Cross-section calculation using QMC and the short-time approximation

4th International Workshop on Quantitative Challenges in Short-Range Correlations and the EMC Effect Research

CEA Paris-Saclay

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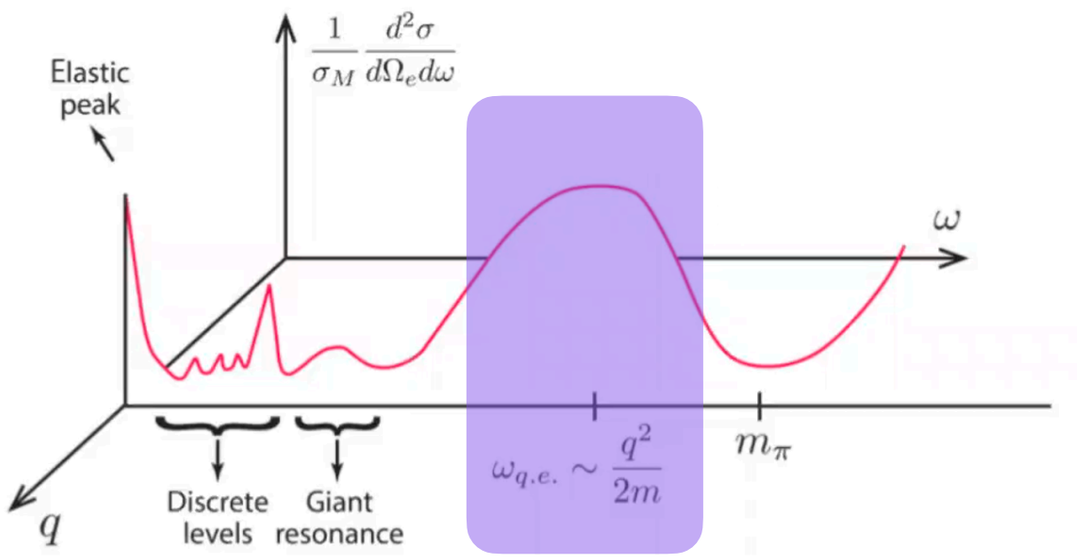
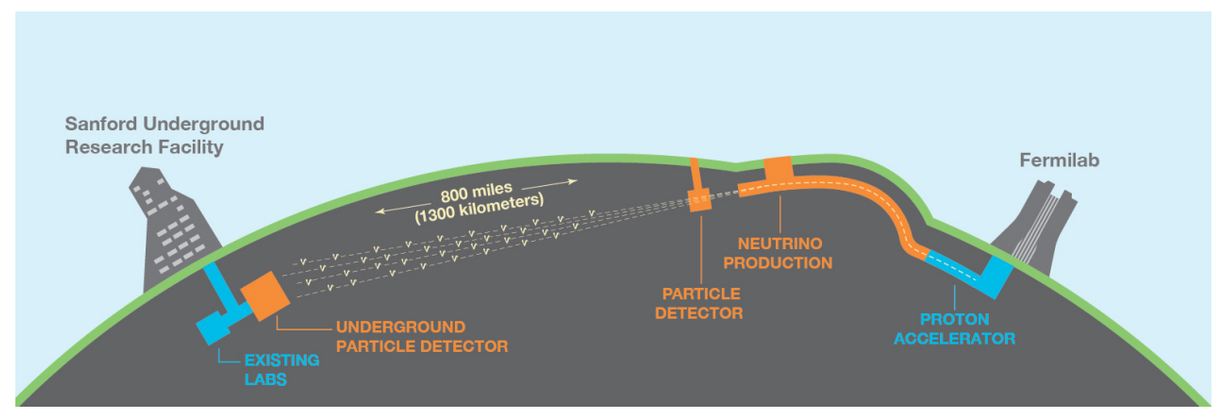
Electron-nucleus scattering

Theoretical understanding of nuclear effects is extremely important for neutrino experimental programs





Lepton-nucleus cross sections $\omega \sim 10^2$ MeV

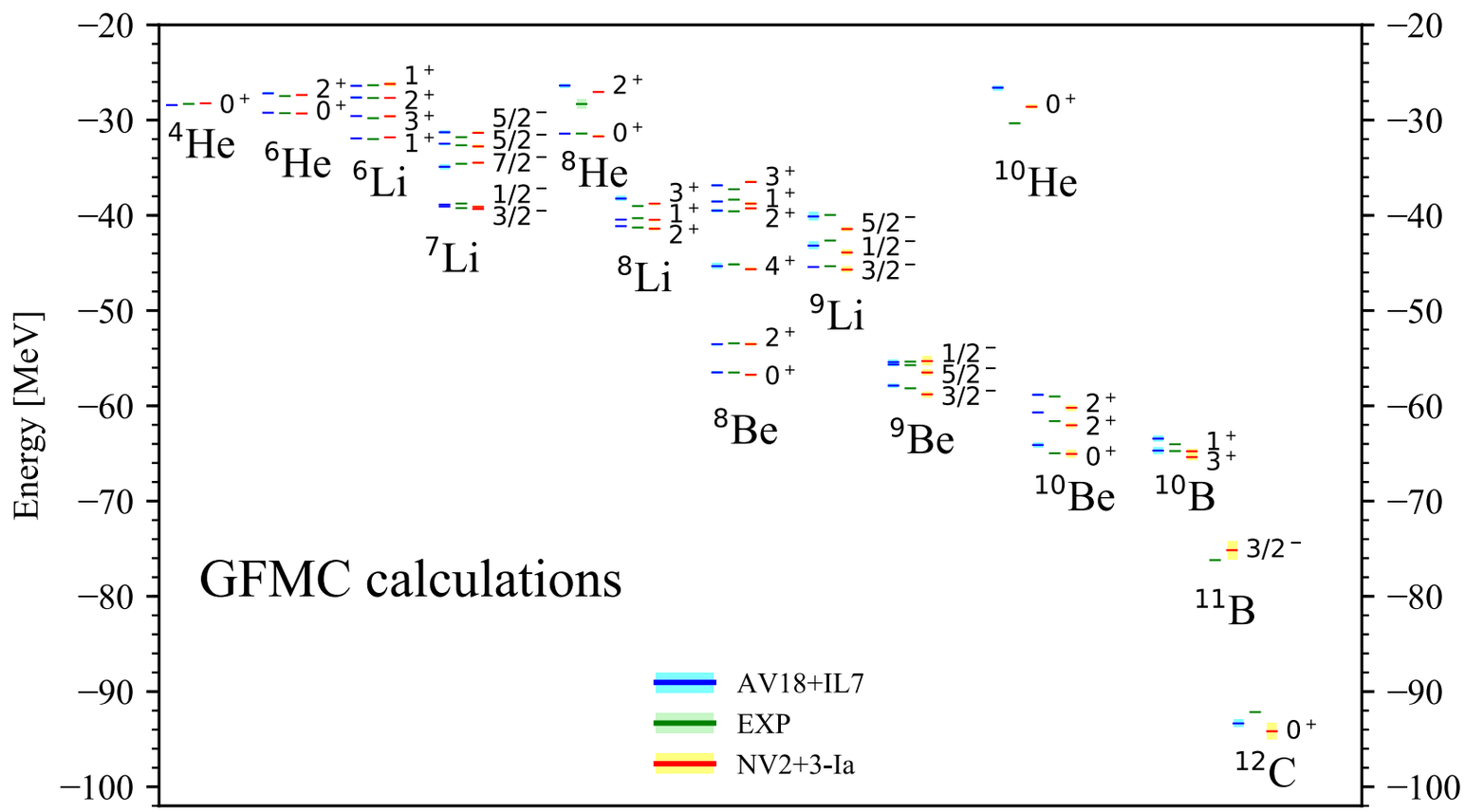
Ab-initio description of nuclei

- Nuclear interaction
- Electroweak interaction of leptons with nucleons and clusters of correlated nucleons
- Computational method

Many-body nuclear interaction

Many-body Nuclear Hamiltonian: Argonne v_{18} + Urbana IX

$$H = \sum_i T_i + \sum_{i<j} v_{ij} + \sum_{i<j<k} v_{ijk}$$



Spectra of light nuclei

Piarulli et al. PRL120(2018)052503

Many-body nuclear interaction

Many-body Nuclear Hamiltonian: Argonne v_{18} + Urbana IX

$$H = \sum_i T_i + \sum_{i<j} v_{ij} + \sum_{i<j<k} v_{ijk}$$

Quantum Monte Carlo methods:
Use nuclear wave functions that minimize the expectation value of E

$$E_V = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \geq E_0$$

The evaluation is performed using Metropolis sampling

Nuclear Wave Functions

Variational wave function for nucleus in J state

$$|\psi\rangle = \mathcal{S}\prod_{i<j}^{A}\left[1 + U_{ij} + \sum_{k\neq i,j}^{A} U_{ijk}\right]\left[\prod_{i<j} f_c(r_{ij})\right]|\Phi(JMTT_3)\rangle$$

