Quantum Monte Carlo calculations of lepton-nucleus scattering in the Short-Time Approximation and uncertainty quantification

Theoretical Physics Uncertainties to Empower Neutrino Experiments

INT WORKSHOP INT-23-86W

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Quantum Monte Carlo Group @ WashU

Garrett King (GS) Jason Bub (GS)

Lorenzo Andreoli (PD)

Anna McCoy

Maria Piarulli and Saori Pastore

Washington University in St. Louis

Lorenzo Andreoli

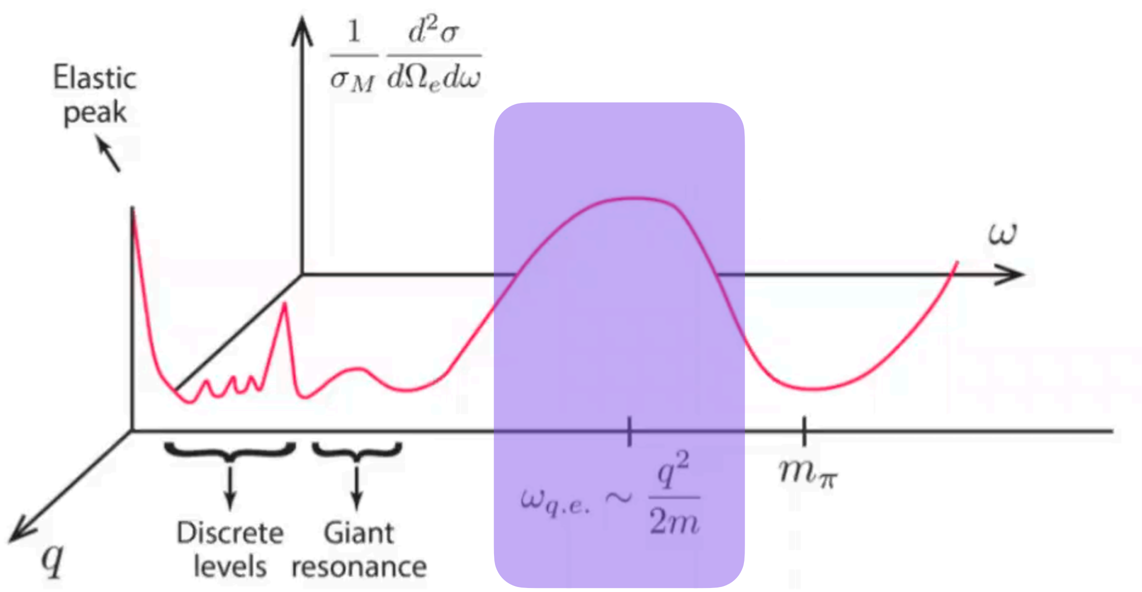
Outline

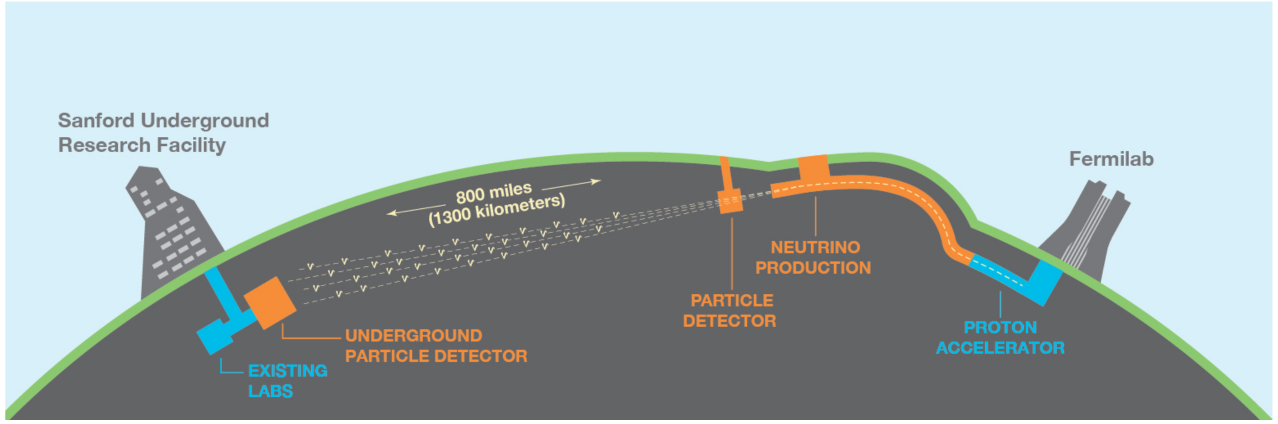
- Quasielastic lepton-nucleus scattering
- Ab initio description of nuclei:
  - Nuclear interaction
  - Electroweak interaction of leptons with nucleons and clusters of correlated nucleons
  - Variational Monte Carlo
- Short-time approximation
- Results
- Conclusions and outlook

Electron-nucleus scattering

Theoretical understanding of nuclear effects is extremely important for neutrino experimental programs: oscillation experiments require accurate calculations of cross sections

Electron scattering can be used to test our nuclear model (same nuclear effects, no need to reconstruct energies, abundant experimental data)





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

Many-body nuclear interaction

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

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

Quantum Monte Carlo method:
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

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

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

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

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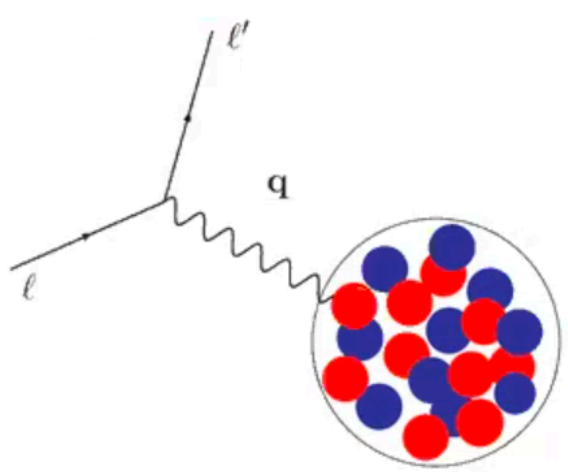
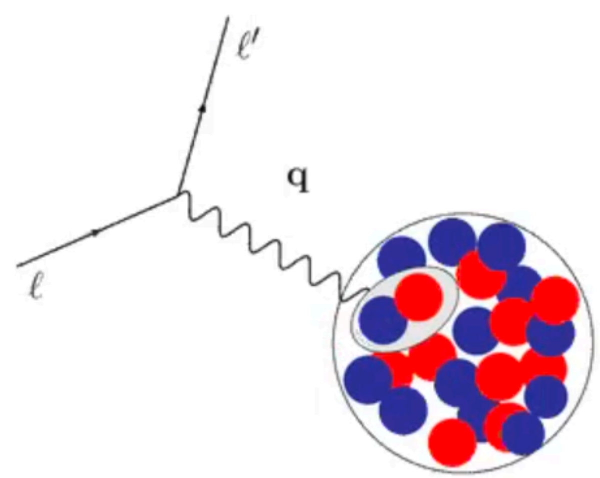
Electromagnetic interactions

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

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

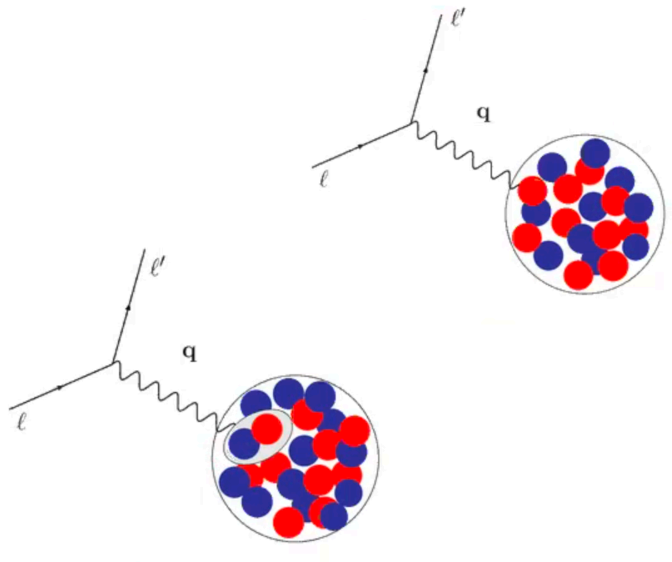
Current operators

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

Two-body currents are a manifestation of two-nucleon correlations

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 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

