Theoretical uncertainty quantification

Joanna Sobczyk

Measuring neutrino interactions for next-generation oscillation experiments
ECT*, 22 October 2024

Cluster of Excellence PRISMA+ Precision Physics, Fundamental Interactions and Structure of Matter

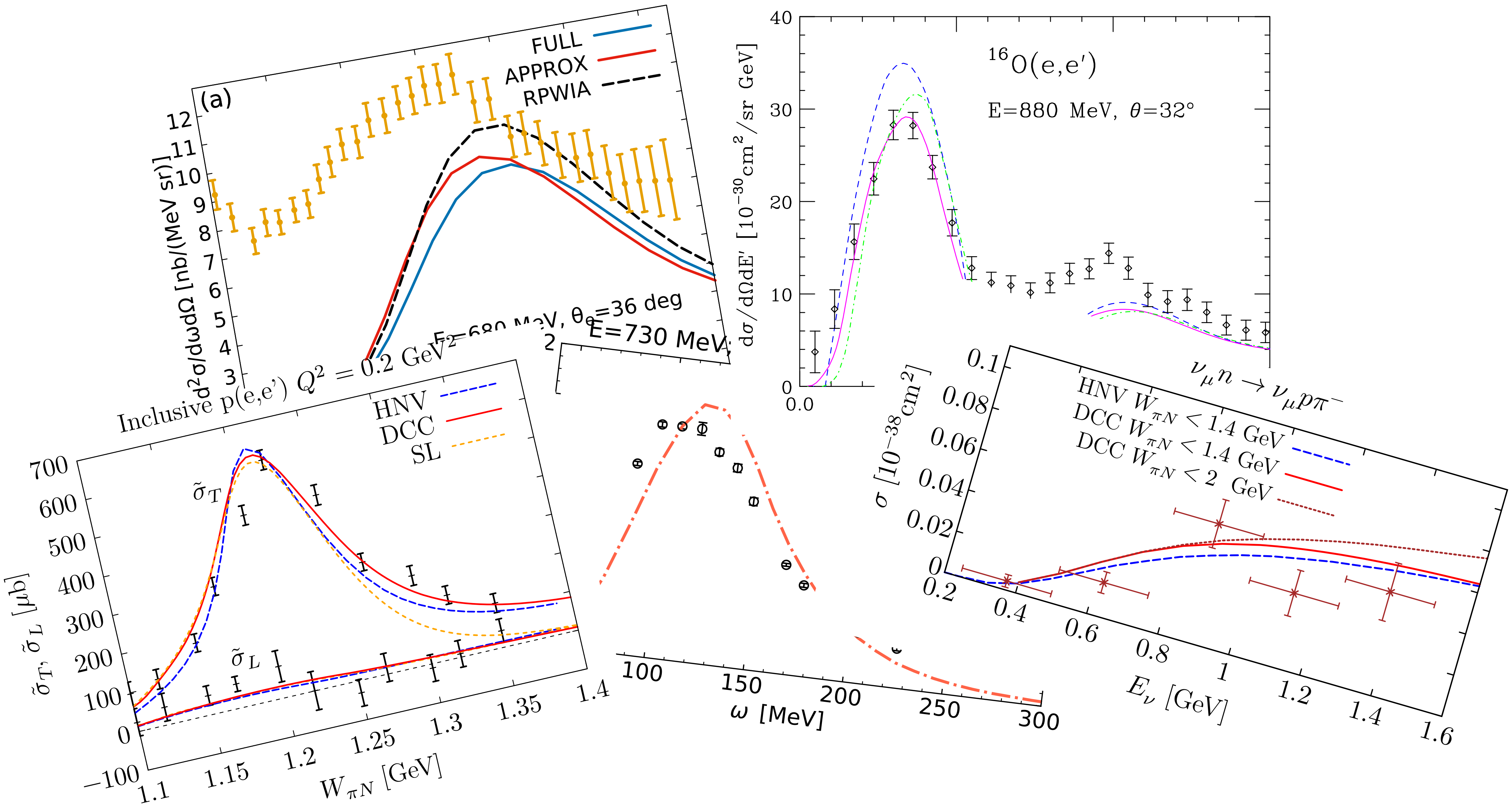
JG|U

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

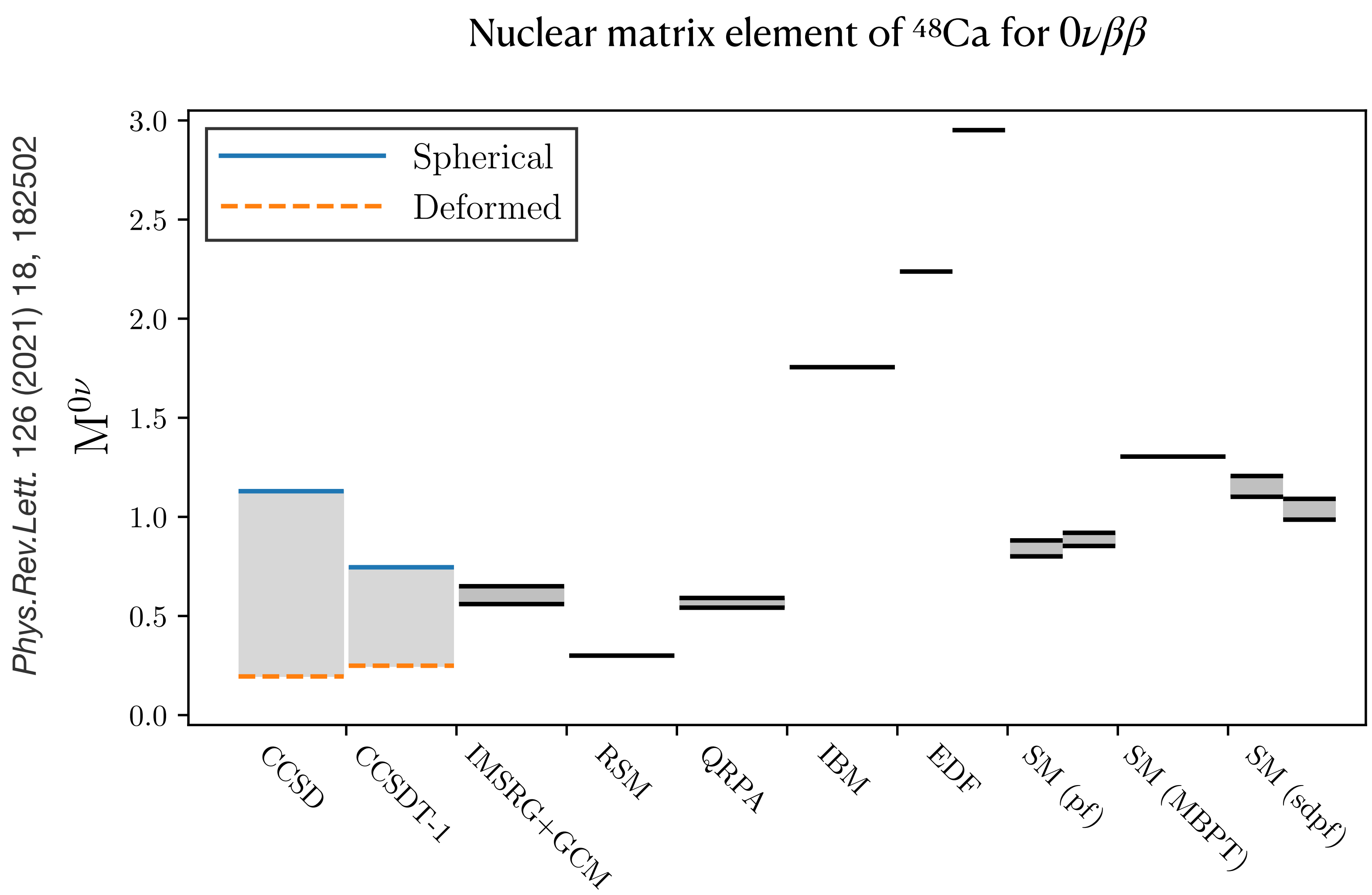


Capturing relevant physics

Small (but estimated) uncertainty

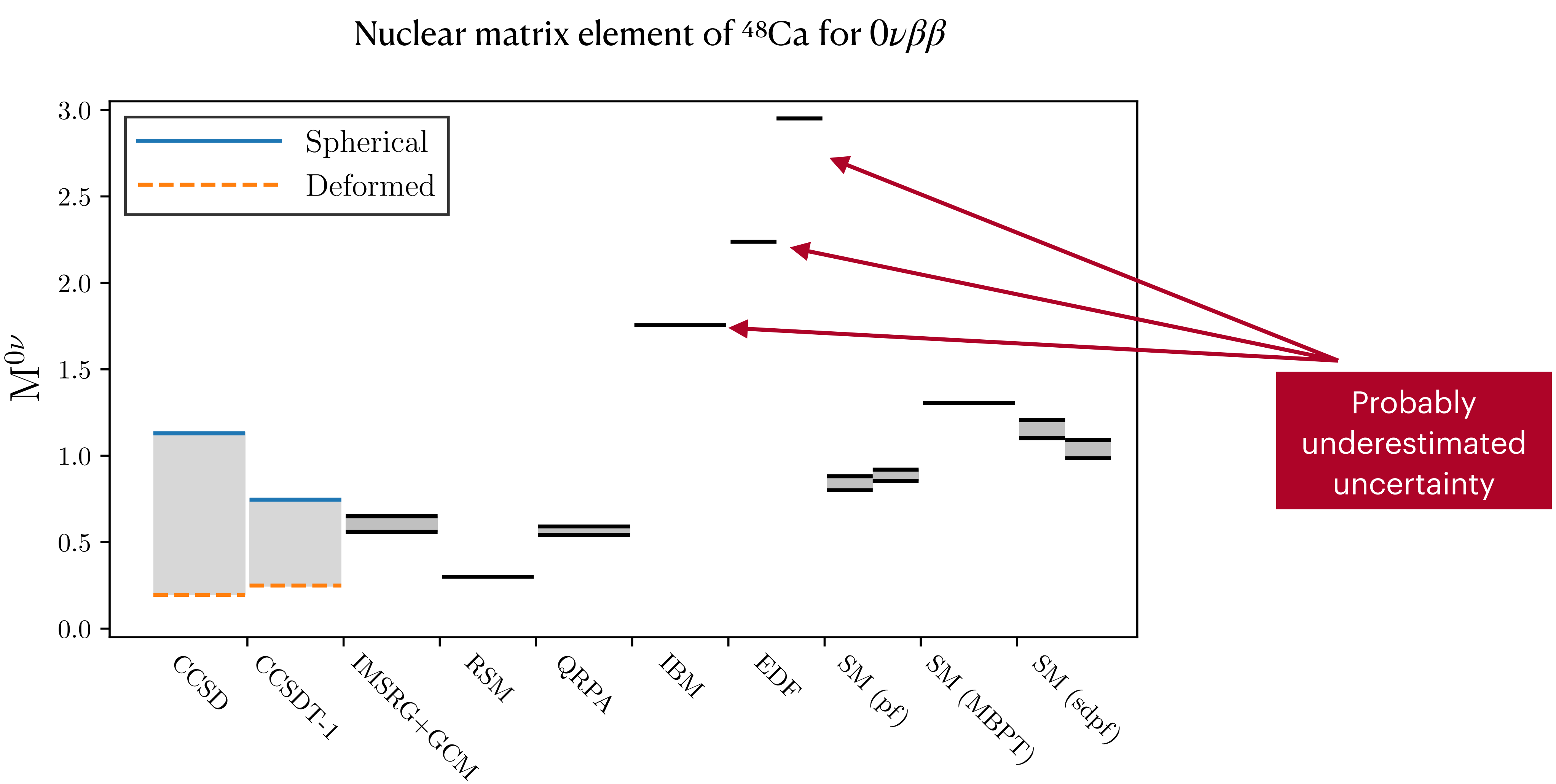
We need **accurate** and **precise** theories

Predictive theories



Predictive theories

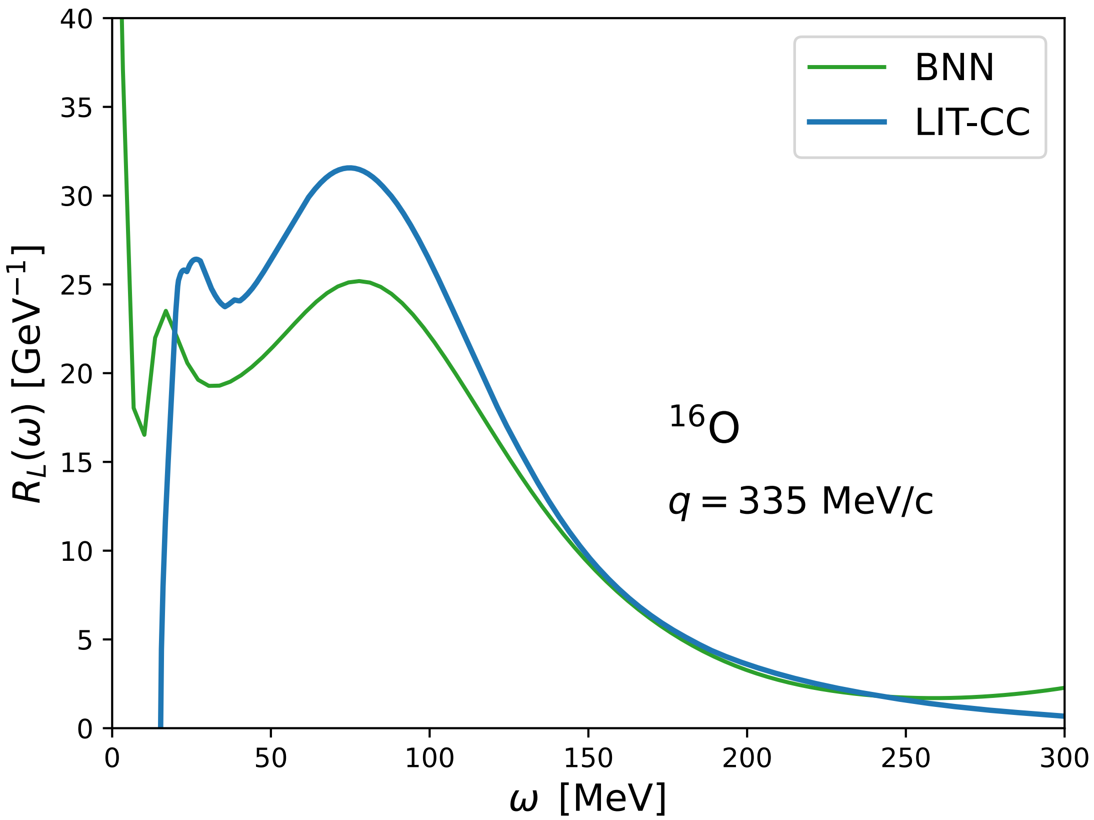
Phys.Rev.Lett. 126 (2021) 18, 182502



Theoretical uncertainty is crucial for predictive models

Predictive theories

What can we learn from estimated uncertainties?



