Uncertainty quantification in coupled cluster theory

Joanna Sobczyk

Theoretical Physics Uncertainties to Empower Neutrino Experiments, 31 Oct 2023

Cluster of Excellence PRISMA+ Precision Physics, Fundamental Interactions and Structure of Matter
JG|U
Alexander von Humboldt Stiftung / Foundation
MARIE CURIE ACTIONS
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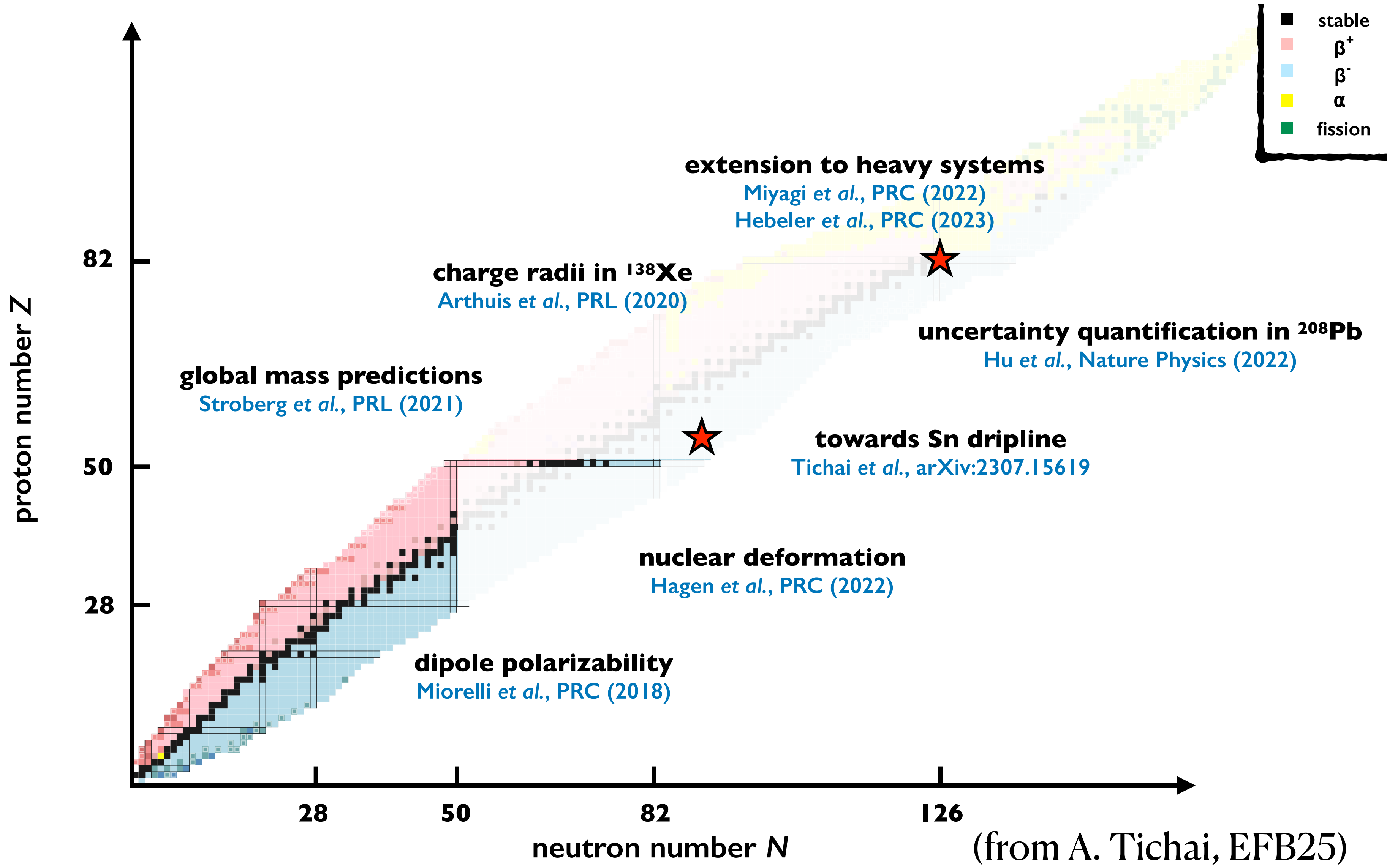
An initio nuclear methods

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

“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



(from A. Tichai, EFB25)

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

Coupled cluster method

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

Include correlations through e^T operator

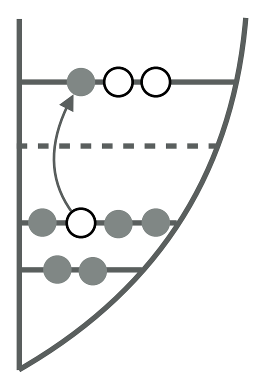
similarity transformed Hamiltonian

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

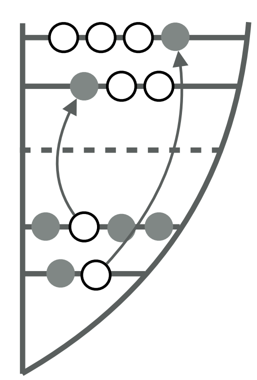
Expansion: $T = \sum t_a^i a_a^\dagger a_i + \sum t_{ab}^{ij} a_a^\dagger a_b^\dagger a_i a_j + \ldots$

←coefficients obtained through coupled cluster equations

singles



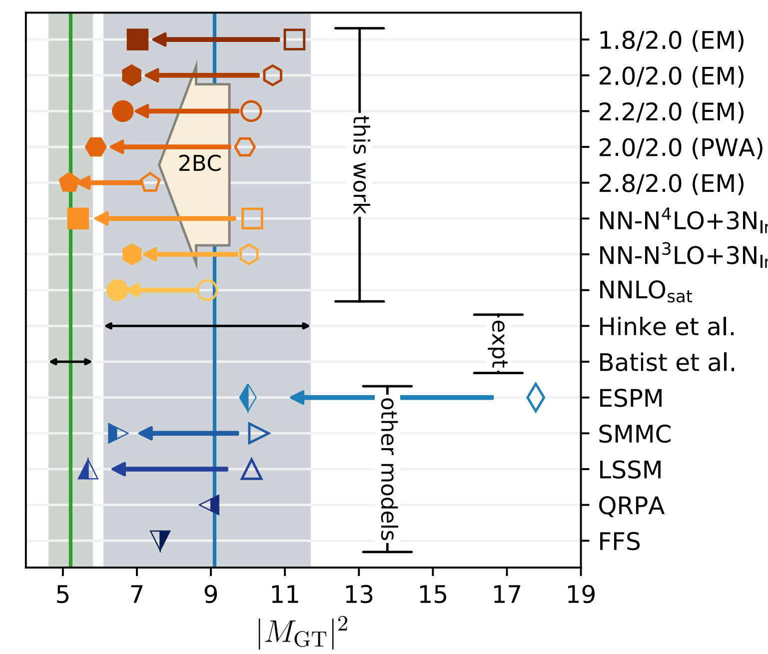
doubles



Coupled cluster method

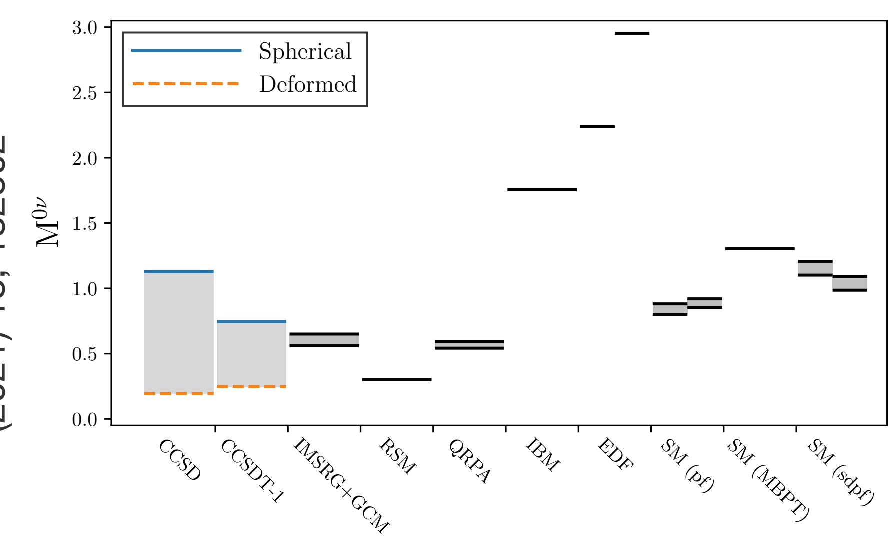
- ✓ Controlled approximation through truncation in T
- ✓ Polynomial scaling with A (predictions for ^{100}Sn, ^{208}Pb)
- ✓ Size extensive
- ✓ Works most efficiently for doubly magic nuclei

Nature Phys. 15 (2019) 5, 428-431



GT strength for β decay of ^{100}Sn

Phys.Rev.Lett. 126 (2021) 18, 182502



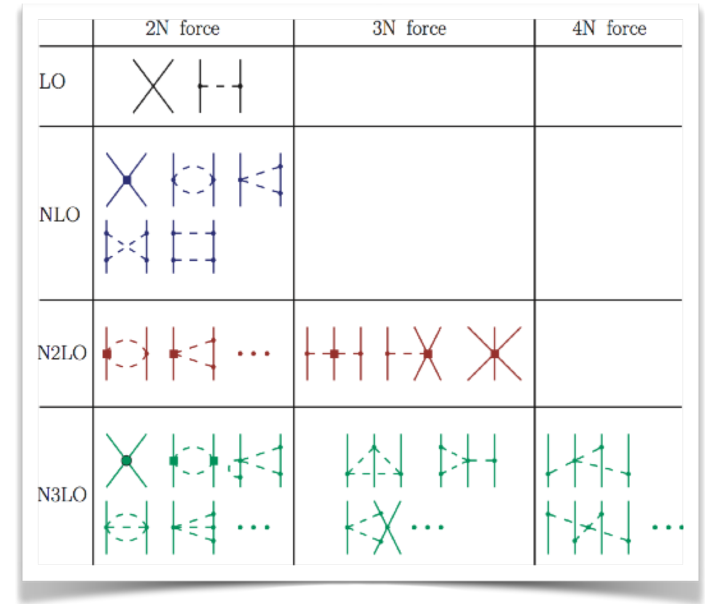
NME of ^{48}Ca for $0\nu\beta\beta$

Ab initio nuclear theory for neutrinos

Nuclear chiral Hamiltonian

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

- ➡ order of expansion
- ➡ low energy constants fit to data



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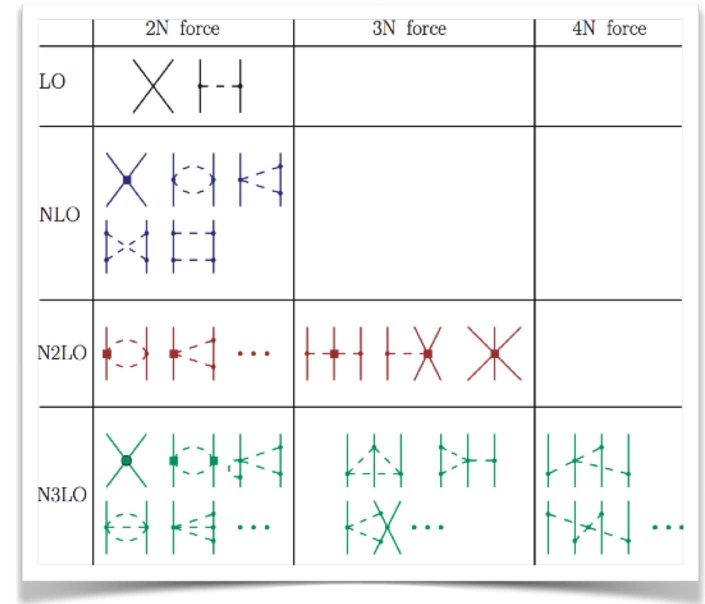

Electroweak currents

$$J^{\mu} = (\rho, \vec{j})$$

- ➡ order of expansion
- ➡ 2-body currents important

Ab initio nuclear theory for neutrinos

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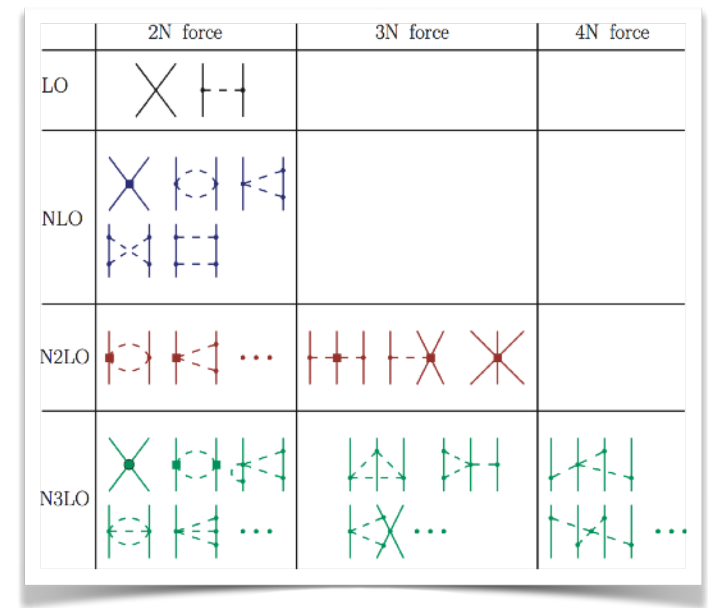