Two-body spin- and isospin-dependent correlations

$$U_{ij} = \sum_p f^p(r_{ij})\, O^p_{ij}$$

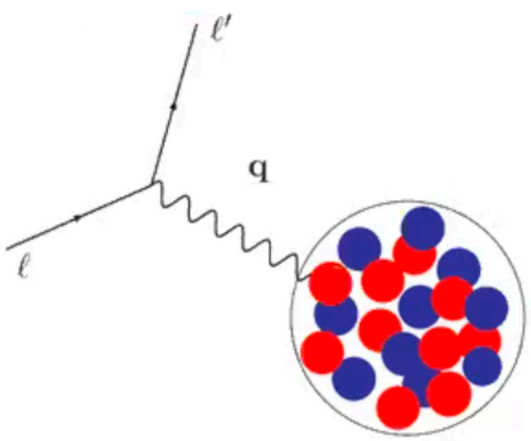
$$O^p_{ij} = [1, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, S_{ij}] \otimes [1, \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j]$$

$$U_{ijk} = \epsilon v_{ijk}(\bar{r}_{ij}, \bar{r}_{jk}, \bar{r}_{ki})$$

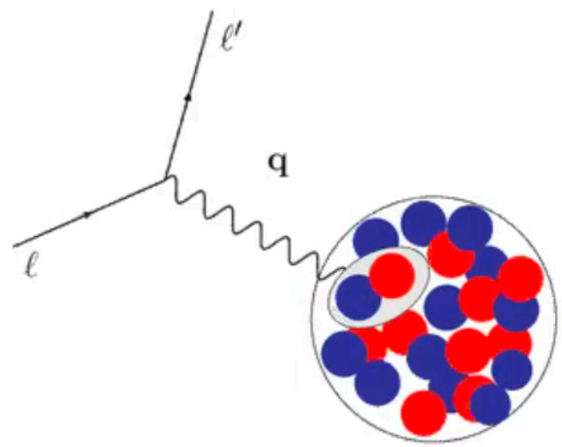
Electromagnetic interactions

Phenomenological Hamiltonian for NN and NNN

The interaction with external probes is described in terms on one- and two-body charge and current operators



one-body



two-body

Charge operators

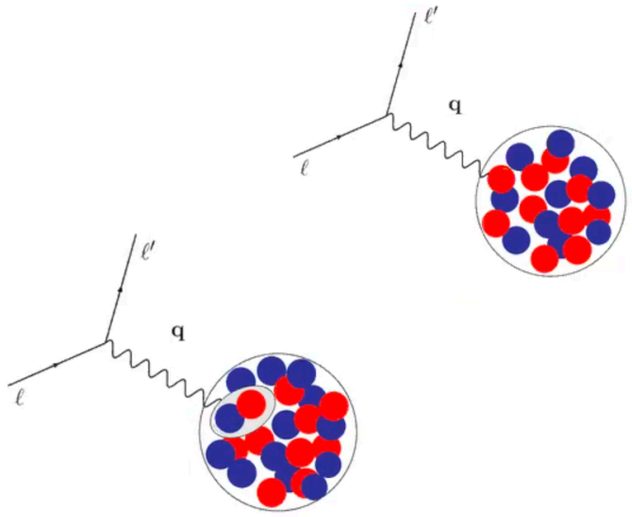
$$\rho = \sum_{i=1}^{A} \rho_i + \sum_{i<j} \rho_{ij} + \dots$$

Current operators

$$\mathbf{j} = \sum_{i=1}^{A} \mathbf{j}_i + \sum_{i<j} \mathbf{j}_{ij} + \dots$$

Electromagnetic interactions

- One body-currents: non-relativistic reduction of covariant nucleons' isoscalar and isovector currents
- Two-body currents: modeled on MEC currents constrained by commutation relation with the nuclear Hamiltonian (Pastore et al. PRC84(2011)024001, PRC87(2013)014006)

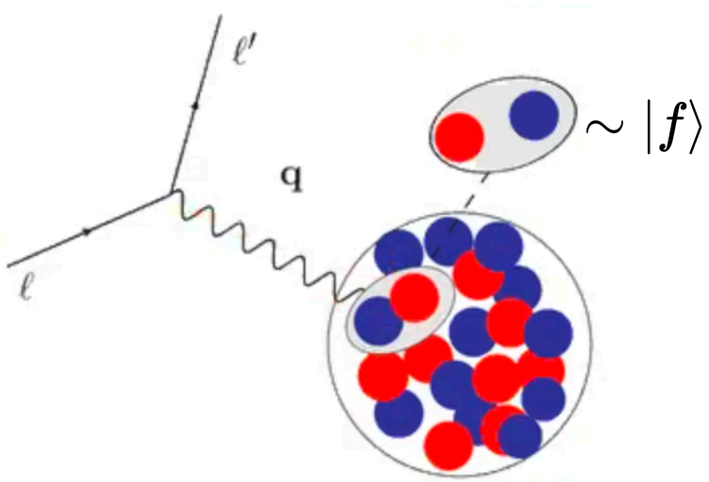


- Argonne v18 two-nucleon and Urbana IX potentials, together with these currents, provide a quantitatively successful description of many nuclear electroweak observables, including charge radii, electromagnetic moments and transition rates, charge and magnetic form factors of nuclei with up to A = 12 nucleons

Short-time approximation

Pastore et al. PRC101(2020)044612

Quasielastic scattering cross sections are expressed in terms of response function



Response functions

$$R_\alpha(q,\omega) = \sum_f \delta(\omega + E_0 - E_f)|\langle f|O_\alpha(\mathbf{q})|0\rangle|^2$$

$$R_\alpha(q,\omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i(\omega+E_i)t} \langle \Psi_i | O_\alpha^\dagger(\mathbf{q}) e^{-iHt} O_\alpha(\mathbf{q}) | \Psi_i \rangle$$

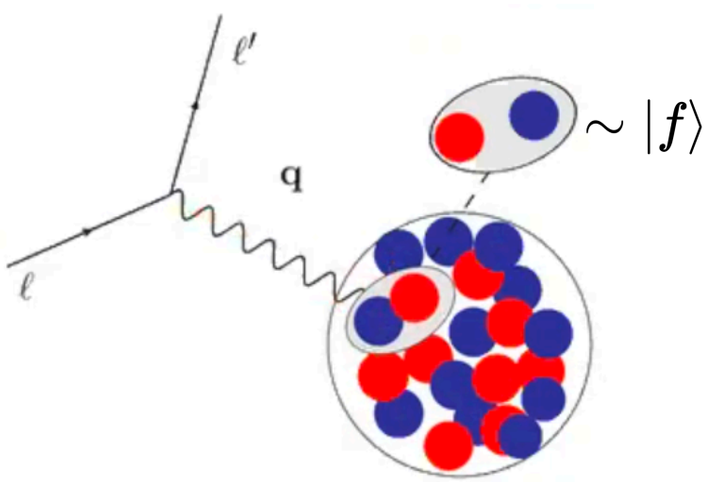
$$\begin{aligned} O^\dagger e^{-iHt} O &= \left(\sum_i O_i^\dagger + \sum_{i<j} O_{ij}^\dagger\right) e^{-iHt} \left(\sum_{i'} O_{i'} + \sum_{i'<j'} O_{i'j'}\right) \\ &= \sum_i O_i^\dagger e^{-iHt} O_i + \sum_{i\neq j} O_i^\dagger e^{-iHt} O_j \\ &\quad + \sum_{i\neq j} \Big(O_i^\dagger e^{-iHt} O_{ij} + O_{ij}^\dagger e^{-iHt} O_i \\ &\quad + O_{ij}^\dagger e^{-iHt} O_{ij} \Big) + \dots \end{aligned}$$

The sum over all final states is replaced by a two nucleon propagator

Short-time approximation

Pastore et al. PRC101(2020)044612

Quasielastic scattering cross sections are expressed in terms of response function



Response functions

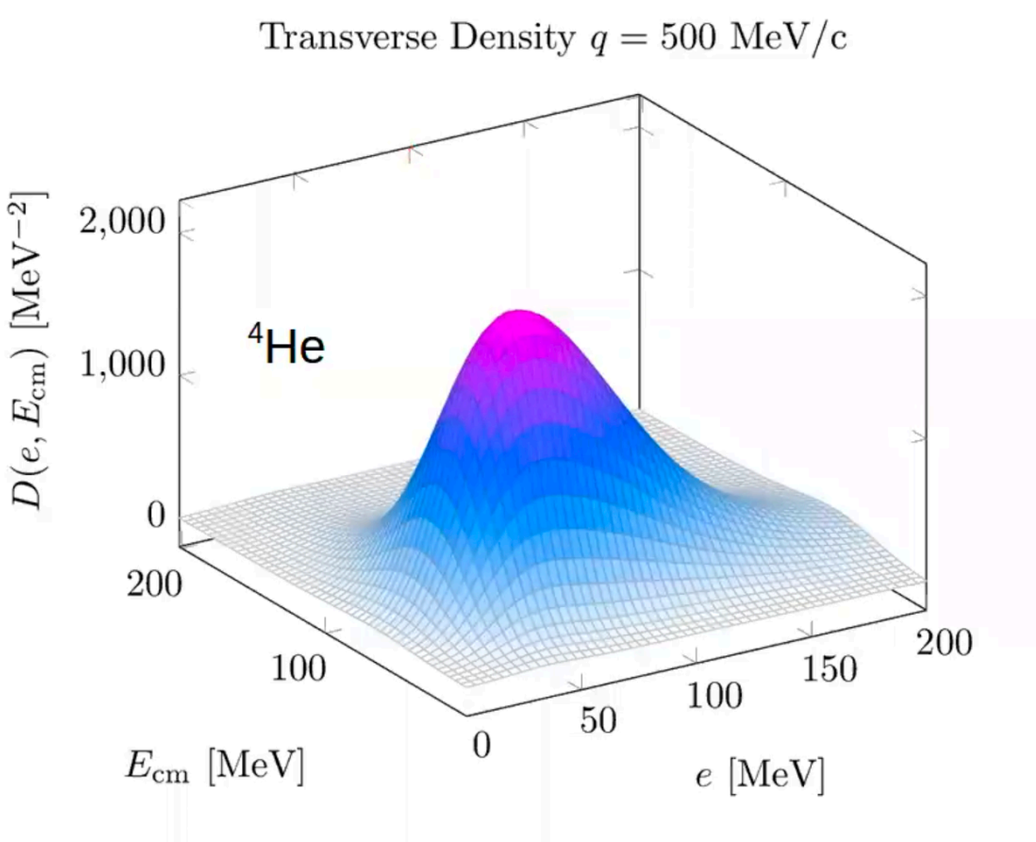
$$R_\alpha(q,\omega) = \sum_f \delta(\omega + E_0 - E_f)|\langle f|O_\alpha(\mathbf{q})|0\rangle|^2$$