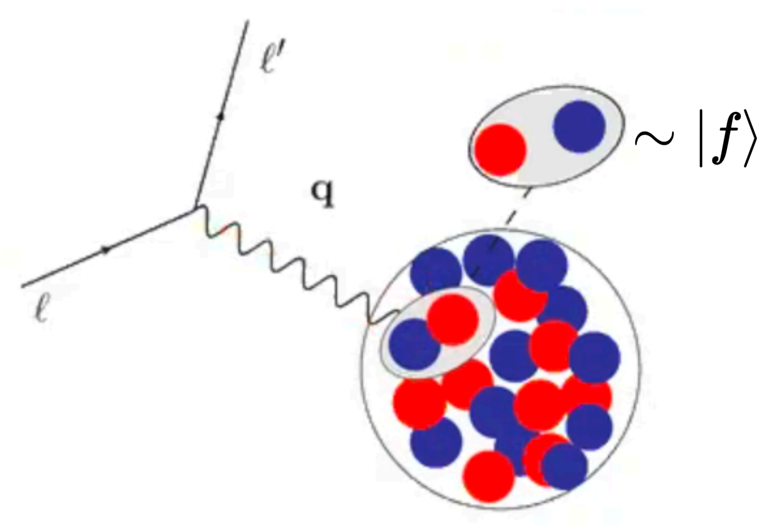


Carlson, Schiavilla 1992. Marcucci et al. 2005

Short-time approximation

S. Pastore, J. Carlson, S. Gandolfi, R. Schiavilla, and R. B. Wiringa PRC101(2020)044612

Quasielastic inclusive scattering cross sections are expressed in terms of response functions



Response functions

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

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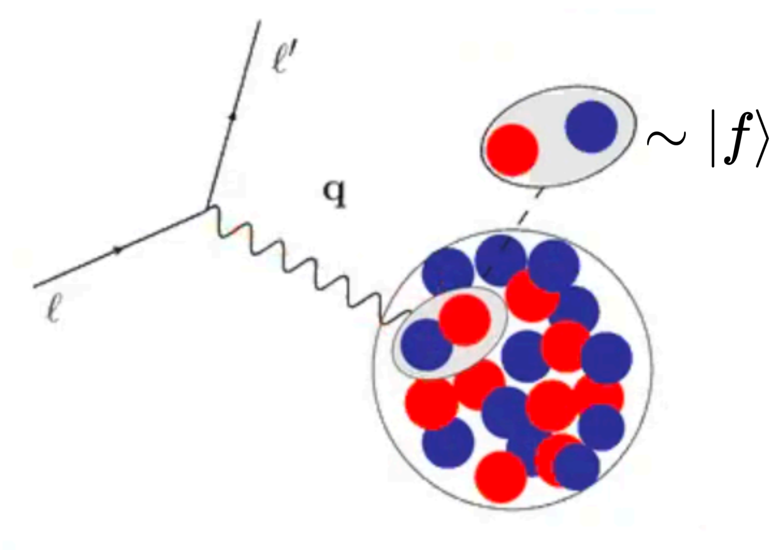

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The sum over all final states is replaced by a two nucleon propagator

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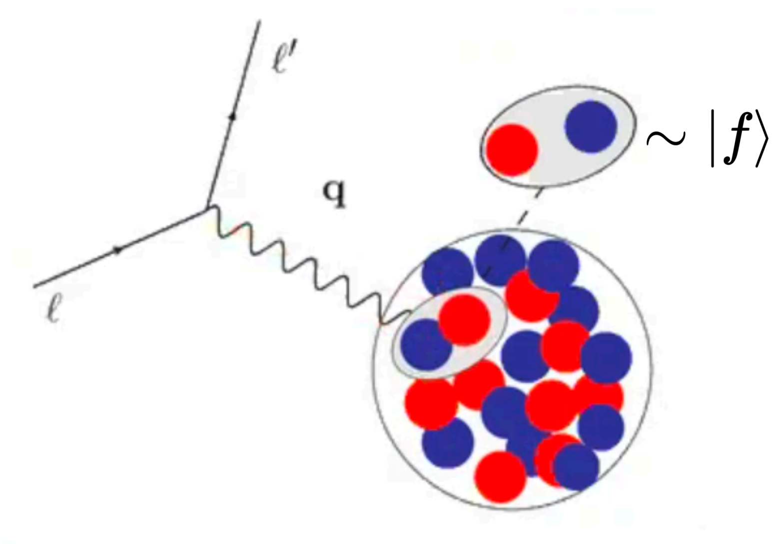

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$$\begin{aligned} O^\dagger e^{-iHt} O &= \left(\sum_i O_i^\dagger + \sum_{i<j} O_{ij}^\dagger \right) e^{-iHt} \left(\sum_{i'} O_{i'} + \sum_{i'<j'} O_{i'j'} \right) \\ &= \sum_i O_i^\dagger e^{-iHt} O_i + \sum_{i \neq j} O_i^\dagger e^{-iHt} O_j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

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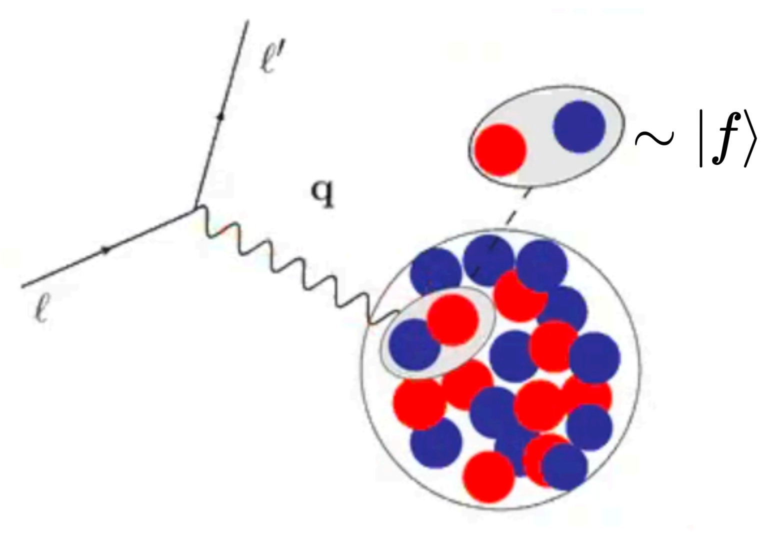

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Response densities

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

STA: scattering of external probes from pairs of correlated nucleons

Validity of the Short Time Approximation

Pastore et al. PRC101(2020)044612

If one expands the propagator to second order

$$e^{-iHt} \approx 1 - i\left(\sum_i T_i + \sum_{ij} V_{ij}\right) t - \frac{1}{2}\left(\sum_i T_i + \sum_{ij} V_{ij}\right)\left(\sum_{i'} T_{i'} + \sum_{i'j'} V_{i'j'}\right) t^2 + \dots$$

And notes that in light nuclei $\frac{T}{A} \sim \frac{2|V|}{A(A-1)} \equiv \epsilon_{\rm nuc}$ we have an energy (and thus time) scale associated with including correlations of A nucleons which is ~20 MeV per nucleon