Electroweak currents

$$J^\mu = (\rho, \vec{j})$$

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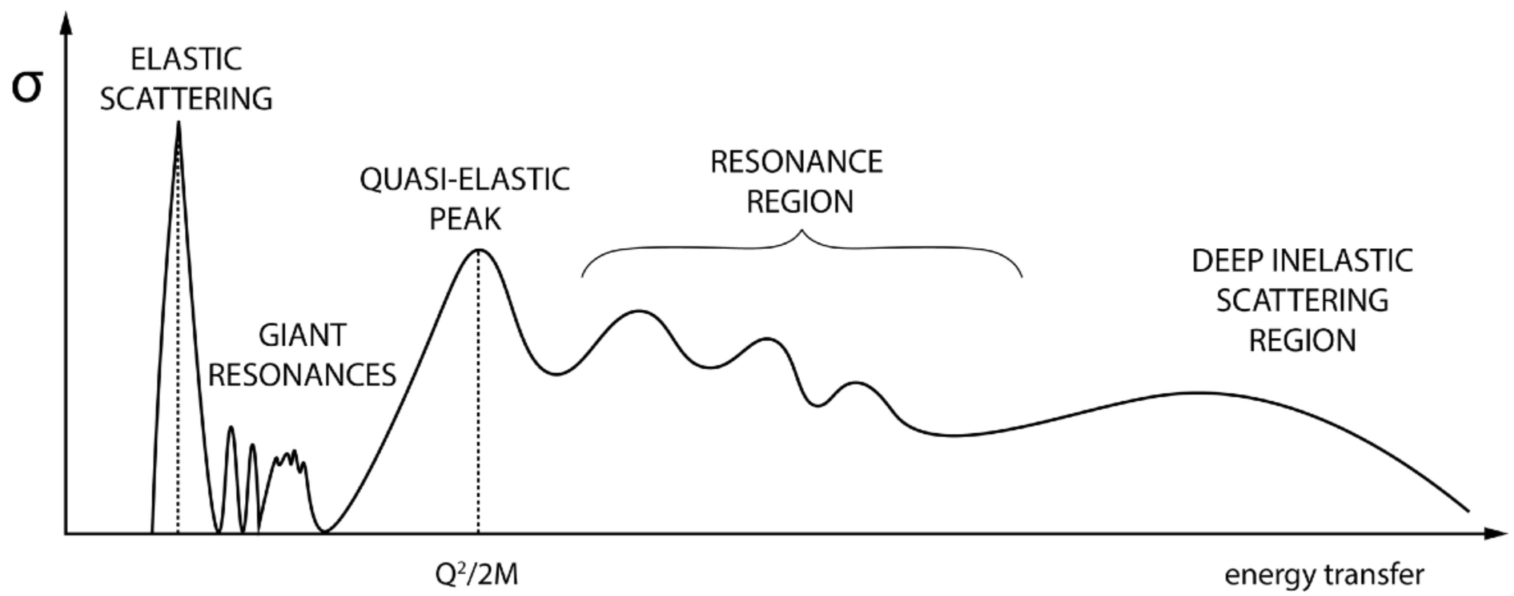
Coupled cluster method

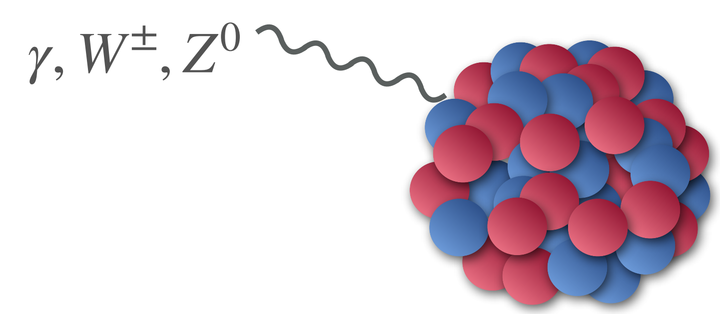
$$\mathscr{A} = \langle \Psi_m\,|\,J_\mu\,|\,\Psi_n\rangle$$

- ➡ truncation in correlations
- ➡ model space dependence

Nuclear response



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

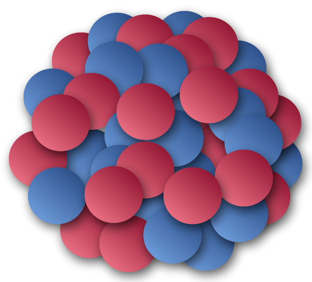


$$\sigma \propto L^{\mu\nu} R_{\mu\nu}$$

lepton tensor — nuclear responses

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

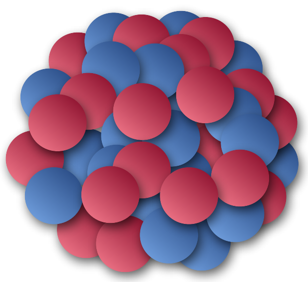
Low/high energies



$$\hat{H}|\psi_A\rangle = E|\psi_A\rangle$$

Many-body problem

Low/high energies



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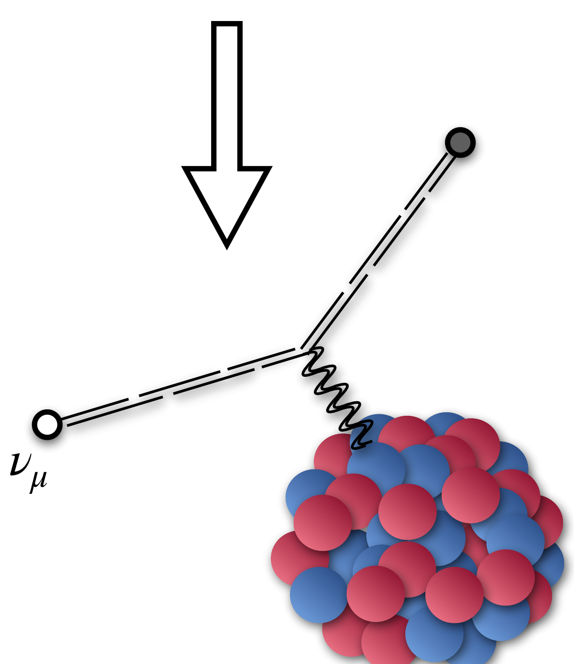
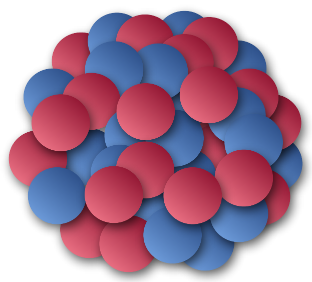


$$\langle\psi_f|\hat{j}|\psi_A\rangle$$

Electroweak responses
consistent FSI treatment

Low/high energies



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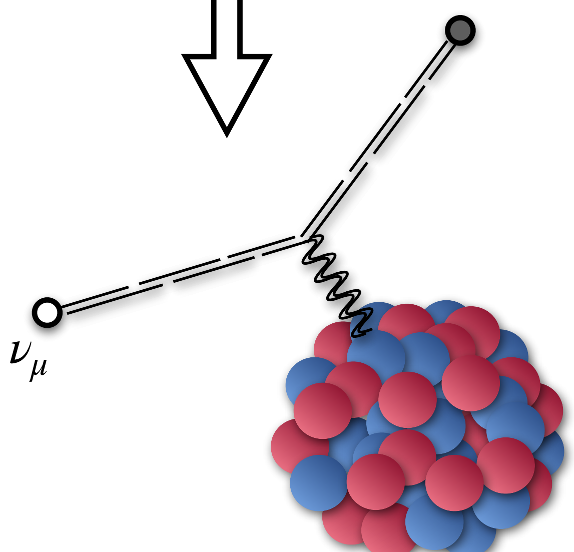

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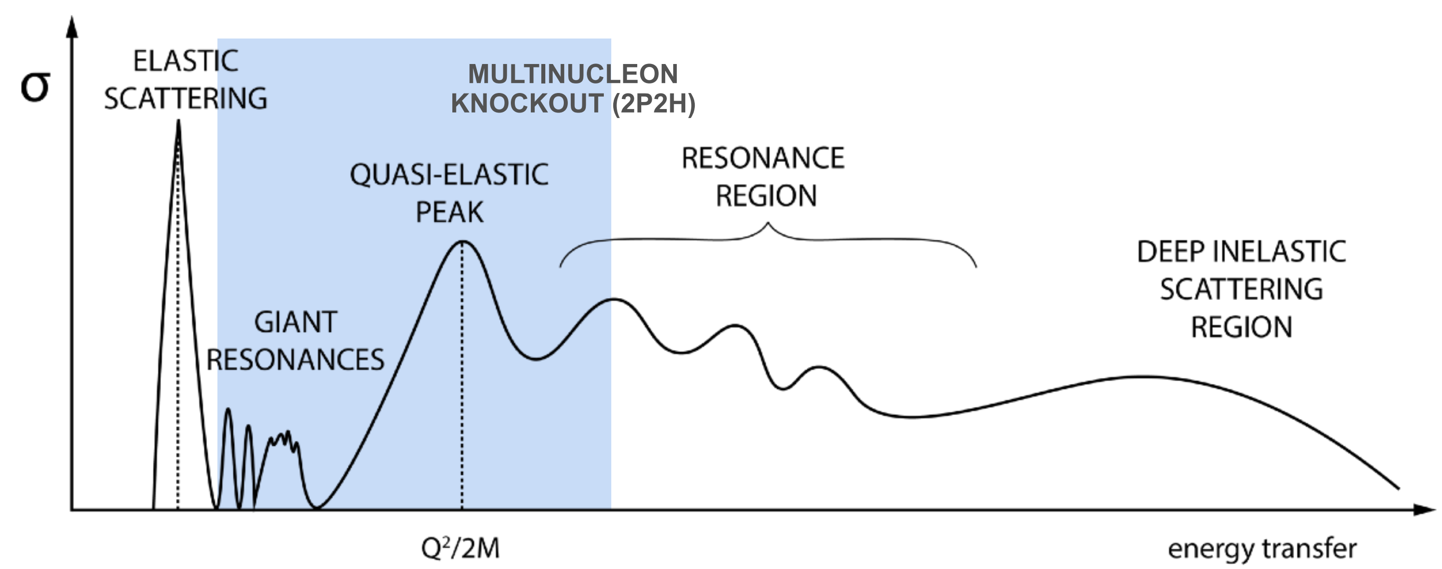

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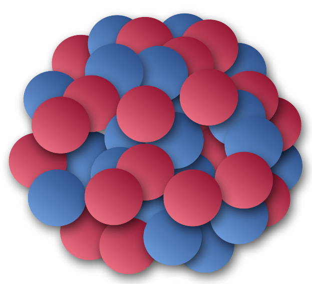

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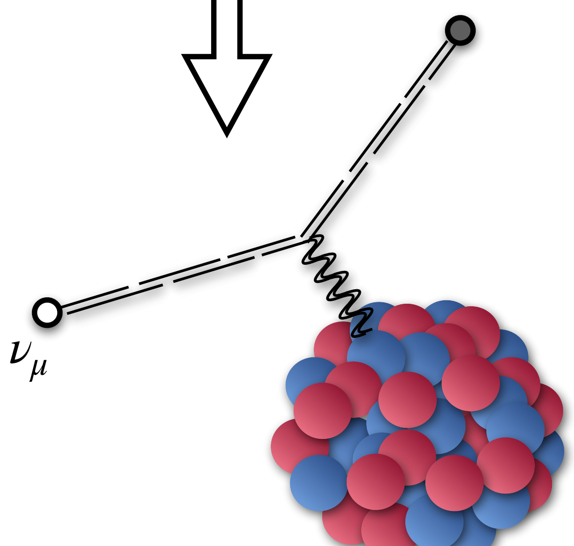

$\langle \psi_f\,|\,\hat{j}\,|\,\psi_A\rangle$

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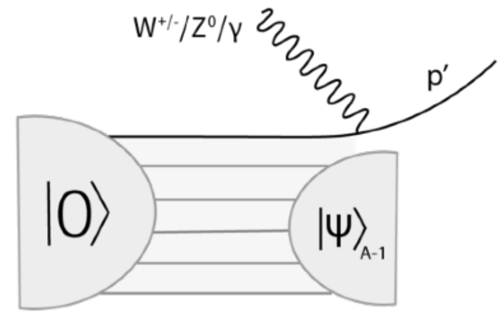
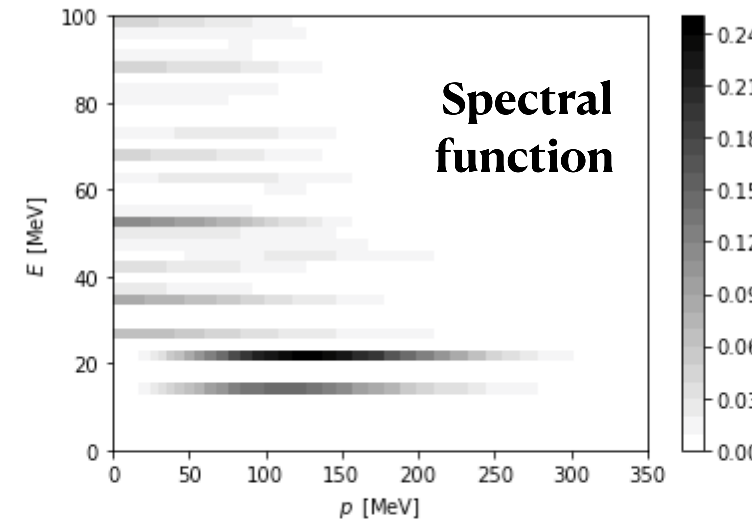
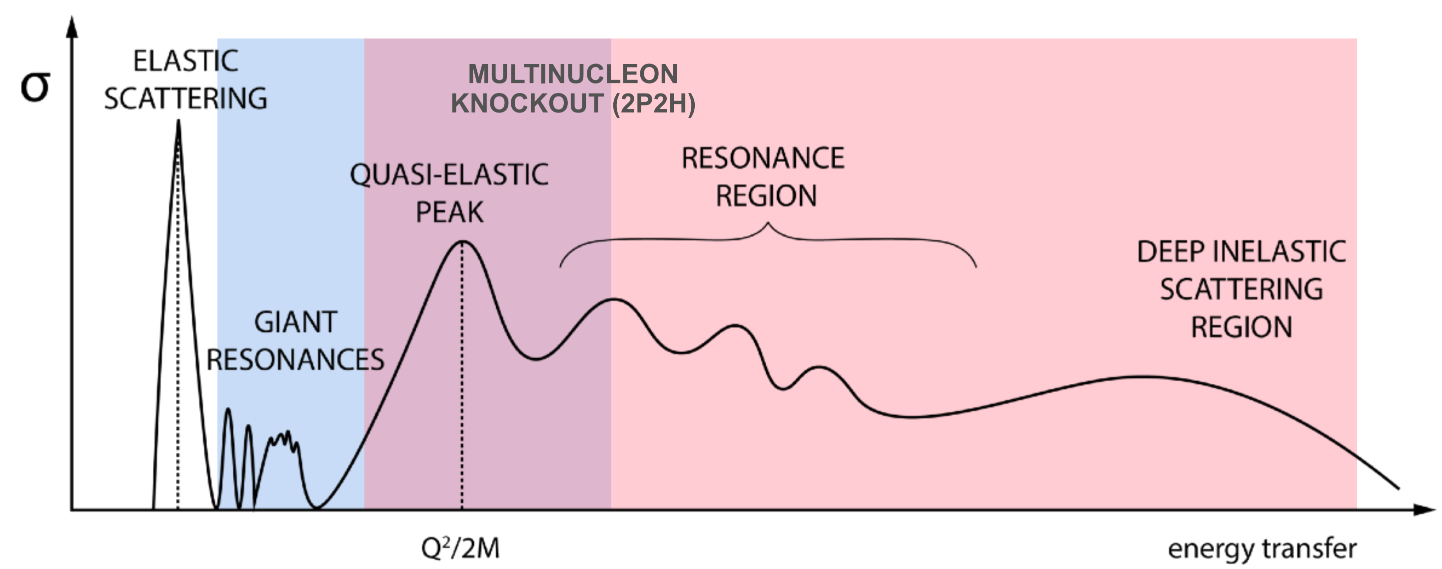