BNN: Bayesian neural network

LIT-CC: ab-initio calculation

B. Acharya, JES, S.Bacca et al. 2410.05962

$$\left.\frac{d\sigma}{dE' d\Omega}\right|_e = \sigma_M \Big(v_L R_L(\omega, \bar{q}) + v_T R_T(\omega, \bar{q}) \Big)$$

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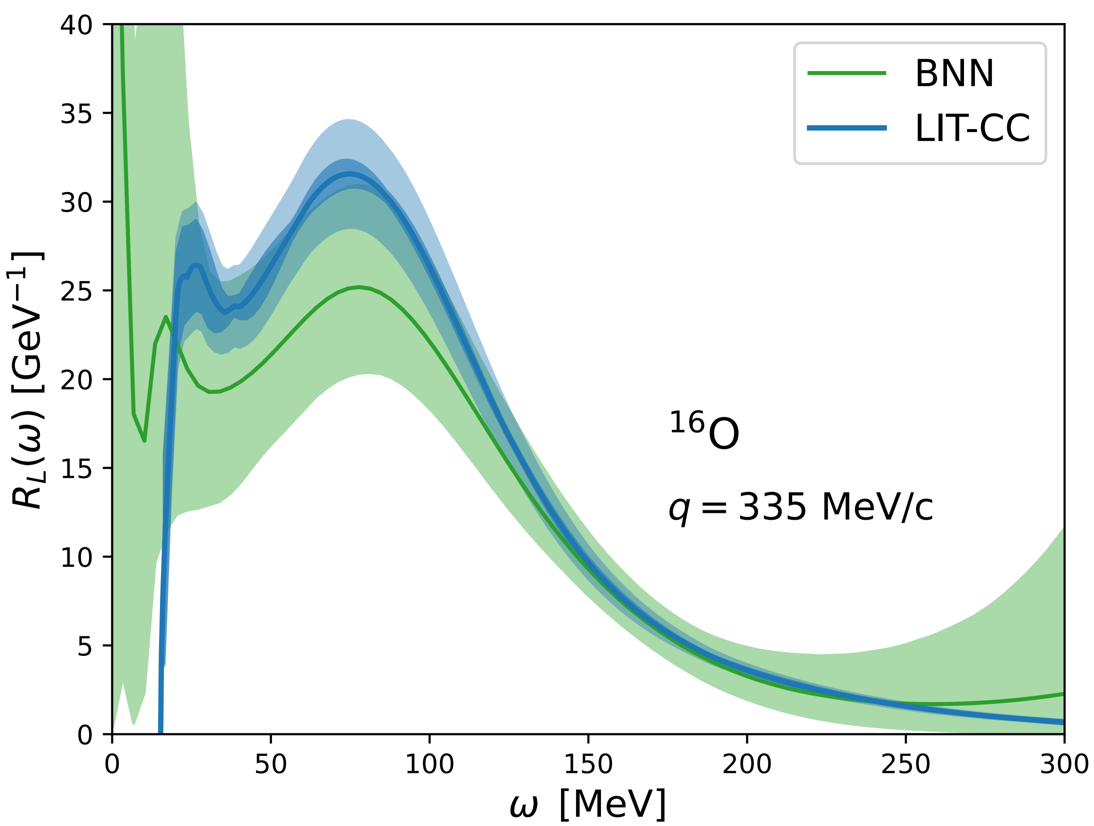

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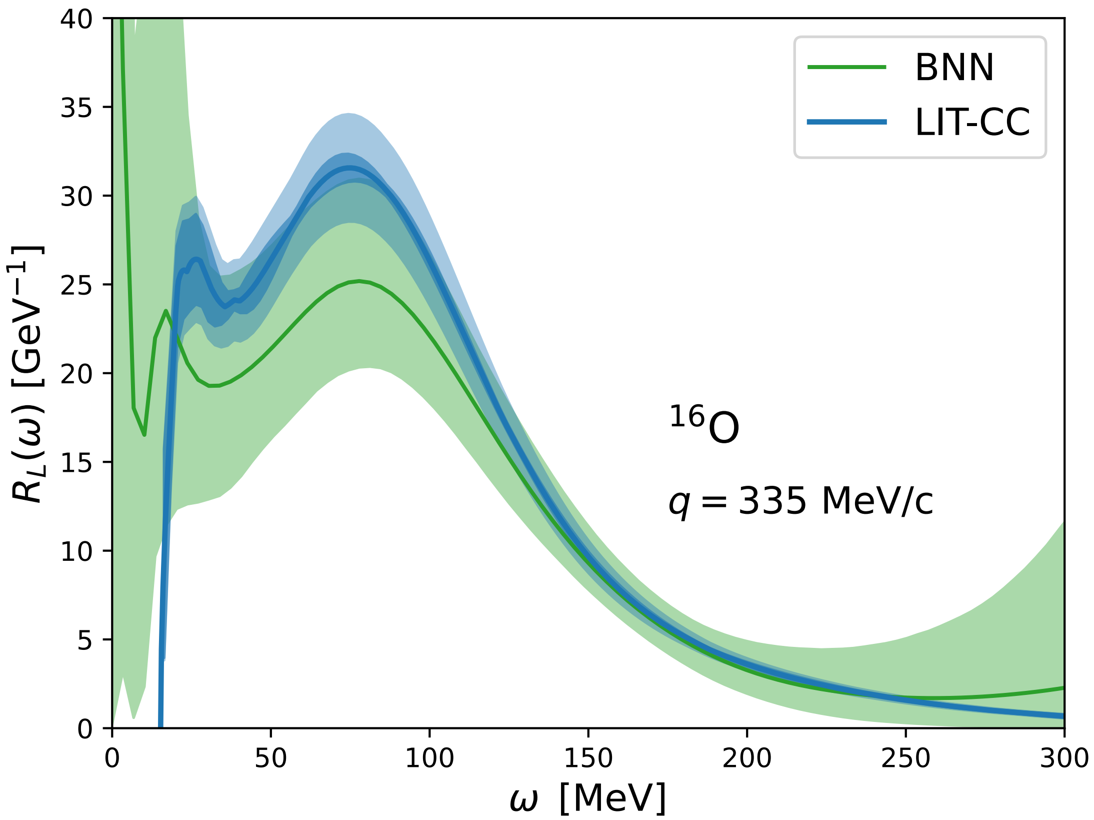

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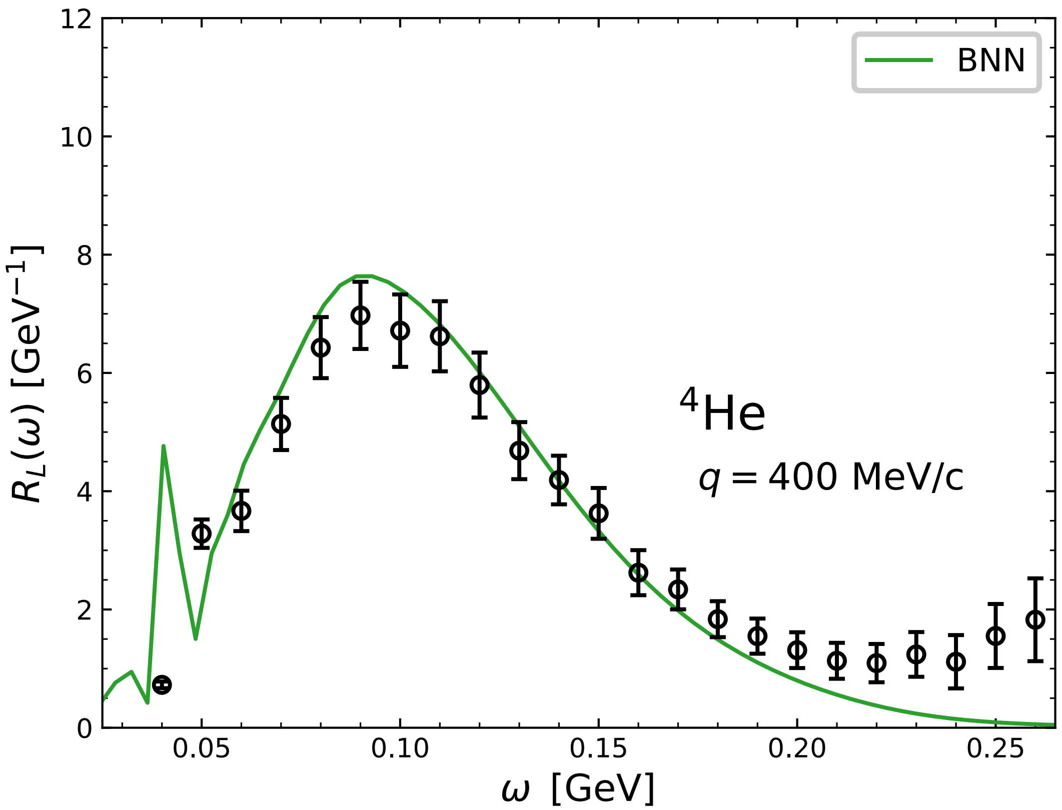

JES, N.Rocco, A.Lovato, 2406.06292

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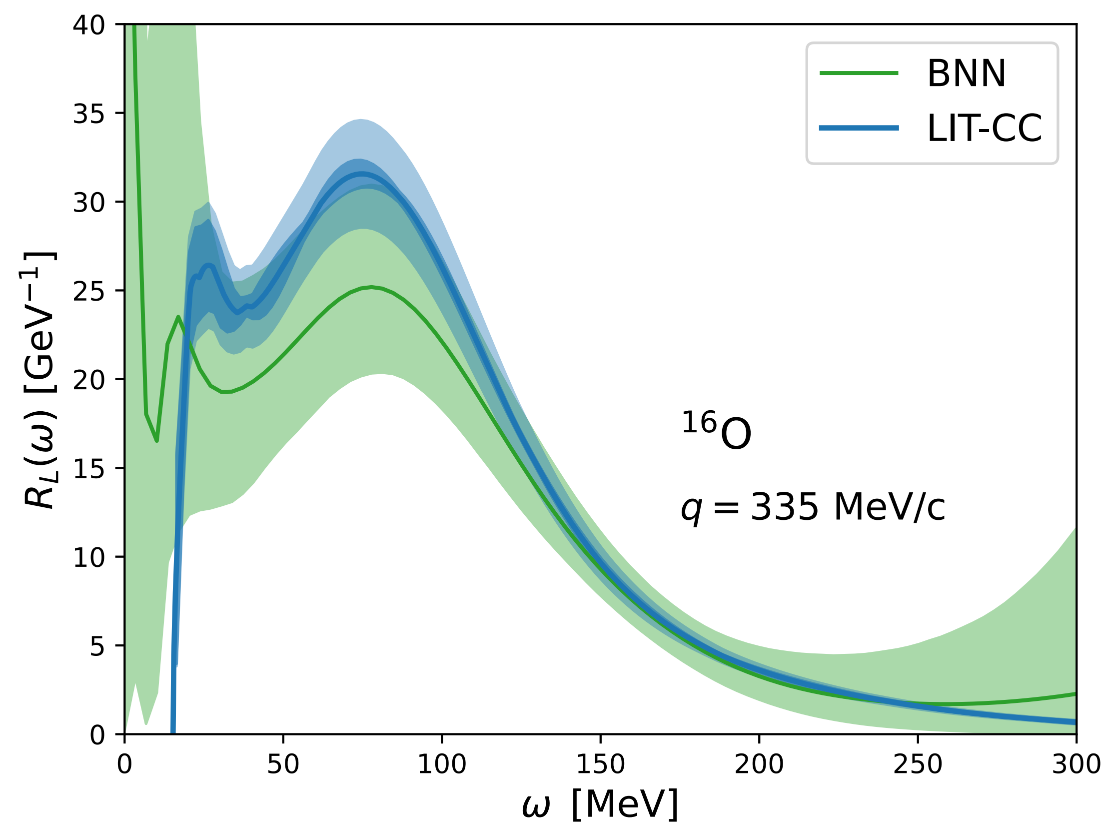