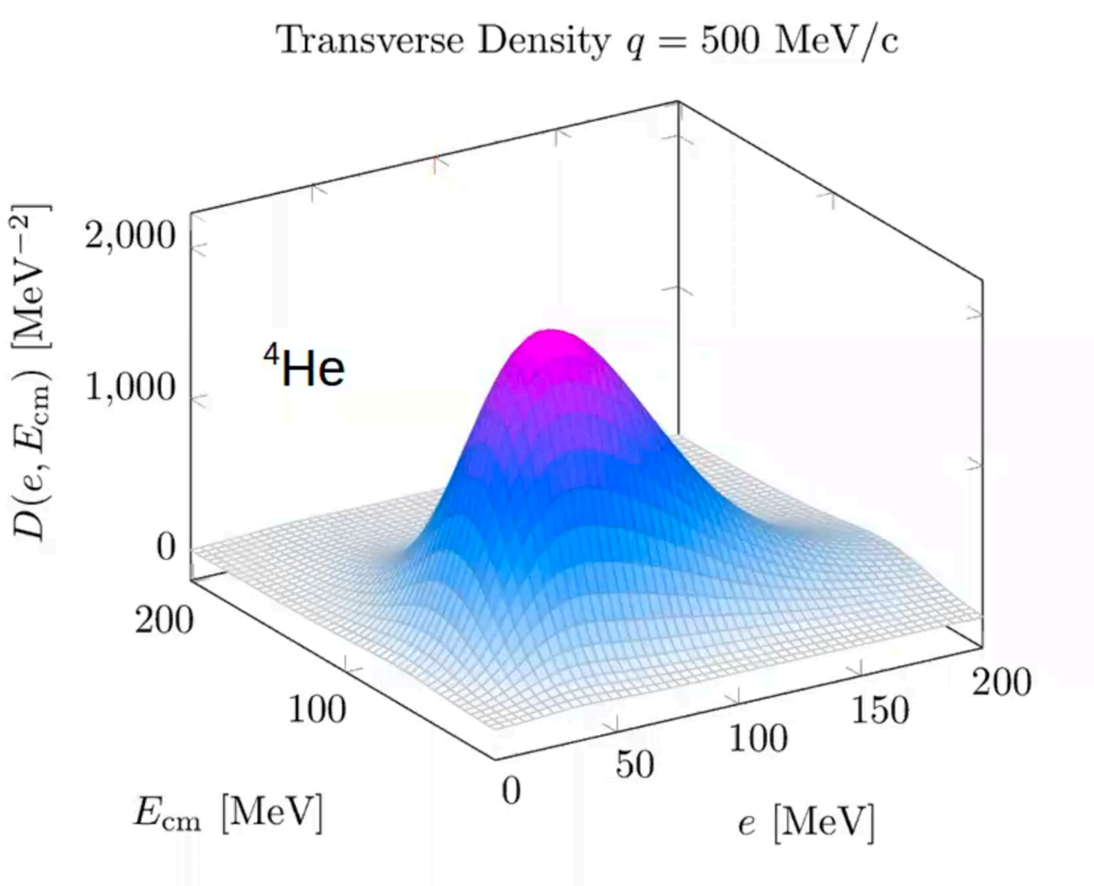
This gives a way to estimate the impact on the description of the quasi-elastic peak $\omega_{qe} = \sqrt{m^2 + q^2} - m$

In the STA, one drops terms of order $\mathcal{O}\left(\frac{\epsilon^2_{\rm nuc}}{\omega^2_{qe}}\right)$ so it is valid at sufficiently high ω and |**q**| w.r.t. epsilon nuc

Consistent with the notion that there is a high probability for the correlated pair to absorb the entirety of |**q**| when the final state mometa are far from the Fermi surface

One may note that the PWIA comes from dropping terms of order $\mathcal{O}\left(\frac{\epsilon_{\rm nuc}}{\omega_{qe}}\right)$

Transverse response density

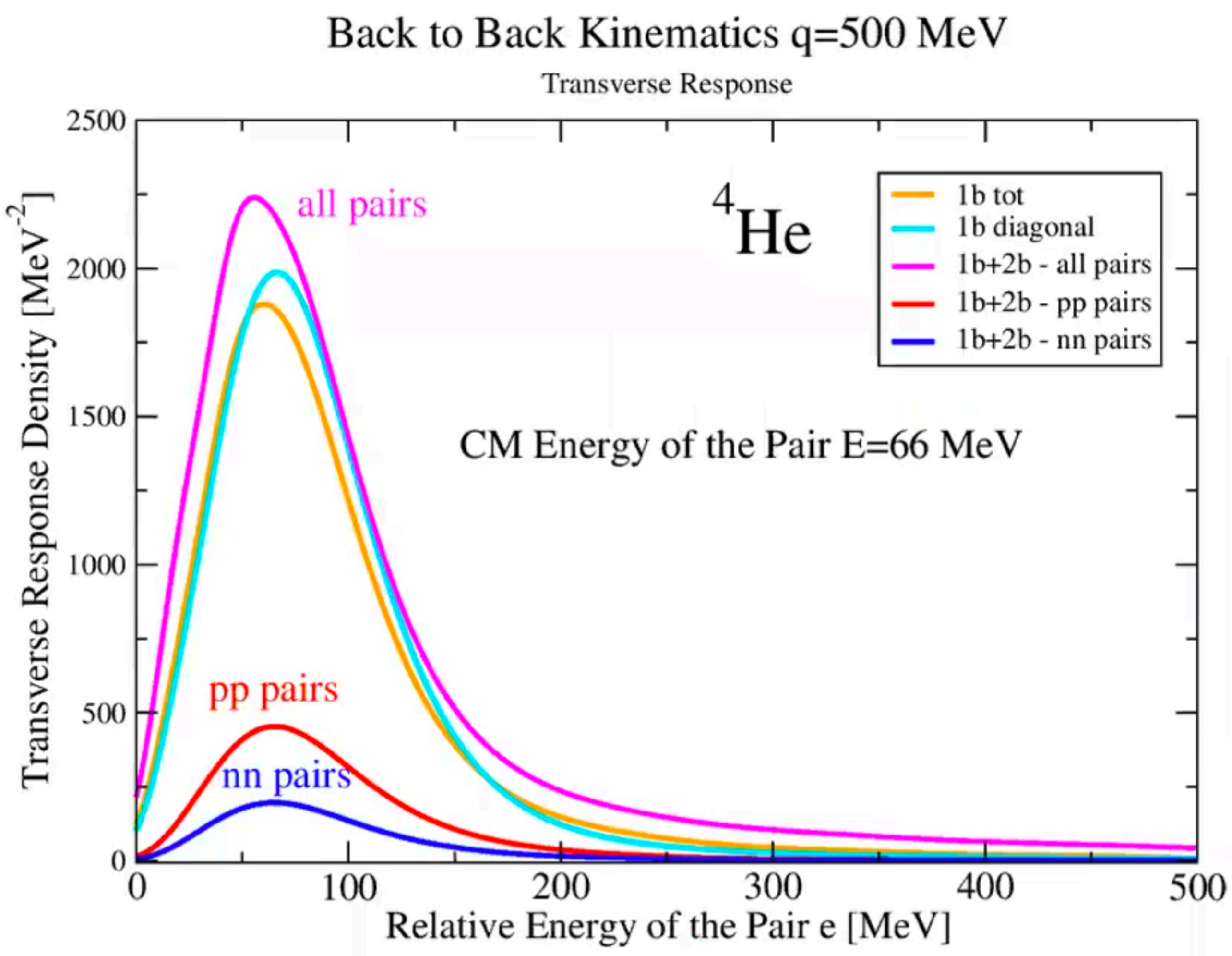


Electron scattering from ^4He in the STA:

- Provides "more" exclusive information in terms of nucleon-pair kinematics via the Response Densities as functions 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

Benchmark

L.A, J. Carlson, A. Lovato, S. Pastore, N. Rocco, RB Wiringa 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