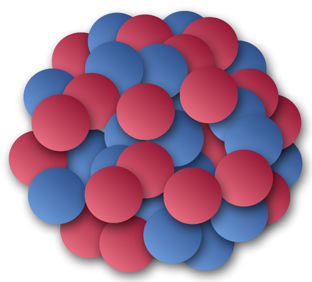
Impulse Approximation



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

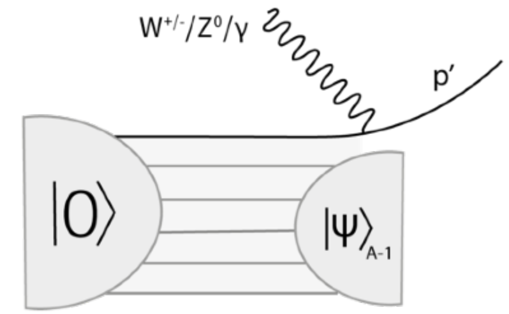


Low/high energies



$$\hat{H}\,|\psi_A\rangle = E\,|\psi_A\rangle$$

Many-body problem



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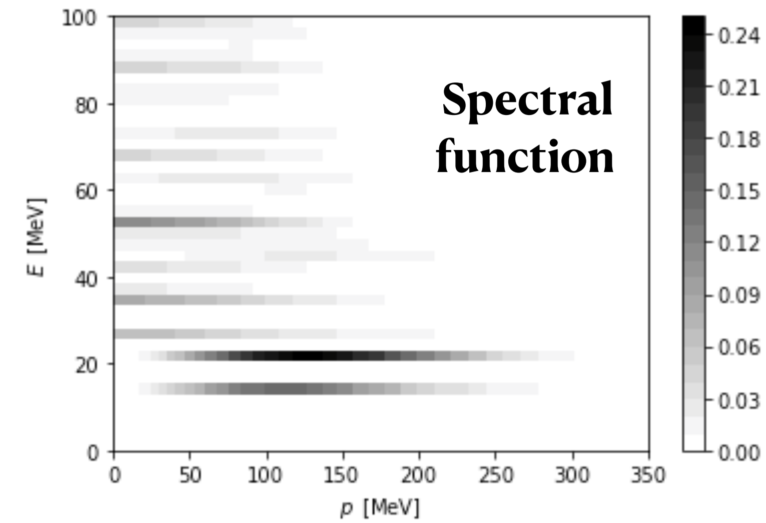
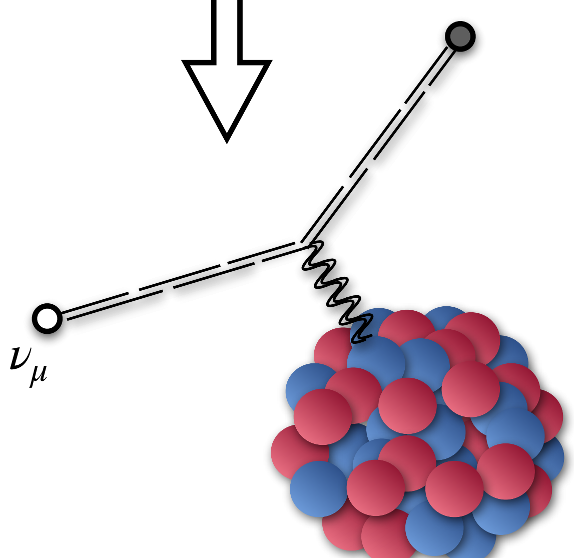
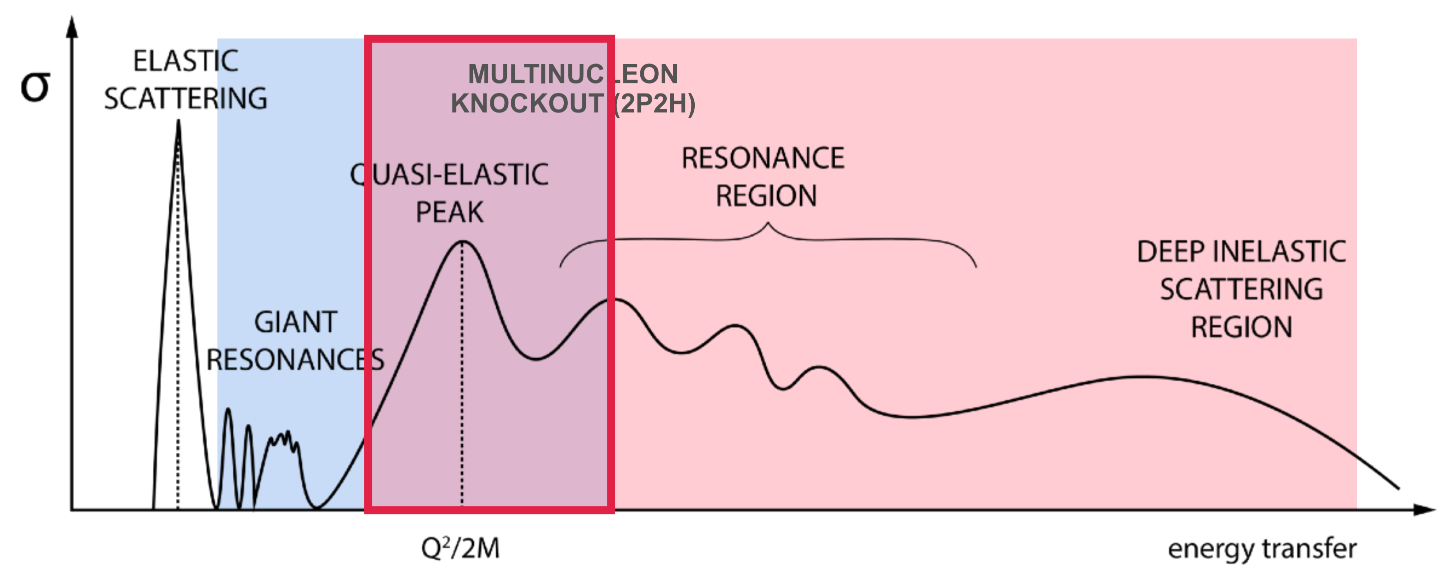


Probability density of finding nucleon $(E, \mathbf{p})$ in ground state nucleus



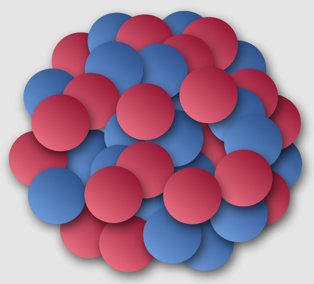
$$\langle\psi_f|\,\hat{j}\,|\psi_A\rangle$$

Electroweak responses
consistent FSI treatment



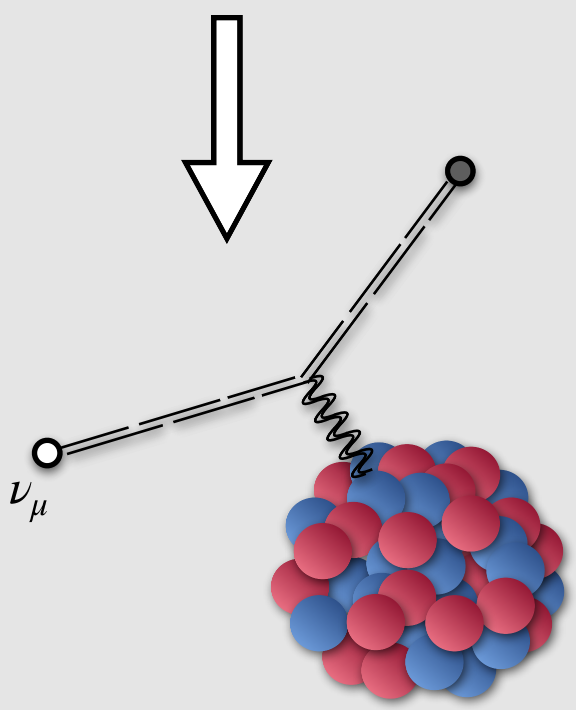
Possible comparison within the same framework

Low/high energies



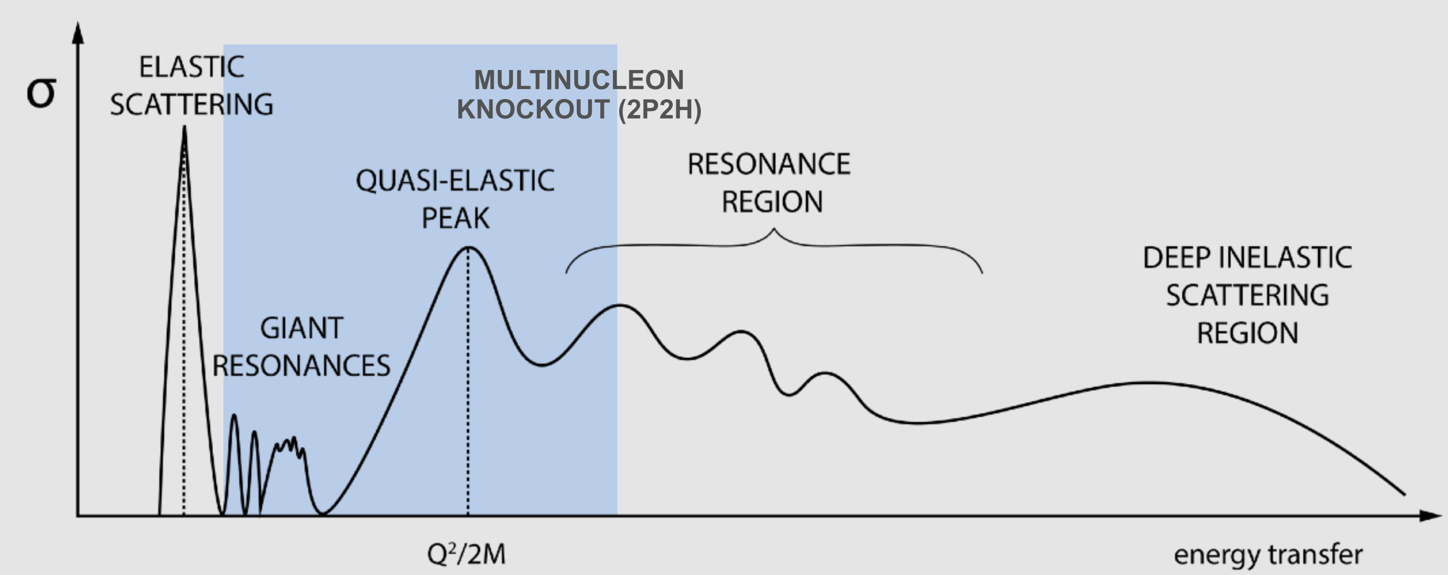
$\hat{H}|\psi_A\rangle = E|\psi_A\rangle$

Many-body problem



$\langle\psi_f|\hat{j}|\psi_A\rangle$

Electroweak responses



Lorentz Integral Transform (LIT)