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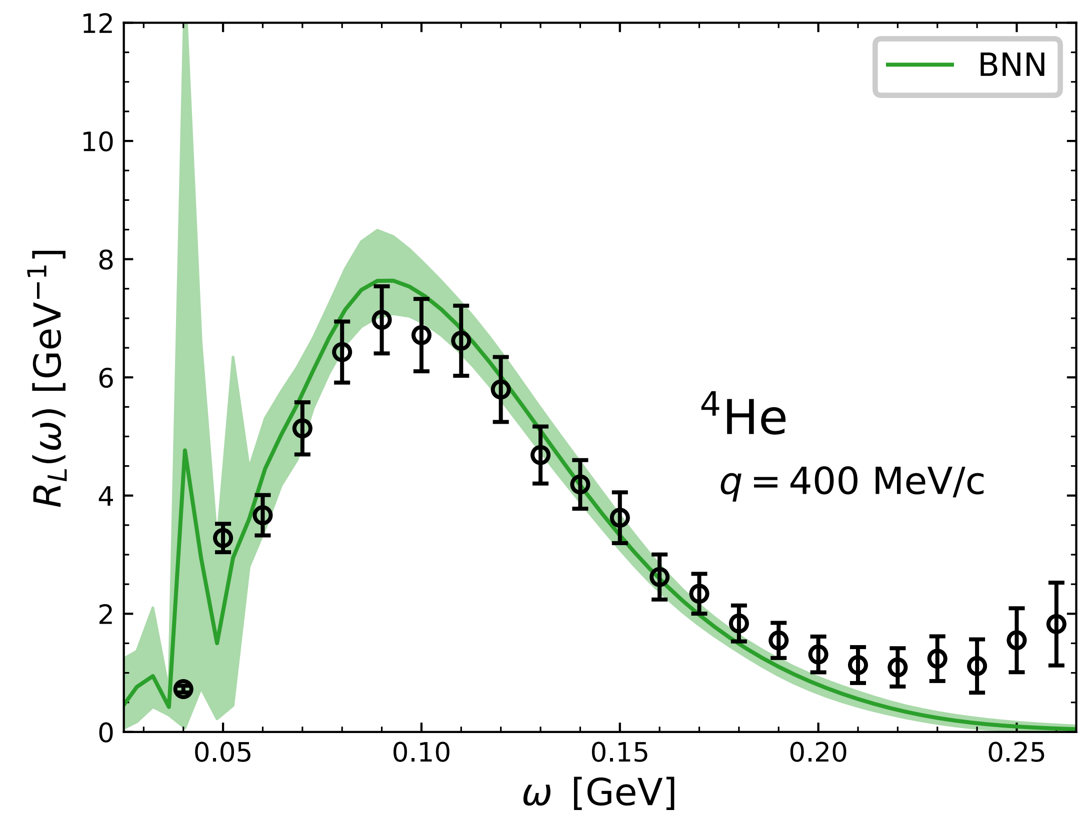

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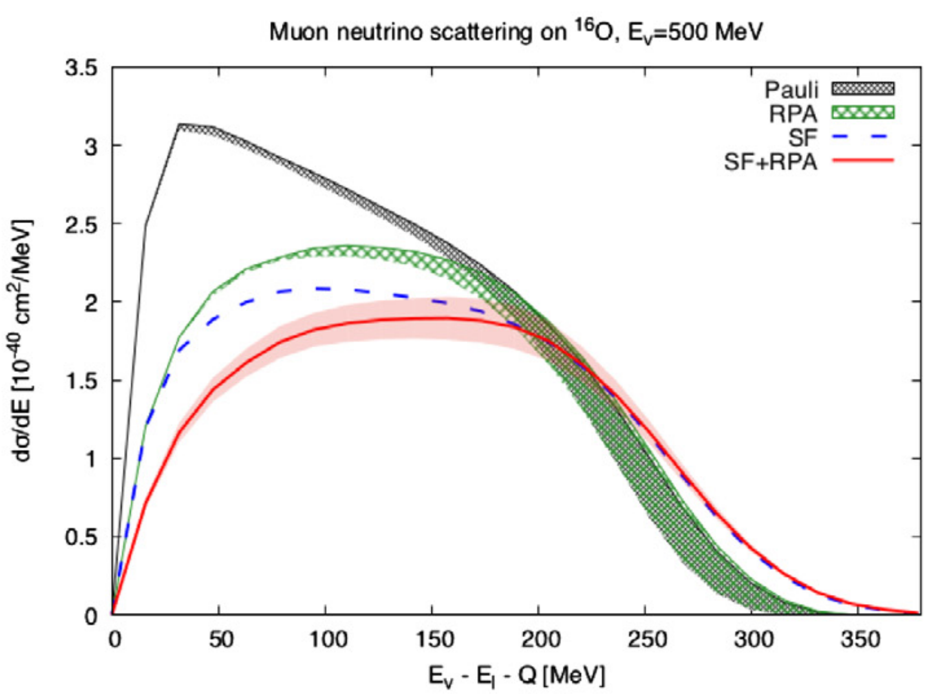
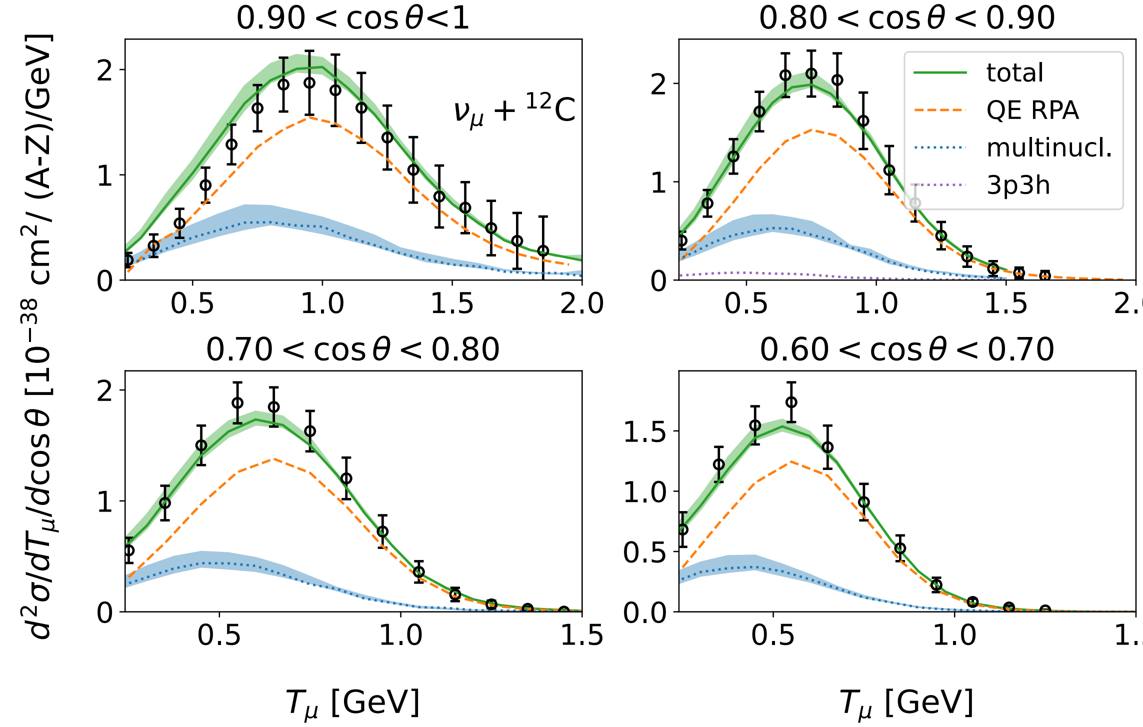
Parametric uncertainties



Variation in RPA parameters (68%CL)



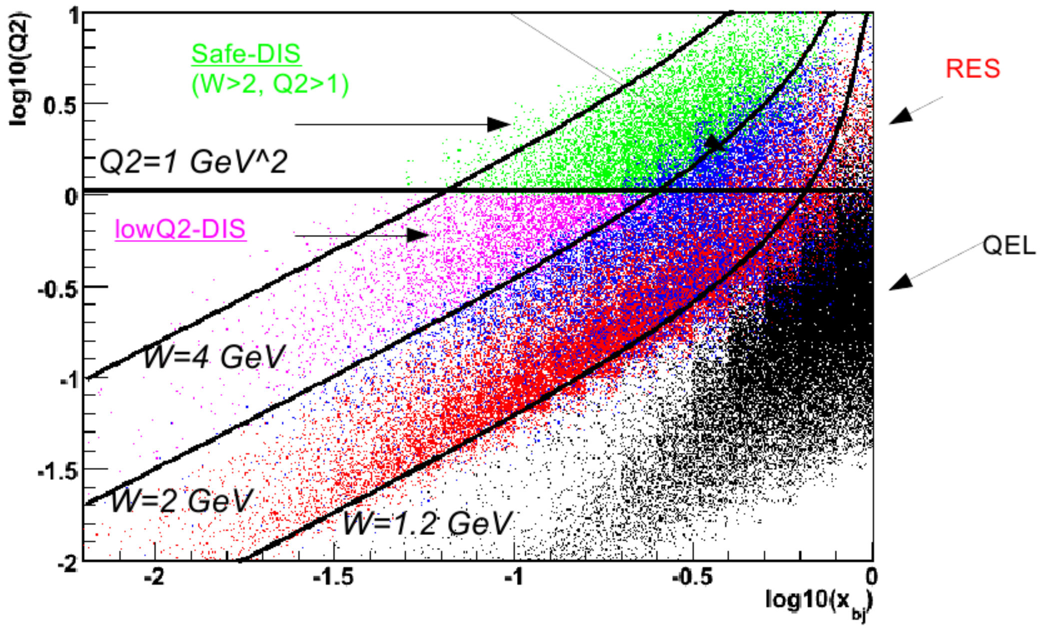
2p2h contribution: uncertainty coming from the Δ treatment

Relatively straightforward to calculate (e.g. assuming Gaussian distribution)

Various parameters: binding energies, Fermi momentum, RPA parameters, parameters of effective interactions…

Model uncertainties

- What is the inherent uncertainty coming from the framework itself (impulse approximation, local density approximation, mean-field, RPA, lack of interference effects...)?
- What is its region of validity (kinematics)?
- Which observables can be described ?

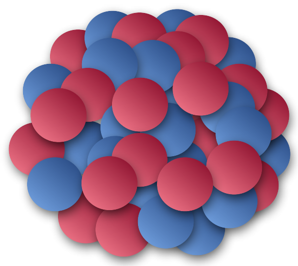


In neutrino oscillation experiments we need various descriptions (models) to cover a large phase-space. How to "stitch" them?

Optimistic example

“Ab initio” nuclear theory

nucleons — degrees of freedom



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

$$\mathscr{H} = \sum_{i=1}^{A} t_{kin} + \sum_{i>j=1}^{A} v_{ij} + \sum_{i>j>k=1}^{A} v_{ijk} + \ldots$$

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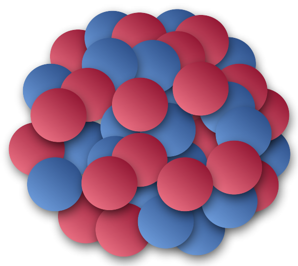

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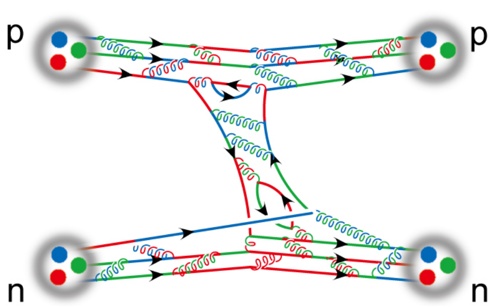
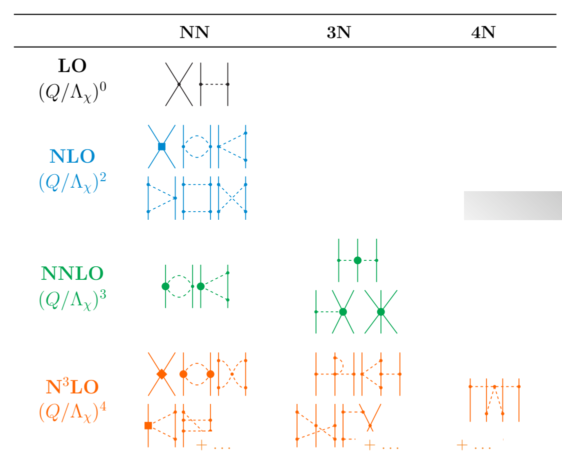
How the **nuclear force** is rooted in the fundamental theory of QCD?