L.A. et al. PRC105(2022)014002

Green's function Monte Carlo

$$|\Psi_0\rangle \propto \lim_{\tau\to\infty} \exp[-(H-E_0)\tau]|\Psi_T\rangle$$

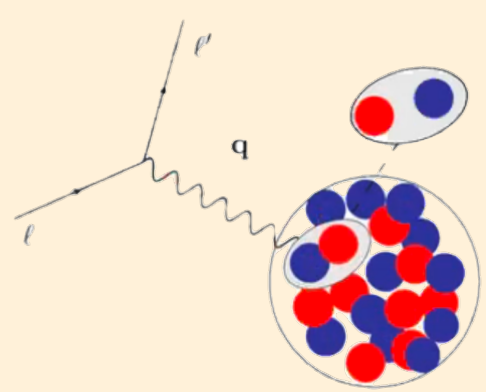
$$E_\alpha(\mathbf{q},\tau) = \int_{\omega_{\rm th}}^{\infty} d\omega e^{-\omega\tau} R_\alpha(\mathbf{q},\omega), \quad \alpha = L, T$$

$$E_\alpha(\mathbf{q},\tau) = \left\langle \Psi_0 \middle| J_\alpha^\dagger(\mathbf{q}) e^{-(H-E_0)\tau} J_\alpha(\mathbf{q}) \middle| \Psi_0 \right\rangle - |F_\alpha(\mathbf{q})|^2 e^{-\omega_{el}\tau}$$

Stort-time approximation

$$R_\alpha(\mathbf{q},\omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} \mathrm{e}^{i(\omega+E_0)t} \times \left\langle \Psi_0 \middle| J_\alpha^\dagger(\mathbf{q}) \mathrm{e}^{-iHt} J_\alpha(\mathbf{q}) \middle| \Psi_0 \right\rangle$$

$$J^\dagger \mathrm{e}^{-iHt} J = \sum_i J_i^\dagger \mathrm{e}^{-iHt} J_i + \sum_{i\neq j} J_i^\dagger \mathrm{e}^{-iHt} J_j + \sum_{i\neq j} \left(J_i^\dagger \mathrm{e}^{-iHt} J_{ij} + J_{ij}^\dagger \mathrm{e}^{-iHt} J_i + J_{ij}^\dagger \mathrm{e}^{-iHt} J_{ij} \right) + \cdots$$



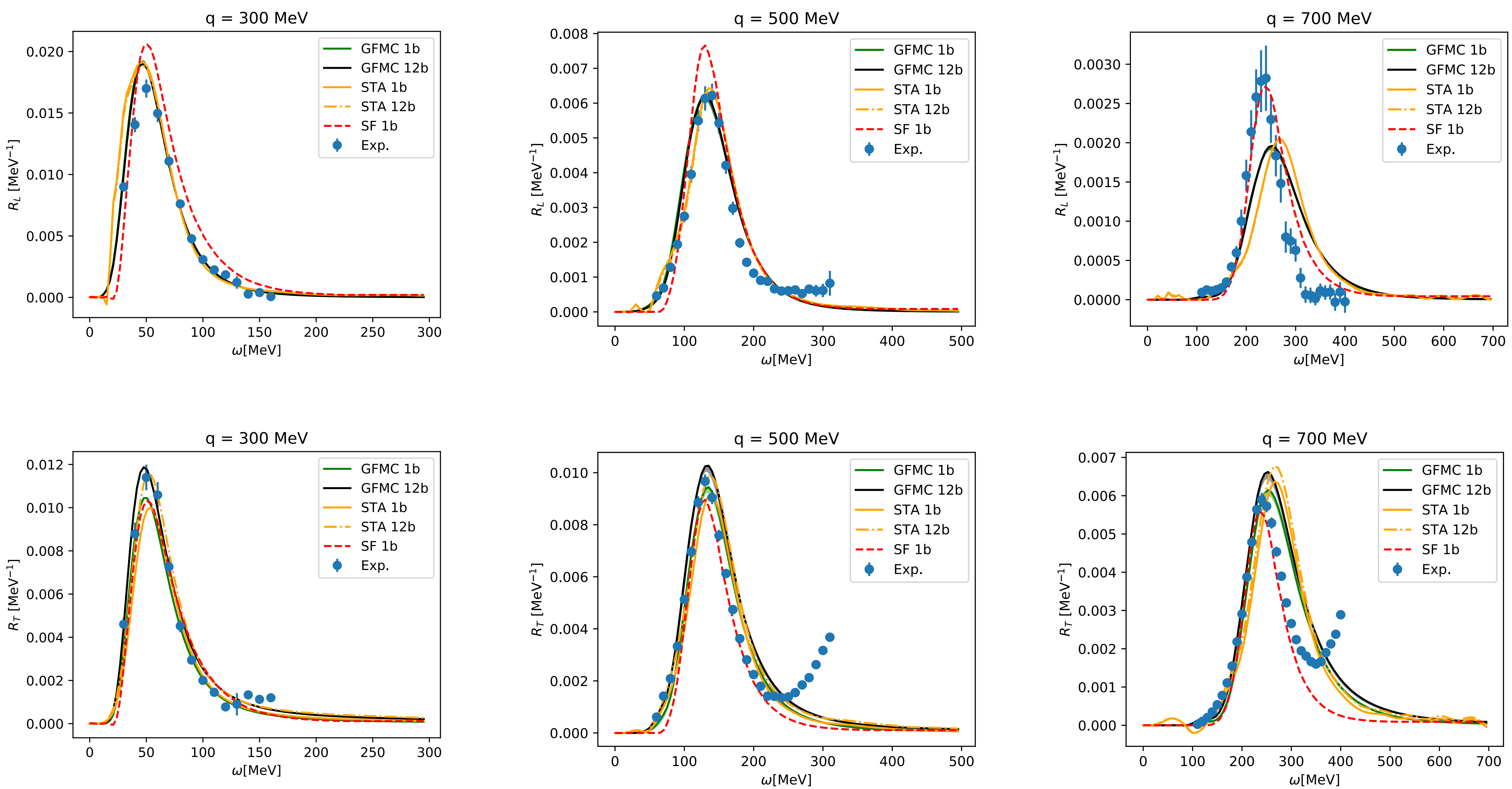
Spectral function

$$|\Psi_f\rangle = |\mathbf{p}\rangle \otimes \left|\Psi_n^{A-1}\right\rangle$$

$$R_\alpha(\mathbf{q},\omega) = \sum_{\tau_k=p,n} \int \frac{d^3k}{(2\pi)^3} dE[P_{\tau_k}(\mathbf{k},E) \times \frac{m_N^2}{e(\mathbf{k})e(\mathbf{k}+\mathbf{q})} \sum_i \left\langle k \middle| j_{i,\alpha}^\dagger \middle| k+q \right\rangle \langle p | j_{i,\alpha} | k \rangle \times \delta(\tilde{\omega} + e(\mathbf{k}) - e(\mathbf{k}+\mathbf{q}))]$$