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

continuum spectrum

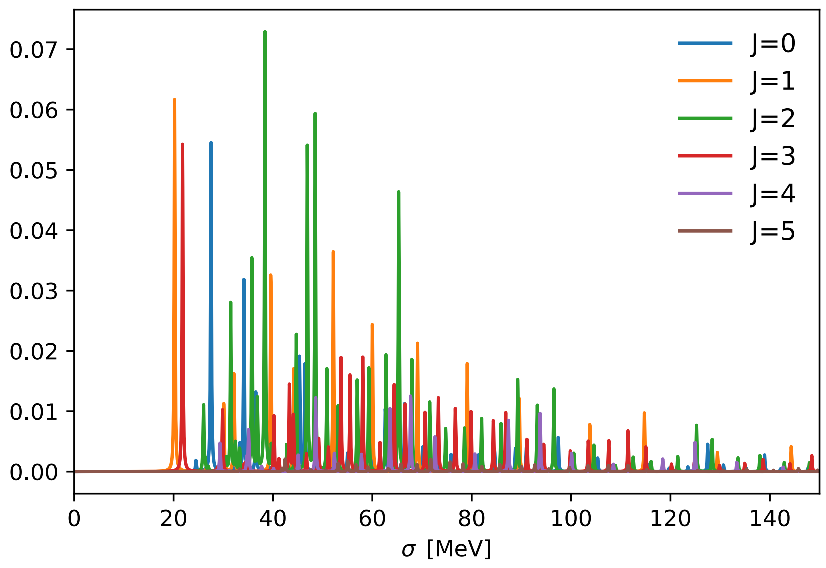
Integral transform

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

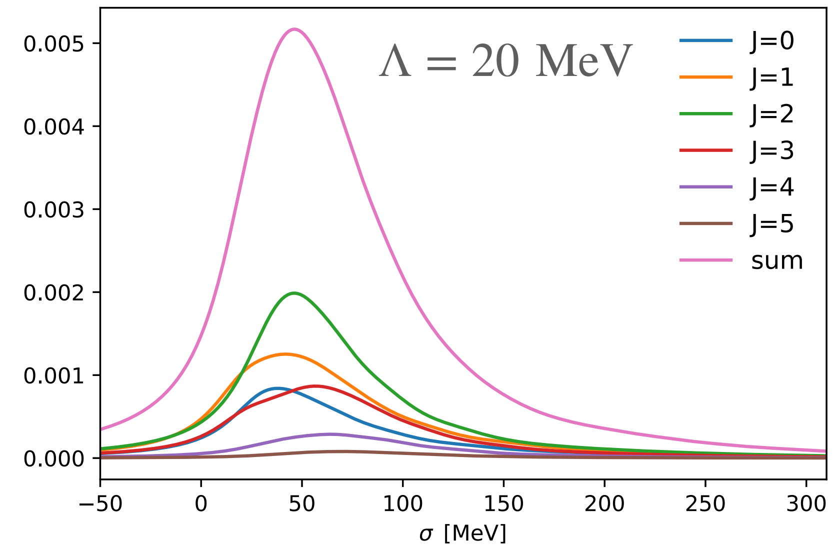
Lorentzian kernel:
$$K_\Lambda(\omega, \sigma) = \frac{1}{\pi} \frac{\Lambda}{\Lambda^2 + (\omega - \sigma)^2}$$

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

Lorentz Integral Transform

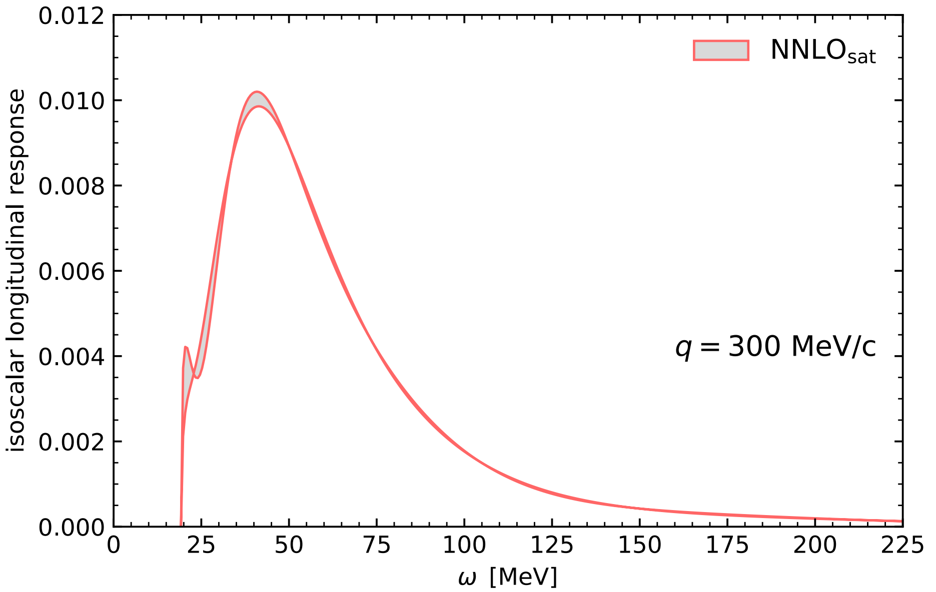


Integral transform



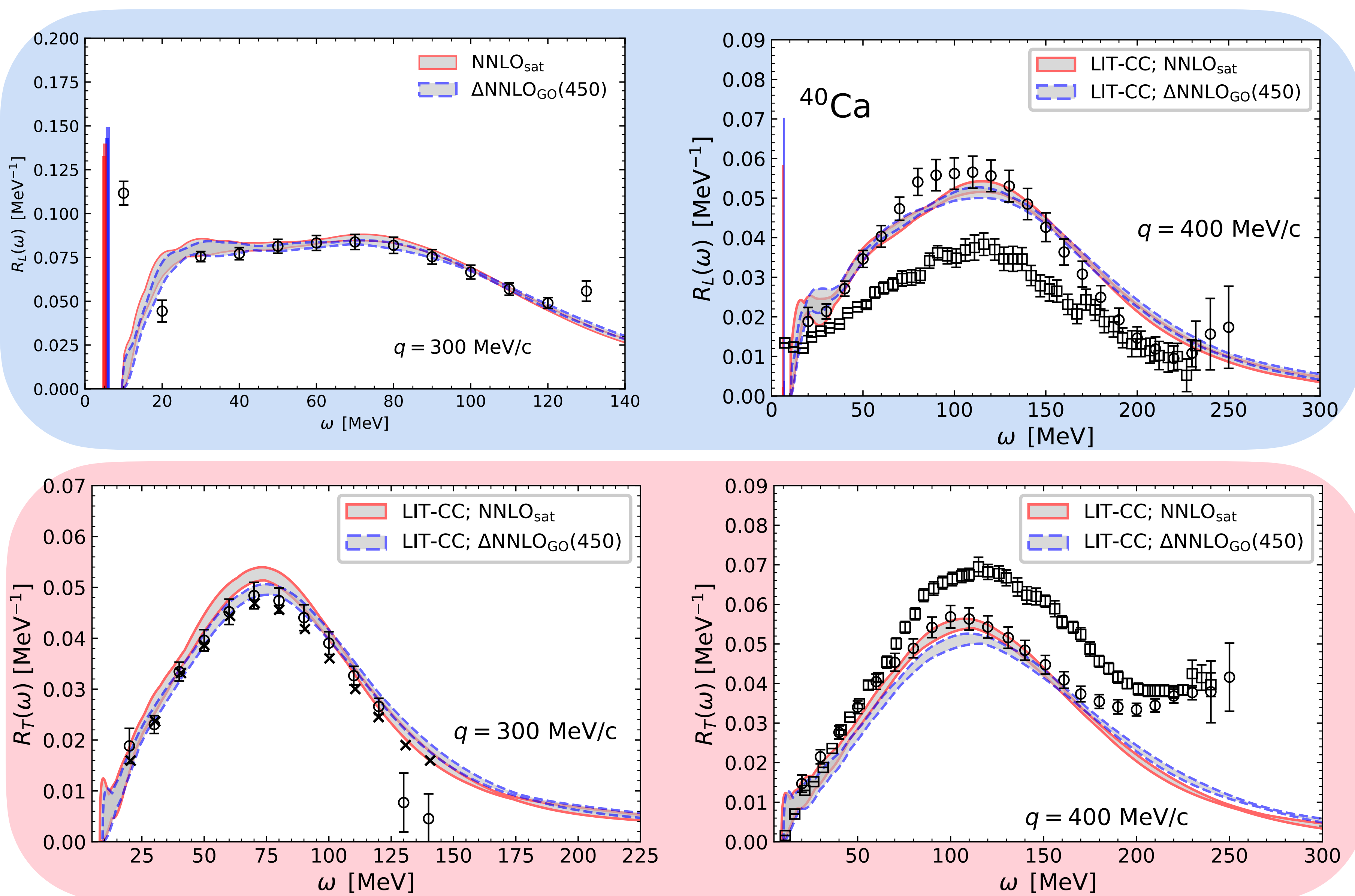
Inversion

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



Electromagnetic responses ^{40}Ca

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

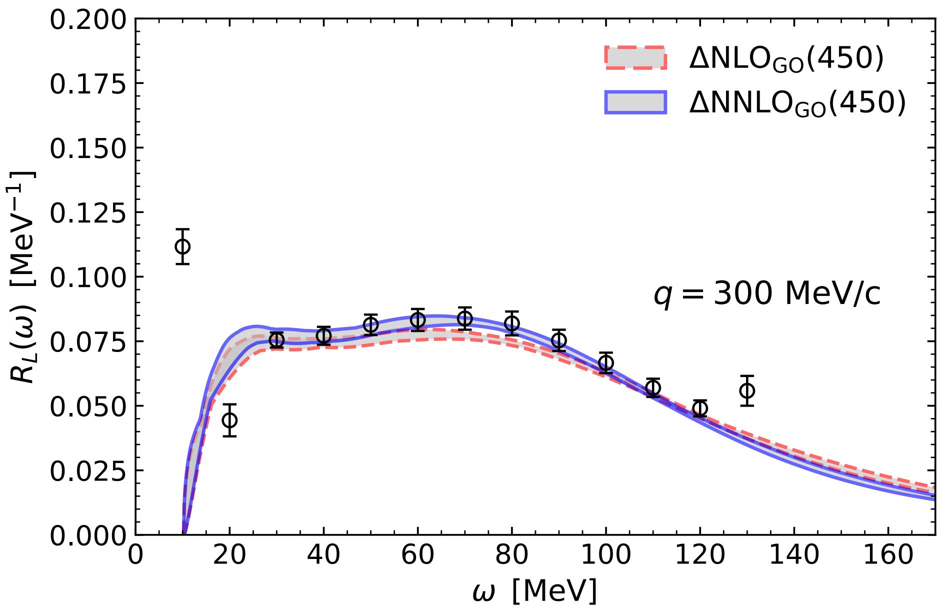


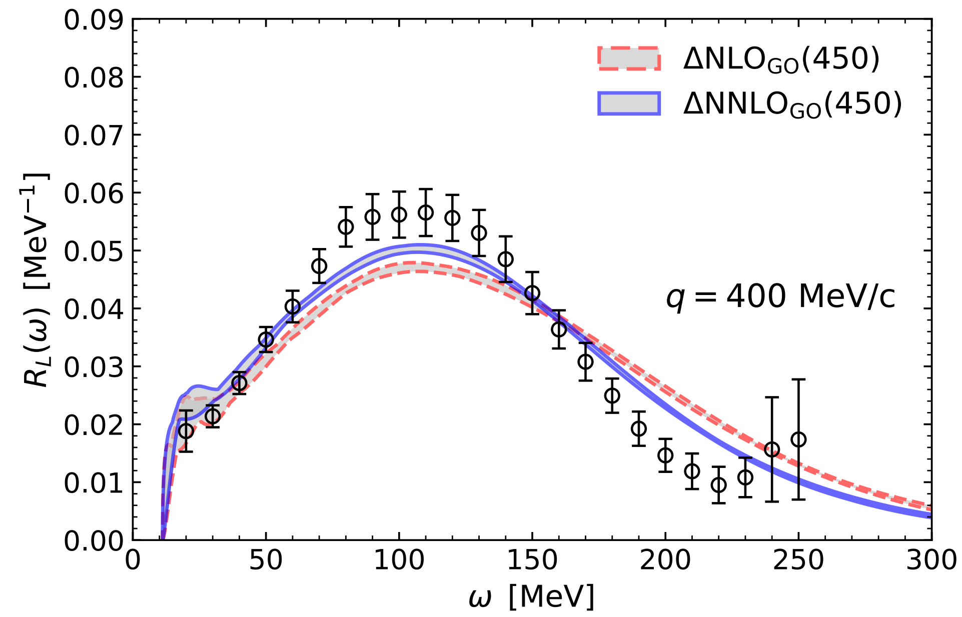
- ✓ CC singles & doubles
- ✓ two different chiral Hamiltonians
- ✓ *inversion procedure*

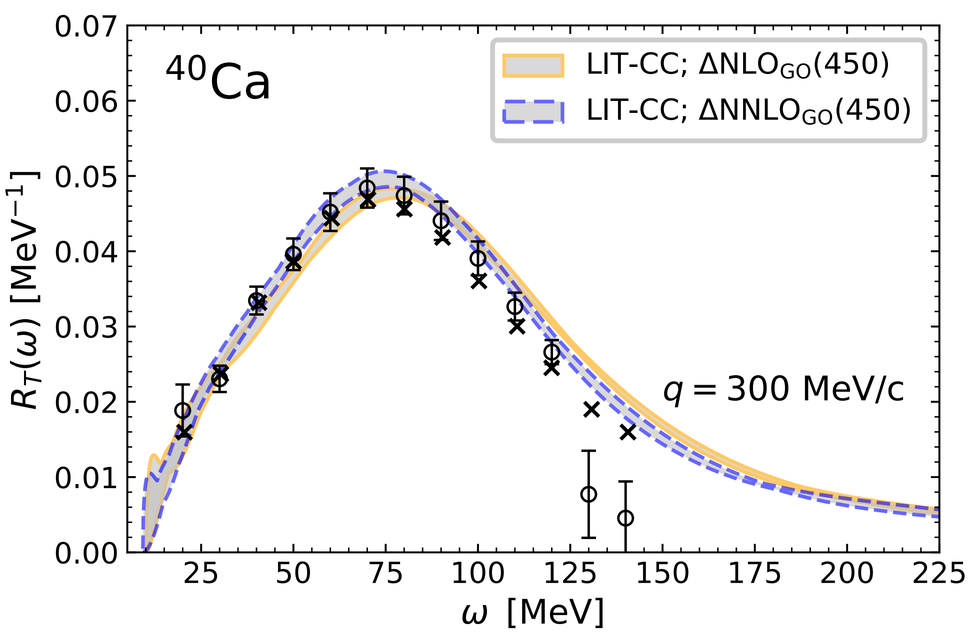
JES, B. Acharya, S. Bacca, G. Hagen; *PRL* 127 (2021) 7, 072501
JES, B. Acharya, S. Bacca, G. Hagen; arXiV: 2310.03109

Chiral expansion for ^{40}Ca

(Electromagnetic responses)