Quantum Chromodynamics



Chiral Effective Field Theory



Nuclei & nuclear matter

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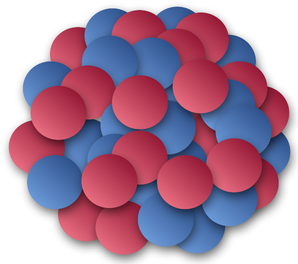

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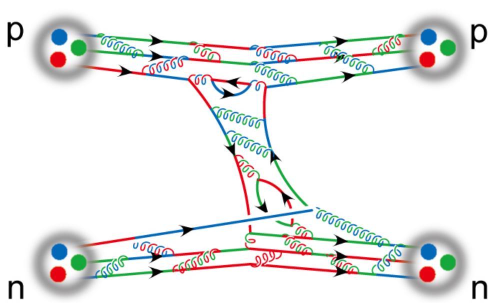

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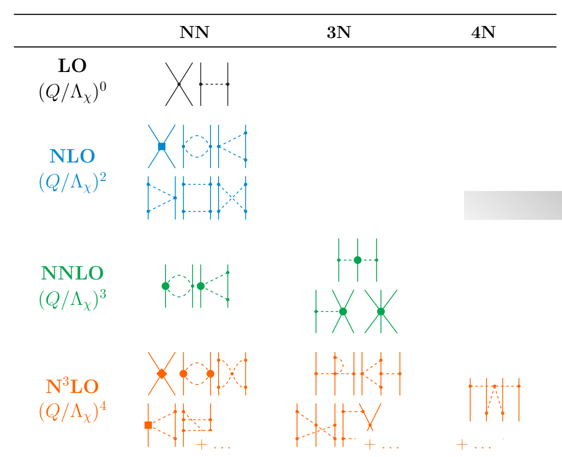
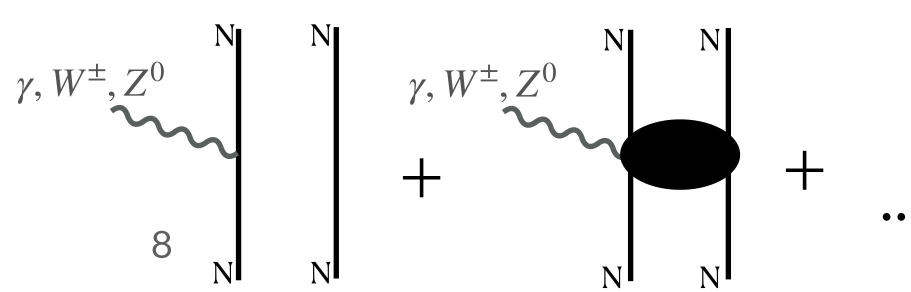


Nuclei & nuclear matter

Allows to construct **electroweak currents** consistently with the chiral potential

$$j = \sum_{i=1}^{A} j_i + \sum_{j<i=1}^{A} j_{ij} + \sum_{k<j<i=1}^{A} j_{ijk} + \ldots$$



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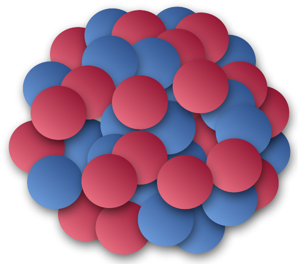

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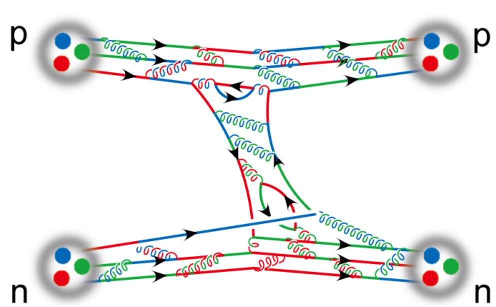

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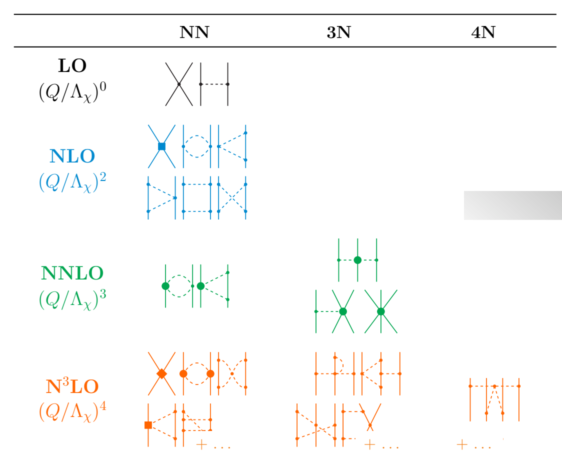

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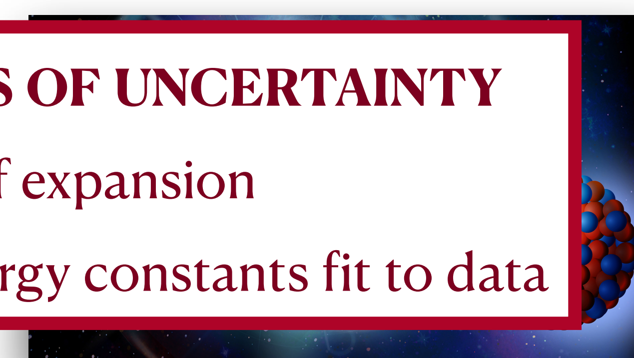

SOURCES OF UNCERTAINTY

- order of expansion
- low energy constants fit to data

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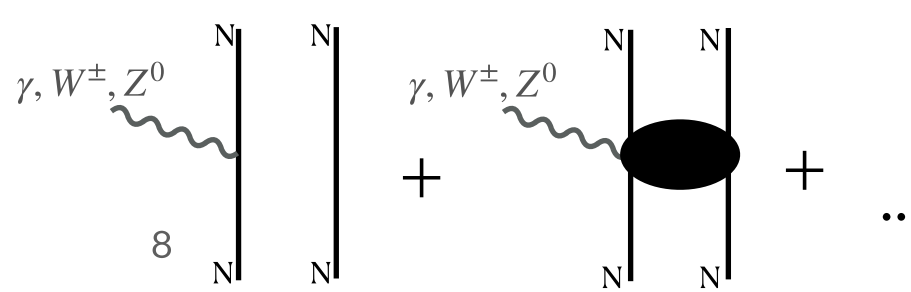

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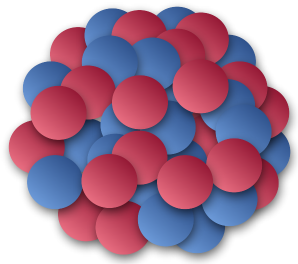

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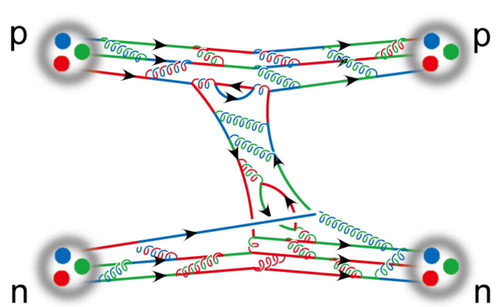

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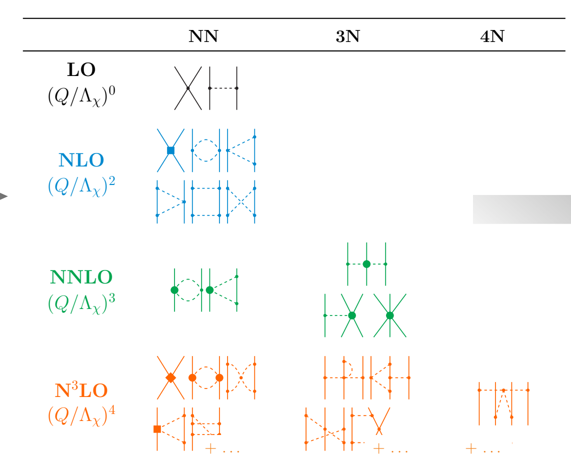

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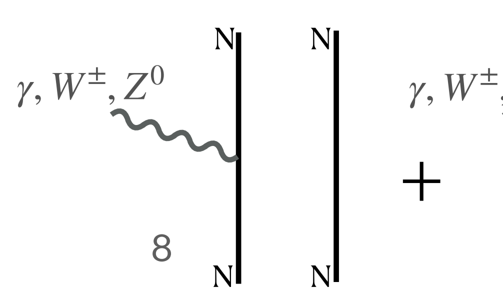
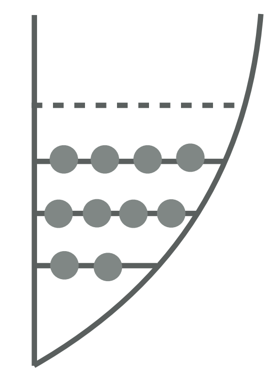


SOURCES OF UNCERTAINTY

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

Coupled cluster theory

Reference state (Hartree-Fock): $|\Psi\rangle = a_i^\dagger a_j^\dagger \ldots a_k^\dagger |0\rangle$



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$$\mathcal{H}_N e^T |\Psi\rangle = E e^T |\Psi\rangle$$

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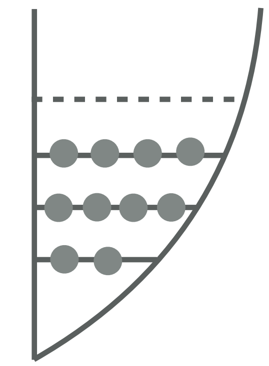

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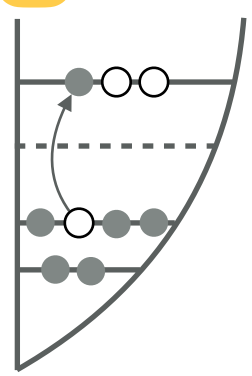
1p1h

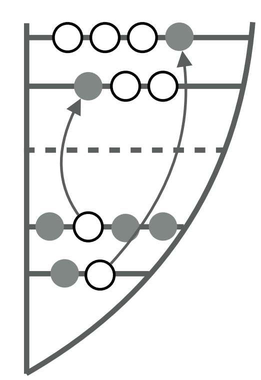
2p2h

Expansion: $T = \sum t_a^i a_a^\dagger a_i + \frac{1}{4} \sum t_{ab}^{ij} a_a^\dagger a_b^\dagger a_i a_j + \ldots$

singles



doubles



G. Hagen, T. Papenbrock, M. Hjorth-Jensen, D. J. Dean, Rep. Prog. Phys. 77, 096302 (2014).

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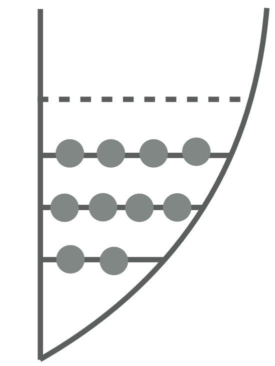

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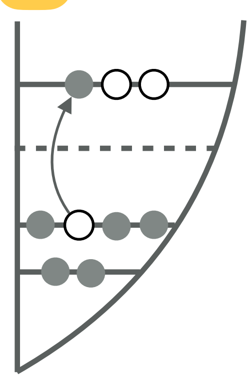

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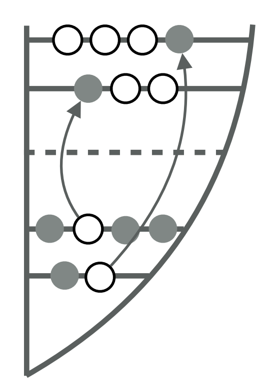

- ✓ Controlled approximation through truncation in T
- ✓ Polynomial scaling with A (predictions for ^{132}Sn and ^{208}Pb)

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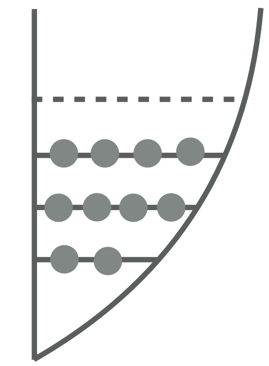

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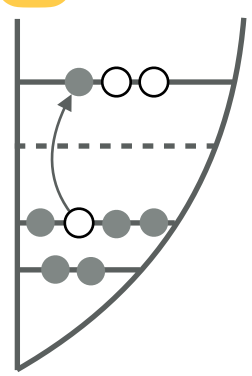

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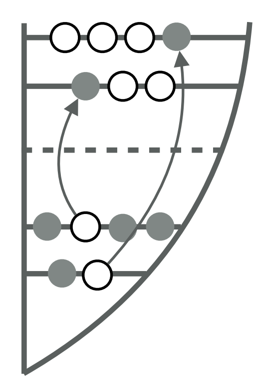

SOURCES OF UNCERTAINTY

➡ truncation in correlations

➡ model space dependence

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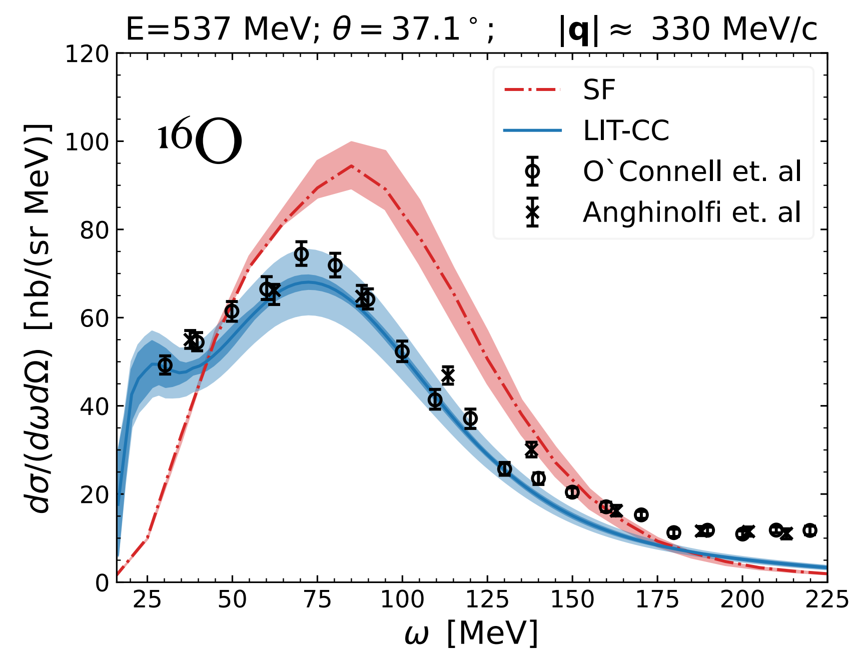
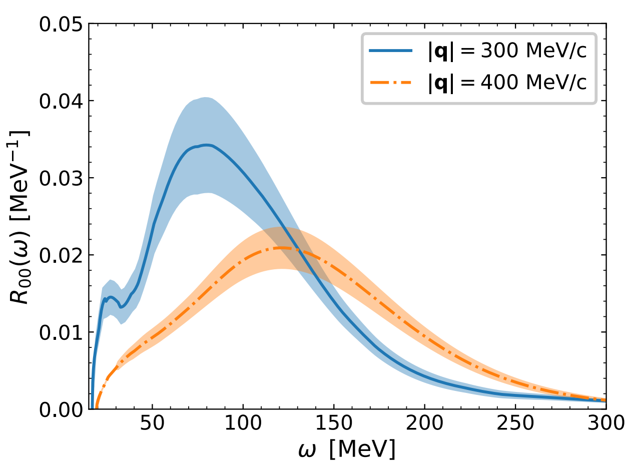
Responses from coupled-cluster