Benchmark

Longitudinal and transverse response function in ^{3}He



L.A. et al. PRC105(2022)014002

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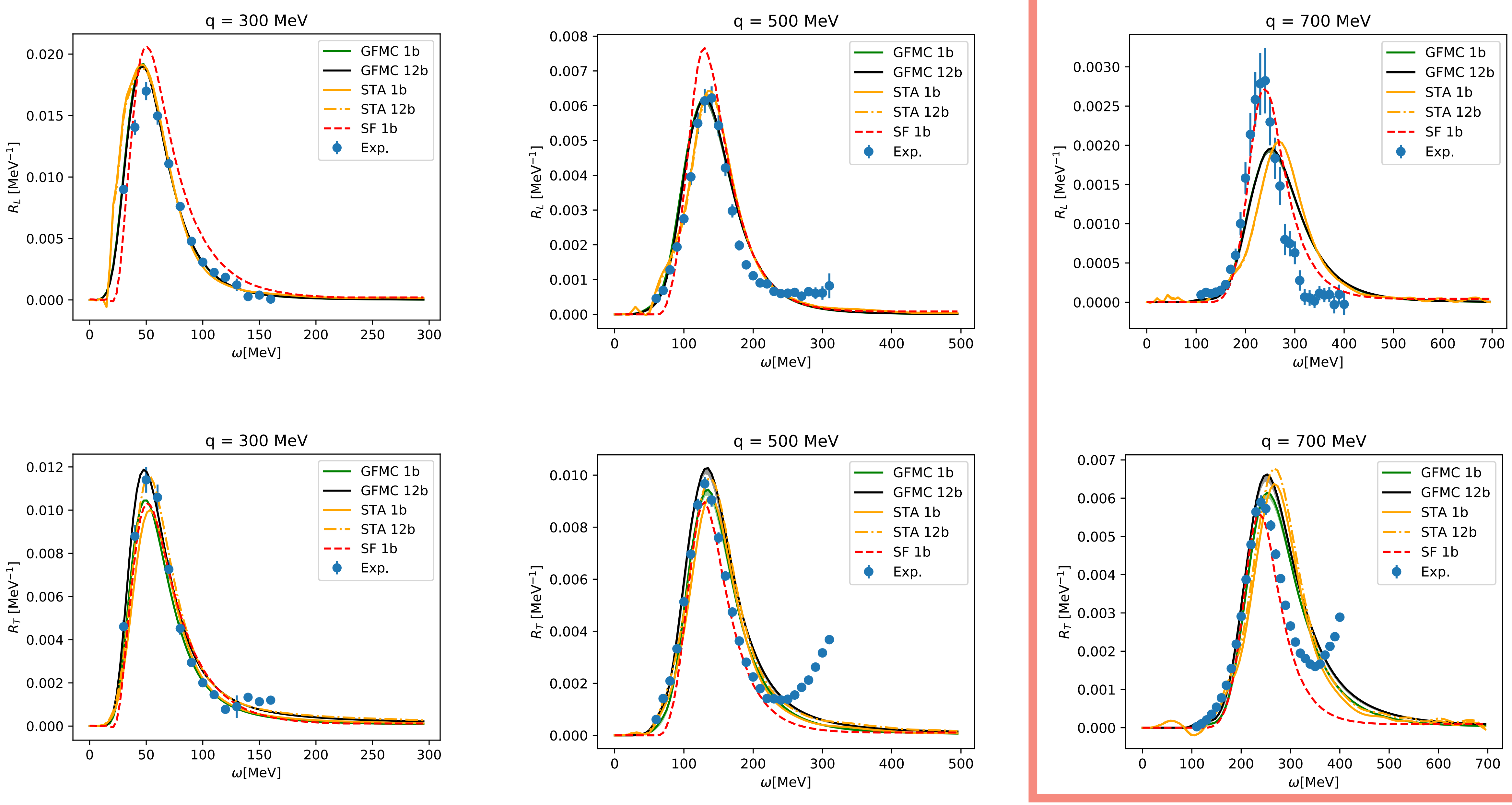

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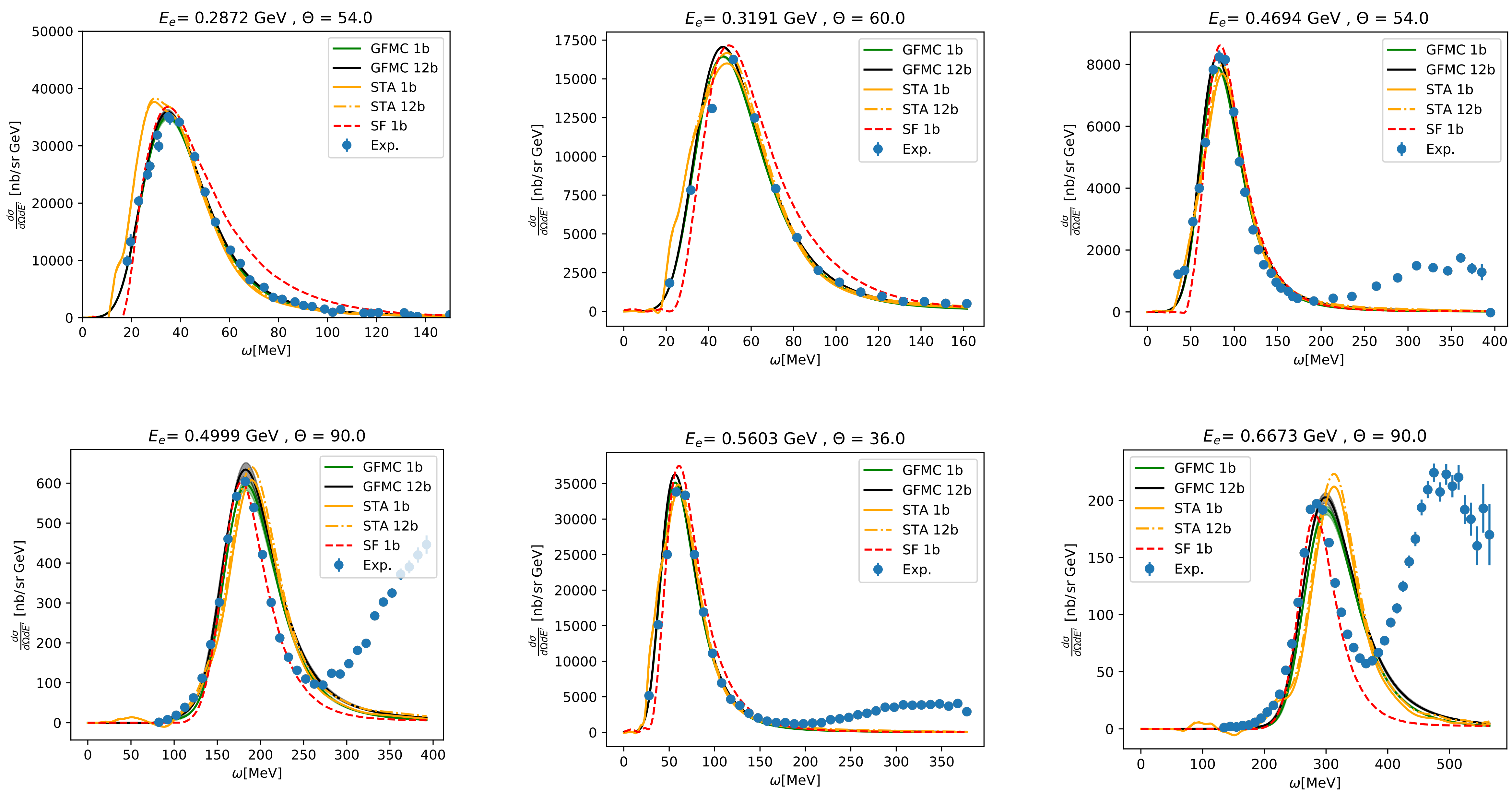
Cross sections

^{3}He



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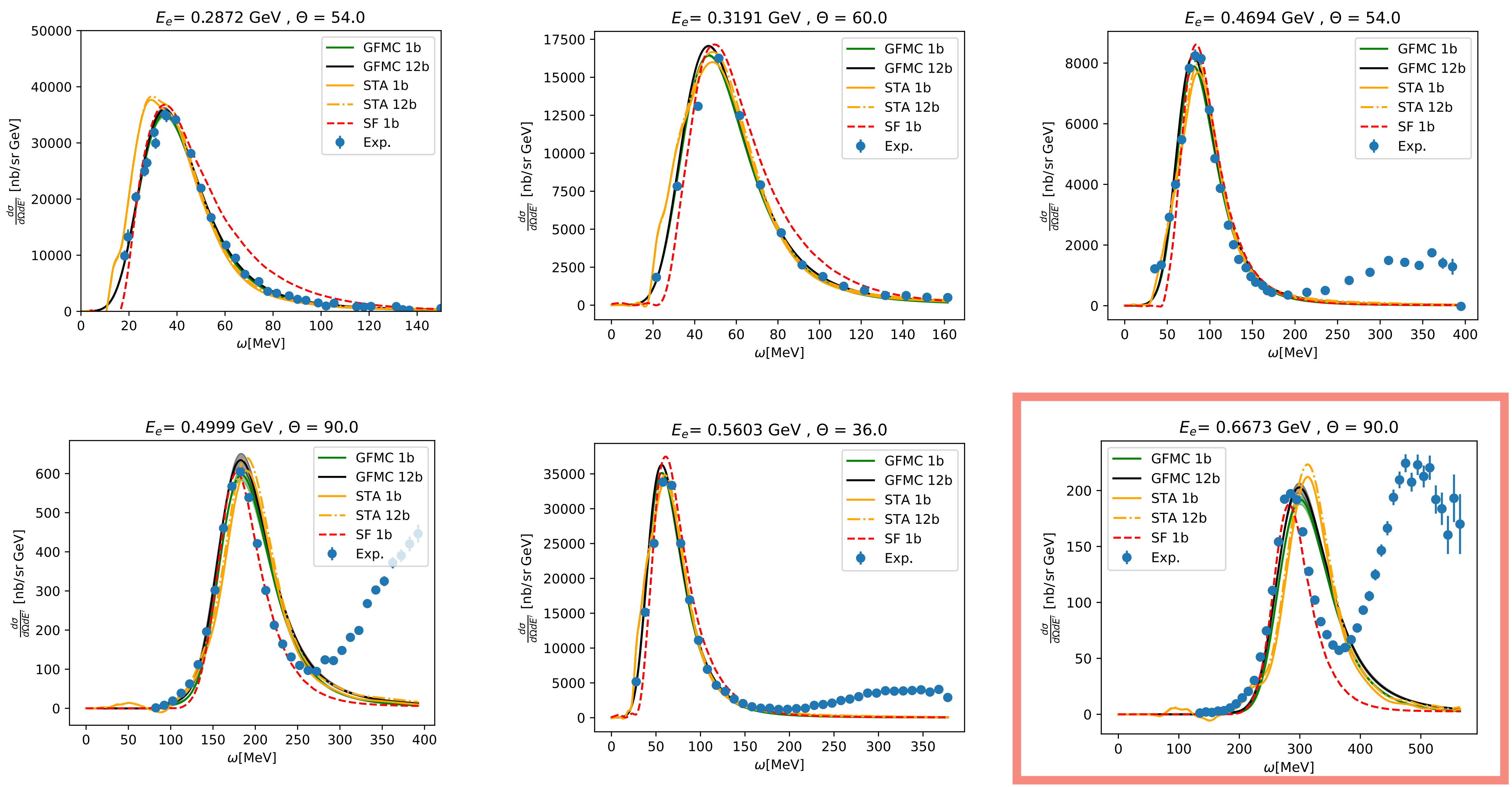

