and ΔNNLO$_{\mathrm{GO}}$(450)

A. Ekström et al. *Phys.Rev.C* 91 (2015) 5, 051301
W. Jiang at al. *Phys.Rev.C* 102 (2020) 5, 054301

Electroweak currents

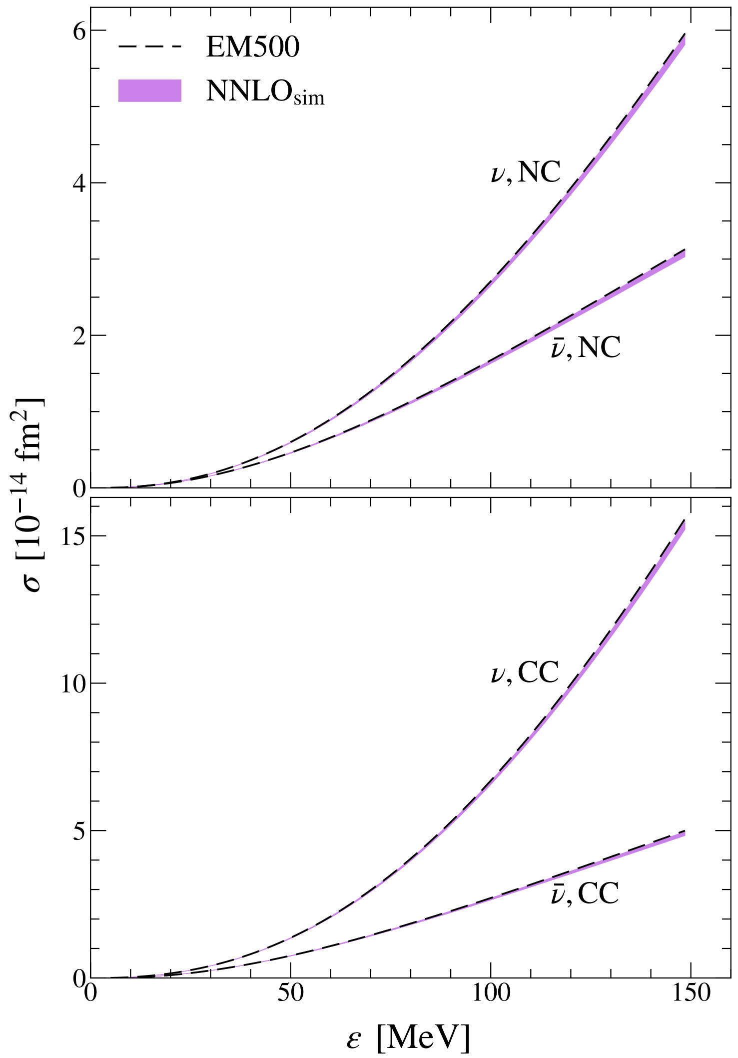
$$J = \sum_i j_i + \sum_{i<j} j_{ij} + \dots$$



known to give significant contribution for neutrino-nucleus scattering

Can be expanded consistently with the chiral Hamiltonian.

$$\nu(\bar{\nu}) + d \to \mu^\pm + X$$



Multipole decomposition for 1- and 2-body EW currents

B. Acharya, S. Bacca
Phys.Rev.C 101 (2020) 1, 015505

Coupled cluster method

Reference state (Hartree-Fock): $|\Psi\rangle$

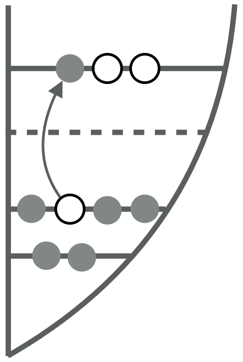
Include correlations through e^{T} operator

similarity transformed Hamiltonian (non-Hermitian)

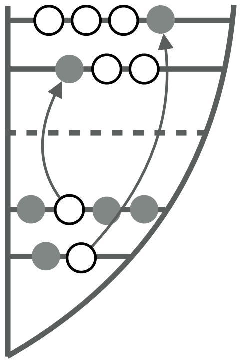
$$e^{-T}\mathscr{H}e^{T}|\Psi\rangle \equiv \bar{\mathscr{H}}|\Psi\rangle = E|\Psi\rangle$$

Expansion: $T = \sum t_a^i a_a^\dagger a_i + \sum t_{ab}^{ij} a_a^\dagger a_b^\dagger a_i a_j + \dots$

←coefficients obtained through coupled cluster equations



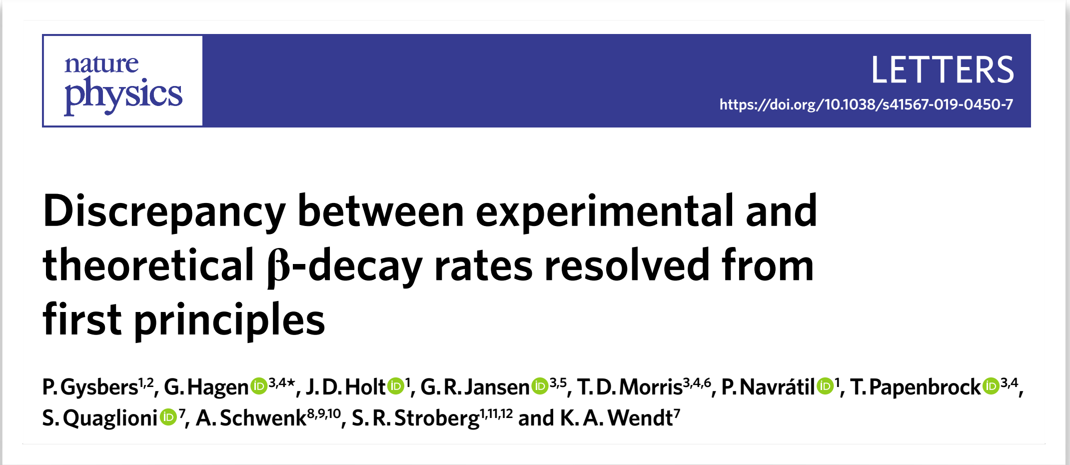
singles



doubles

Coupled cluster method

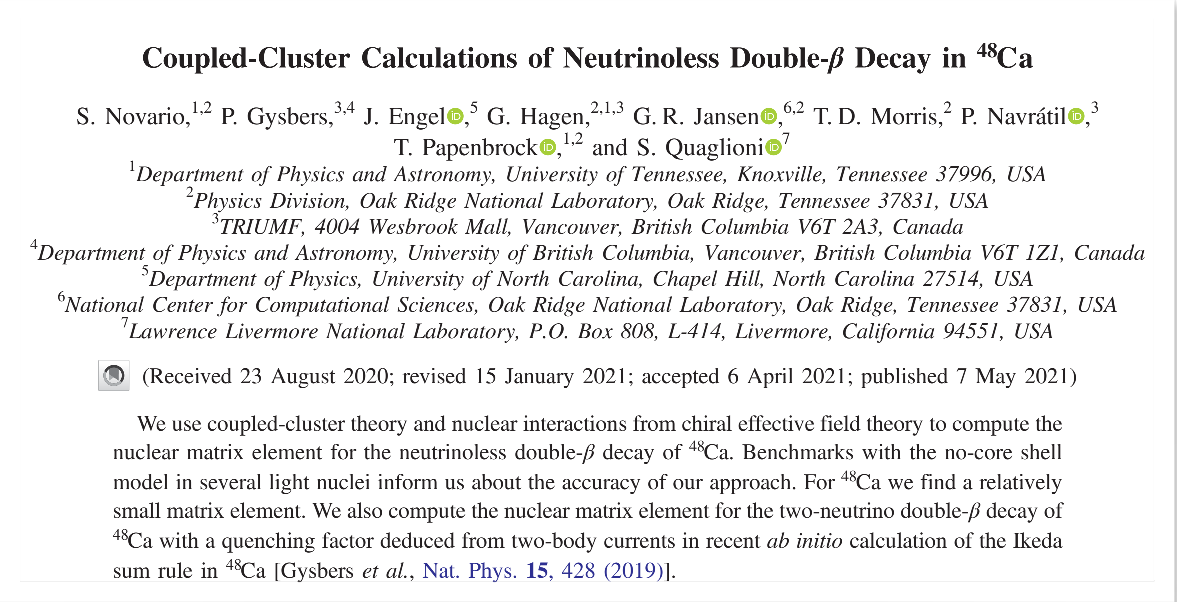
- ✓ Controlled approximation through truncation in T
- ✓ Polynomial scaling with A (predictions for ^{132}Sn and ^{208}Pb)
- ✓ Works most efficiently for doubly magic nuclei



nature physics
LETTERS
https://doi.org/10.1038/s41567-019-0450-7

Discrepancy between experimental and theoretical β-decay rates resolved from first principles

P. Gysbers[1,2], G. Hagen[3,4*], J. D. Holt[1], G. R. Jansen[3,5], T. D. Morris[3,4,6], P. Navrátil[1], T. Papenbrock[3,4], S. Quaglioni[7], A. Schwenk[8,9,10], S. R. Stroberg[1,11,12] and K. A. Wendt[7]