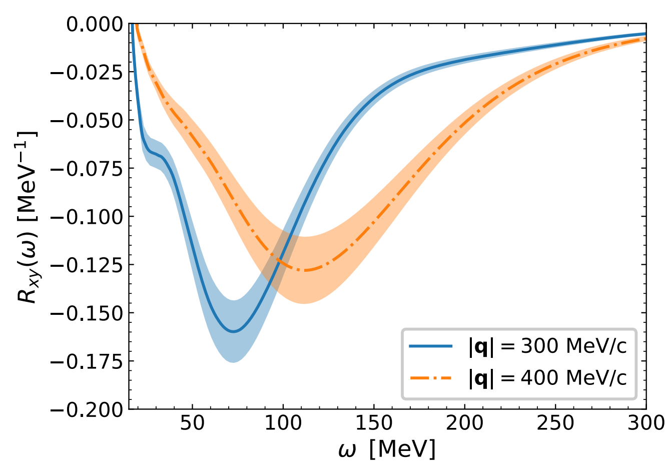
- **Parametric uncertainties:**
  low energy constants of the chiral effective theory

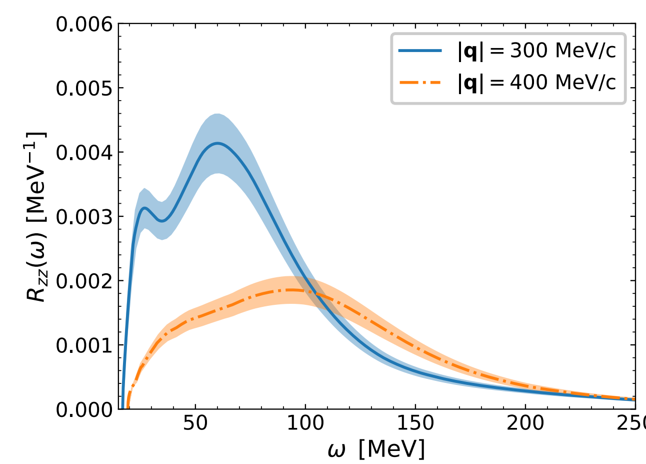
- **Model uncertainties:**
  - many-body method error
  - order of chiral expansion of Hamiltonian
  - integral transform inversion



LIT-CC error: truncation in chiral expansion + inversion procedure







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No unique model

Short-range correlations

- In quantum mechanics operators or wave-functions are **not observables!**

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$$U H U^{\dagger} U|\Psi\rangle = E U|\Psi\rangle$$

U-unitary transformation

- Operators also evolve: $J^{\mu}|\Psi\rangle \rightarrow U J^{\mu} U^{\dagger} U|\Psi\rangle$

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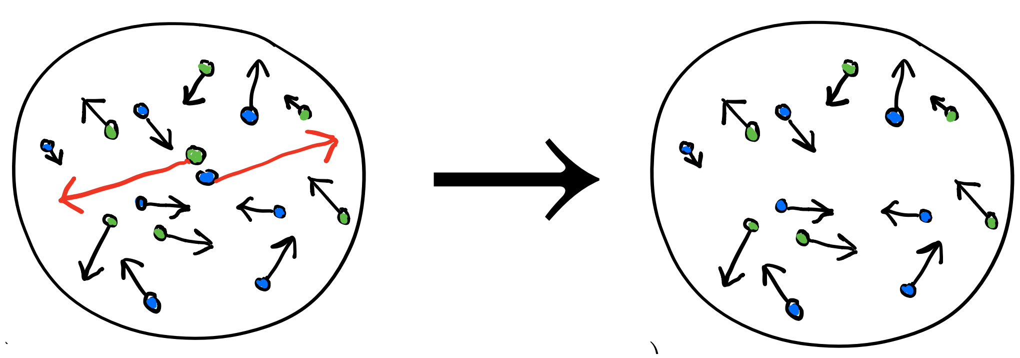

"Hard" (high-resolution) wave-function

"Soft" wave-function

El-weak operators

Evolved (more complicated) operators

No unique model

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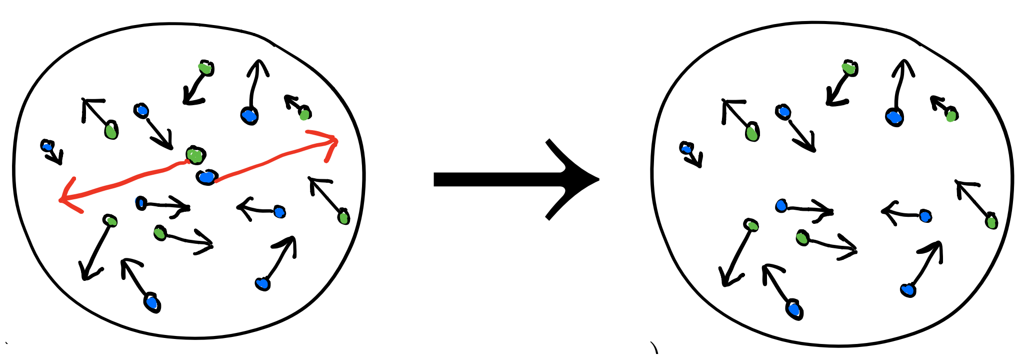

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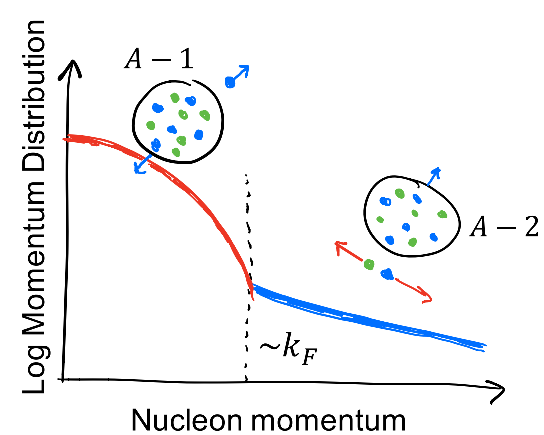

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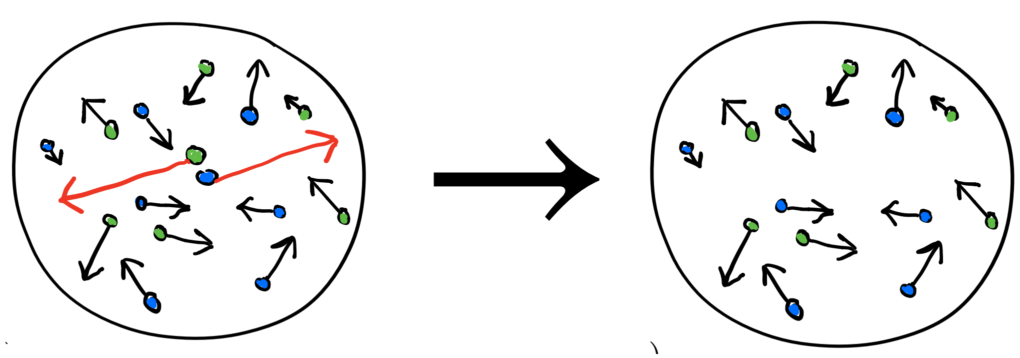

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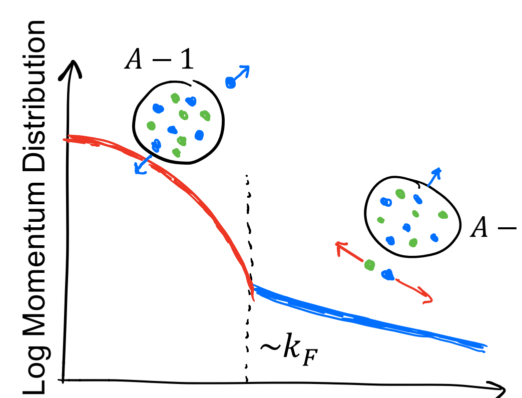
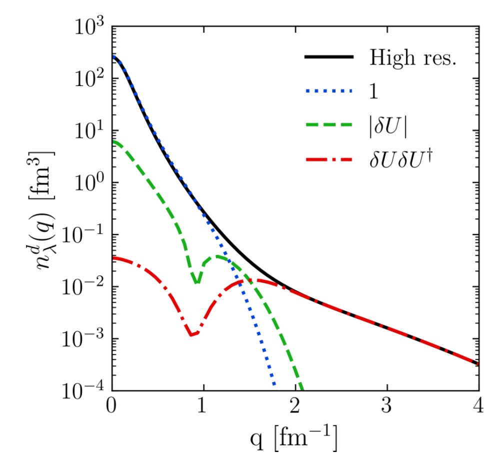
El-weak operators

Evolved (more complicated) operators



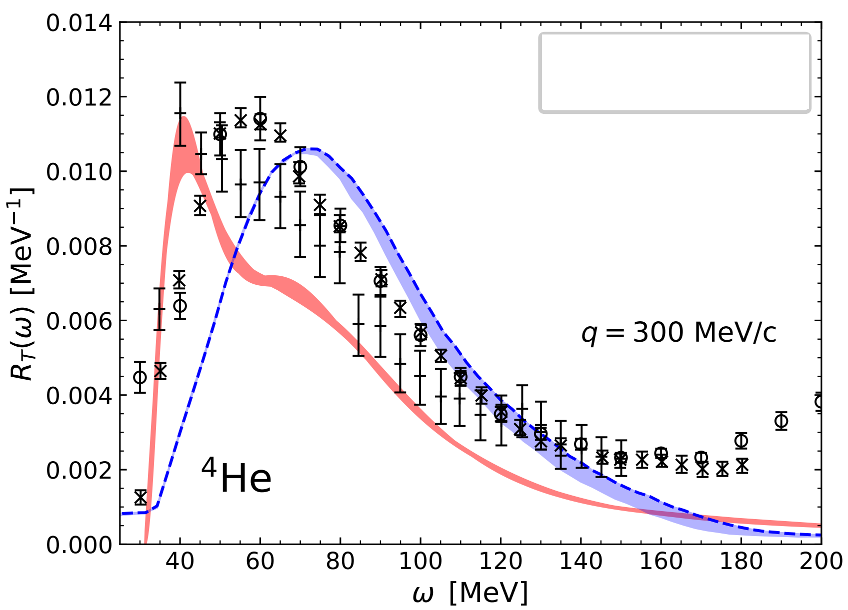


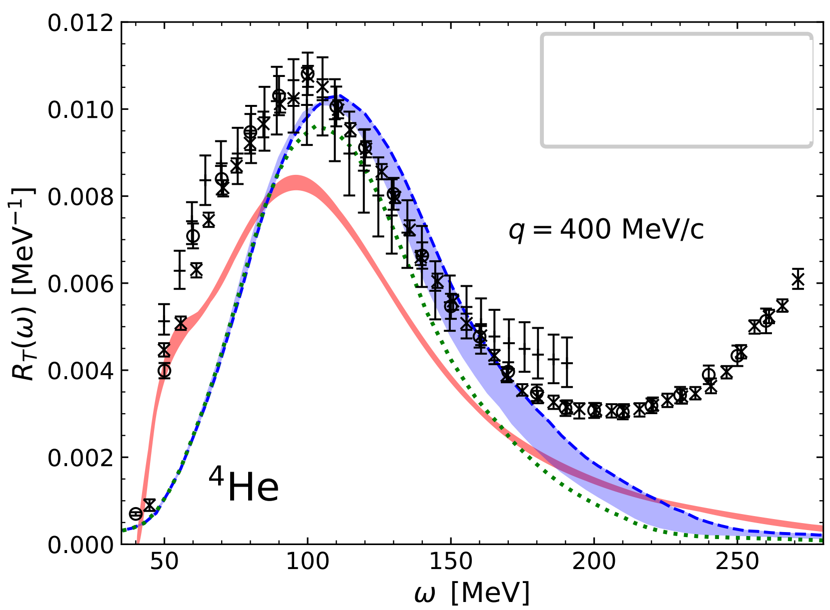
High-momentum tail is generated by evolved operators

Short-range correlation physics at low renormalization group resolution
J. Tropiano , S. K. Bogner, and R. J. Furnstahl *Phys. Rev. C 104, 034311*

Theoretical insight needed

Disentangle different sources of uncertainty





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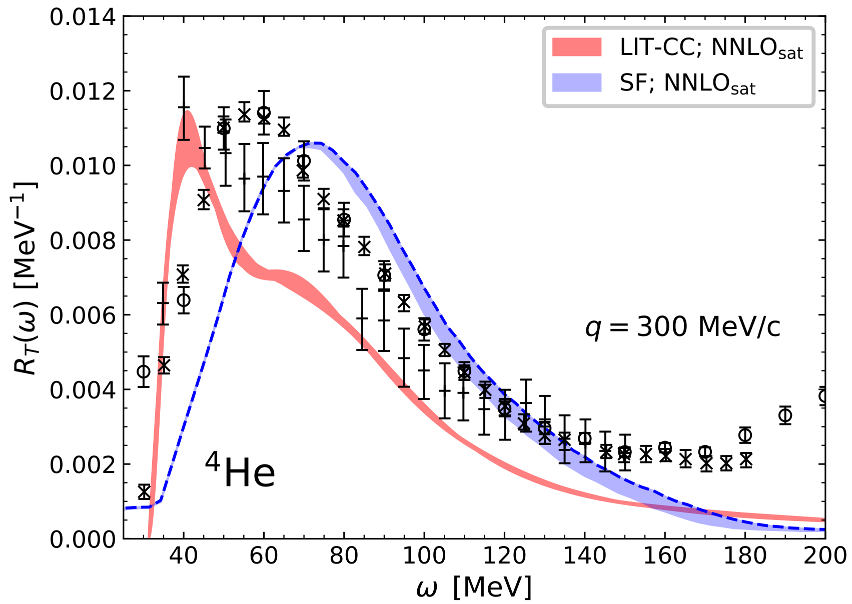