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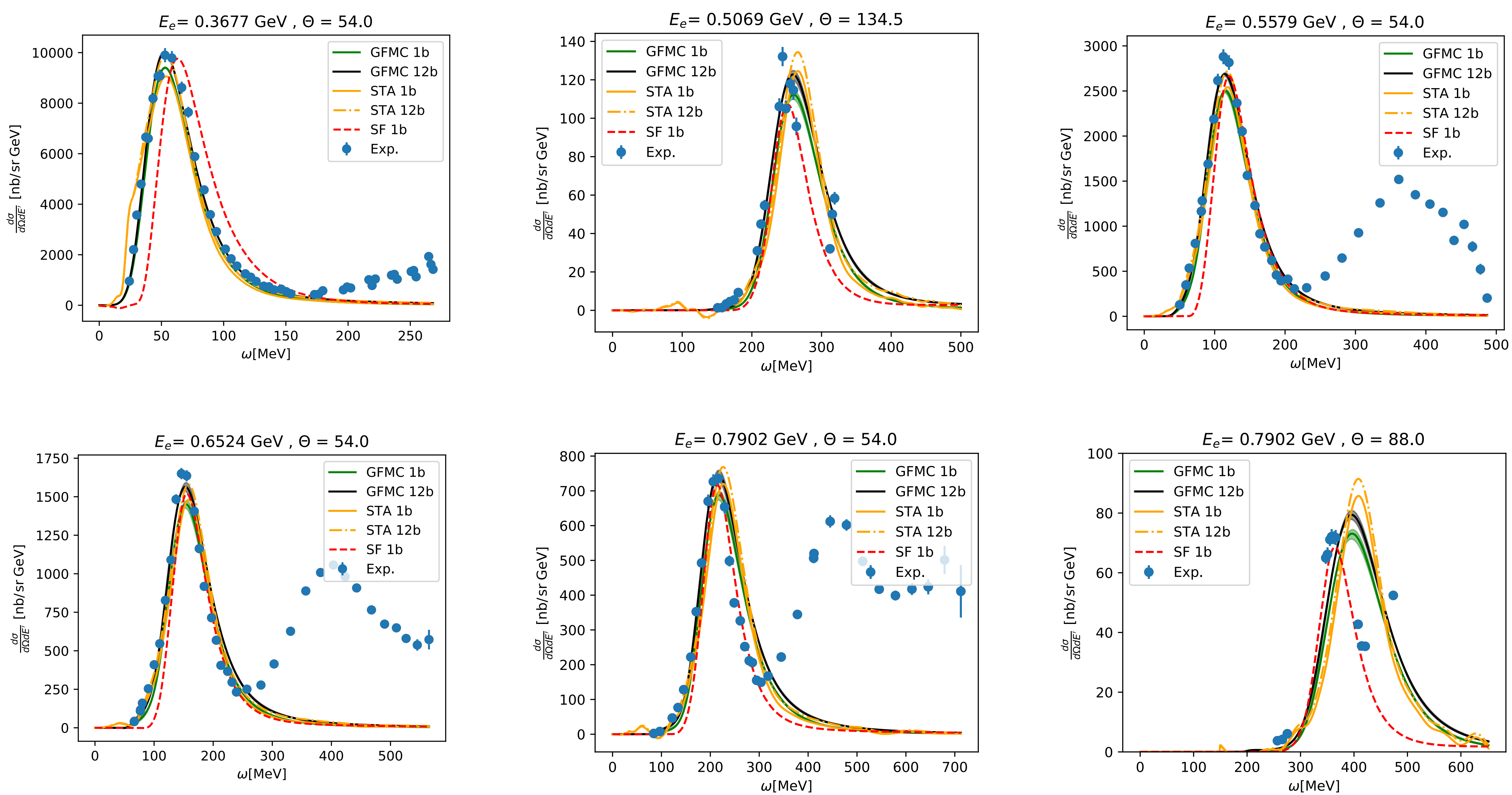

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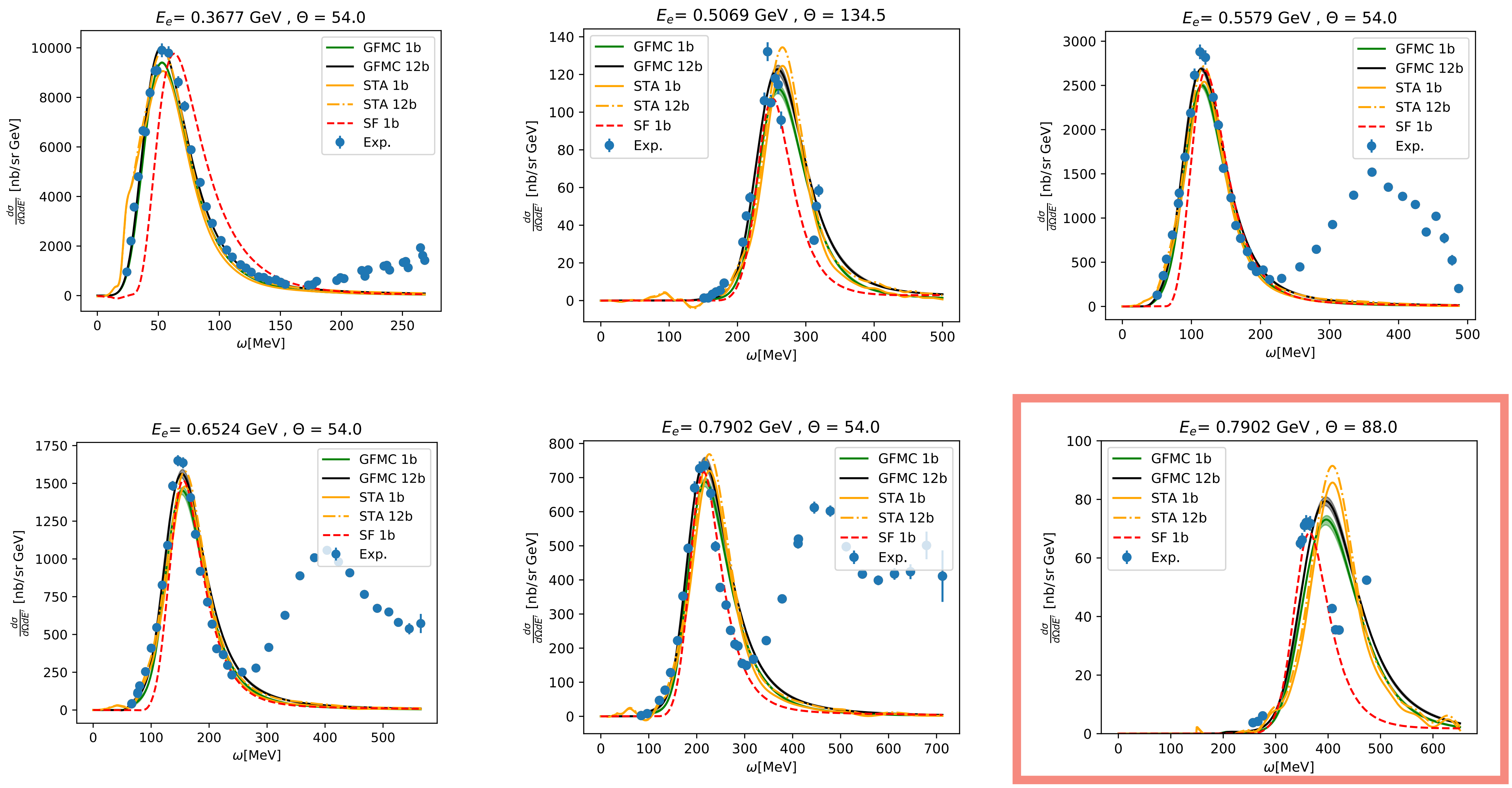
Cross sections