Coupled-Cluster Calculations of Neutrinoless Double-β Decay in ^{48}Ca

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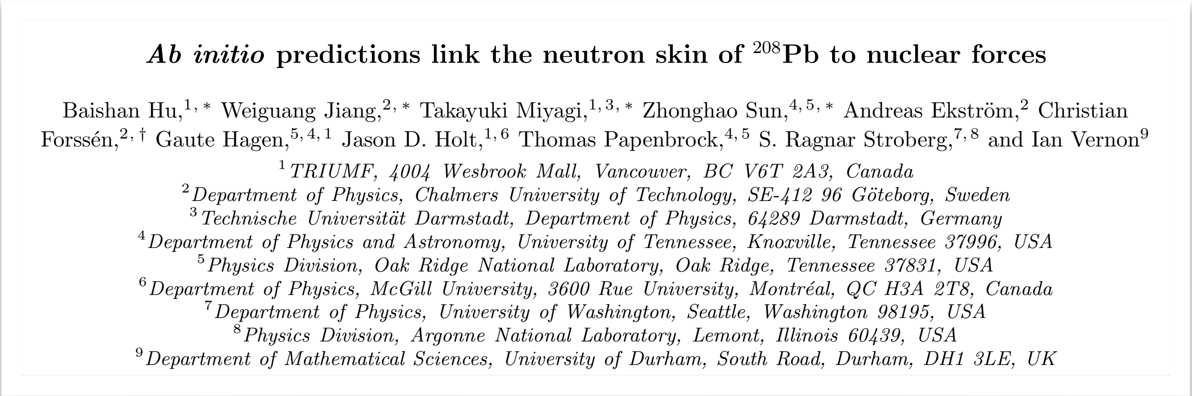
(Received 23 August 2020; revised 15 January 2021; accepted 6 April 2021; published 7 May 2021)

We use coupled-cluster theory and nuclear interactions from chiral effective field theory to compute the nuclear matrix element for the neutrinoless double-β decay of ^{48}Ca. Benchmarks with the no-core shell model in several light nuclei inform us about the accuracy of our approach. For ^{48}Ca we find a relatively small matrix element. We also compute the nuclear matrix element for the two-neutrino double-β decay of ^{48}Ca with a quenching factor deduced from two-body currents in recent *ab initio* calculation of the Ikeda sum rule in ^{48}Ca [Gysbers *et al.*, Nat. Phys. **15**, 428 (2019)].



***Ab initio* predictions link the neutron skin of ^{208}Pb to nuclear forces**

Baishan Hu,[1,*] Weiguang Jiang,[2,*] Takayuki Miyagi,[1,3,*] Zhonghao Sun,[4,5,*] Andreas Ekström,[2] Christian Forssén,[2,†] Gaute Hagen,[5,4,1] Jason D. Holt,[1,6] Thomas Papenbrock,[4,5] S. Ragnar Stroberg,[7,8] and Ian Vernon[9]
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CC for nuclear matter —> used for SRC theoretical studies:

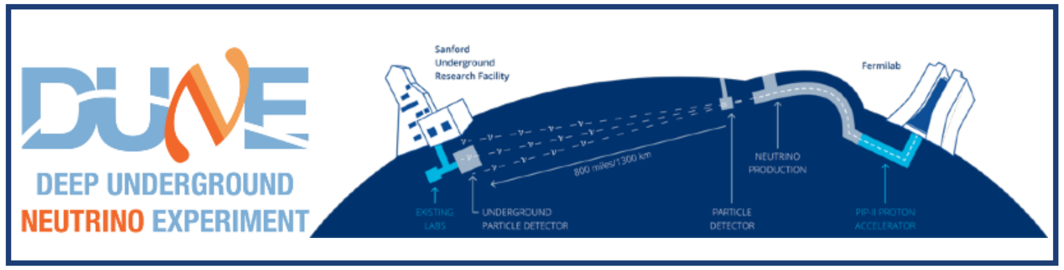
S. Beck, R. Weiss, N. Barnea, *Phys.Rev.C* 107 (2023) 6, 064306

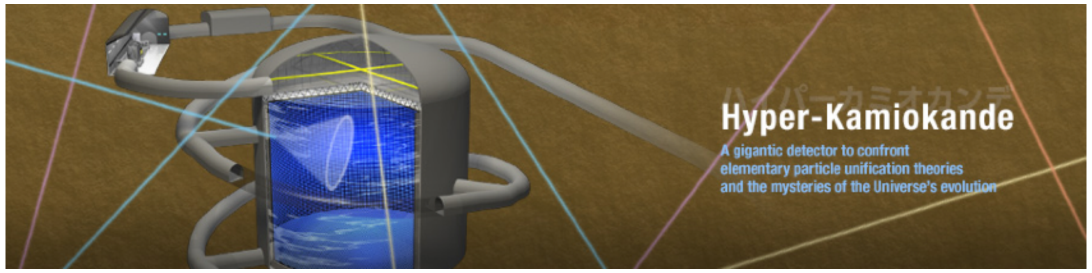
S. Beck, R. Weiss, N. Barnea, arXiv:2305.17649

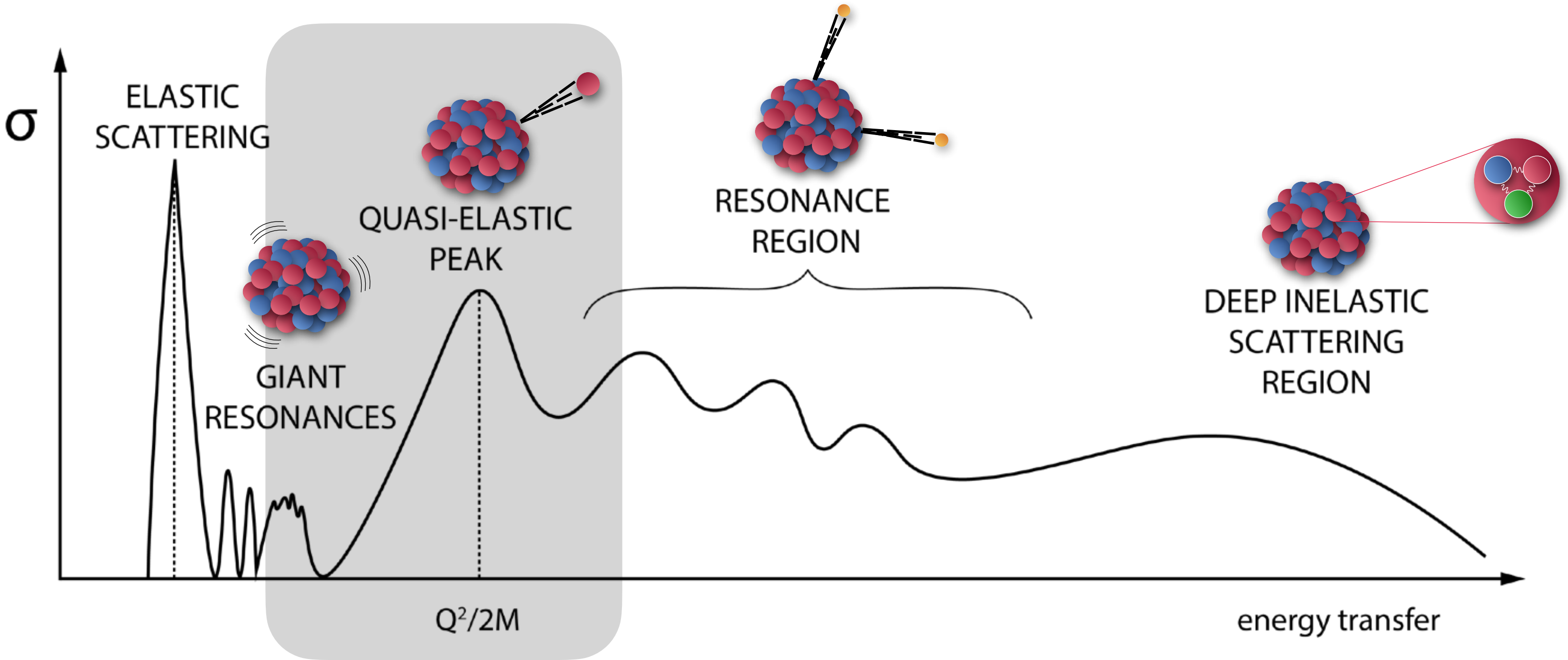
Quasielastic response

Long-baseline ν experiments

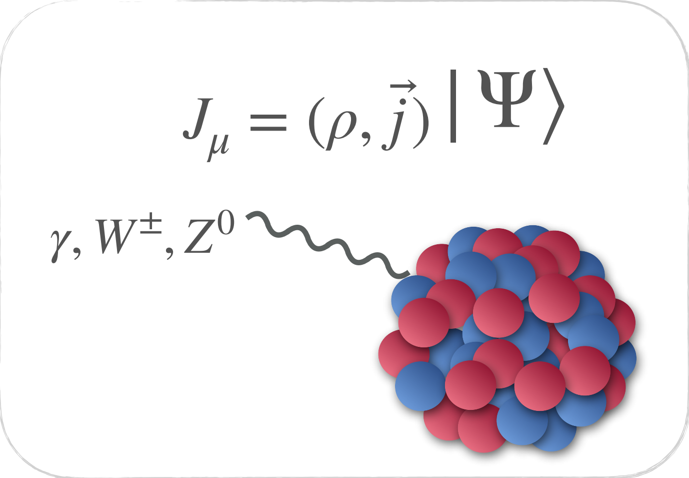
- ✓ Momentum transfer ~hundreds MeV
- ✓ Upper limit for ab initio methods
- ✓ Important mechanism for HyperK, DUNE
- ✓ Role of final state interactions
- ✓ Role of 1-body and 2-body currents







Electrons & neutrinos



$$J_\mu = (\rho, \vec{j})\,|\,\Psi\rangle$$

Inclusive cross-section $\sigma \propto L^{\mu\nu}\ R_{\mu\nu}$

$$\left.\frac{d\sigma}{d\omega dq}\right|_e = \sigma_M\Big(v_L R_L + v_T R_T\Big)$$