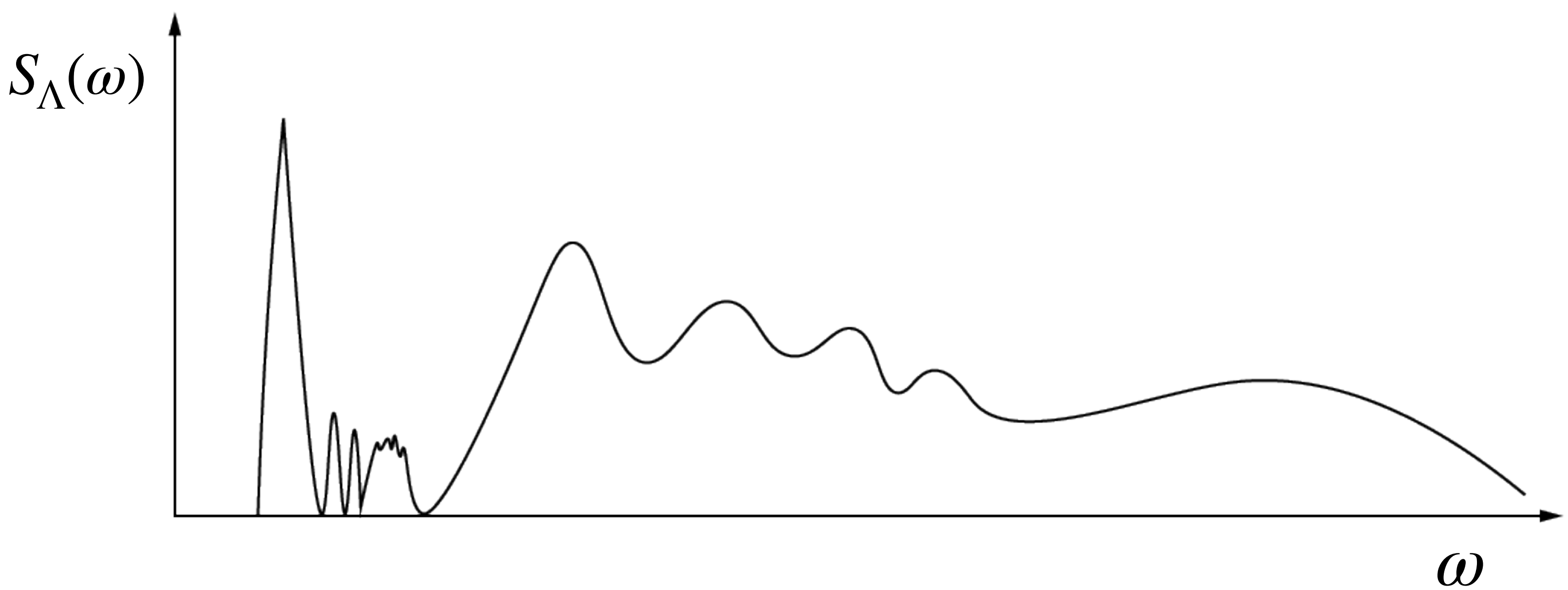
- ✓ Two orders of chiral expansion
- ✓ Convergence better for lower q (as expected)
- ✓ Higher order brings results closer to the data

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

JES, B. Acharya, S. Bacca, G. Hagen; arXiV: 2310.03109

ChEK method

Chebyshev Expansion of integral Kernel



Integral transform

$$S_\Lambda(\omega') = \int K_\Lambda(\omega', \omega) R(\omega) d\omega$$

Gaussian, Lorentzian, etc.

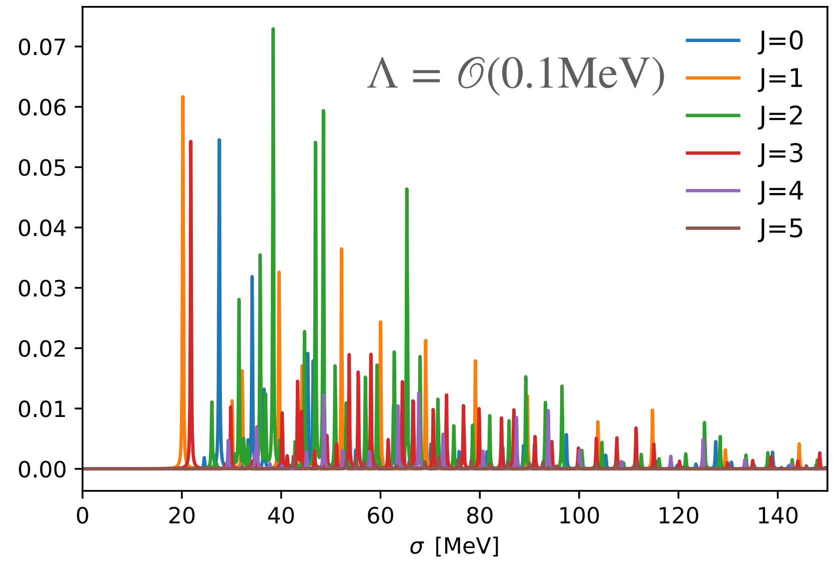
expansion in Chebyshev polynomials

$$K_\Lambda(\omega, \sigma) = \sum_k c_k(\sigma) T_k(\omega)$$

A. Roggero Phys.Rev.A 102 (2020) 2, 022409
JES, A. Roggero Phys.Rev.E 105 (2022) 055310

Histograms using ChEK

Integral transform expanded in Chebyshev polynomials

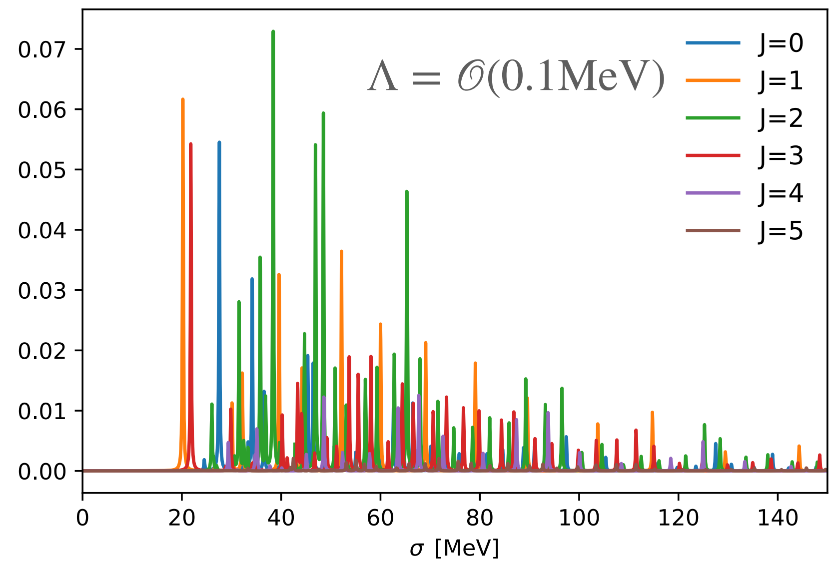


$$\Phi \approx \tilde{\Phi} = \int f(\omega') \int K_\Lambda(\omega', \omega) R(\omega) d\omega d\omega'$$

- Sum-rules
- Flux folding
- Histogram
- ...

Histograms using ChEK

Integral transform expanded in Chebyshev polynomials

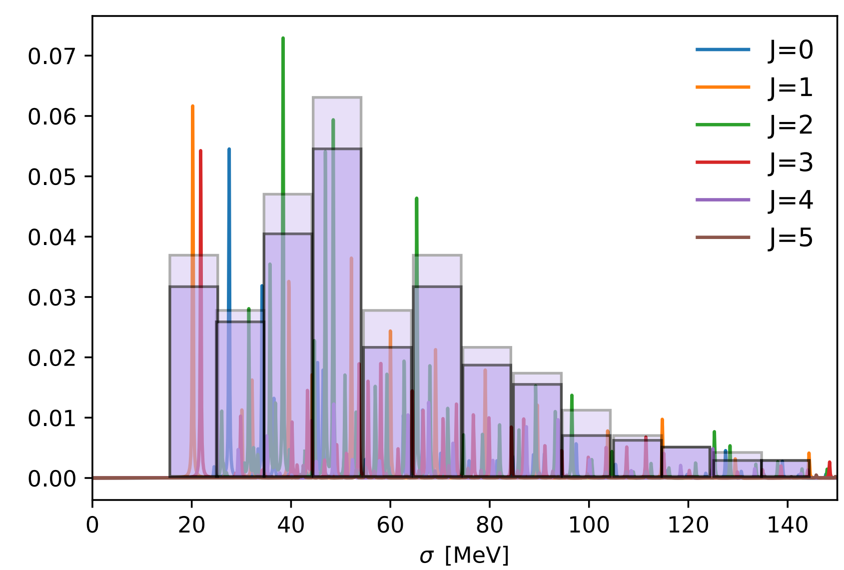


$$\Phi \approx \tilde{\Phi} = \int f(\omega') \int K_\Lambda(\omega', \omega) R(\omega) d\omega d\omega'$$

- Sum-rules
- Flux folding
- Histogram
- ...

Build histogram

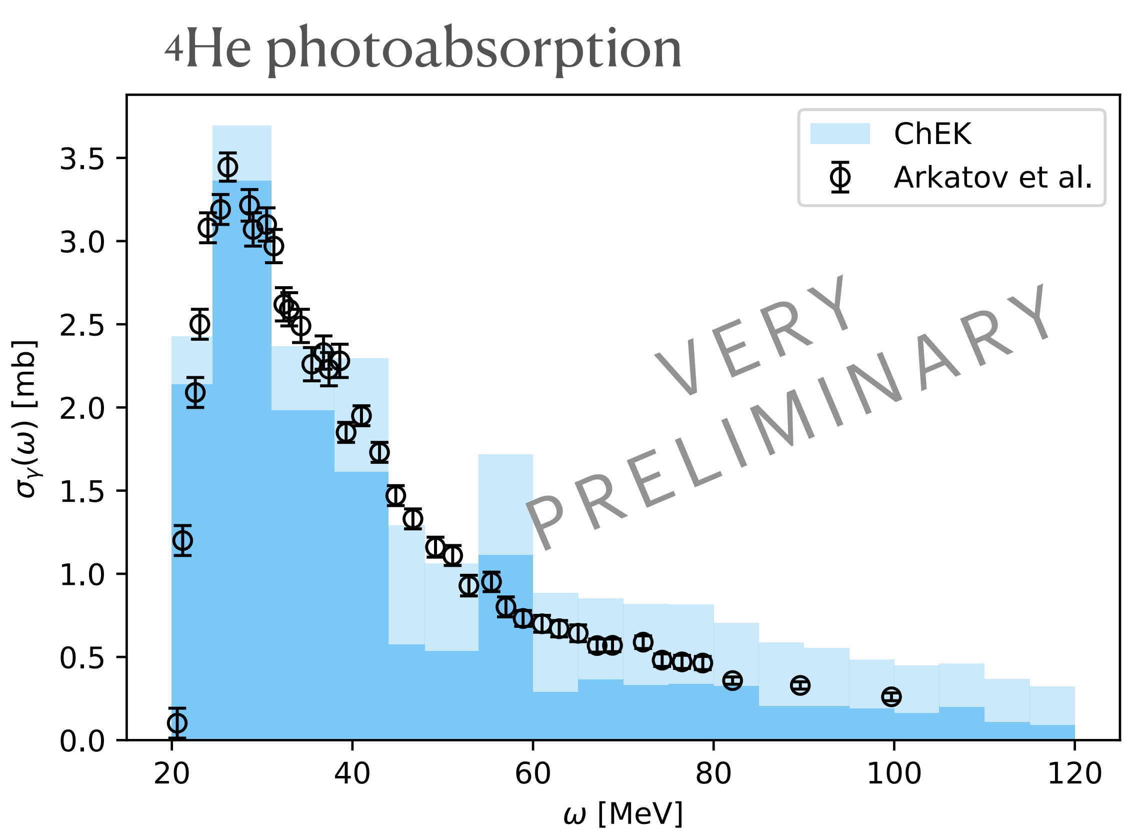
$$\Phi = \int f(\omega) R(\omega) d\omega$$

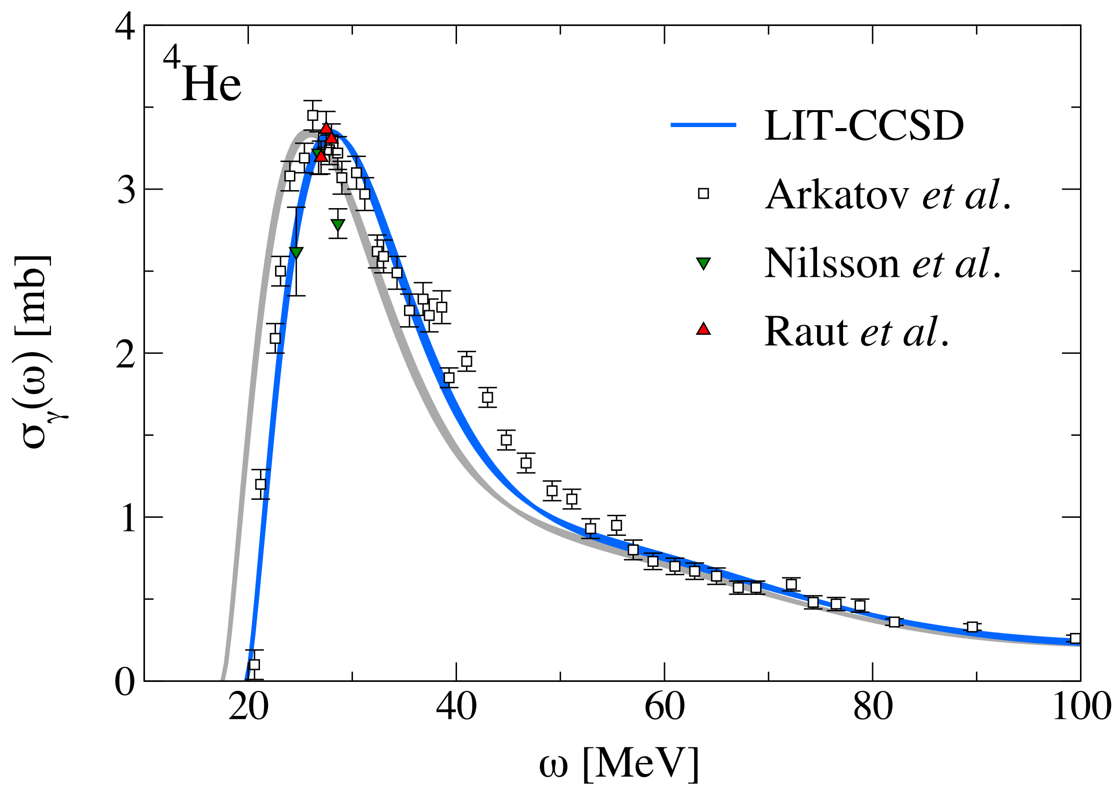


estimated error $|\Phi - \tilde{\Phi}| < \epsilon$

ChEK method

Chebyshev Expansion of integral Kernel





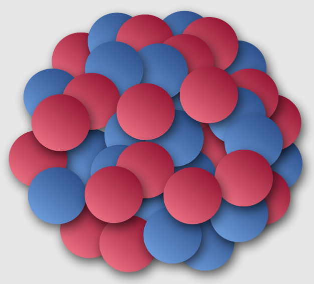
S. Bacca, N. Barnea, G. Hagen, G. Orlandini; *Phys.Rev.C* 90 (2014) 6