^3H



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Relativistic corrections

Necessary to include relativistic correction at higher momentum q.

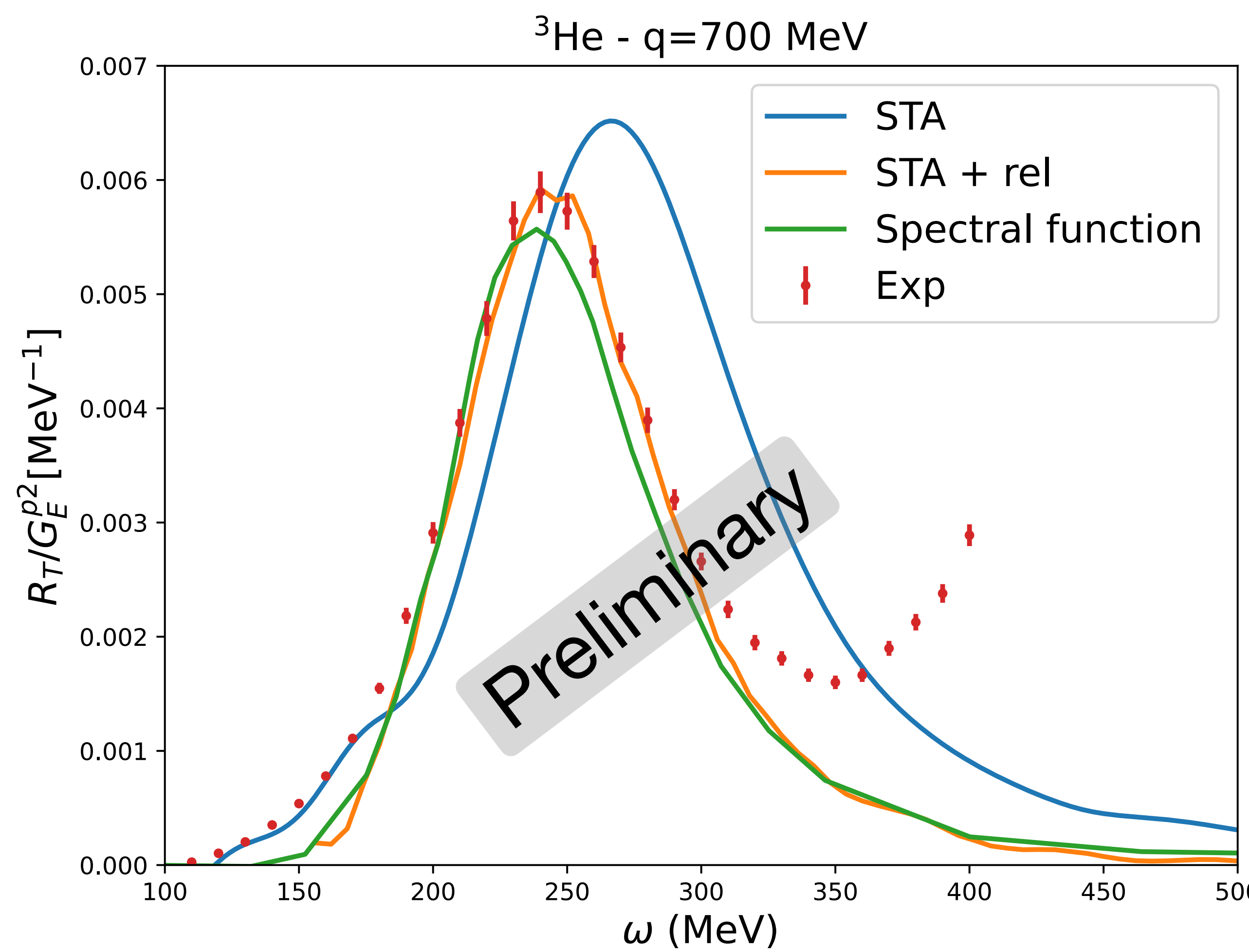
We are currently working on including relativistic corrections within the STA formalism:

R. Weiss, J. Carlson (LANL)

- Relativistic kinematic: allowed by STA factorization scheme
- Relativistic currents: expansion for a large value of the momentum transfer **q**

$$j^\mu = e\bar{u}(\boldsymbol{p}'s')\left(e_N\gamma^\mu + \frac{i\kappa_N}{2m_N}\sigma^{\mu\nu}q_\nu\right)u(\boldsymbol{p}s)$$

$$\boldsymbol{p}' = \boldsymbol{p} + \boldsymbol{q}$$

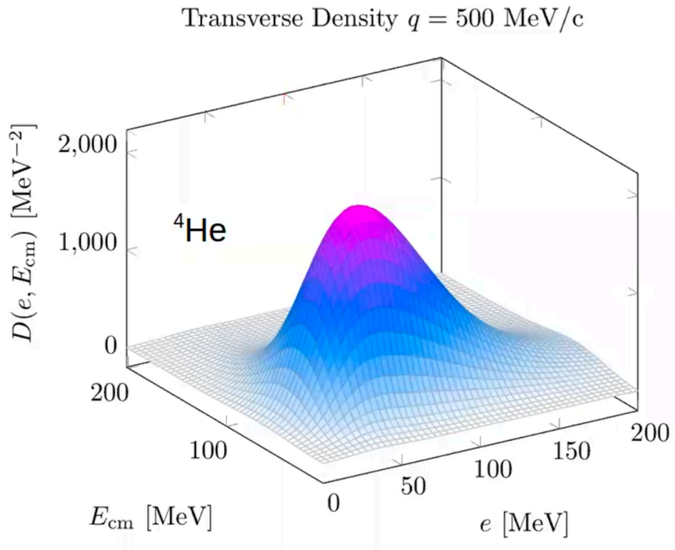


Heavier nuclei

Computational complexity of response functions and densities:

Wave-function		^4He	^{12}C
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



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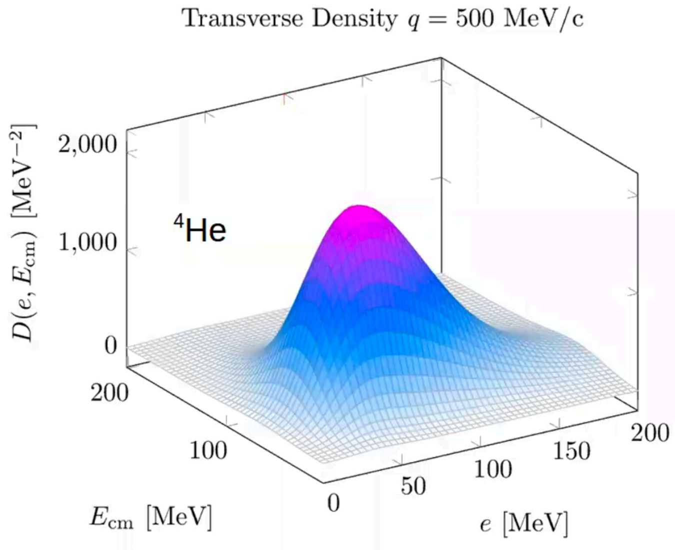