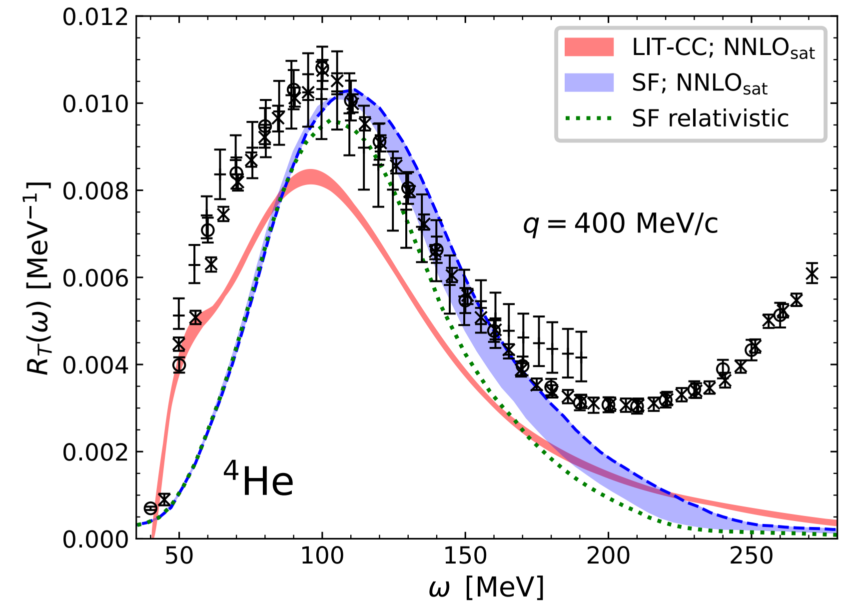

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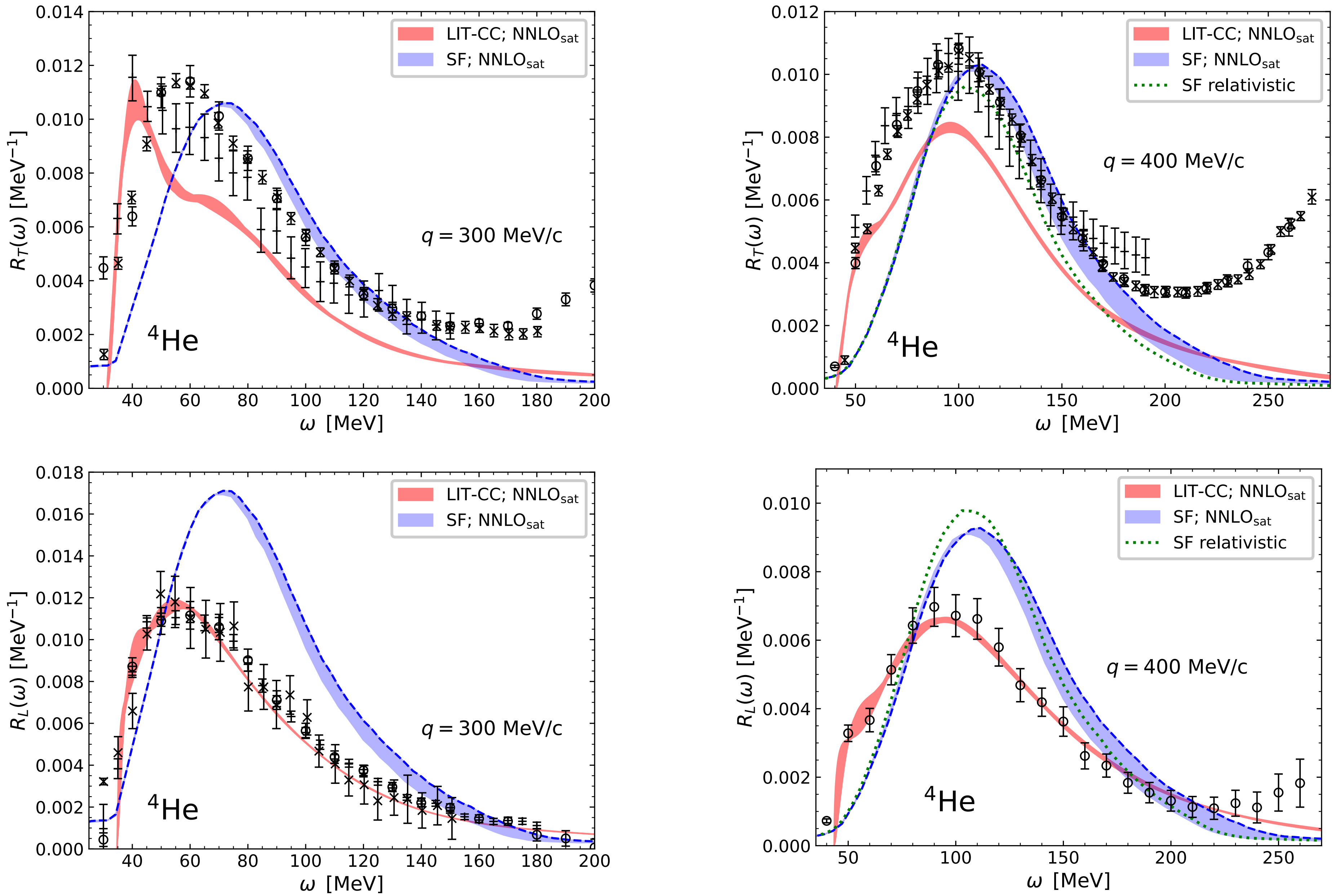
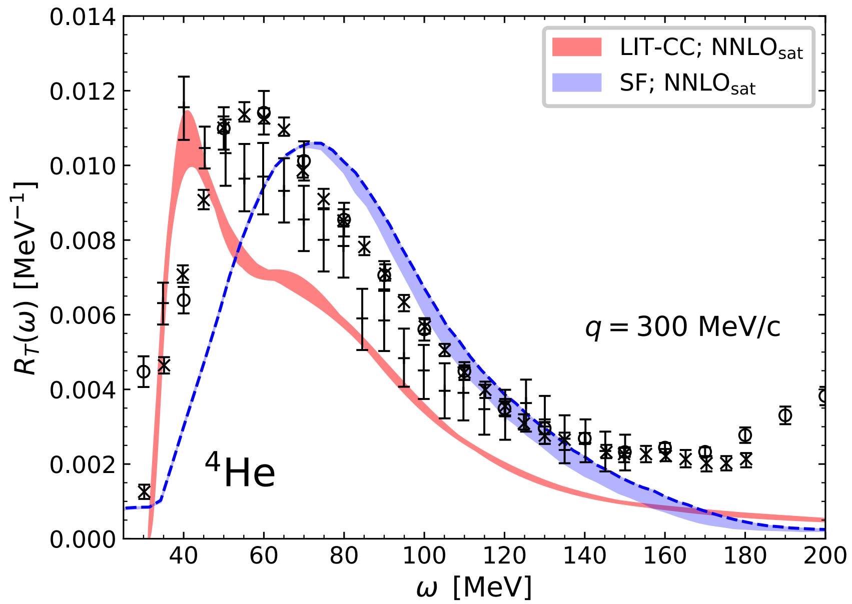


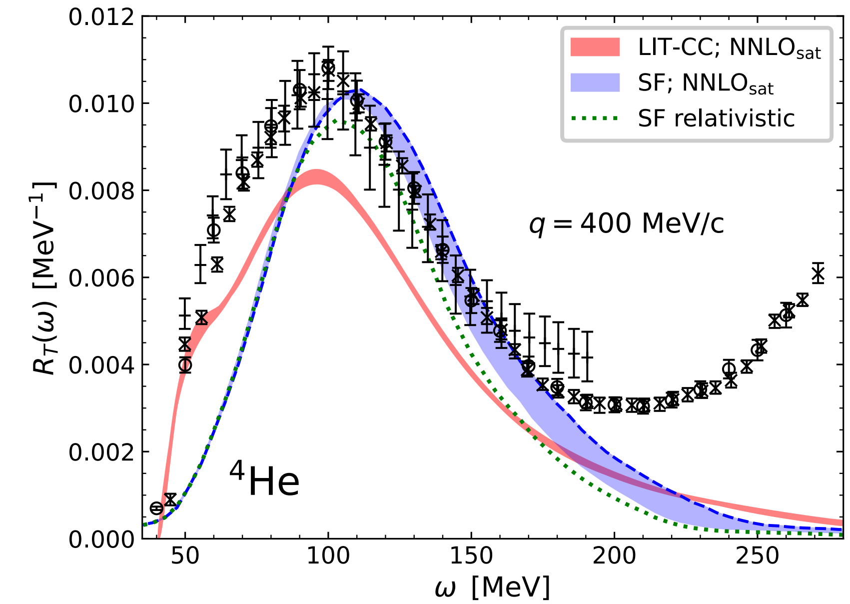
Theoretical insight needed

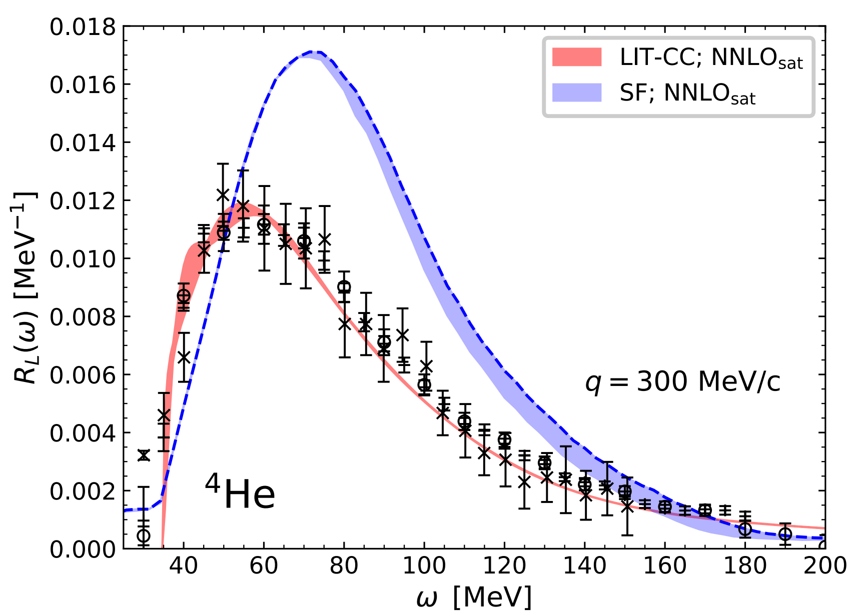
Disentangle different sources of uncertainty

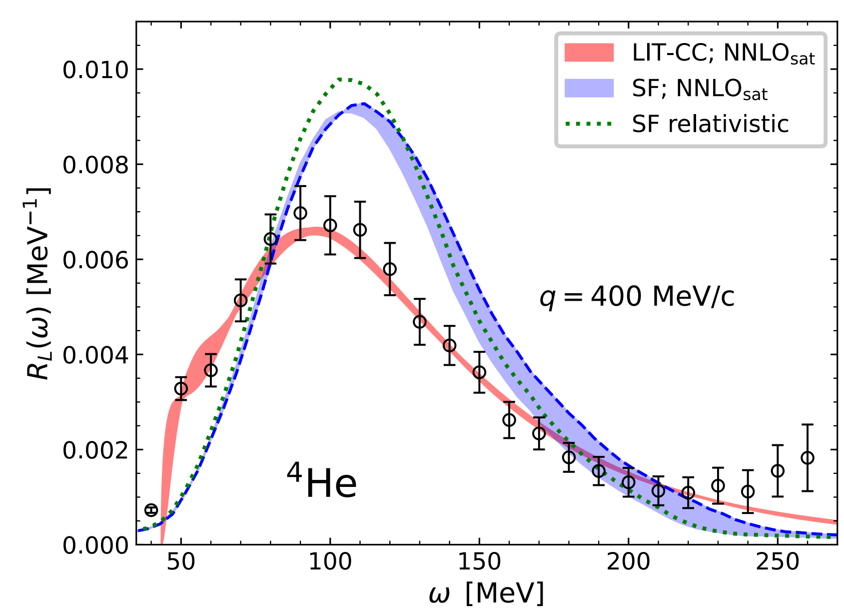
Calculations do not contain 2-body currents