Response densities

$$R^{\mathrm{STA}}(q,\omega) \sim \int \delta(\omega + E_0 - E_f) de\, dE_{cm} \mathcal{D}(e, E_{cm}; q)$$

STA: scattering of external probes from pairs of correlated nucleons

Transverse response density

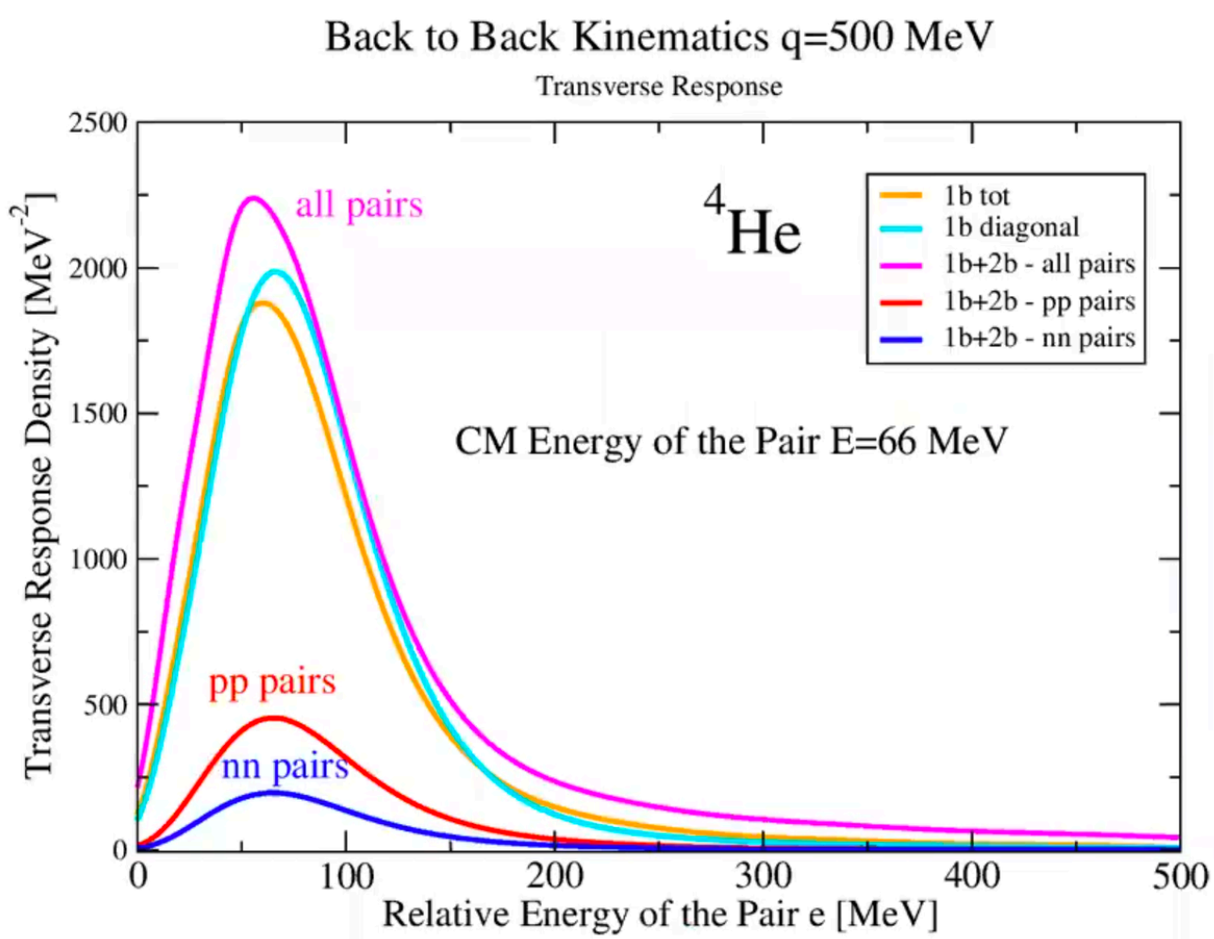


Electron scattering from $^4\mathrm{He}$:

- Response density as a function of (E,e)
- Give access to particular kinematics for the struck nucleon pair

Pastore et al. PRC101(2020)044612

Back-to-back kinematic



We can select a particular kinematic, and assess the contributions from different particle identities

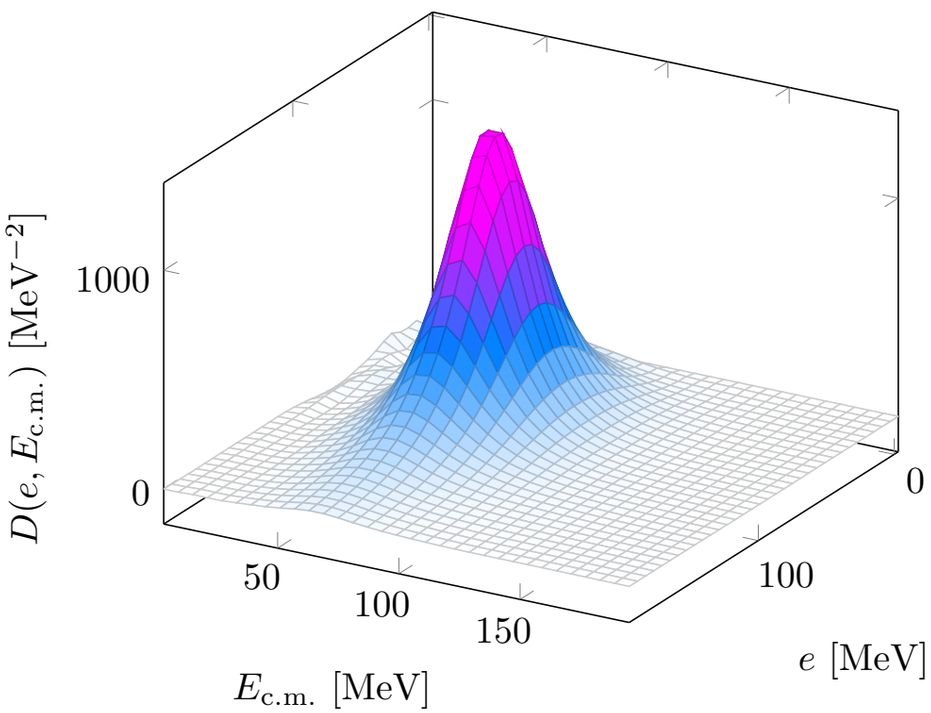
Pastore et al. PRC101(2020)044612

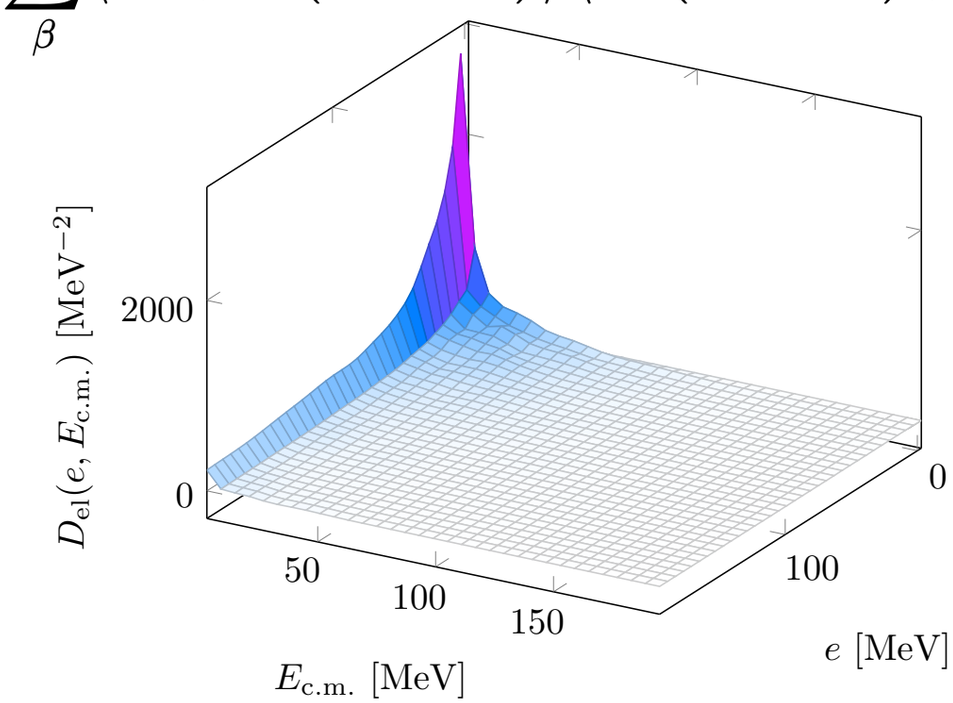
Longitudinal response density: elastic peak removal

$$R^{\mathrm{STA}}(q,\omega) \sim \int \delta(\omega + E_0 - E_f)de\, dE_{cm}\mathcal{D}(e, E_{cm}; q)$$

$$\mathcal{D}(e, E_{\mathrm{cm}}) - \mathcal{D}_{\mathrm{el}}(e, E_{\mathrm{cm}})$$

$$\mathcal{D}_{el}(\mathbf{q}, \mathbf{p}', \mathbf{P}') = |\langle \Psi_0 | J(\mathbf{q}) | \Psi_0 \rangle|^2 \times \sum_{\beta} \langle \Psi_0 \mid \Psi_2(\mathbf{p}', \mathbf{P}', \beta) \rangle \langle \Psi_2(\mathbf{p}', \mathbf{P}', \beta) \mid \Psi_0 \rangle$$