➡ No assumption about the shape of the response

➡ Rigorous error estimation

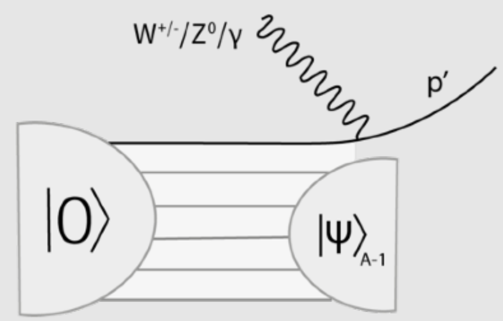
➡ Convenient when the response has a complicated structure

Low/high energies

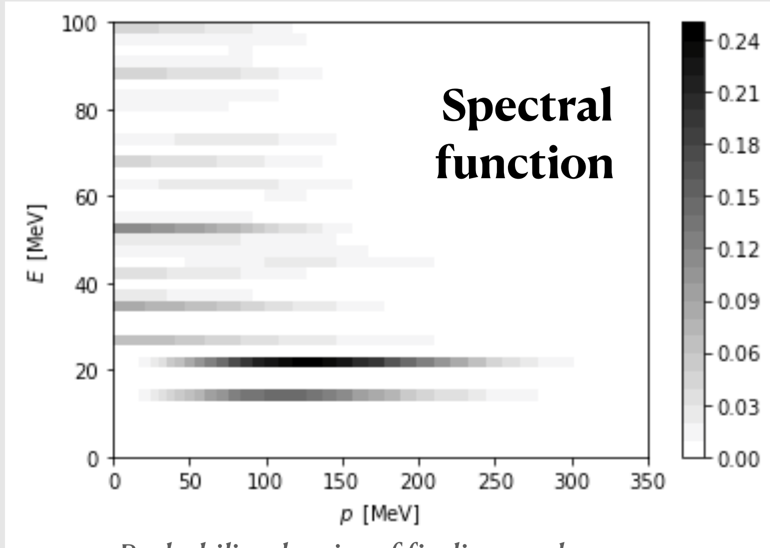


$$\hat{H}|\psi_A\rangle = E|\psi_A\rangle$$

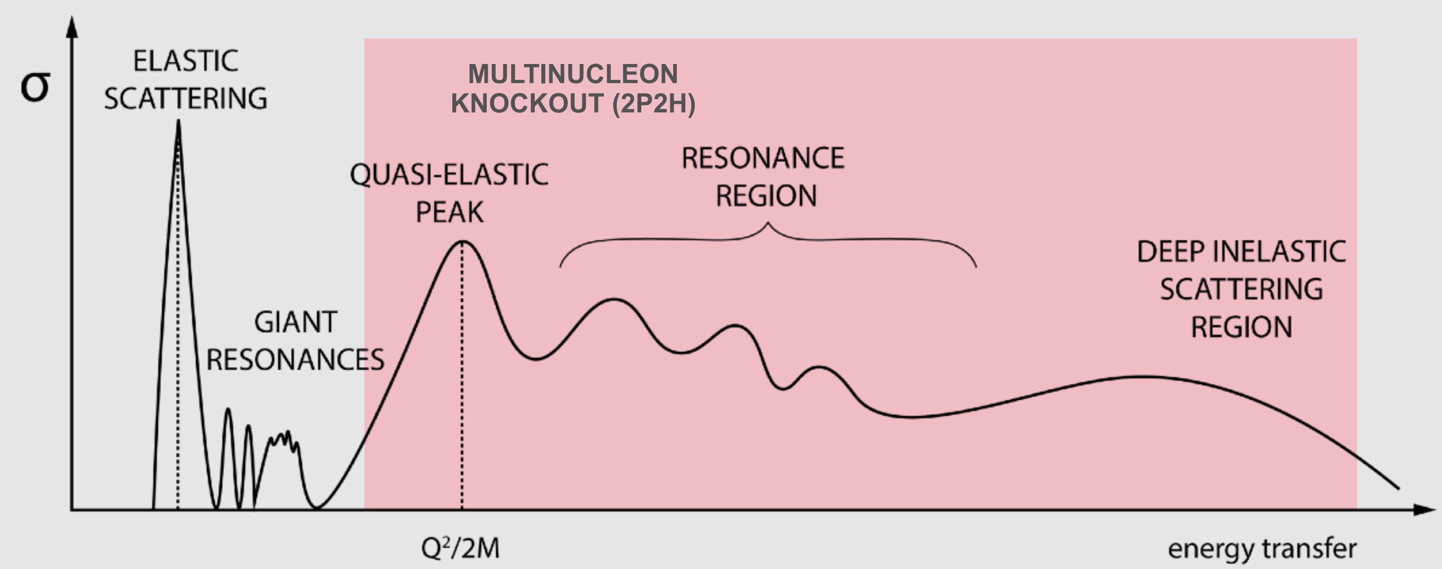
Many-body problem



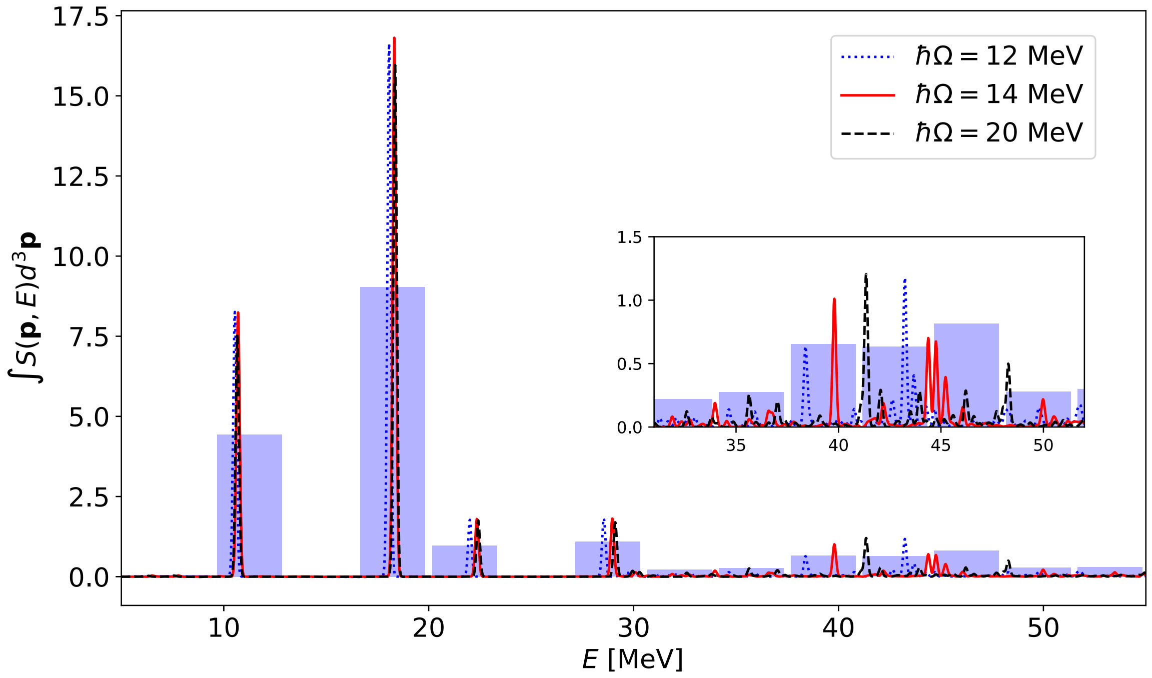
Impulse Approximation



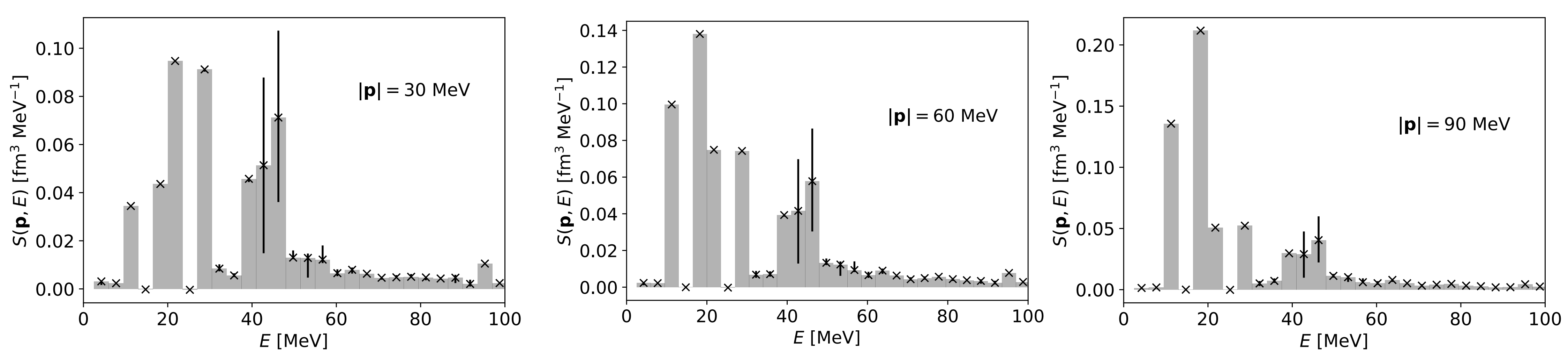
Probability density of finding nucleon $(E, \mathbf{p})$ *in ground state nucleus*



^{16}O spectral function

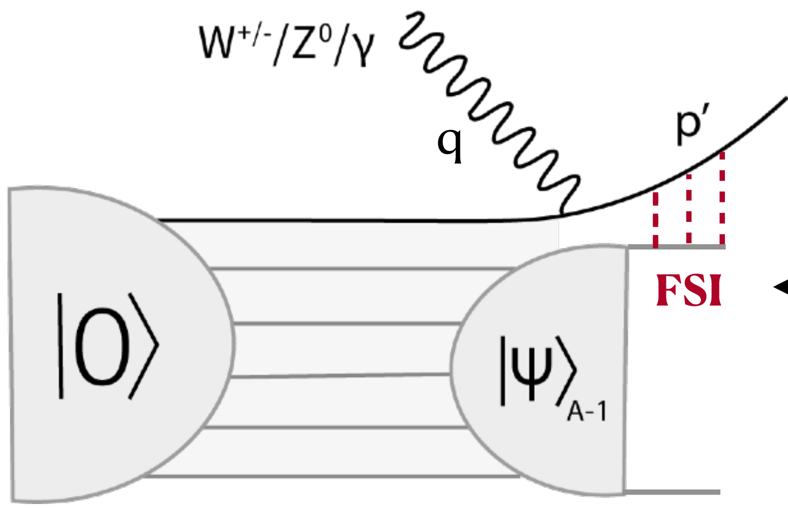


- Spectral reconstruction using expansion in Chebyshev polynomials + building histograms
- Uncertainty sources:
  - ✓ $K(\omega, \sigma) = \sum_{k=0}^{N} c_k(\sigma) T_k(\omega)$
  - ✓ Kernel's width Λ