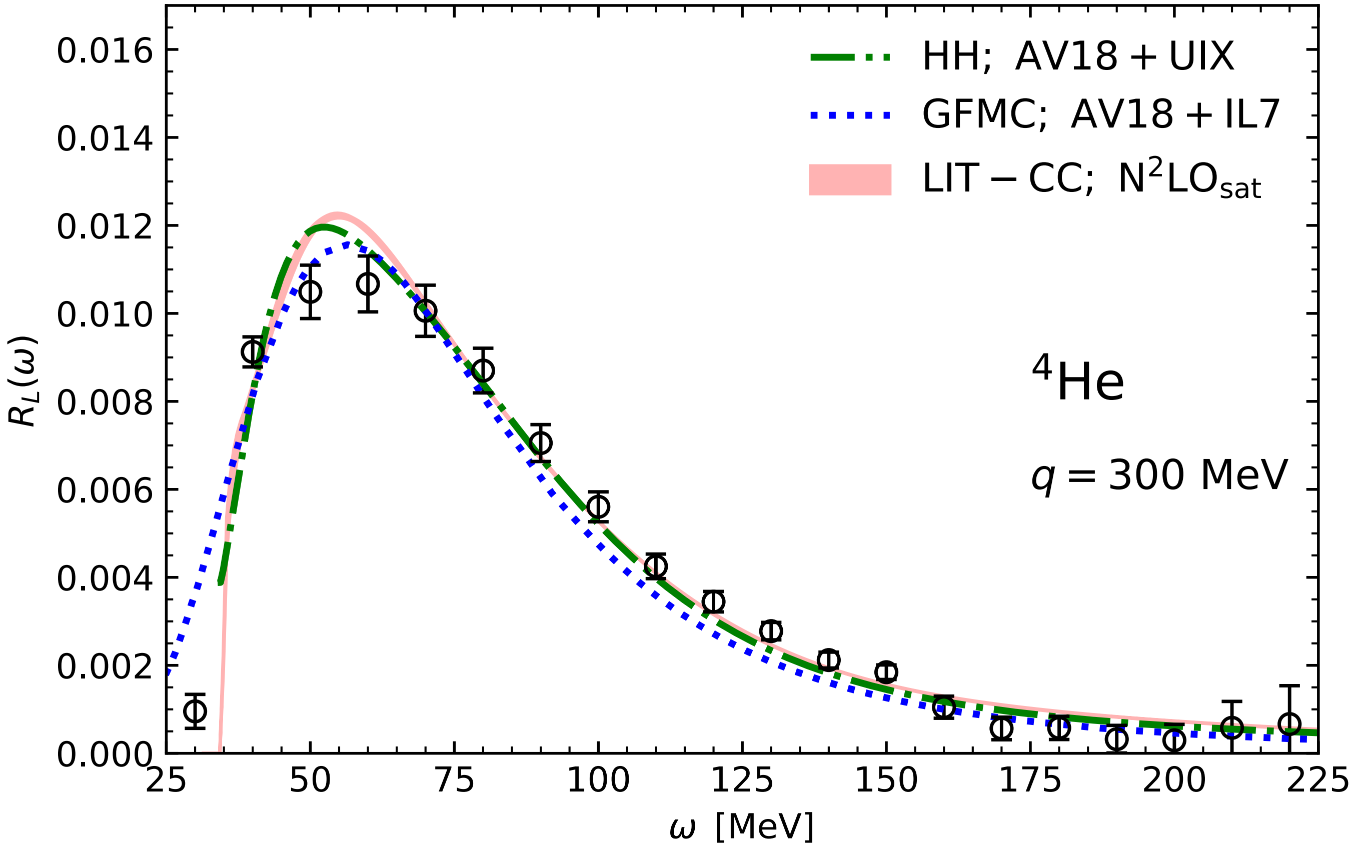
$$\left.\frac{d\sigma}{d\omega dq}\right|_{\nu/\bar{\nu}} = \sigma_0\Big(v_{CC}R_{CC} + v_{CL}R_{CL} + v_{LL}R_{LL} + v_T R_T \pm v_{T'}R_{T'}\Big)$$

Nuclear responses:

$$R_{\mu\nu}(\omega, q) = \sum_f \langle\Psi\,|\,J_\mu^\dagger(q)\,|\,\Psi_f\rangle\langle\Psi_f\,|\,J_\nu(q)\,|\,\Psi\rangle\delta(E_0 + \omega - E_f)$$

Longitudinal response

Lorentz Integral Transform + Coupled Cluster



JES, B. Acharya, S. Bacca, G. Hagen; *PRL* 127 (2021) 7, 072501

charge operator

$$\hat{\rho}(q) = \sum_{j=1}^{Z} e^{iqz'_j}$$

Uncertainty band: inversion procedure

$$R_{\mu\nu}(\omega, q) = \sum\!\!\!\!\!\!\int_f \langle \Psi | J_\mu^\dagger | \Psi_f \rangle \langle \Psi_f | J_\nu | \Psi \rangle \delta(E_0 + \omega - E_f)$$

Consistent treatment of final state interactions.

Lorentz Integral Transform (LIT)

$$R_{\mu\nu}(\omega, q) = \sum_f \langle \Psi | J_\mu^\dagger | \Psi_f \rangle \langle \Psi_f | J_\nu | \Psi \rangle \delta(E_0 + \omega - E_f)$$

continuum spectrum

Integral
transform

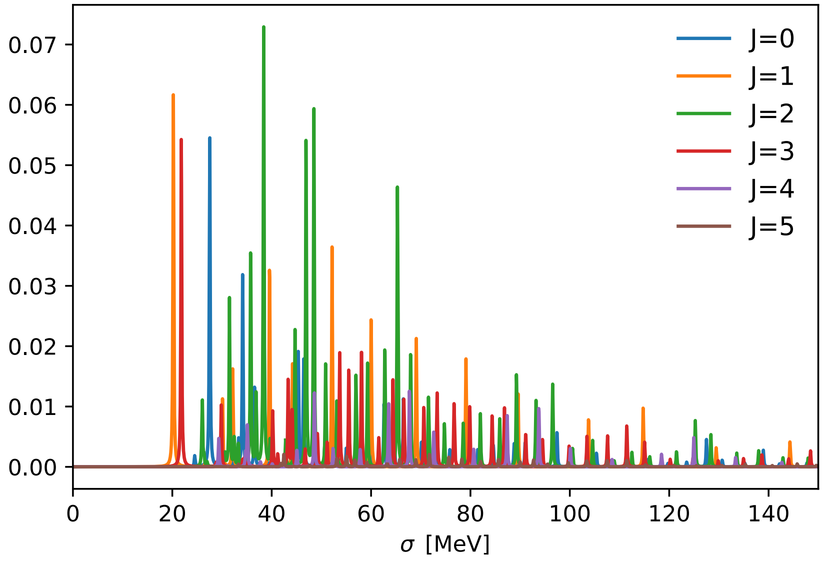
$$S_{\mu\nu}(\sigma, q) = \int d\omega K(\omega, \sigma) R_{\mu\nu}(\omega, q) = \langle \Psi | J_\mu^\dagger \, K(\mathscr{H} - E_0, \sigma) \, J_\nu | \Psi \rangle$$

Lorentzian kernel:

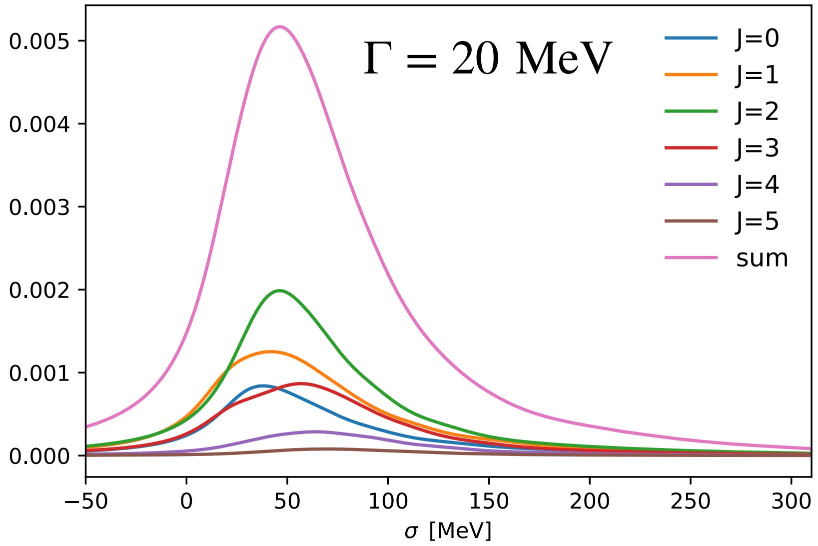
$$K_\Gamma(\omega, \sigma) = \frac{1}{\pi} \frac{\Gamma}{\Gamma^2 + (\omega - \sigma)^2}$$