^{3}H Longitudinal response at 300 MeV

L.A., S. Pastore, N. Rocco, et al. PRC105(2022)014002

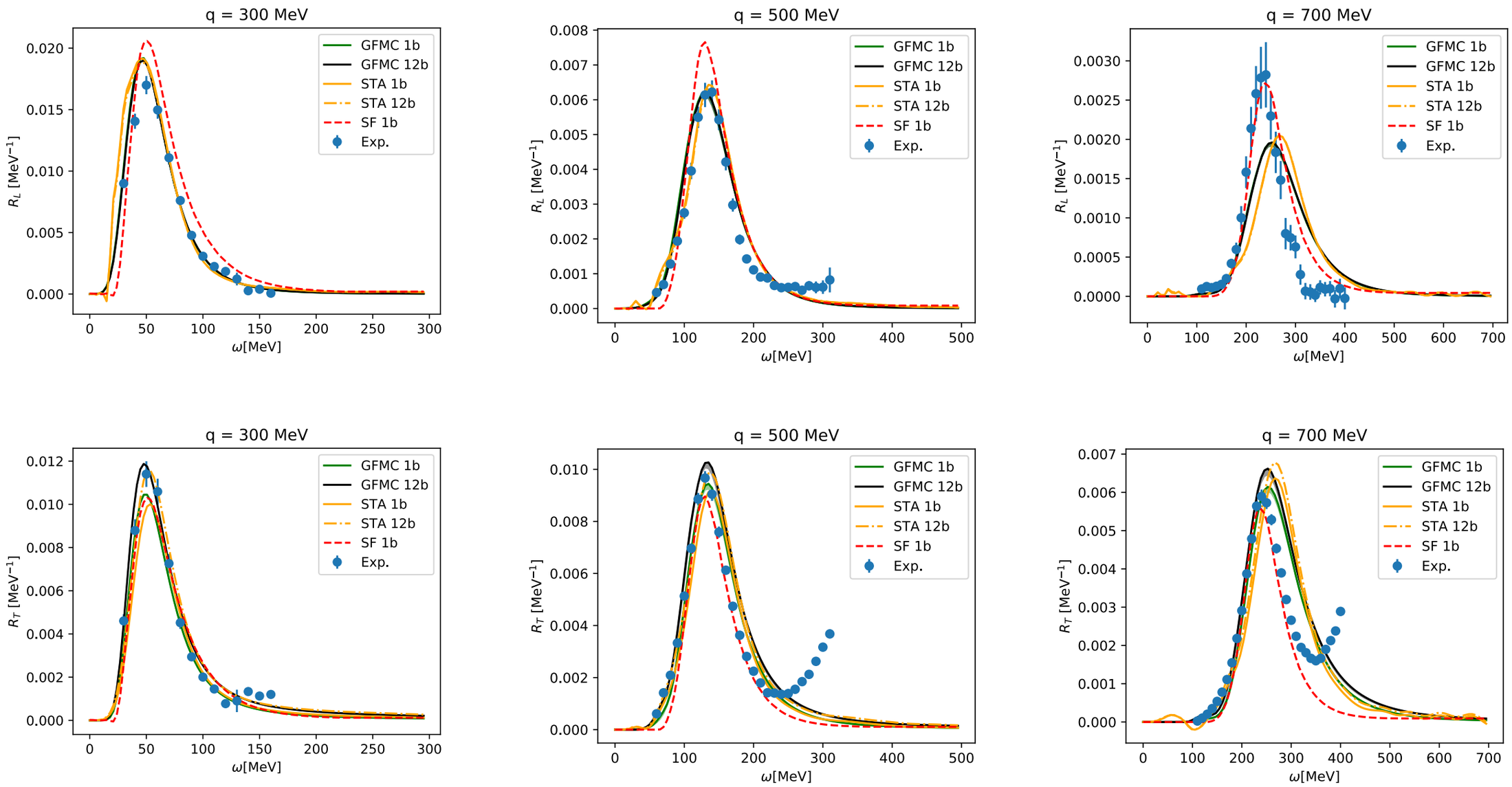
Benchmark

L.A., S. Pastore, N. Rocco, et al. PRC105(2022)014002

- We benchmarked three different methods based on the same description of nuclear dynamics of the initial target state
- Compared to the experimental data for the longitudinal and transverse electromagnetic response functions of ^{3}He, and the inclusive cross sections of both ^{3}He and ^{3}H
- Comparing the results allows for a precise quantification of the uncertainties inherent to factorization schemes

Benchmark

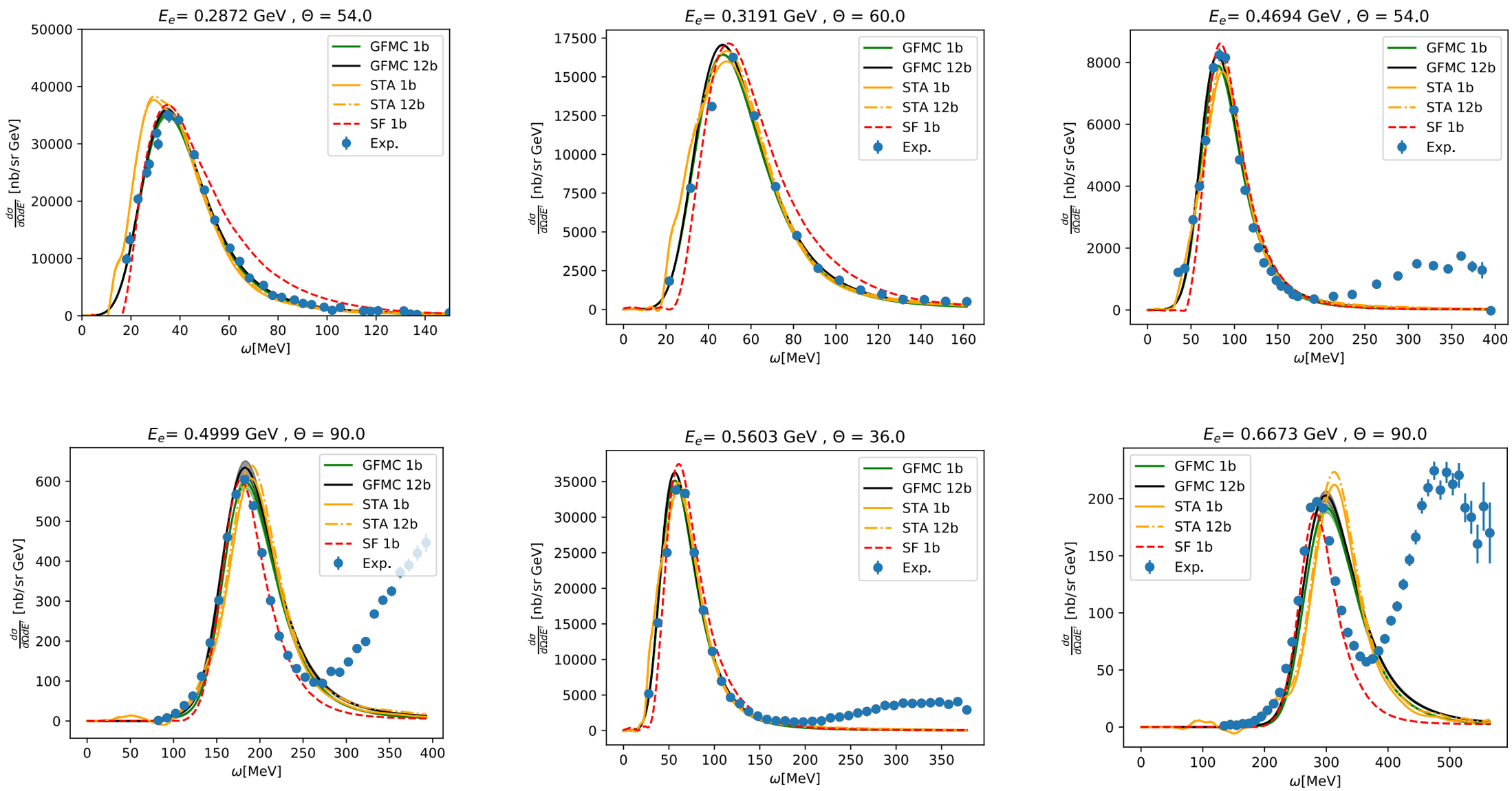
Longitudinal and transverse response function in ^{3}He