LIT-CC accounts for FSI









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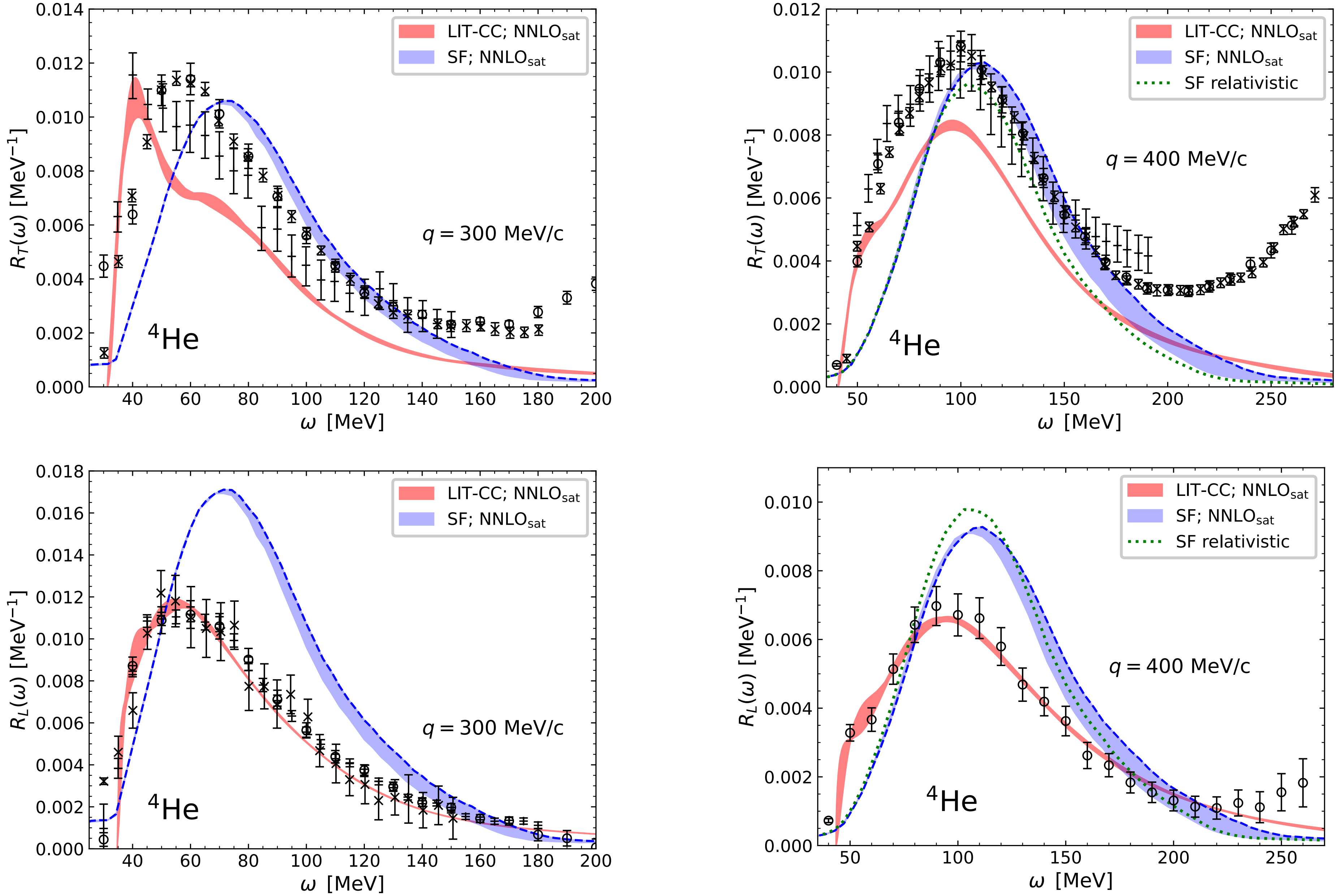
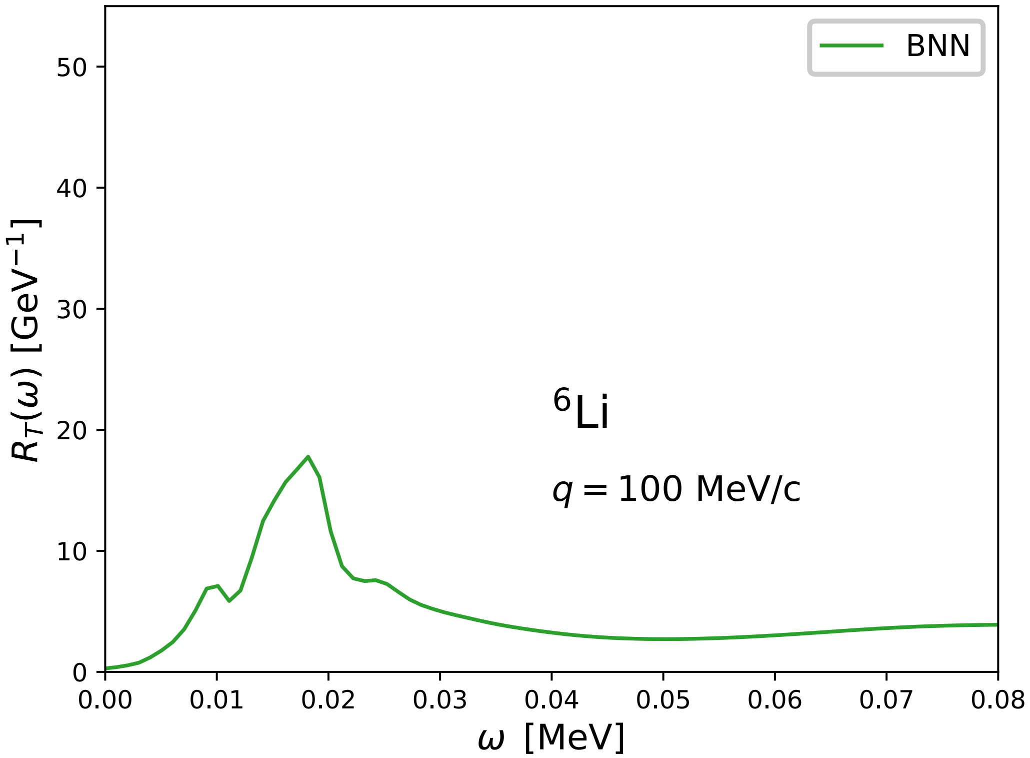


For kinematics where R_T dominates the SF might seem to work well (FSI & 2-B currents cancel)!

Going beyond region of applicability

What can we say about responses of ^{6}Li at very low momentum transfers?



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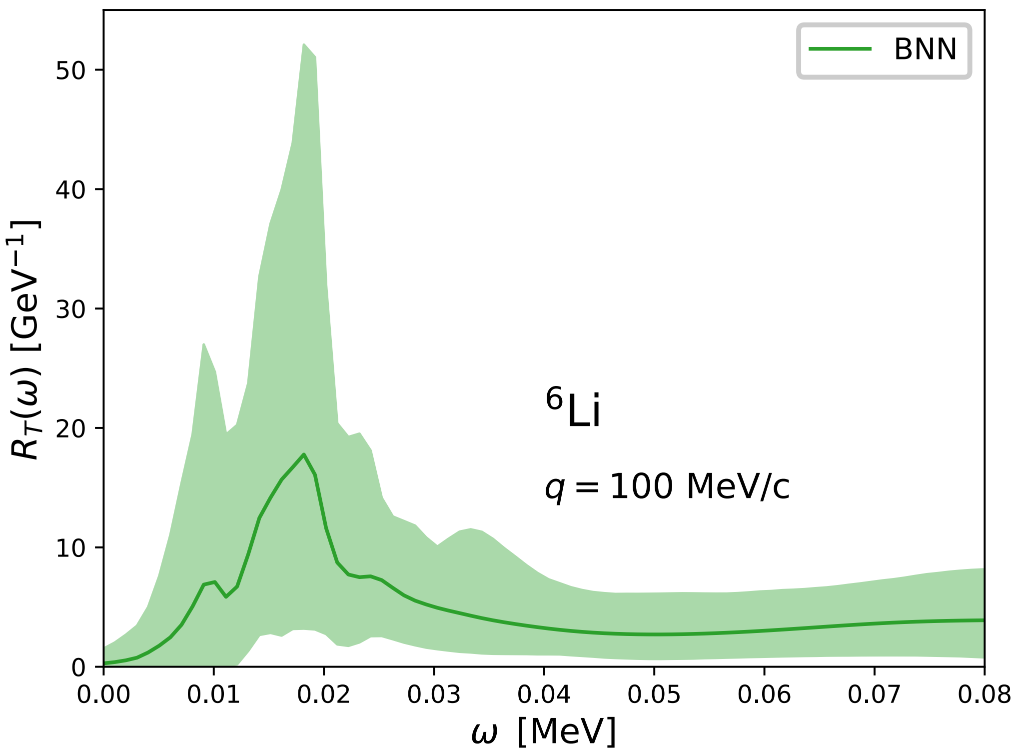

Uncertainty is "data driven"

Going beyond region of applicability

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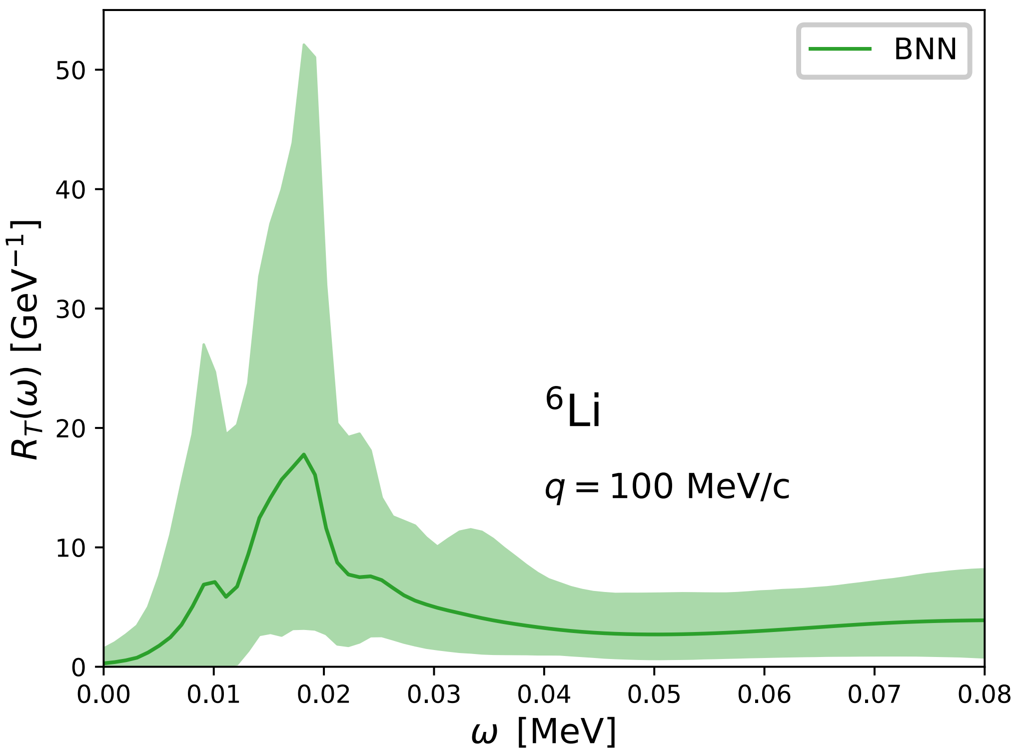
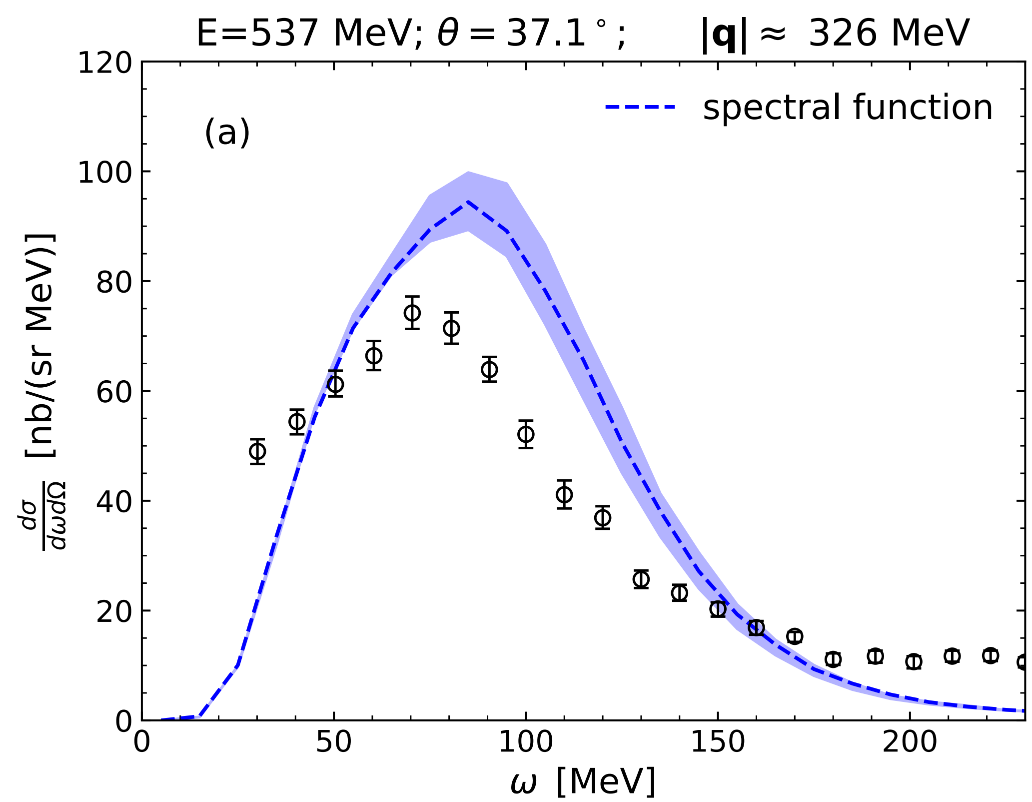


Uncertainty is "data driven"

How important are final state interactions at low momenta?