$S_{\mu\nu}$ has to be inverted to get access to $R_{\mu\nu}$

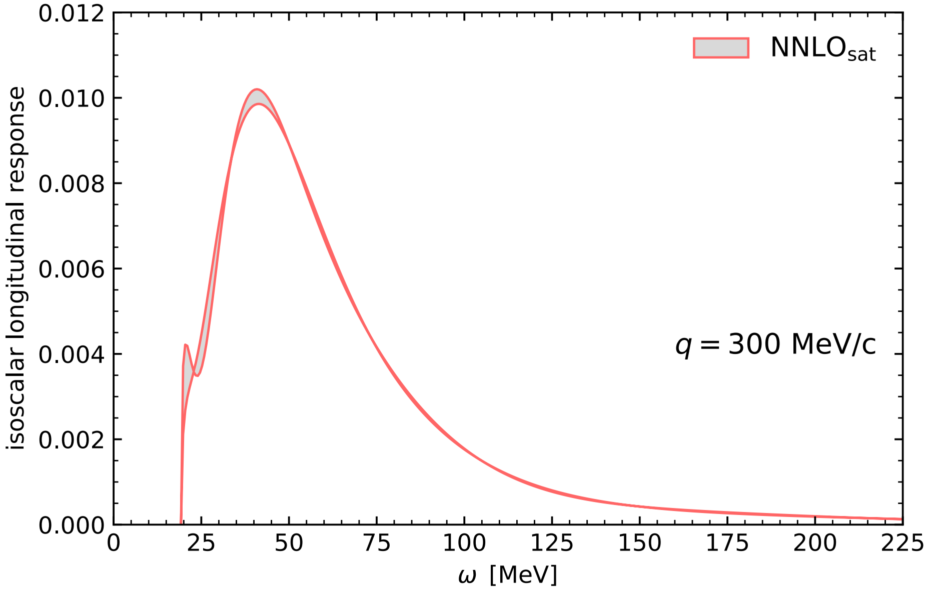
Lorentz Integral Transform



Integral transform



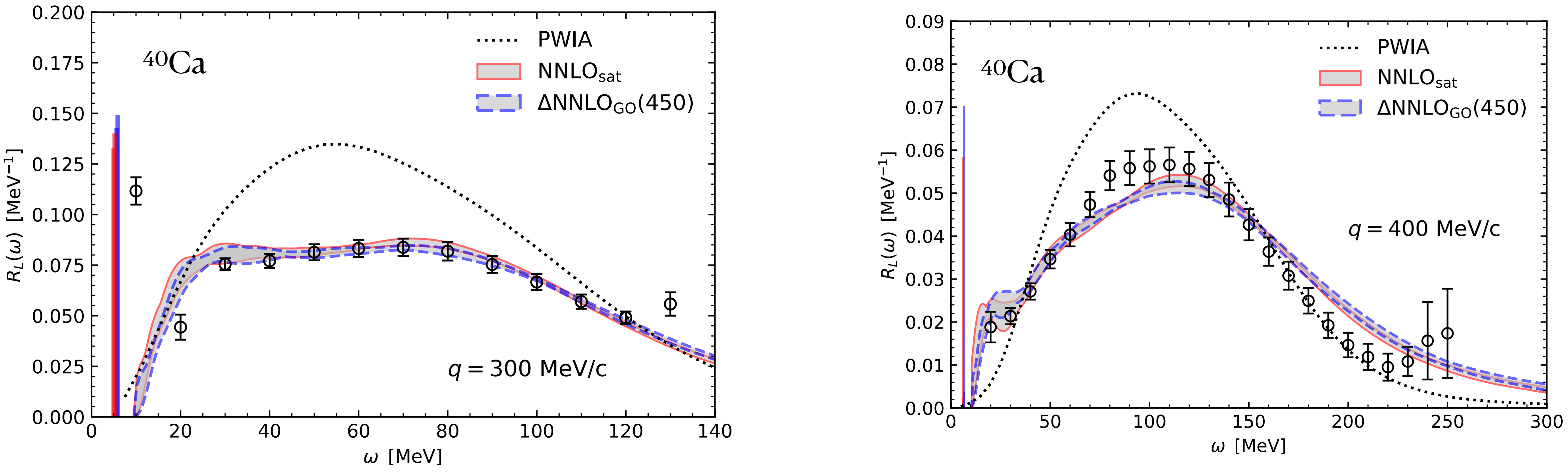
Inversion



Longitudinal isoscalar
response on ^{4}He
at q=300 MeV

Longitudinal response ^{40}Ca

Lorentz Integral Transform + Coupled Cluster



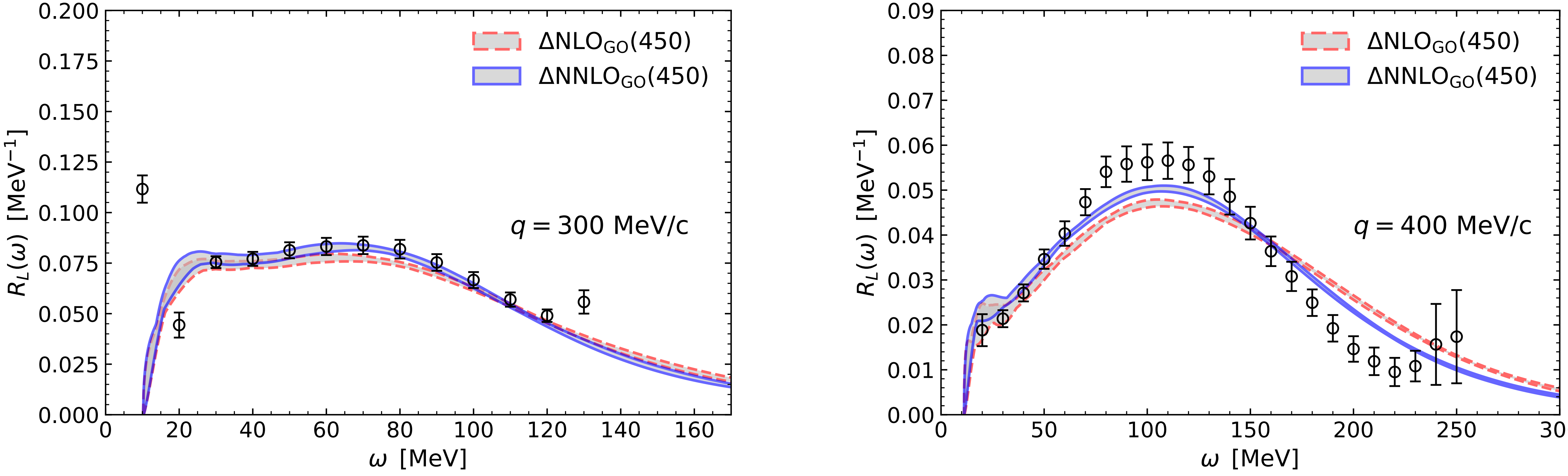
JES, B. Acharya, S. Bacca, G. Hagen; *PRL* 127 (2021) 7, 072501

- ✓ CC singles & doubles
- ✓ varying underlying harmonic oscillator frequency
- ✓ two different chiral Hamiltonians
- ✓ *inversion procedure*

First ab-initio results for many-body system of 40 nucleons

Chiral expansion for ^{40}Ca

(Longitudinal response)

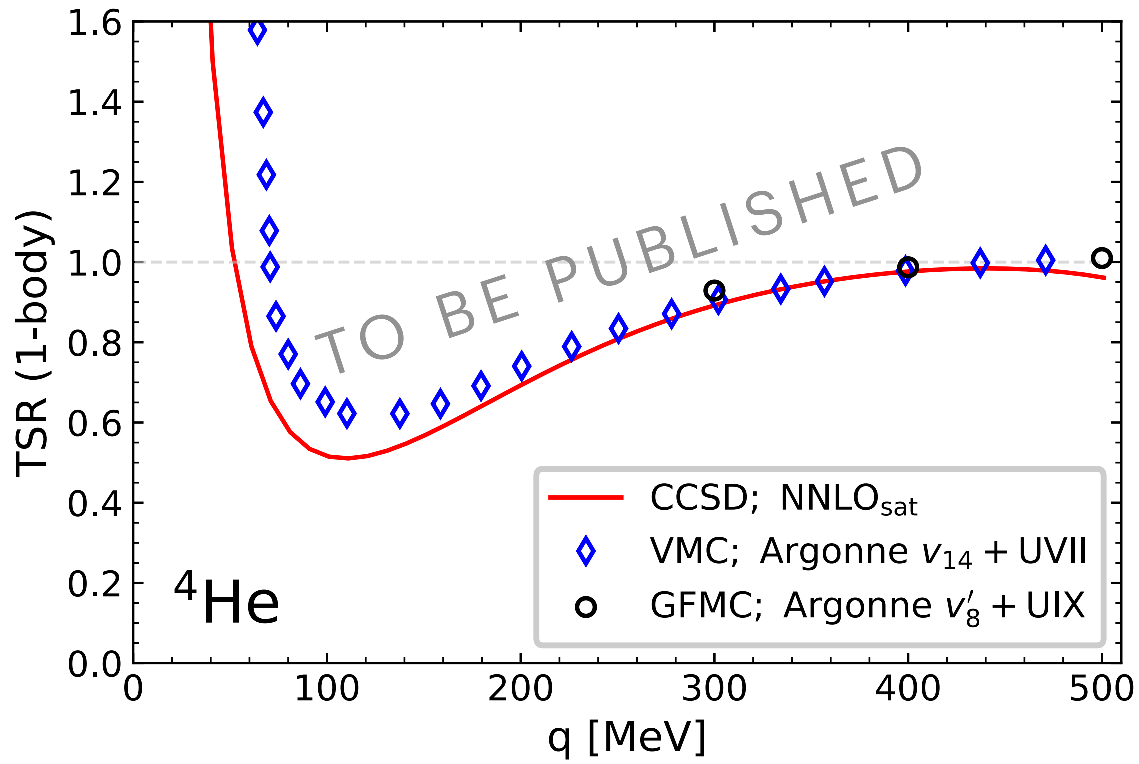


B. Acharya, S. Bacca, JES et al. Front. Phys. 1066035(2022)

- ✓ Two orders of chiral expansion
- ✓ Convergence better for lower q (as expected)
- ✓ Higher order brings results closer to the data

Transverse response

$$\mathrm{TSR}(q) = \frac{2m^2}{Z\mu_p^2 + N\mu_n^2}\frac{1}{q^2}\Big(\langle\Psi|\hat{j}^\dagger\hat{j}\Psi\rangle - |\langle\Psi|\hat{j}|\Psi\rangle|^2\Big)$$