L.A., S. Pastore, N. Rocco, et al. PRC105(2022)014002

Cross sections

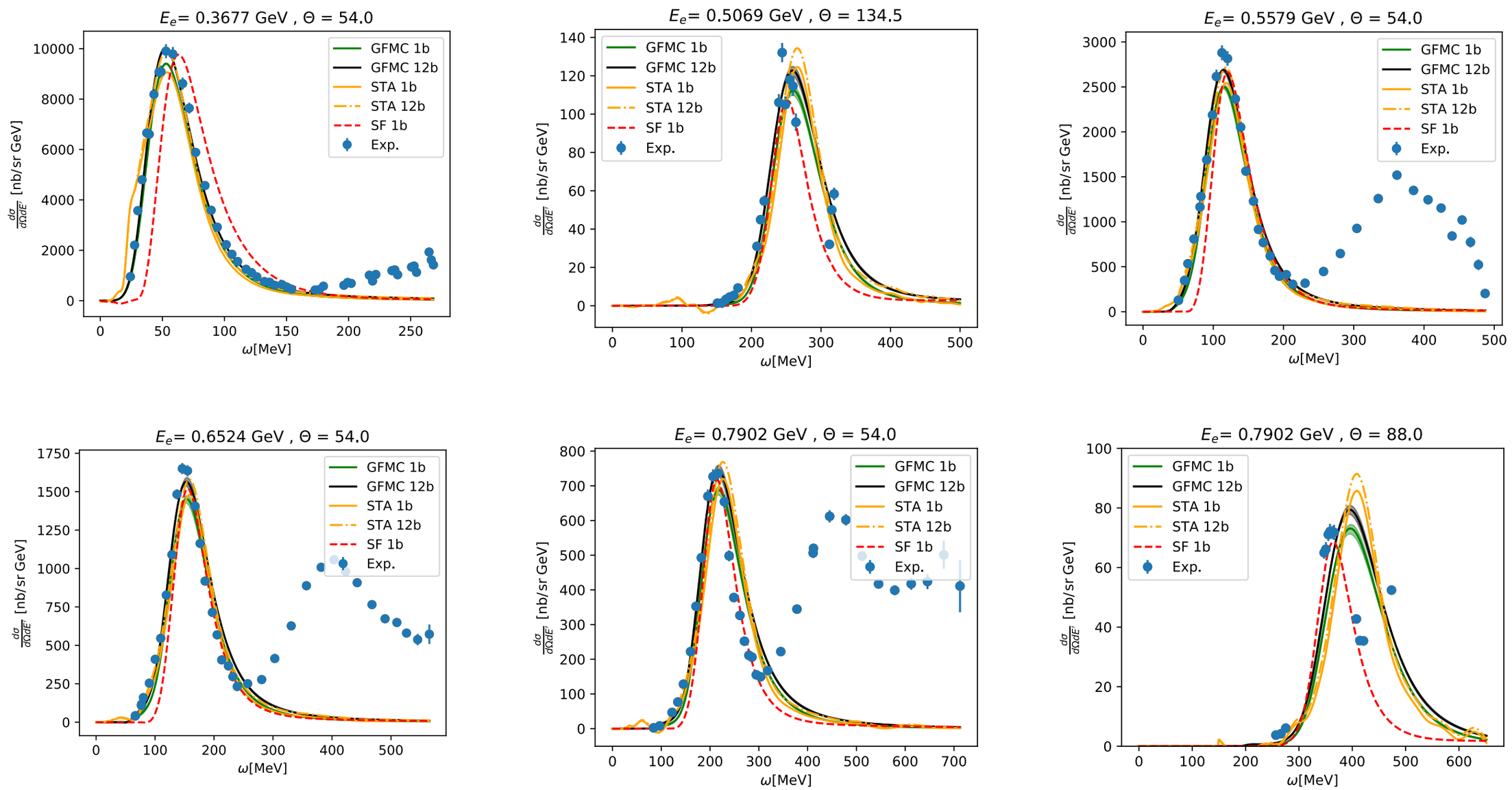
^{3}He



L.A., S. Pastore, N. Rocco, et al. PRC105(2022)014002

Cross sections

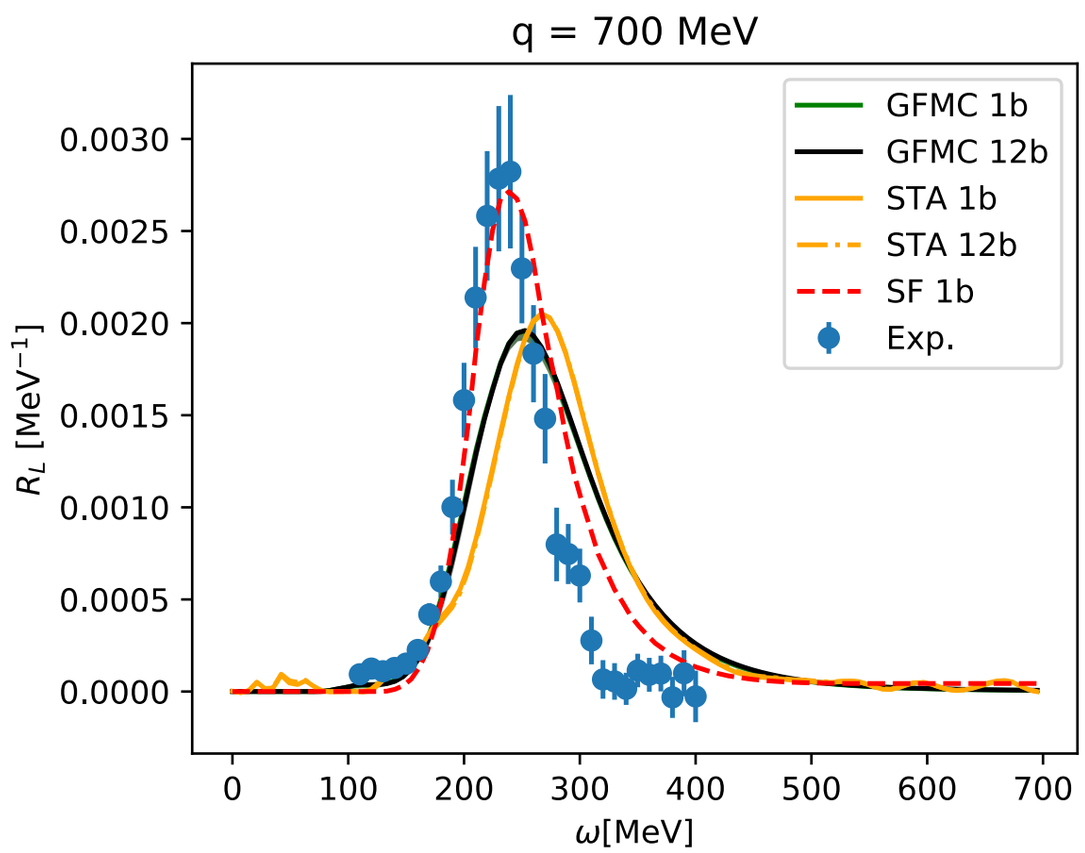
^{3}H



L.A., S. Pastore, N. Rocco, et al. PRC105(2022)014002

Relativistic corrections

Necessary to include relativistic correction at higher momentum q



L.A., S. Pastore, N. Rocco, et al. PRC105(2022)014002

Relativistic corrections

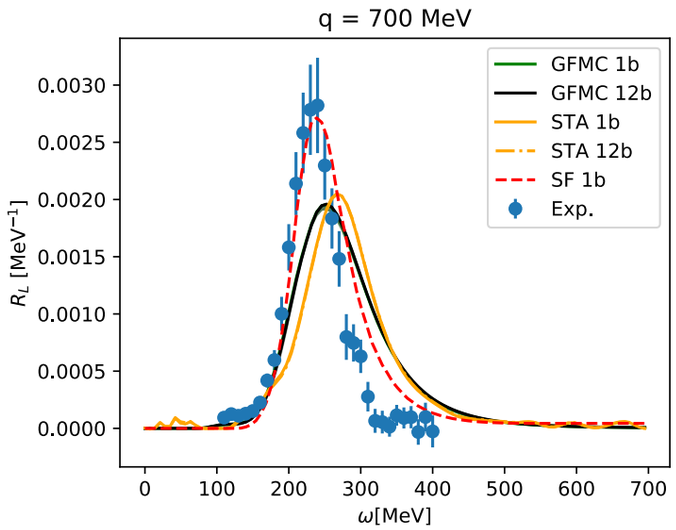
We are currently working on including relativistic corrections within the STA formalism:

R. Weiss, S. Pastore, J. Carlson

- Relativistic kinematic
- Relativistic currents

Relativistic corrections

- Relativistic kinematic
- Relativistic currents



$$E_{NR} \to E(\boldsymbol{p}, \boldsymbol{P}) = \sqrt{\left(\frac{\boldsymbol{P}}{2} - \boldsymbol{p}\right)^2 + m^2} + \sqrt{\left(\frac{\boldsymbol{P}}{2} + \boldsymbol{p}\right)^2 + m^2} - 2m = \sqrt{\frac{P^2}{4} - Pp\cos(\theta) + p^2 + m^2} + \sqrt{\frac{P^2}{4} + Pp\cos(\theta) + p^2 + m^2} - 2m$$

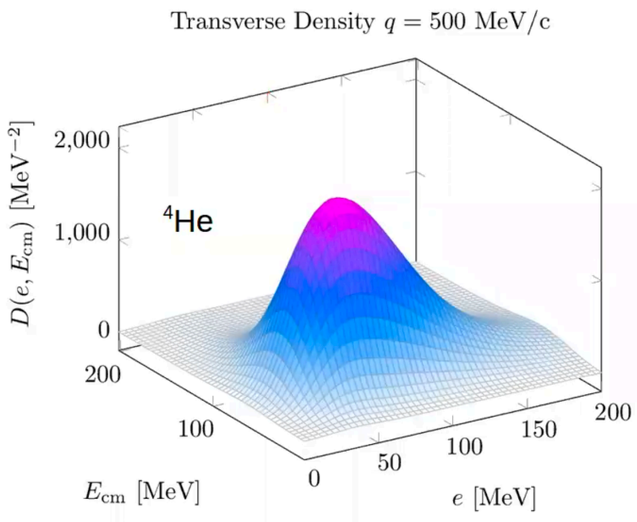
$$\begin{aligned} R_\alpha(\boldsymbol{q}, \omega) = & \\ & \cdots \\ & \cdots \\ & \cdots \\ & = \int \frac{d^3K}{(2\pi)^3} \int \frac{d^3k}{(2\pi)^3} \left[\sum_{M_i} \sum_{\alpha_{A-2}, \alpha} \int d^3R_{A-2} \left\langle \Psi_i \middle| O_L^\dagger(\boldsymbol{q}) \middle| \boldsymbol{K}\boldsymbol{k}\alpha, \boldsymbol{R}_{A-2}, \alpha_{A-2} \right\rangle \langle \boldsymbol{K}\boldsymbol{k}\alpha, \boldsymbol{R}_{A-2}, \alpha_{A-2} | O_R(\boldsymbol{q}) | \Psi_i \rangle \right] \delta(\omega + E_i - E(\boldsymbol{k}, \boldsymbol{K})) \end{aligned}$$

Heavier nuclei

Computational complexity of response functions and densities:

		^4He	^{12}C
Wave-function			
Spin	2^A	16	4096
Isospin	$\frac{A!}{Z!(A-Z)!}$	6	924
Pairs	$A(A-1)/2$	6	66