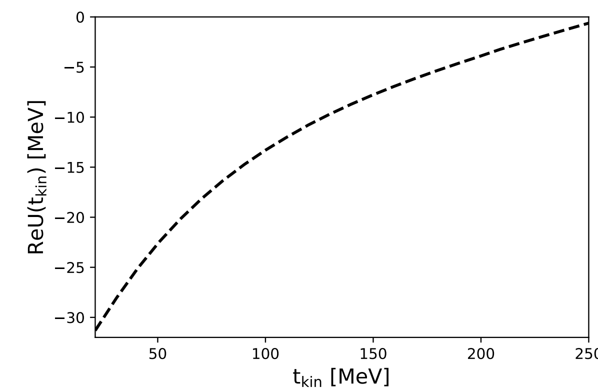
^{16}O spectral function

Error propagation to cross sections



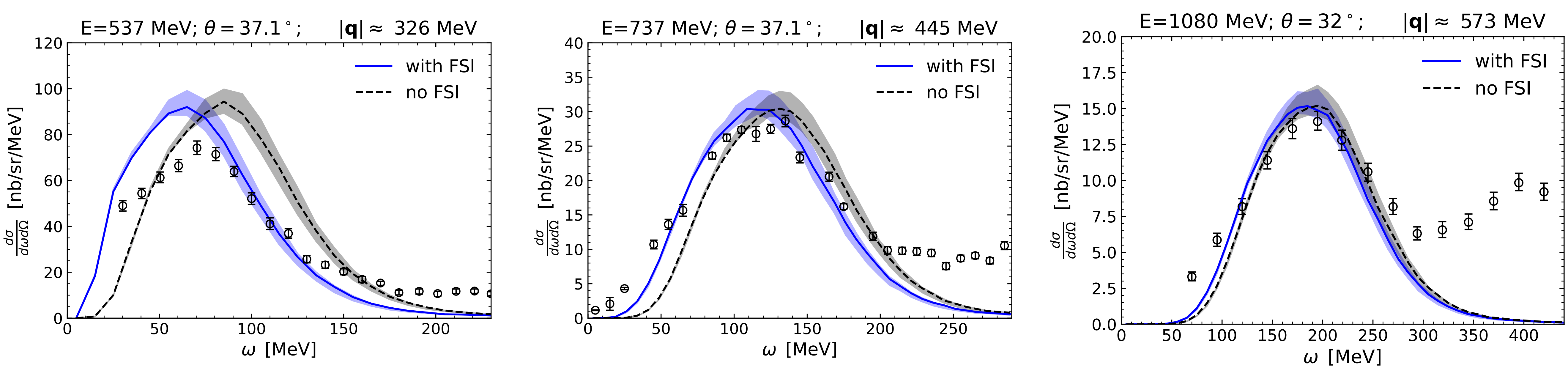
Phenomenological optical potential

$$E_{p+q} \rightarrow E_{p+q} + \mathrm{Re}U(t_{kin})$$



E. D. Cooper et al. *Phys.Rev.C 47, 297–311*

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



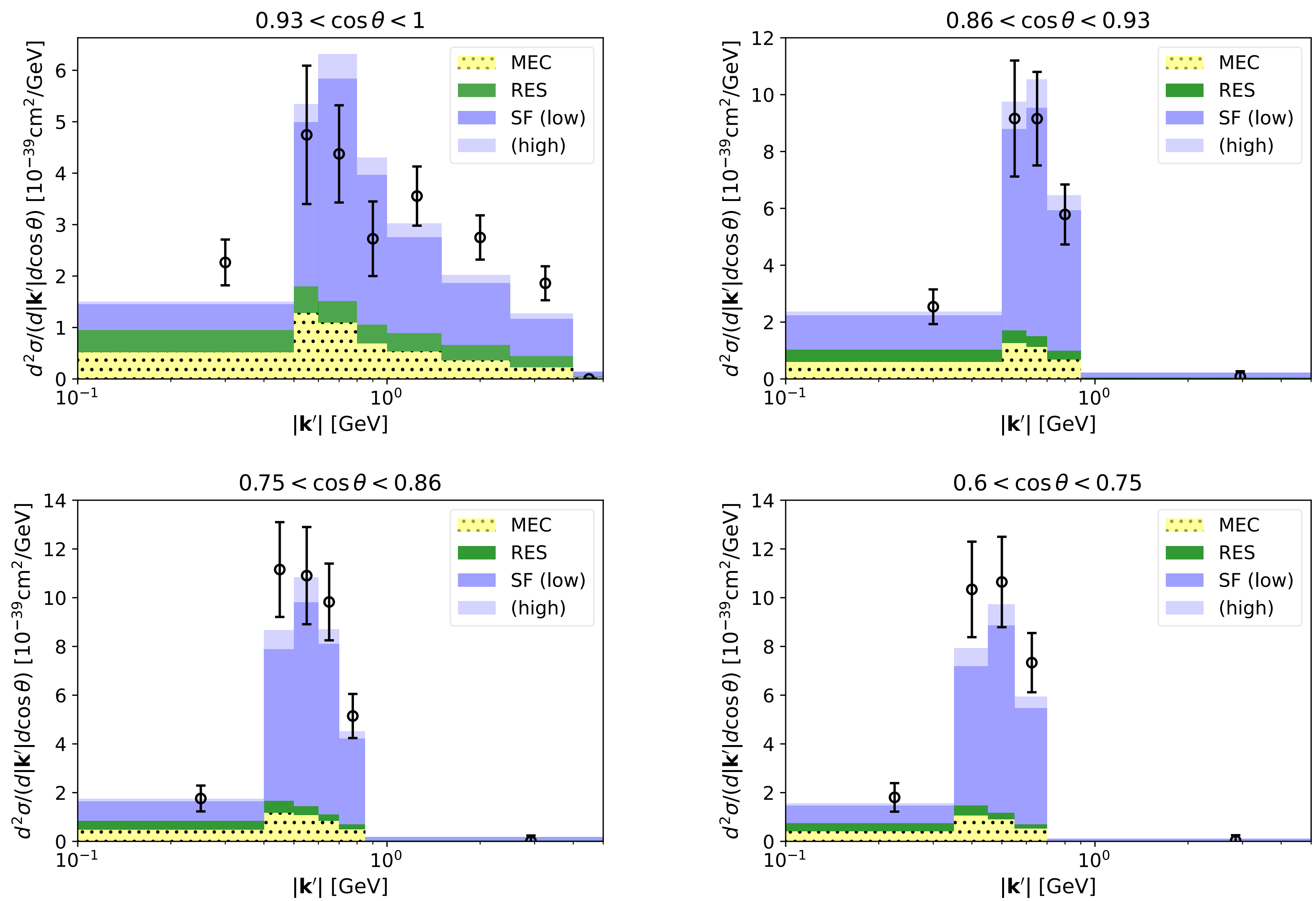
^{16}O spectral function

Error propagation to cross sections

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

- Comparison with T2K long baseline ν oscillation experiment
- CC0π events
- Spectral function implemented into NuWro Monte Carlo generator

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



JES , S. Bacca arXiv:2309.00355

Robust uncertainty quantification

ARTICLES
https://doi.org/10.1038/s41567-022-01715-8
nature physics

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

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- **Bayesian inference**: explore the space of 17 low energy constants of nuclear Hamiltonian

$$\mathrm{pr}(\theta \,|\, D) \propto \mathcal{L}(\theta)\mathrm{pr}(\theta)$$

Posterior probability density function

Likelihood $\mathcal{L}(\theta) \equiv \mathrm{pr}(D \,|\, \theta)$

- posterior predictive distributions

$$\{y(\theta) : \theta \sim \mathrm{pr}(\theta \,|\, D)\}$$

Robust uncertainty quantification

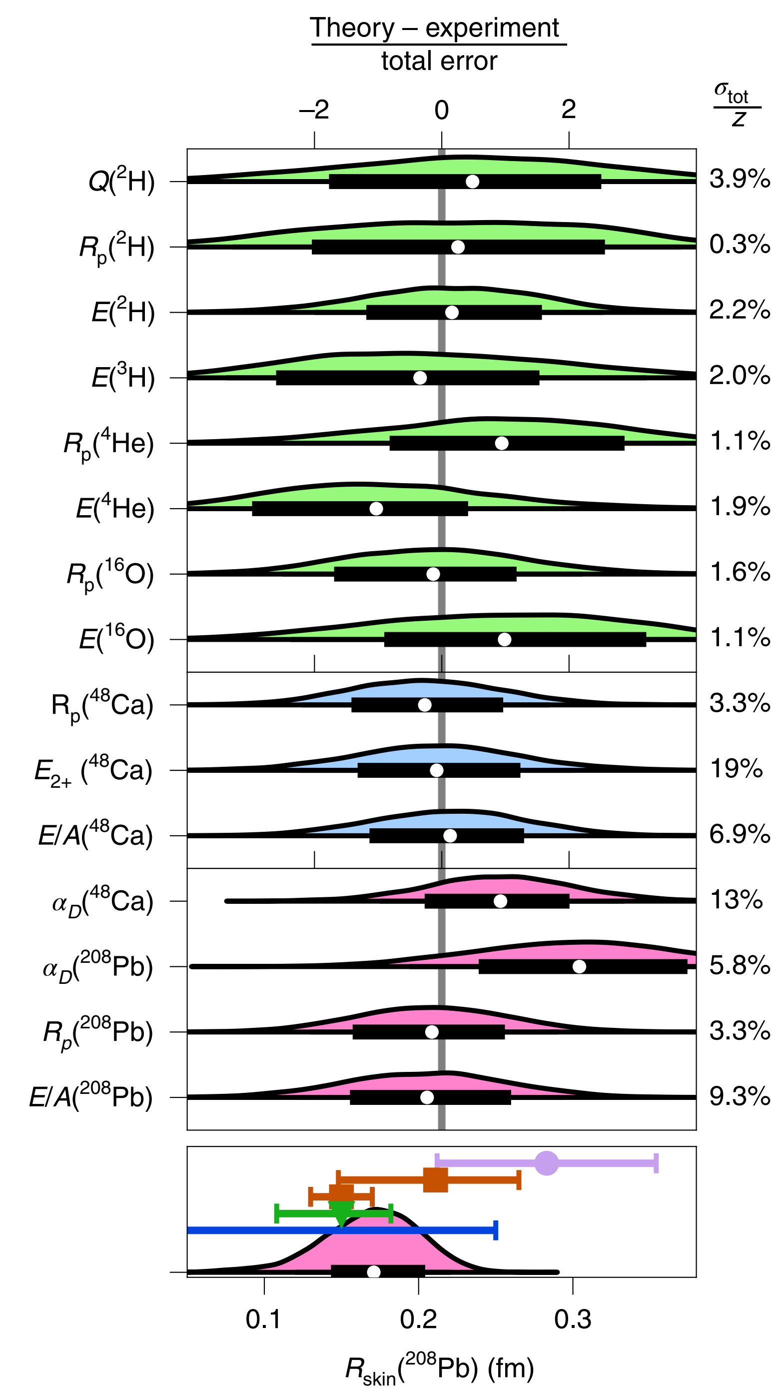
Various sources of uncertainty taken into account

$$y = y_k + \epsilon_{\text{method}} + \epsilon_{\text{model}}$$

$$y_{\text{ref}} \left(\sum_{i=0}^{k} c_i Q^i + \sum_{i=k+1}^{\infty} c_i Q^i \right)$$

Truncation error in chiral expansion

Model space truncation, ab initio many-body solver errors



Posterior predictive distributions

Outlook

- Bayesian analysis of nuclear responses
- Spectral reconstruction method (LIT / ChEK)
- Role played by 2-body currents in LIT-CC predictions
- Spectral function (accounting for FSI, 2-body currents)
- Extension of the formalism to ^{40}Ar

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https://indico.mitp.uni-mainz.de/event/357

Thank you for attention!

Backup

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

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

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

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

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

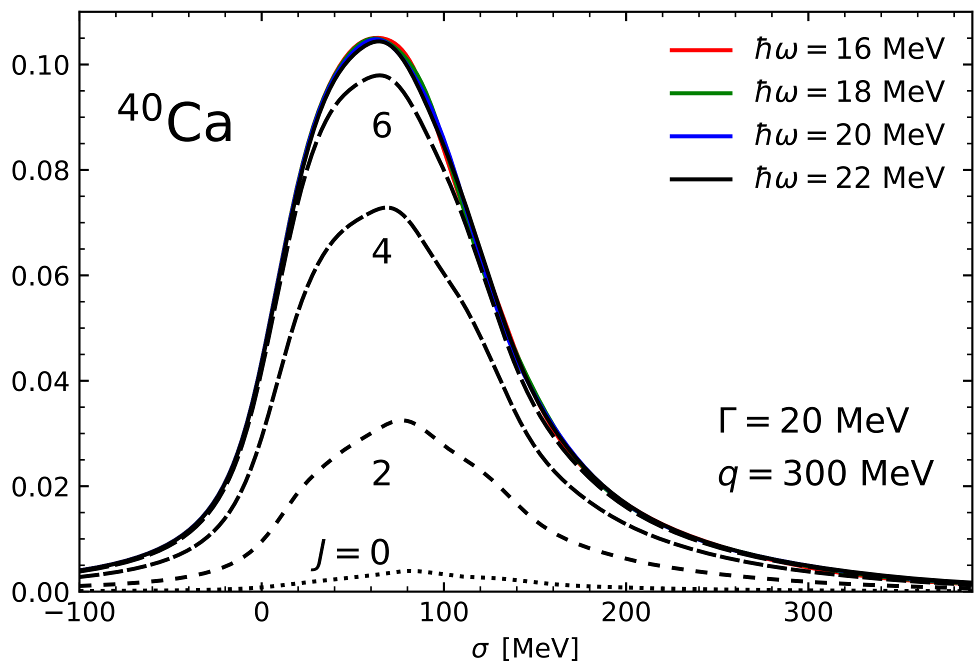
$$\langle \tilde{\Psi} | \qquad\qquad | \tilde{\Psi} \rangle$$

We need to solve

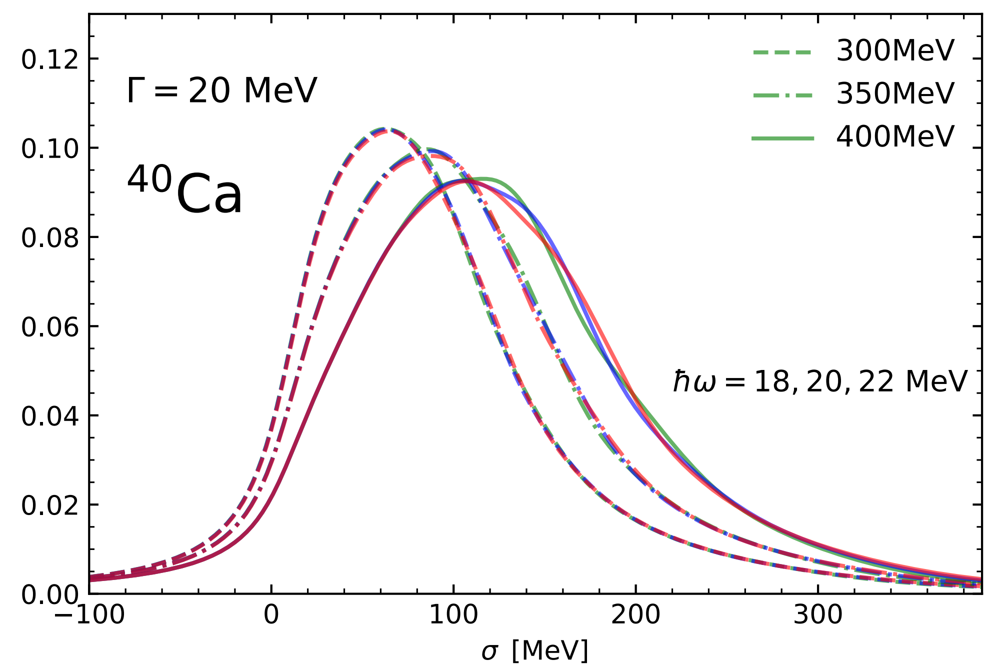
$$(H - E_0 + \tilde{\sigma}) | \tilde{\Psi} \rangle = \rho | \Psi \rangle$$