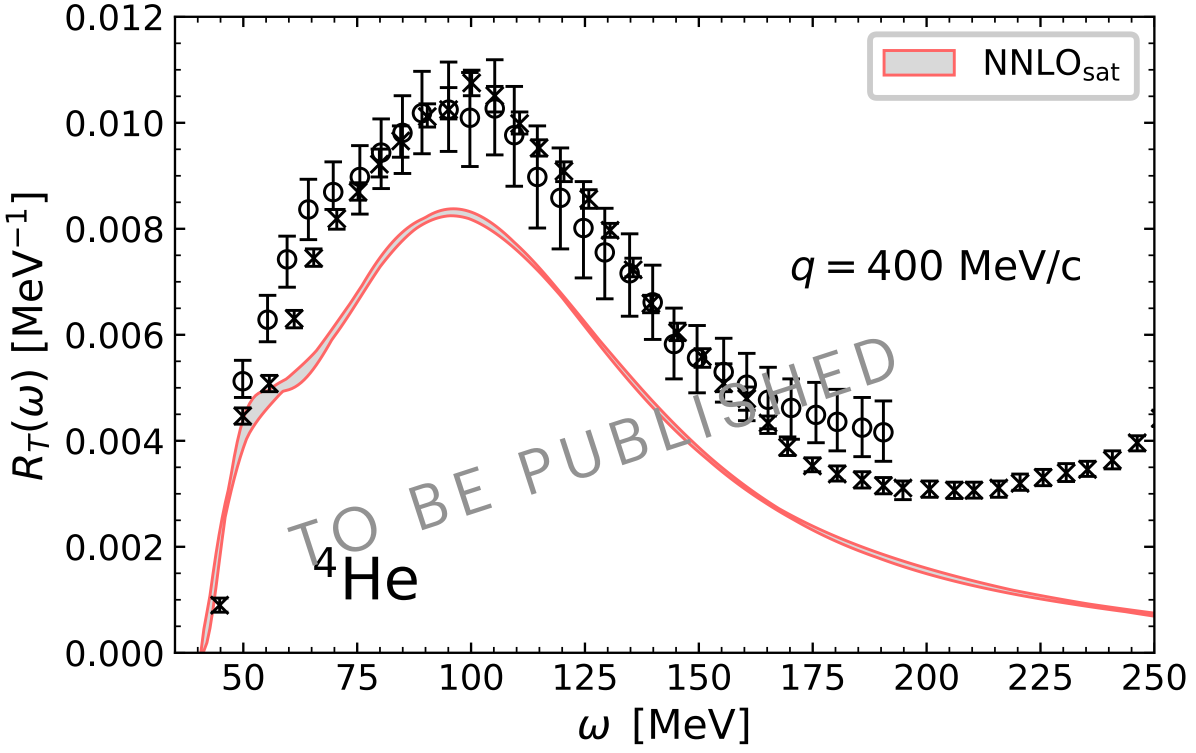


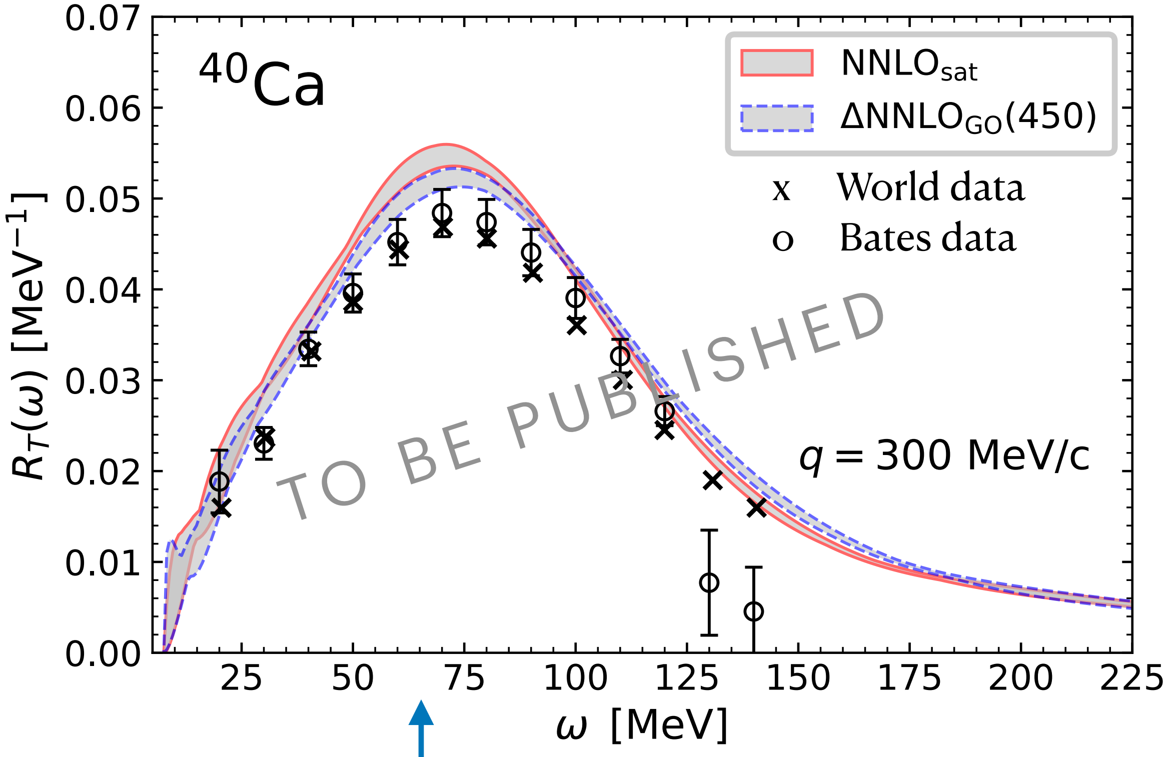
$\mathrm{TSR}(q \to 0) \propto$ kinetic energy

$\mathrm{TSR}(q \to \infty) = 1$

$$\boxed{\mathbf{j}(\mathbf{q}) = \sum_i \frac{1}{2m}\epsilon_i\{\mathbf{p_i}, e^{i\mathbf{q}\mathbf{r}_\mathrm{i}}\} - \frac{i}{2m}\mu_i\mathbf{q}\times\sigma_i e^{i\mathbf{q}\mathbf{r}_\mathrm{i}}}$$

Transverse response





- ➡ This allows to predict electron-nucleus cross-section
- ➡ Currently only 1-body current

2-body currents important for 4He

→ more correlations needed?

→ 2-b currents strength depends on nucleus?

Exclusive cross-sections

- LIT-CC calculations for $q \lesssim 450$ MeV
- Inclusive cross sections
- No pion production

$$\Downarrow$$

- Ideas (and approximations) needed to address relevant physics for ν oscillation experiments
- STA (L. Andreoli) and SF (O. Benhar)

Exclusive cross-sections

- LIT-CC calculations for $q \lesssim 450$ MeV
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$$\Downarrow$$

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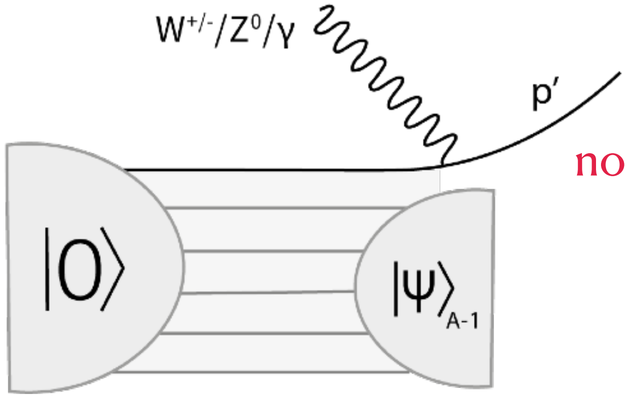
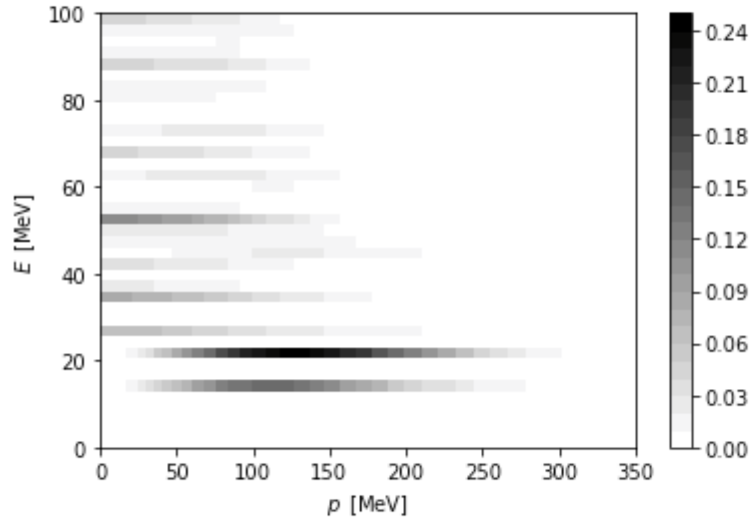
SPECTRAL FUNCTION