Response densities: E, e grid



$$R_\alpha(q,\omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i(\omega+E_i)t} \left\langle \Psi_i \middle| O_\alpha^\dagger(\mathbf{q}) e^{-iHt} O_\alpha(\mathbf{q}) \middle| \Psi_i \right\rangle$$

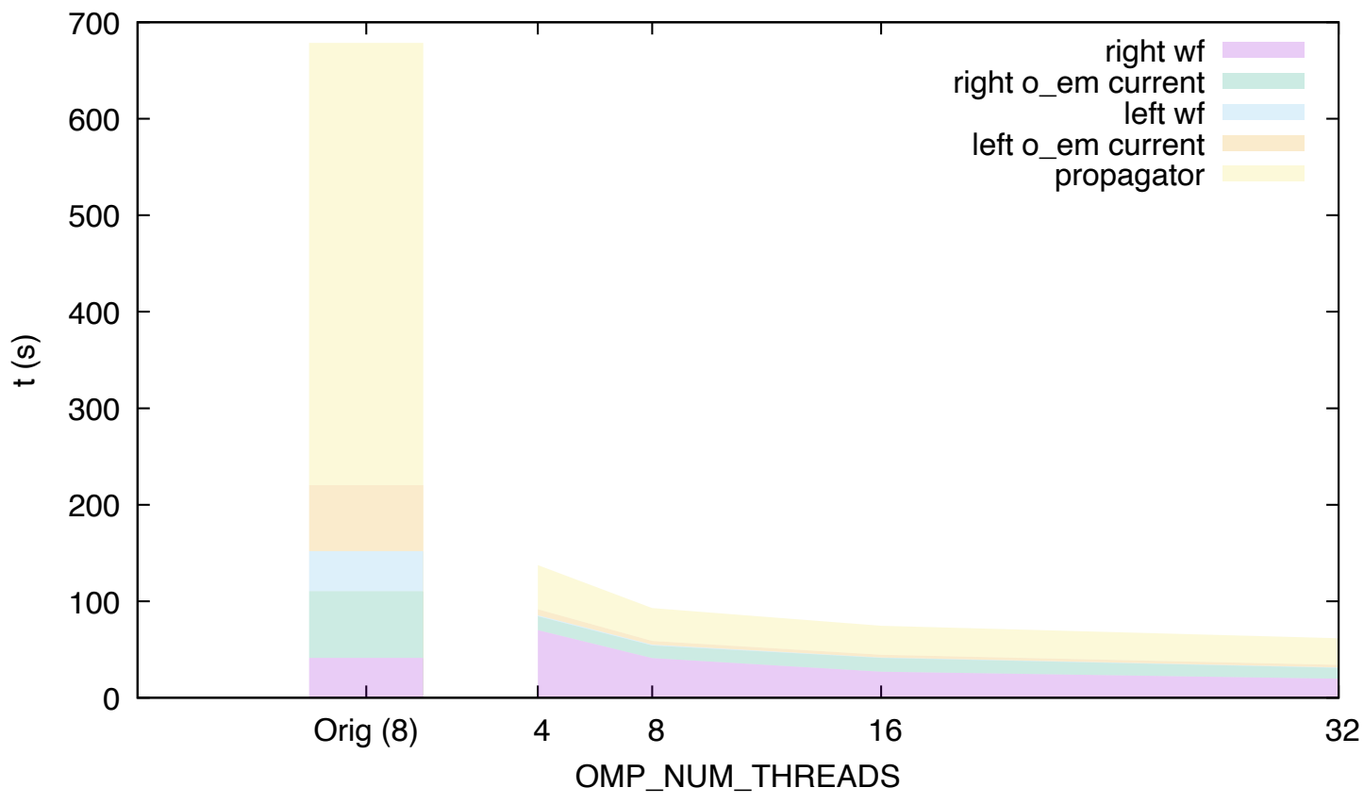
Heavier nuclei

Optimization was necessary to tackle heavier nuclei

$$R_\alpha(q,\omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i(\omega+E_i)t} \left\langle \Psi_i \middle| O_\alpha^\dagger(\mathbf{q}) e^{-iHt} O_\alpha(\mathbf{q}) \middle| \Psi_i \right\rangle$$

- Parallelization - MPI and OpenMP:
  Variational Monte Carlo is almost perfectly parallelizable, but with increased system size memory becomes a constrain
- Refactoring of the code
- Computational algorithms and approximations:
  variation of integration ranges *(r, R)* for struck nucleon pair

Heavier nuclei: ^{12}C



Optimization specific to ^{12}C was needed in oder to perform full response densities calculations:

- **parallelization**
- **refactoring of the code**
- **reduction of memory usage**
- computational algorithms and approximations

$$R_\alpha(q,\omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i(\omega+E_i)t} \langle \Psi_i | O_\alpha^\dagger(\mathbf{q}) e^{-iHt} O_\alpha(\mathbf{q}) | \Psi_i \rangle$$

Heavier nuclei

Comparison for ^3H, 72k MC configurations, 40x40 points in r, R integration

Original:

- ~15k core hours
  (LA et al arXiv:2108.10824)

After optimization:

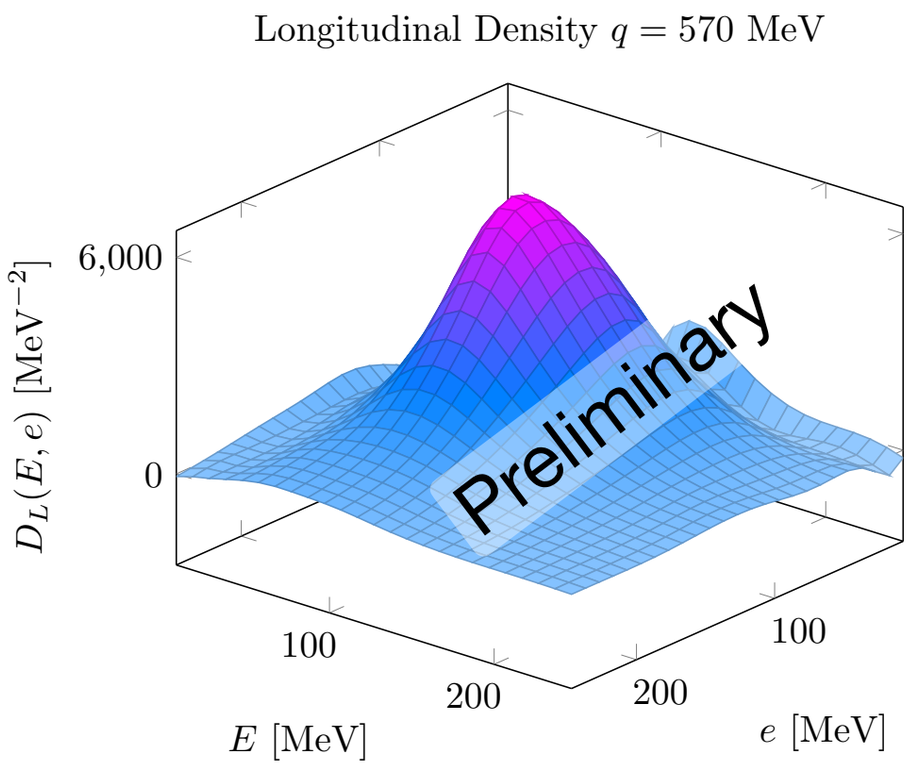
- ~1.8k core hours

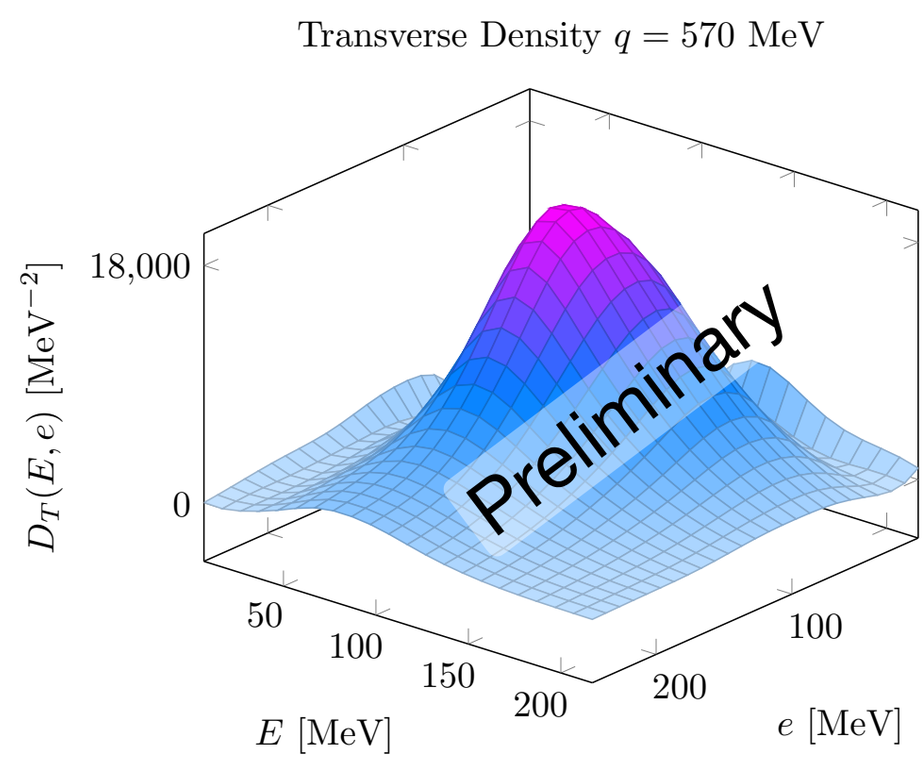
Additional approximations reduce the computation time:

r, R integration up to 8, 5 fm

reduction of grid spacing in relative energy *e*

Response densities for ^{12}C

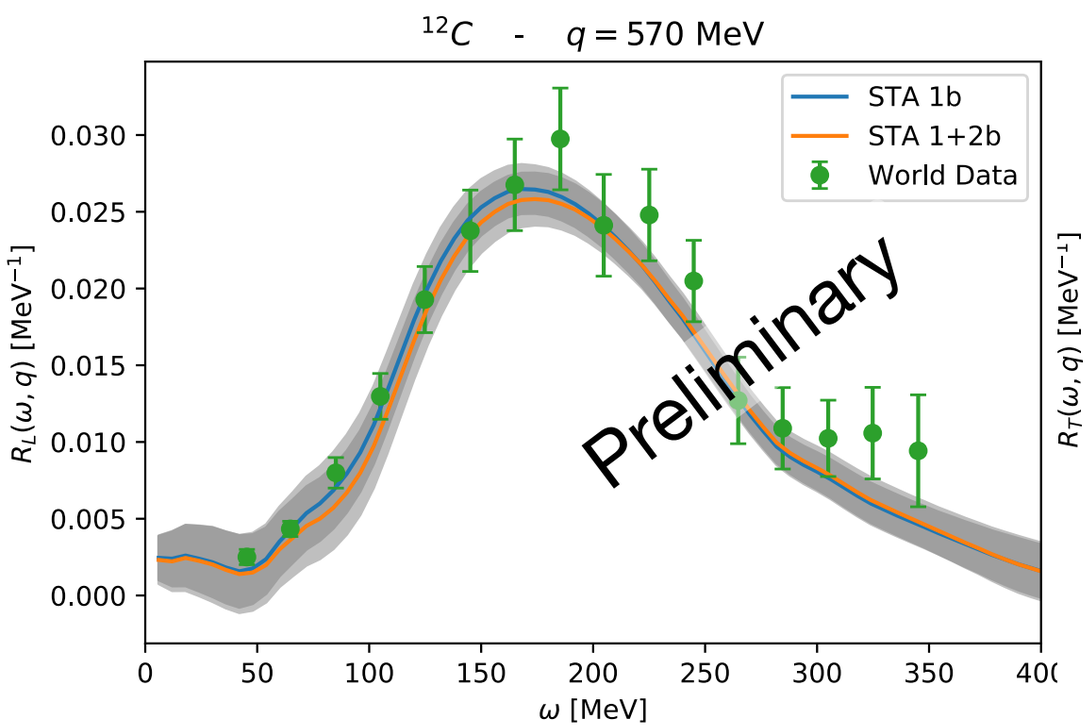


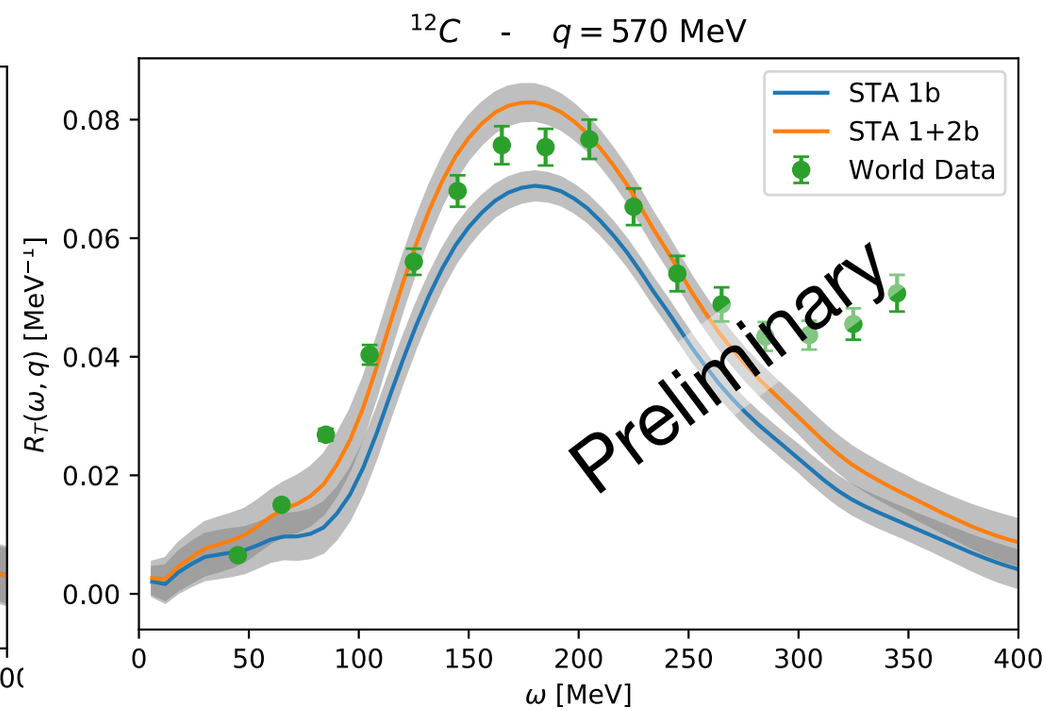


Longitudinal and transverse response densities in ^{12}C

q = 570 MeV

Response functions for ^{12}C



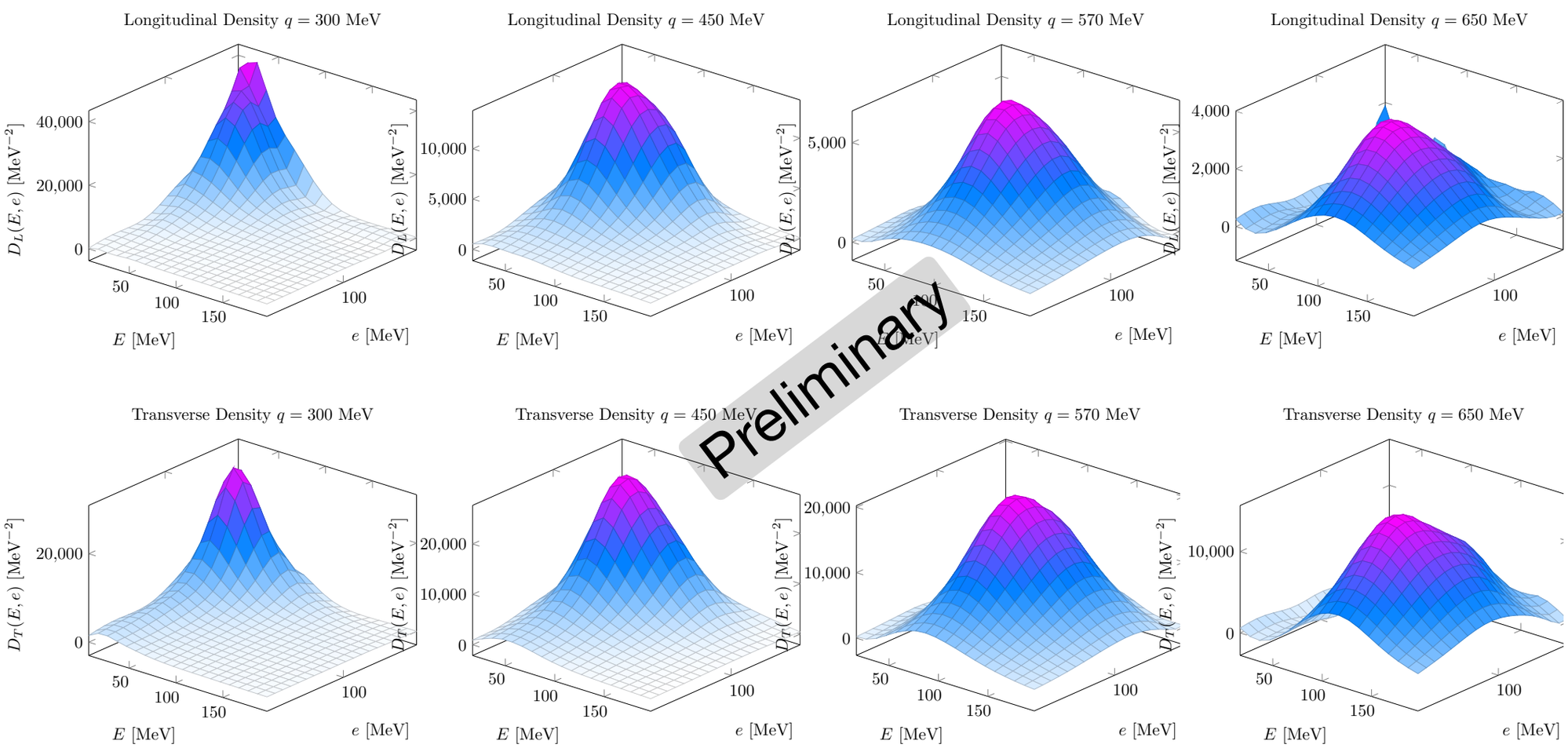


Preliminary results for longitudinal and transverse response functions in ^{12}C

q = 570 MeV

Responses for ^{12}C

Longitudinal and transverse response for **300 < q < 650 MeV**:



Cross sections: Interpolation schemes

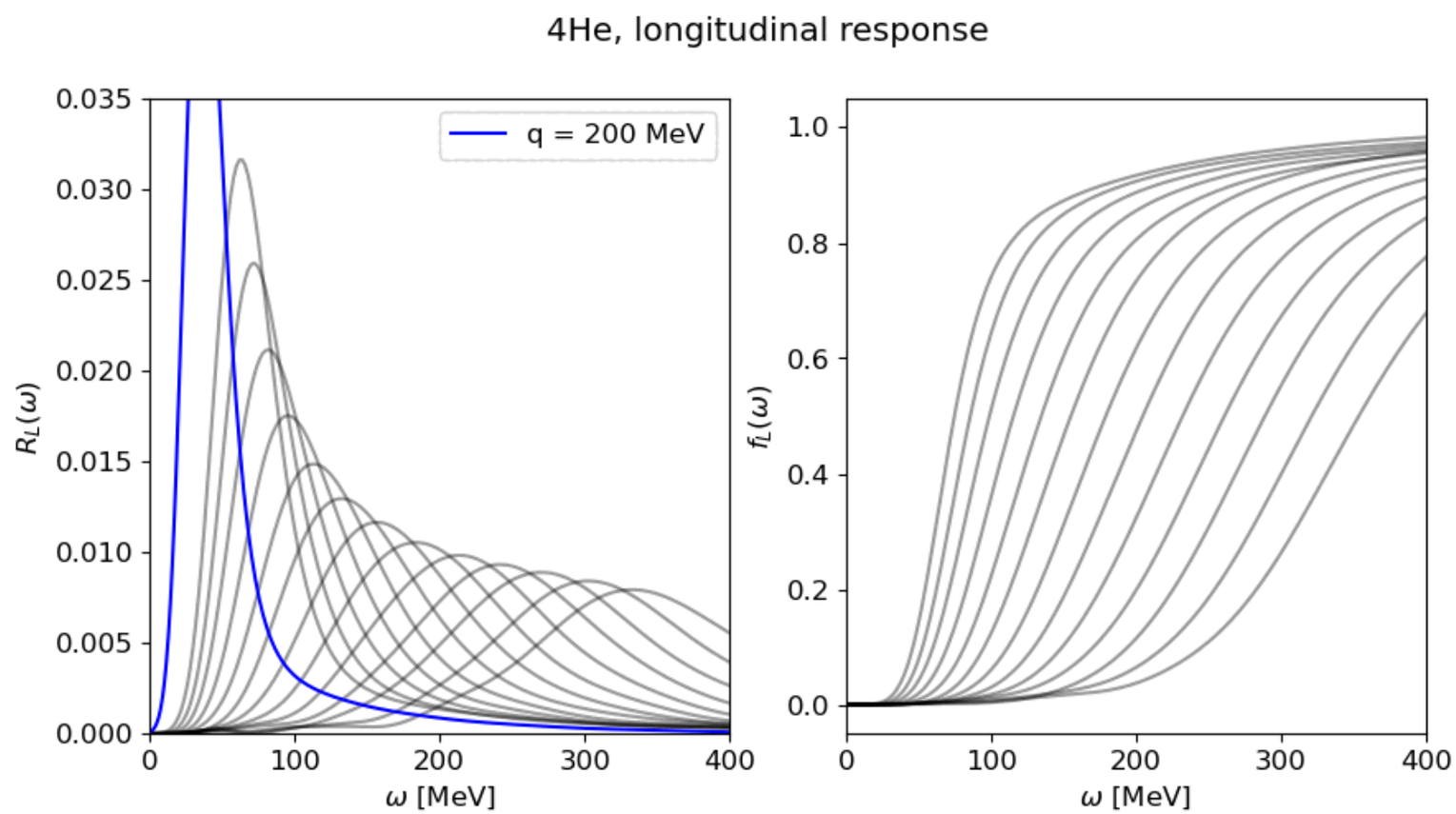
- Cross sections weakly dependent on interpolation scheme in 4He, but relevant in 12C
- We tested various interpolation schemes on 4He, where we can evaluate responses for an arbitrary fine grid of values of q.

Cross sections: Interpolation schemes

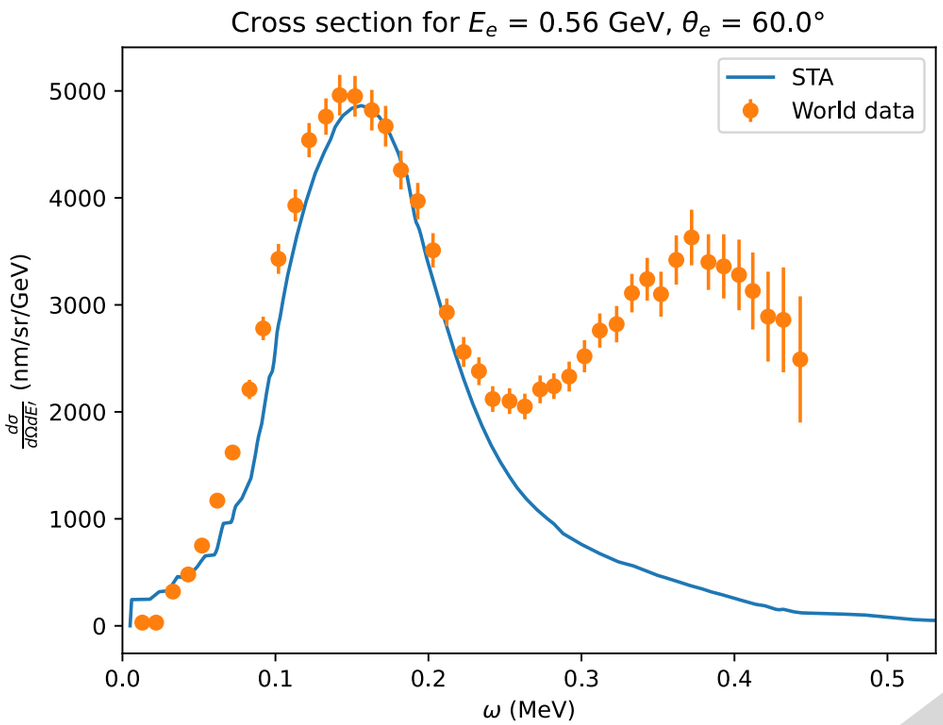
- We **interpolate** in between cumulative integrals of responses, using information from the sum rules

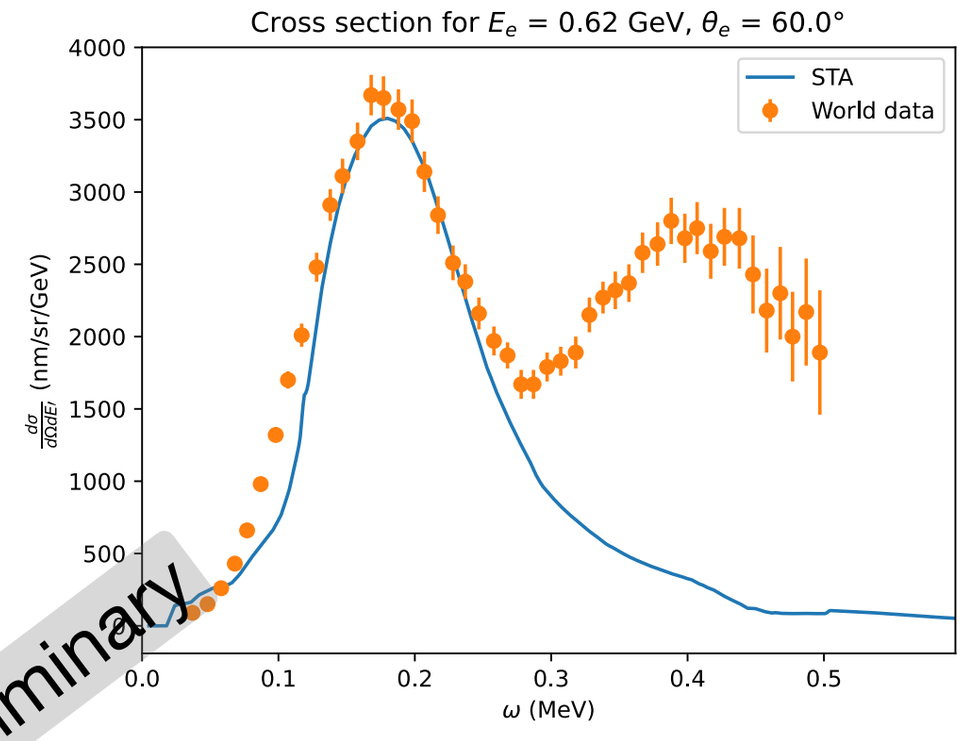
- Outside the range (q < 300 MeV and q > 650 MeV), we use **scaling functions**

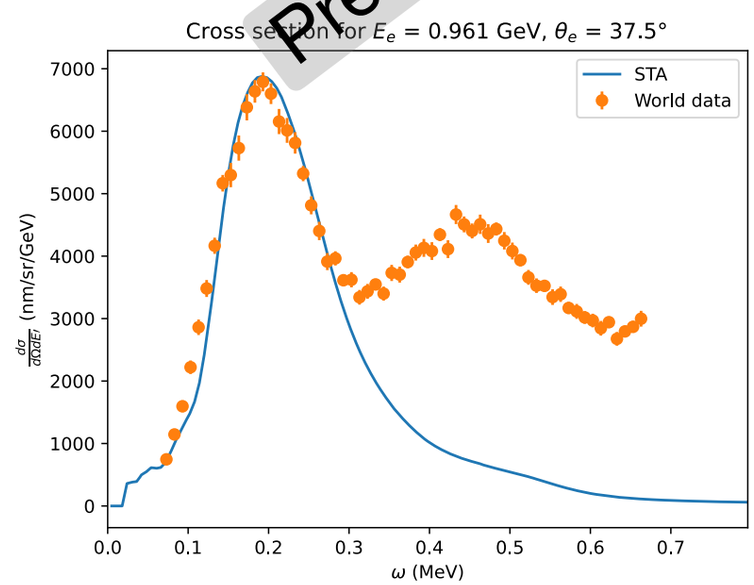
$$\psi'_{\rm nr} = \frac{m_N}{|\mathbf{q}|k_F}\left(\omega - \frac{|\mathbf{q}|^2}{2m_N} - \varepsilon\right)$$



Cross sections results







Conclusion:

- The STA responses for 12C are in good agreement with the data
- Given the computational complexity of evaluating cross sections, a novel interpolation scheme was adopted for the calculation of cross sections

EW interactions:

- The current work on EM interactions allows for a thorough evaluation of the method, and a comparison with the abundant experimental data for electron-nucleus scattering
- Use of information from response densities in event generators.

Collaborators:

S. Pastore, M. Piarulli

Thank you!

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URA

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