Schrodinger-like equation

Longitudinal response ^{40}Ca

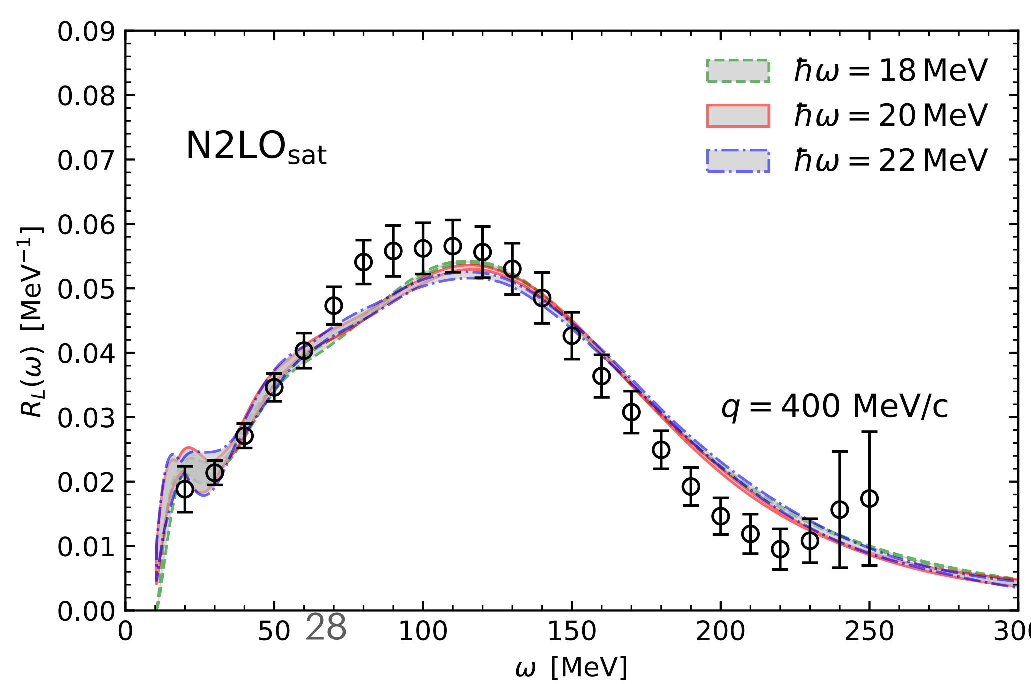


Sum over multipoles



Underlying oscillator frequency

Inversion

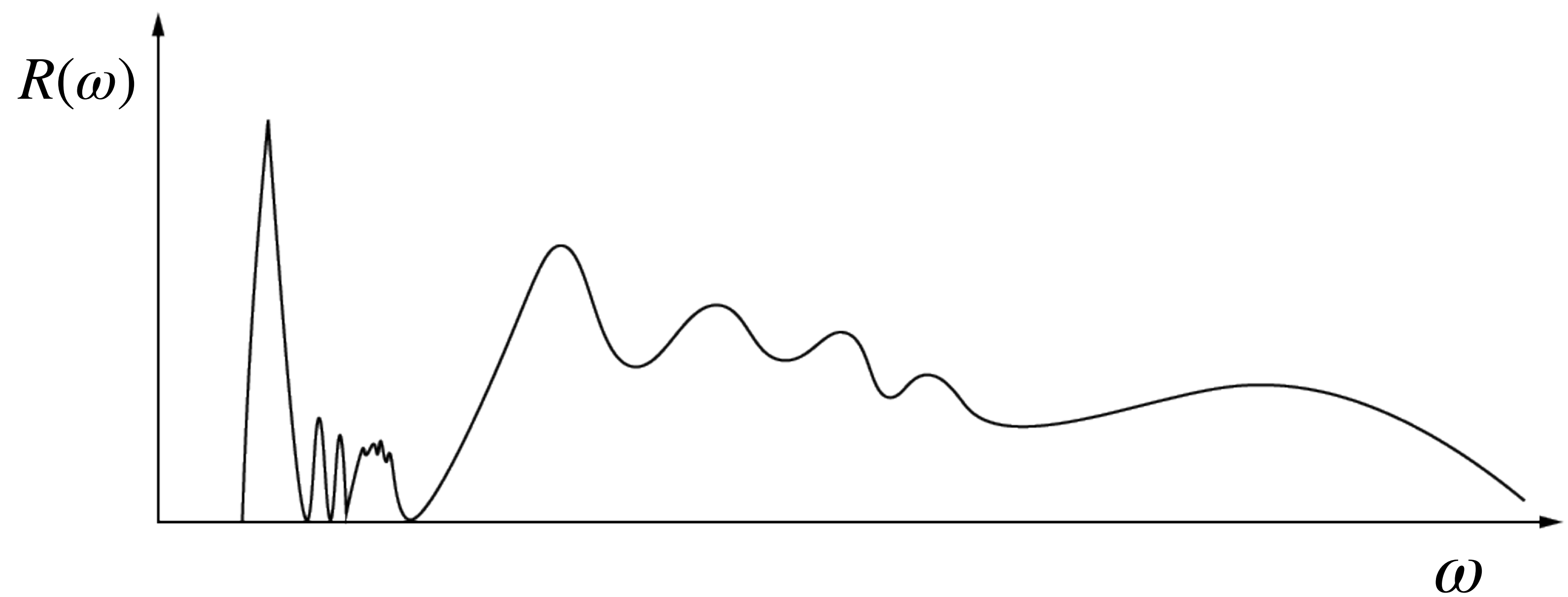


ChEK method

Chebyshev Expansion of integral Kernel

$$\Phi = \int f(\omega) R(\omega) d\omega$$

- Sum-rules
- Flux folding
- Histogram
- ...



$$\Phi \approx \tilde{\Phi} = \int f(\omega') \int K_\Lambda(\omega', \omega) R(\omega) d\omega d\omega'$$

expansion in Chebyshev polynomials $K_\Lambda(\omega, \sigma) = \sum_k c_k(\sigma) T_k(\omega)$

estimated error $|\Phi - \tilde{\Phi}| < \epsilon$

A. Roggero Phys.Rev.A 102 (2020) 2, 022409
JES, A. Roggero Phys.Rev.E 105 (2022) 055310

Nuclear hamiltonian

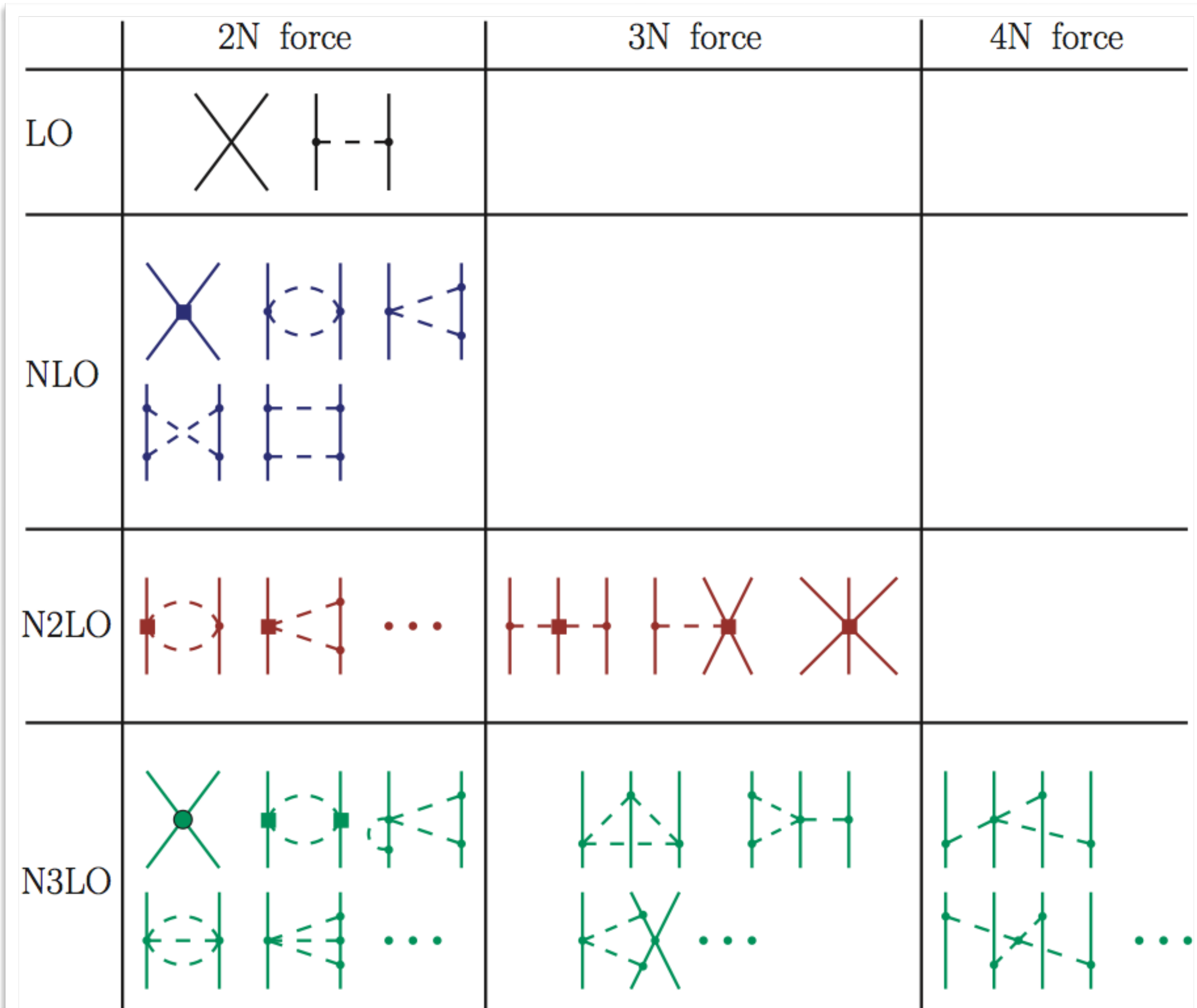
$$\mathscr{H} = \sum_i \frac{p_i^2}{2m} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk} + \dots$$

$n = 0$

$n = 2$

$n = 3$

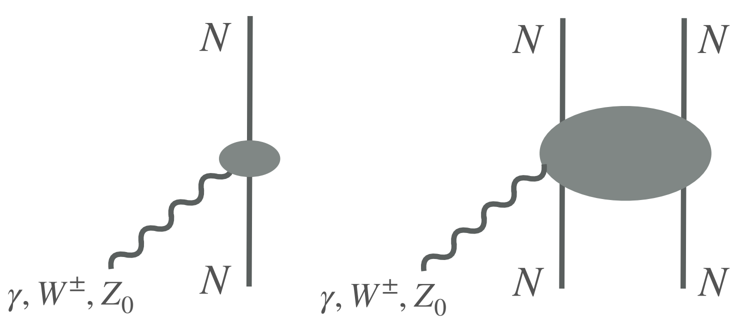
$n = 4$



- ✓ Chiral Hamiltonians exploiting chiral symmetry (QCD); $\pi, N, (\Delta)$ degrees of freedom
- ✓ counting scheme in $\left(\frac{Q}{\Lambda}\right)^n$
- ✓ low energy constants (LEC) fit to data
- ✓ uncertainty assessment

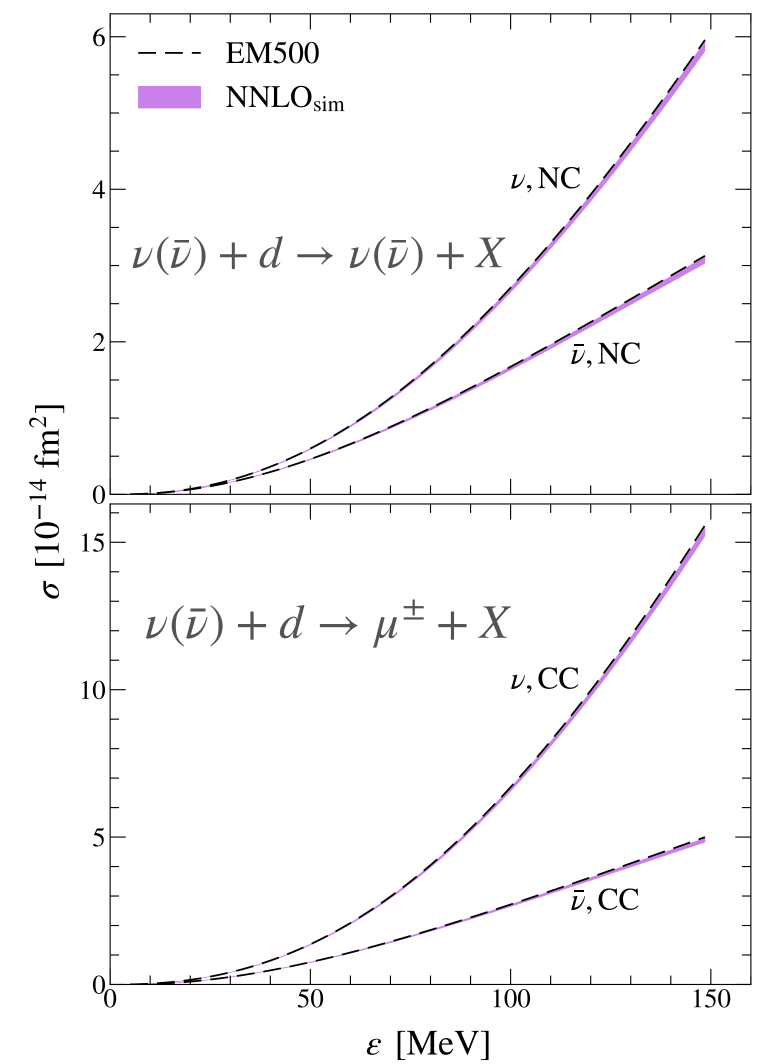
Electroweak currents

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



known to give significant contribution for neutrino-nucleus scattering

Current decomposition into multipoles needed for various *ab initio* methods: CC, No Core Shell Model, In-Medium Similarity Renormalization Group



Multipole decomposition for 1- and 2-body EW currents

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