no FSI

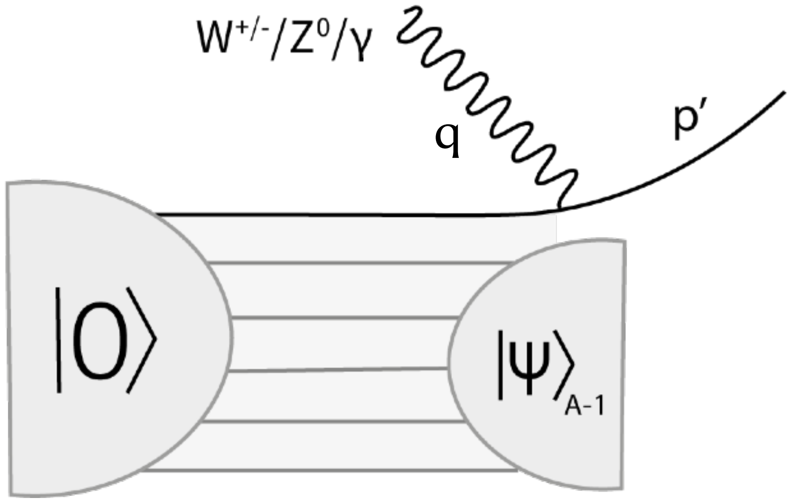
Impulse Approximation



Probability density of finding nucleon $(E, \mathbf{p})$ in ground state nucleus

Spectral functions

Coupled Cluster + ChEK method

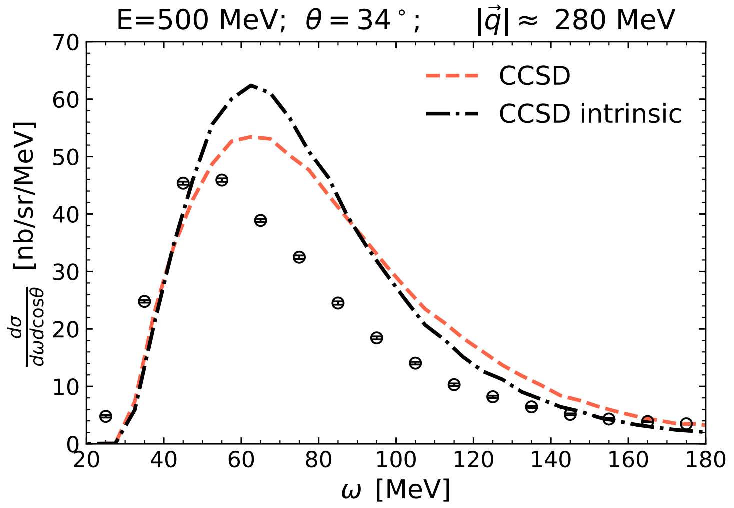


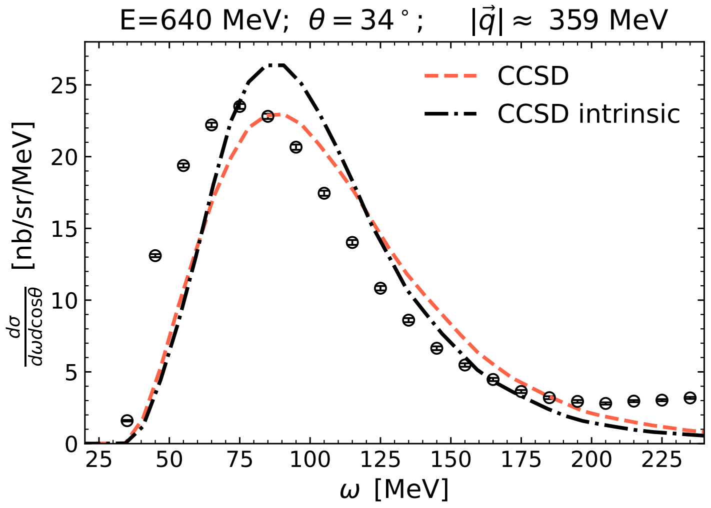
$$\sigma \propto |\mathcal{M}|^2 S(E,p)$$

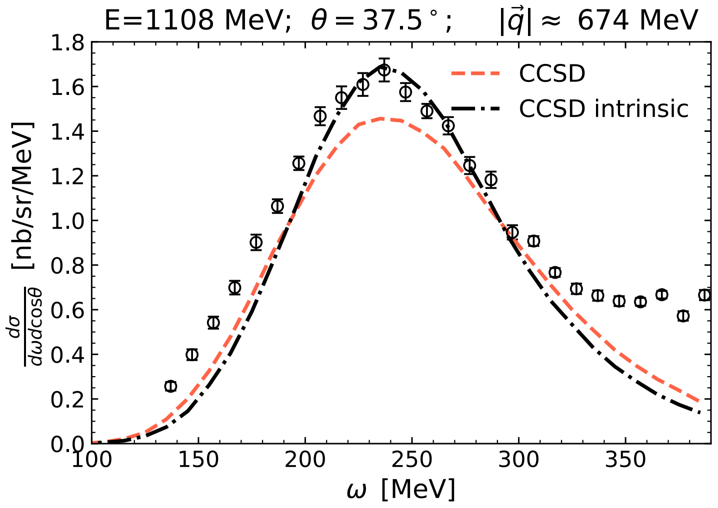
Factorized interaction vertex (relativistic, pion production...)

Spectral function - nuclear information

growing **q** momentum transfer → final state interactions play minor role

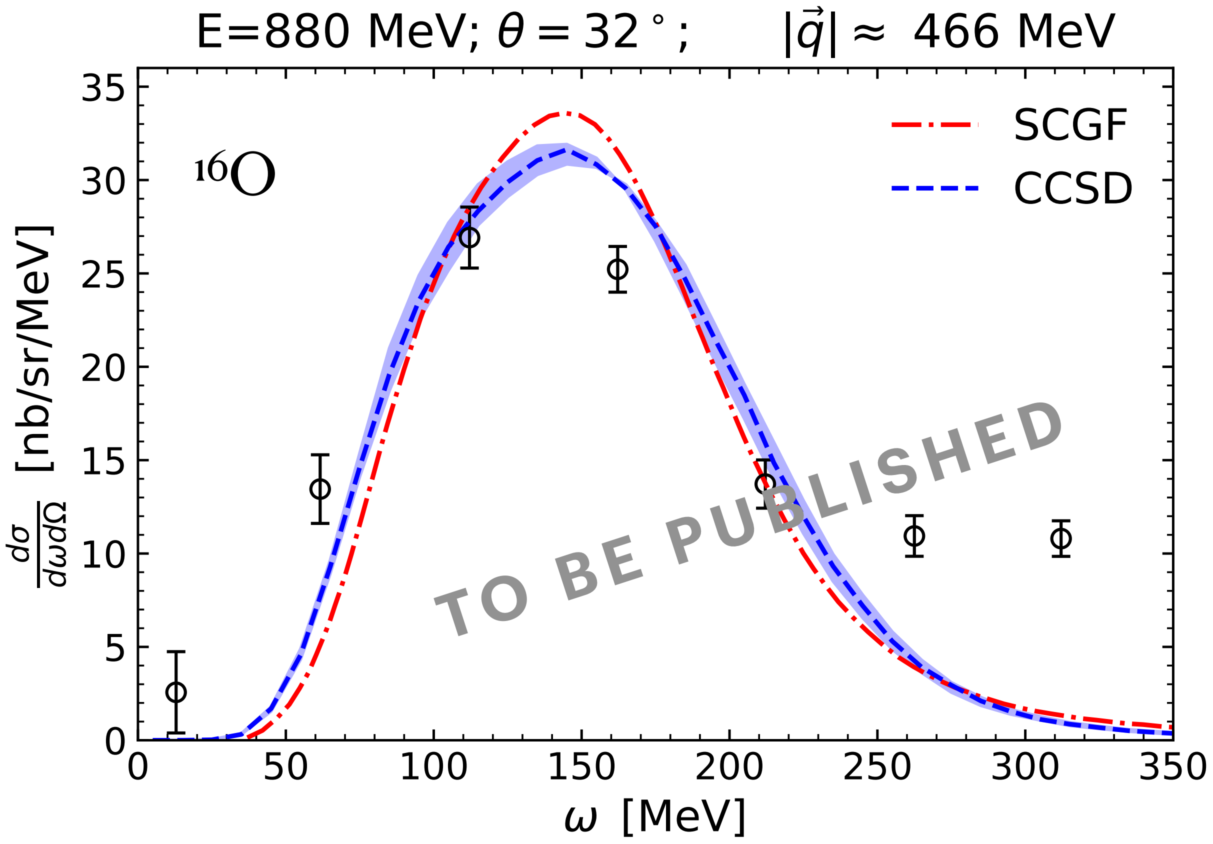


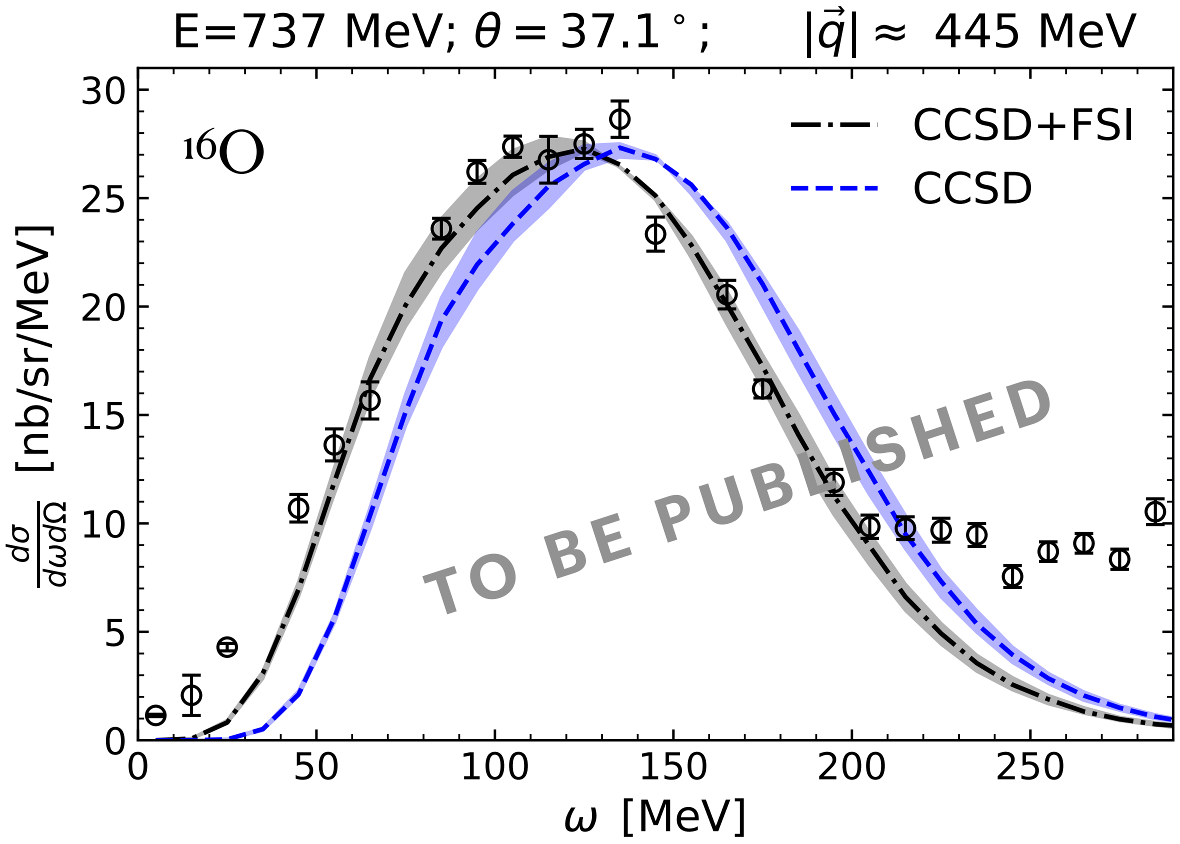




JES, S. Bacca, G. Hagen, T. Papenbrock *Phys.Rev.C* 106 (2022) 3, 034310

Final state interactions





JES et al, in preparation (2023)