Model discrepancy — we should work hard to estimate uncertainties (e.g. using data or other more reliable theories)

Going beyond region of applicability

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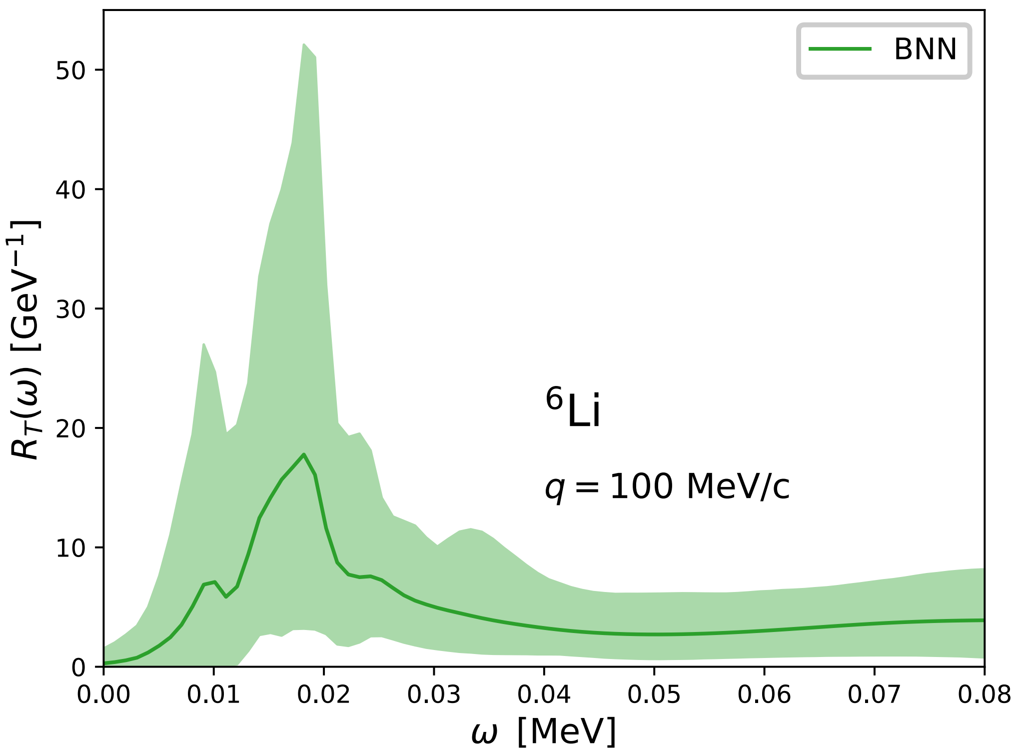

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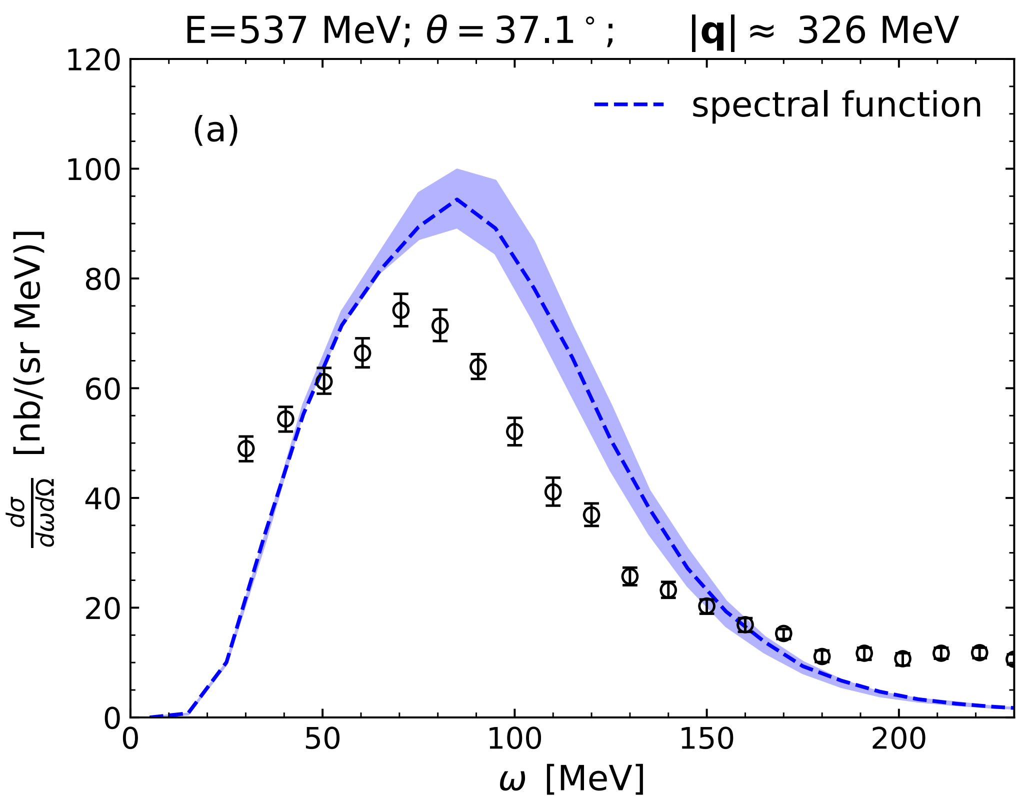


Model discrepancy — we should work hard to estimate uncertainties (e.g. using data or other more reliable theories)

That's a common situation in MC event generators

Final questions and comments

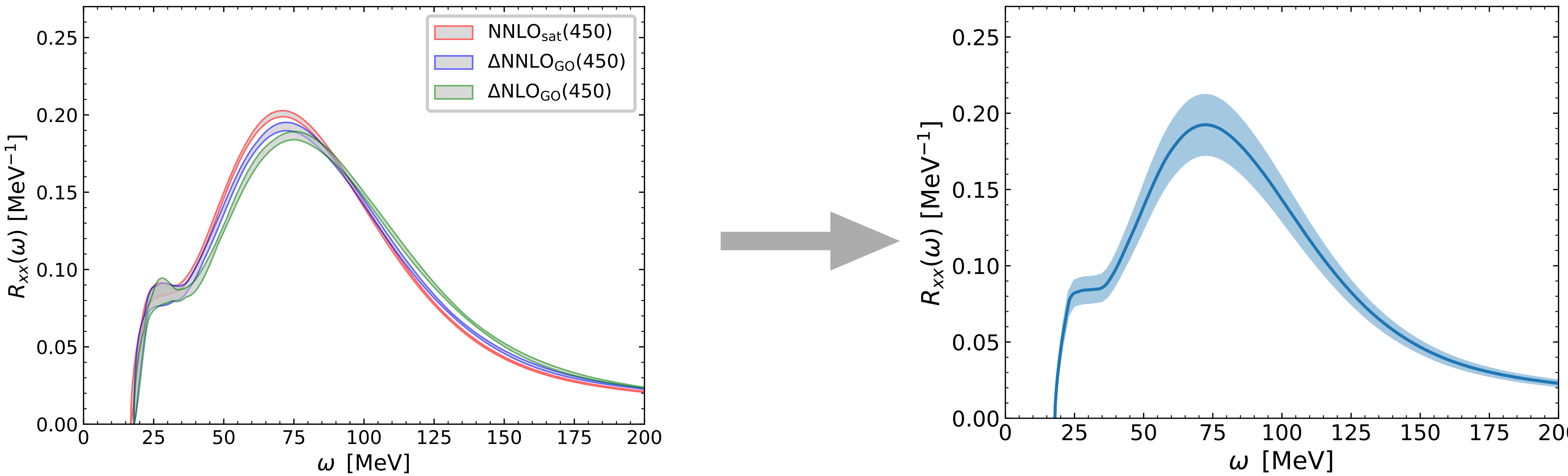
- Estimating theoretical uncertainties is crucial for next-generation experiments (but very challenging!)
- More comparisons between models would be helpful. Examples:
  M. Martini, N. Jachowicz, et al Phys. Rev. C 94 (2016) no.1, 015501
  J.E.S., E. Hernandez, S.X. Nakamura, J. Nieves, T. Sato, Phys. Rev. D 98 (2018) no.7, 073001
- How to stitch different models? (Bayesian model mixing?)
- How to address model discrepancy?
- How to include model uncertainties in intra-nuclear cascade?

Thank you!

Backup

Uncertainty estimation (responses)

Assessing EFT truncation error



Gaussian process (GP) to assess chiral truncation using 2 orders of expansion

Order k EFT prediction: $y_k(p) = y_{\mathrm{ref}}(p) \sum_{n=0}^{k} c_n(p) \left(\frac{p}{\Lambda}\right)^n$

EFT truncation error: $\delta y_k(p) = y_{\mathrm{ref}}(p) \sum_{n=k+1}^{\infty} c_n(p) \left(\frac{p}{\Lambda}\right)^n$

Draws from an underlying GP

Robust uncertainty quantification

ARTICLES
https://doi.org/10.1038/s41567-022-01715-8
nature physics
Check for updates
OPEN

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

Baishan Hu[1,11], Weiguang Jiang[2,11], Takayuki Miyagi[1,3,4,11], Zhonghao Sun[5,6,11], Andreas Ekström[2], Christian Forssén[2] ✉, Gaute Hagen[1,5,6], Jason D. Holt[1,7], Thomas Papenbrock[5,6], S. Ragnar Stroberg[8,9] and Ian Vernon[10]

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

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

Posterior probability density function

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

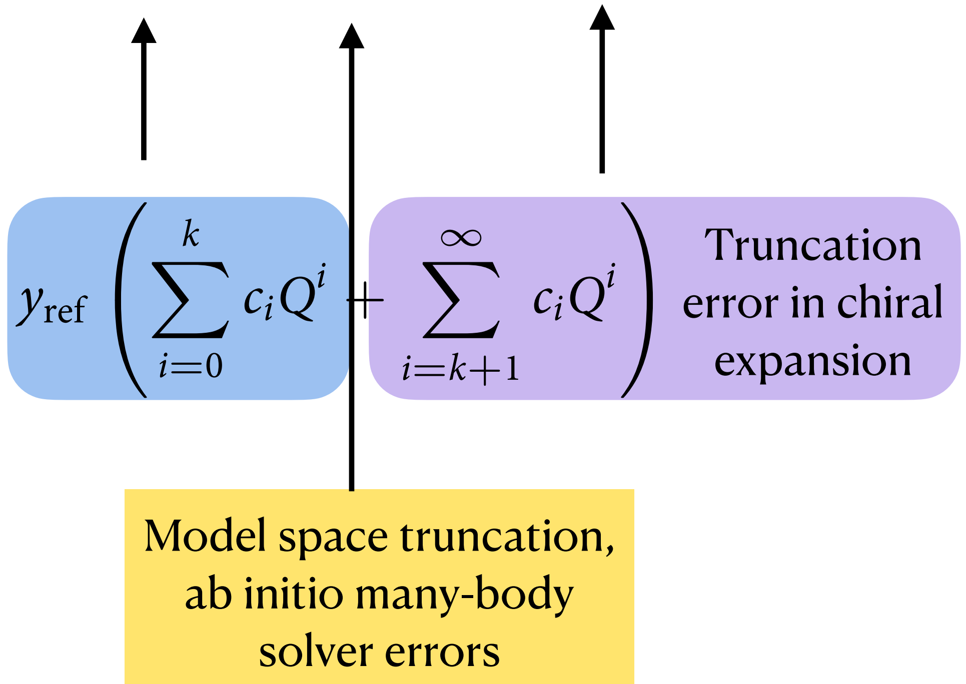
- posterior predictive distributions

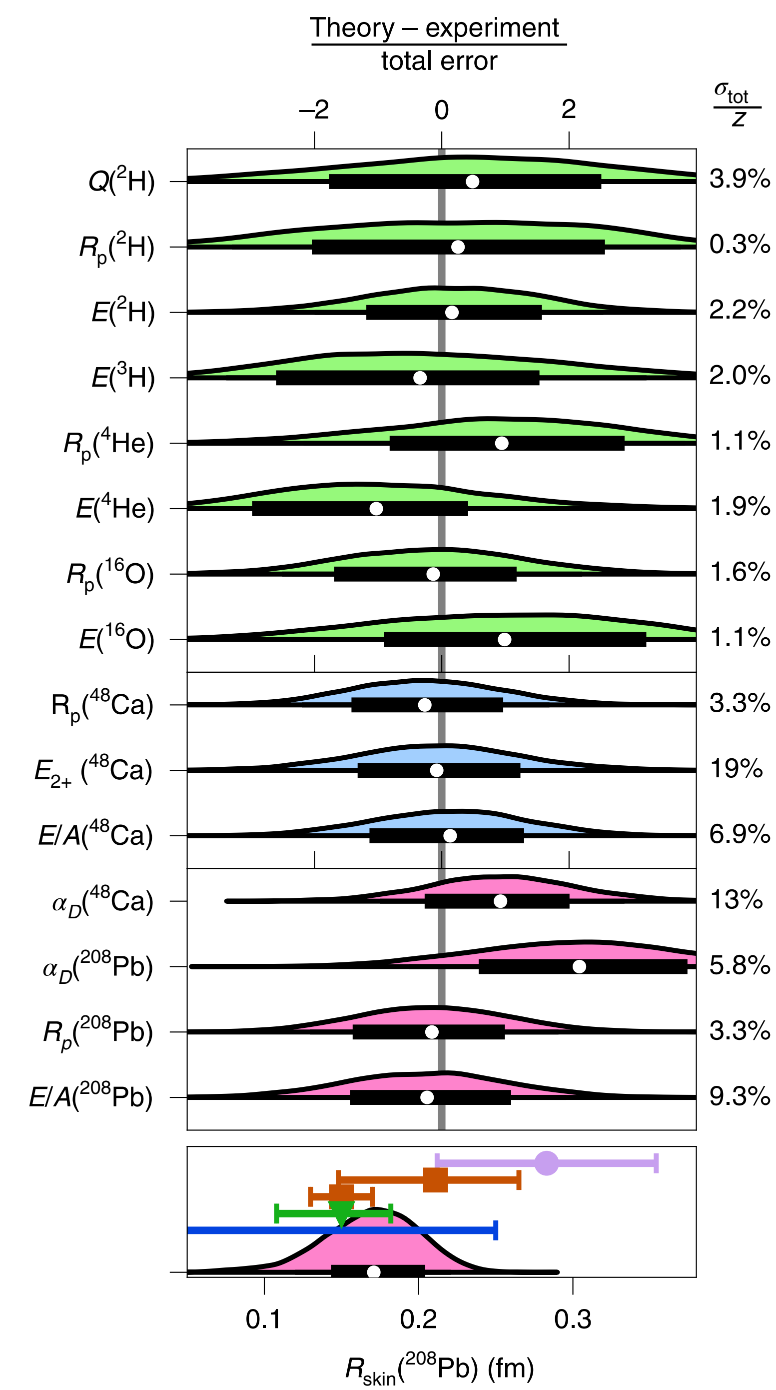
$$\{y(\theta) : \theta \sim \mathrm{pr}(\theta \,|\, D)\}$$

Robust uncertainty quantification

Various sources of uncertainty taken into account

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





Posterior predictive distributions