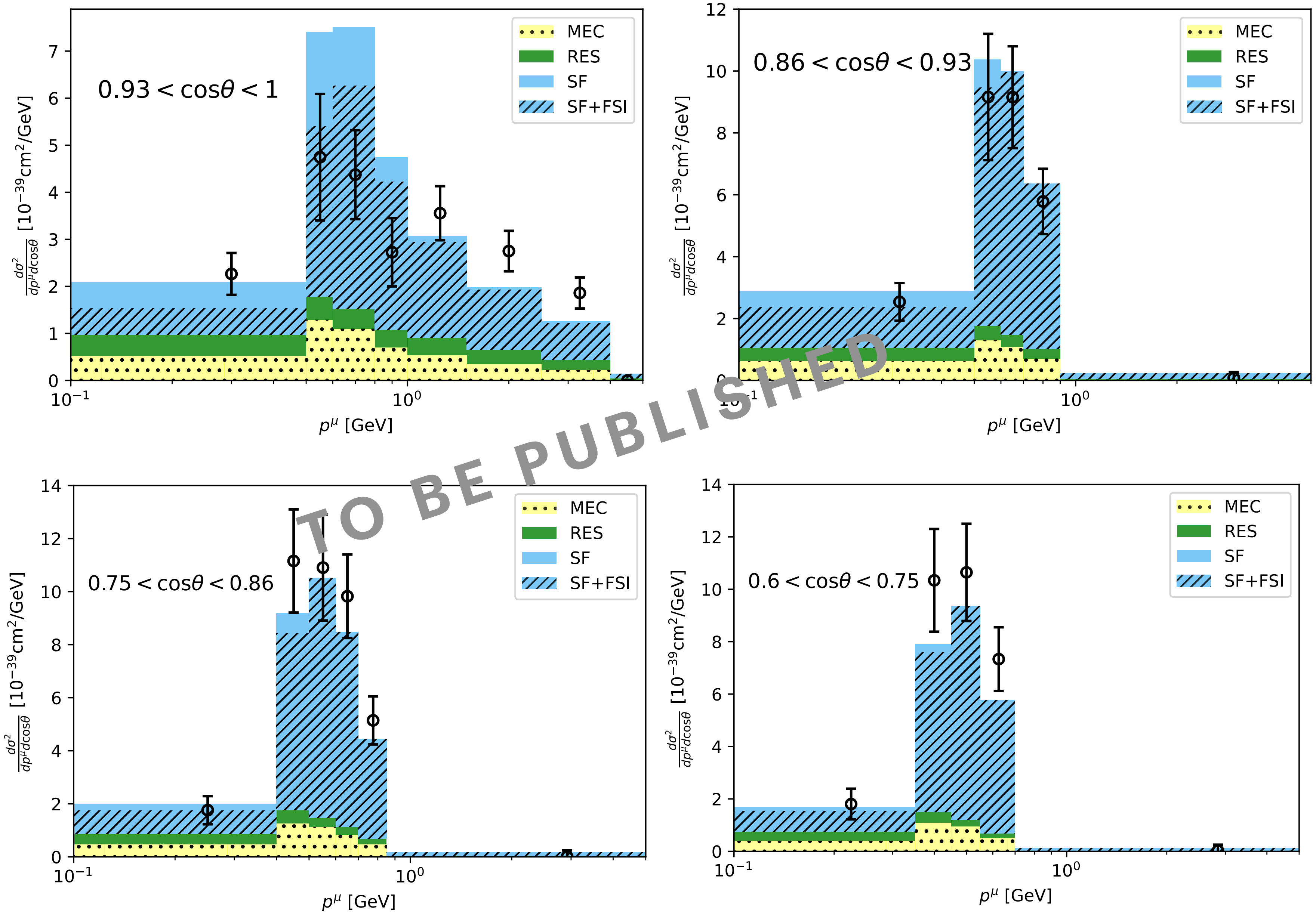
How to account for the FSI? Optical potential for the outgoing nucleon

Spectral function for neutrinos

$$\nu_\mu + ^{16}\mathrm{O} \rightarrow \mu^- + X$$

- Comparison with T2K long baseline ν oscillation experiment
- $\mathrm{CC}0\pi$ events
- Spectral function implemented into NuWro Monte Carlo generator

Data: Phys. Rev. D 101, 112004 (2020)



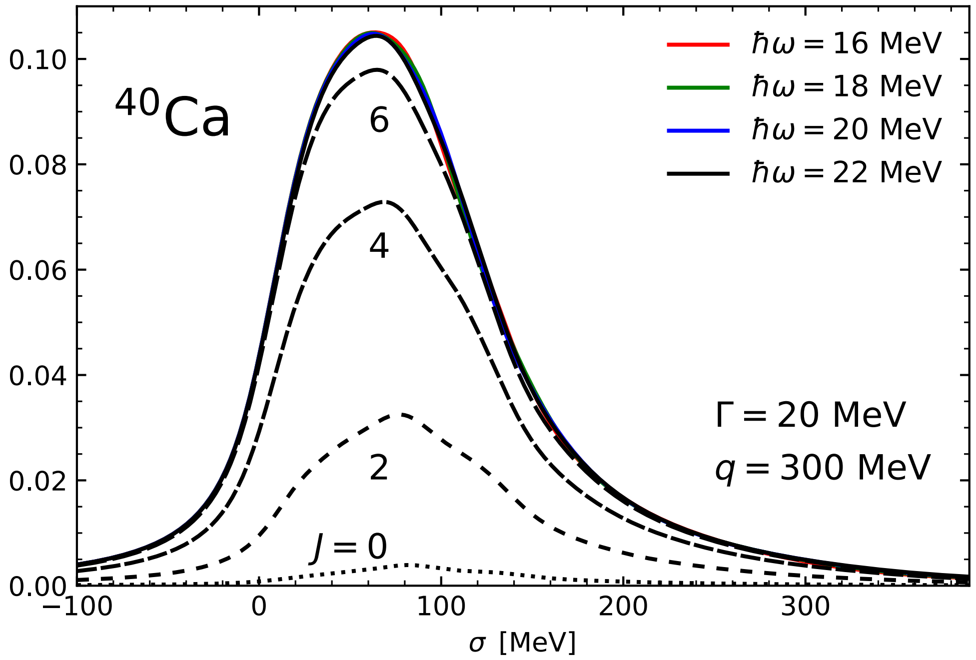
JES et al, in preparation (2023)

Outlook

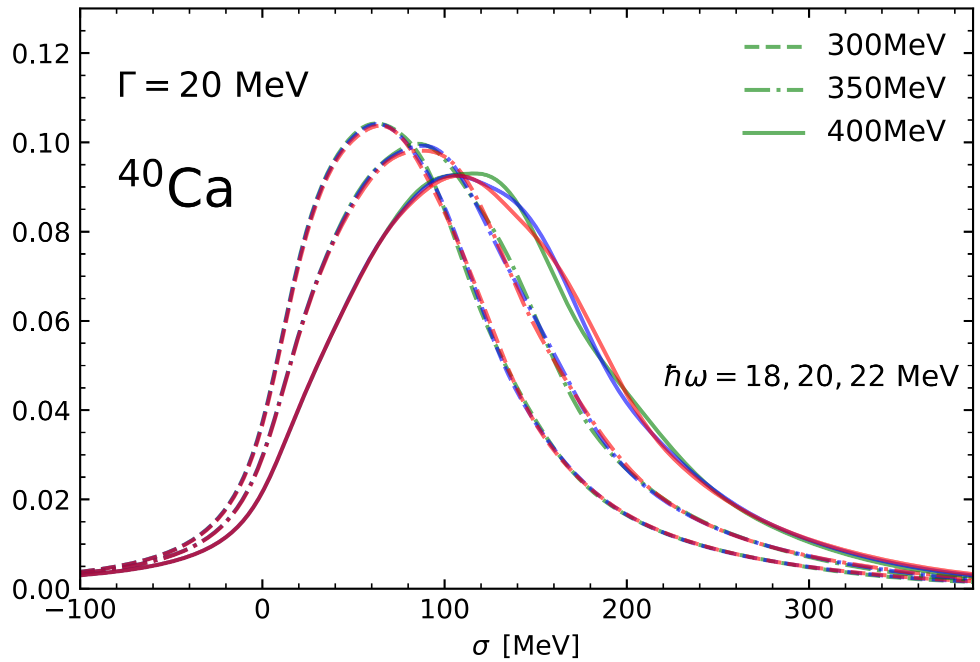
- LIT-CC benchmark for electron scattering → ready for neutrino
- Role of 2-body currents for medium-mass nuclei
- Extending the response calculation to ^{40}Ar
- Spectral functions (within Impulse Approximation):
  - Relativistic regime
  - Semi-inclusive processes
  - Further steps: 2-body spectral functions?, accounting for FSI

Thank you for attention

Longitudinal response ^{40}Ca

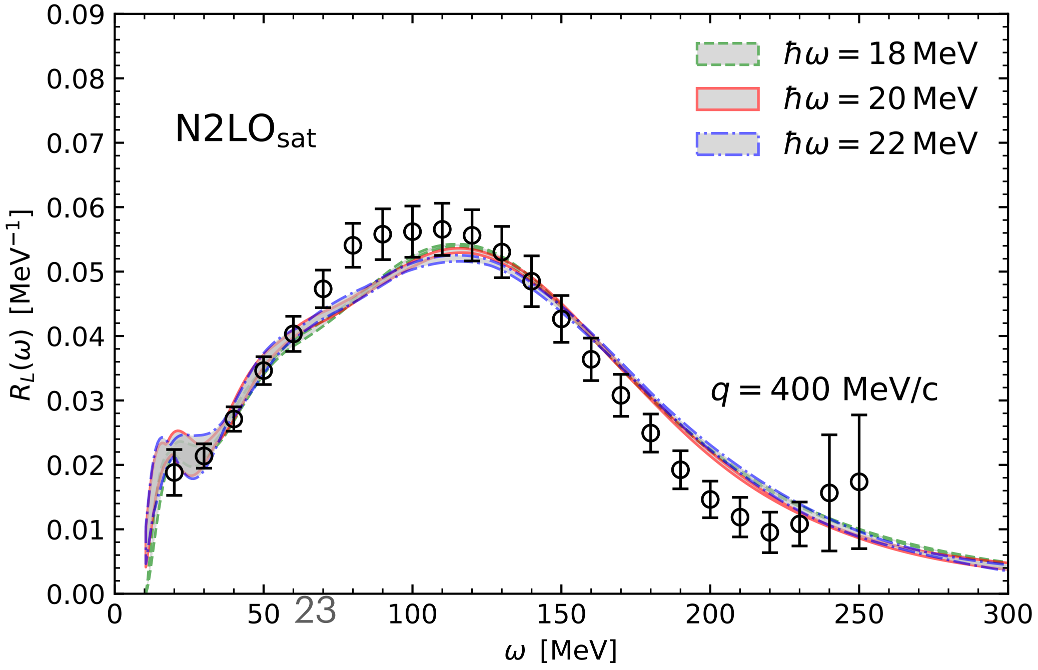


Sum over multipoles



Underlying oscillator frequency

Inversion



Coulomb sum rule

Project out spurious states: $\hat{\rho}\,|\Psi\rangle = |\Psi_{phys}\rangle + |\Psi_{spur}\rangle$

It has been shown that to good approximation the ground state factorizes:

$$|\Psi\rangle = |\Psi_I\rangle\,|\Psi_{CoM}\rangle$$

center of mass wave function is a Gaussian

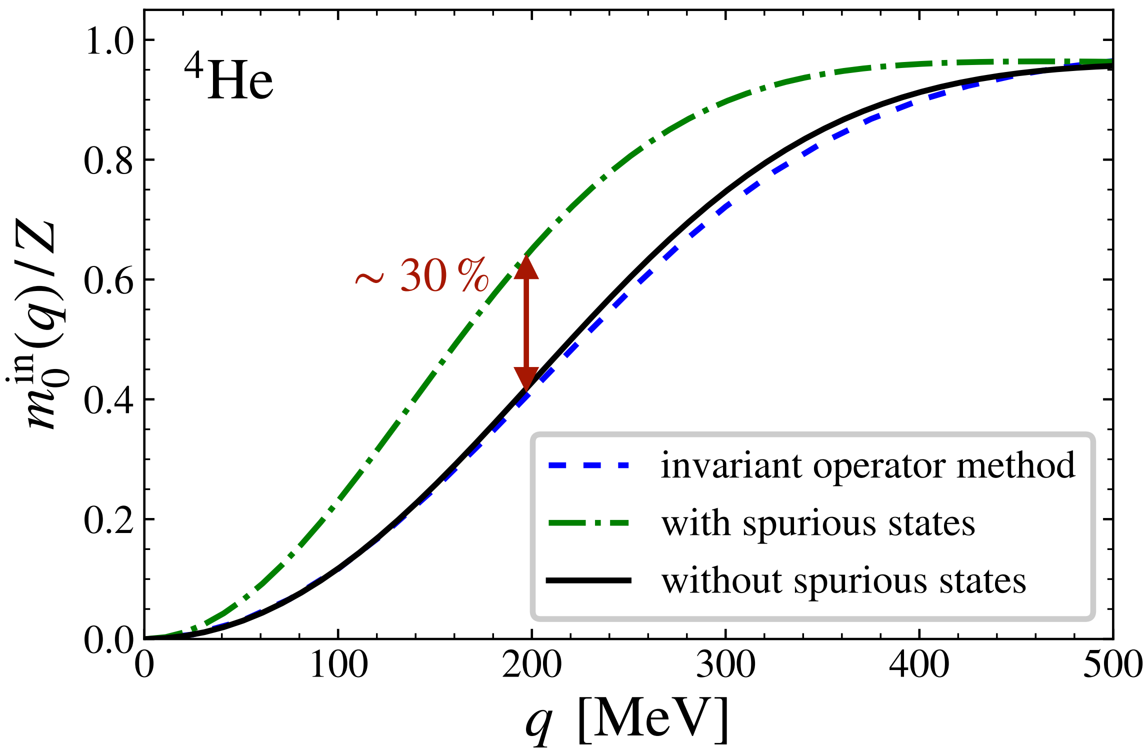
G. Hagen, T. Papenbrock, D. Dean
Phys.Rev.Lett. 103 (2009) 062503

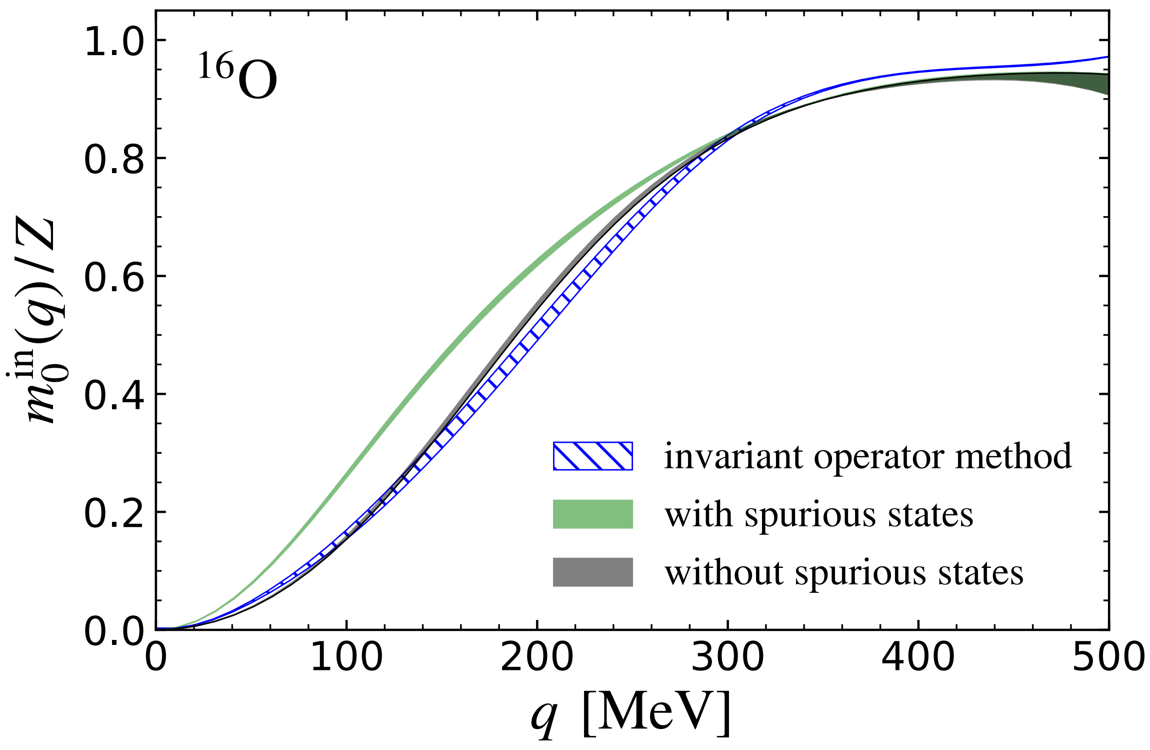
We follow a similar ansatz for the excited states:

$$\hat{\rho}\,|\Psi\rangle = |\Psi_I^{exc}\rangle\,|\Psi_{CoM}\rangle + |\Psi_I\rangle\,\cancel{|\Psi_{CoM}^{exc}\rangle}$$

spurious

Coulomb sum rule





J.E.S. B. Acharya, S.Bacca, G. Hagen
Phys.Rev.C 102 (2020) 064312

CoM spurious states dominate for light nuclei

Details on inversion procedure

- Basis functions

$$R_L(\omega) = \sum_{i=1}^{N} c_i \omega^{n_0} e^{-\frac{\omega}{\beta_i}}$$

- Stability of the inversion procedure:
  - Vary the parameters n_0, β_i and number of basis functions N (6-9)
  - Use LITs of various width Γ (5, 10, 20 MeV)

Lorentz integral transform

$$L(\sigma) = \int \frac{R(\omega)}{(\omega-\sigma)^2+\Gamma^2} d\omega = \int \frac{R(\omega)}{(\omega+\tilde{\sigma}^*)(\omega+\tilde{\sigma})} d\omega$$

$$L(\sigma) = \int d\omega \sum_f \langle \Psi_0 | \rho^\dagger \frac{1}{\omega+\tilde{\sigma}^*} | \Psi_f \rangle \langle \Psi_f | \frac{1}{\omega+\tilde{\sigma}} \rho | \Psi_0 \rangle \delta(\omega + E_0 - E_f)$$

$$L(\sigma) = \sum_f \langle \Psi_0 | \rho^\dagger \frac{1}{E_f - E_0 + \tilde{\sigma}^*} | \Psi_f \rangle \langle \Psi_f | \frac{1}{E_f - E_0 + \tilde{\sigma}} \rho | \Psi_0 \rangle$$

$$L(\sigma) = \sum_f \underbrace{\langle \Psi_0 | \rho^\dagger \frac{1}{H - E_0 + \tilde{\sigma}^*}}_{\langle \tilde{\Psi} |} | \Psi_f \rangle \langle \Psi_f | \underbrace{\frac{1}{H - E_0 + \tilde{\sigma}} \rho | \Psi_0 \rangle}_{| \tilde{\Psi} \rangle}$$

We need to solve

$$(H - E_0 + \tilde{\sigma}) | \tilde{\Psi} \rangle = \rho | \Psi \rangle$$

Schrodinger-like equation