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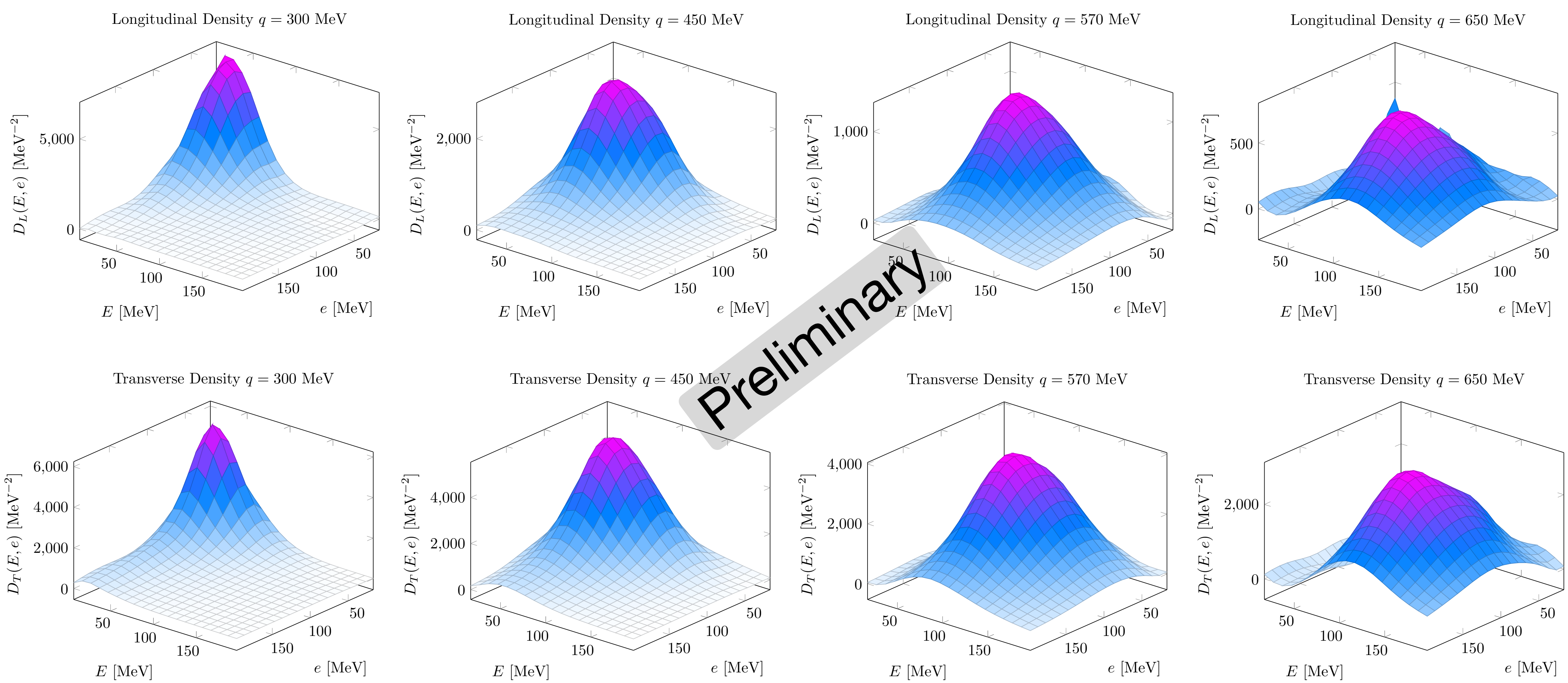
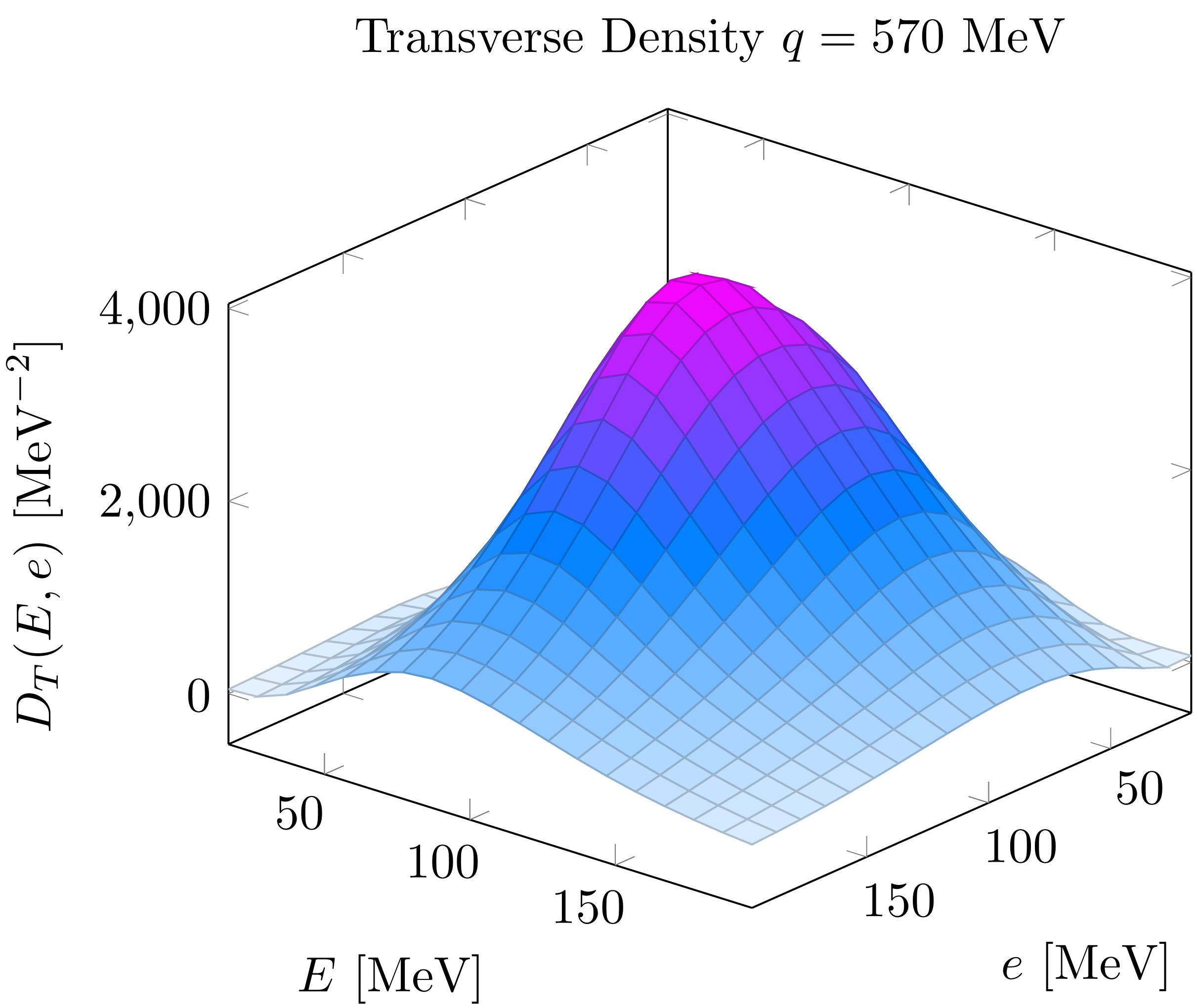
Responses for ^{12}C

Longitudinal and transverse response for **300 < q < 800 MeV**:



Transverse response density



Electron scattering from ^{12}C in the STA:

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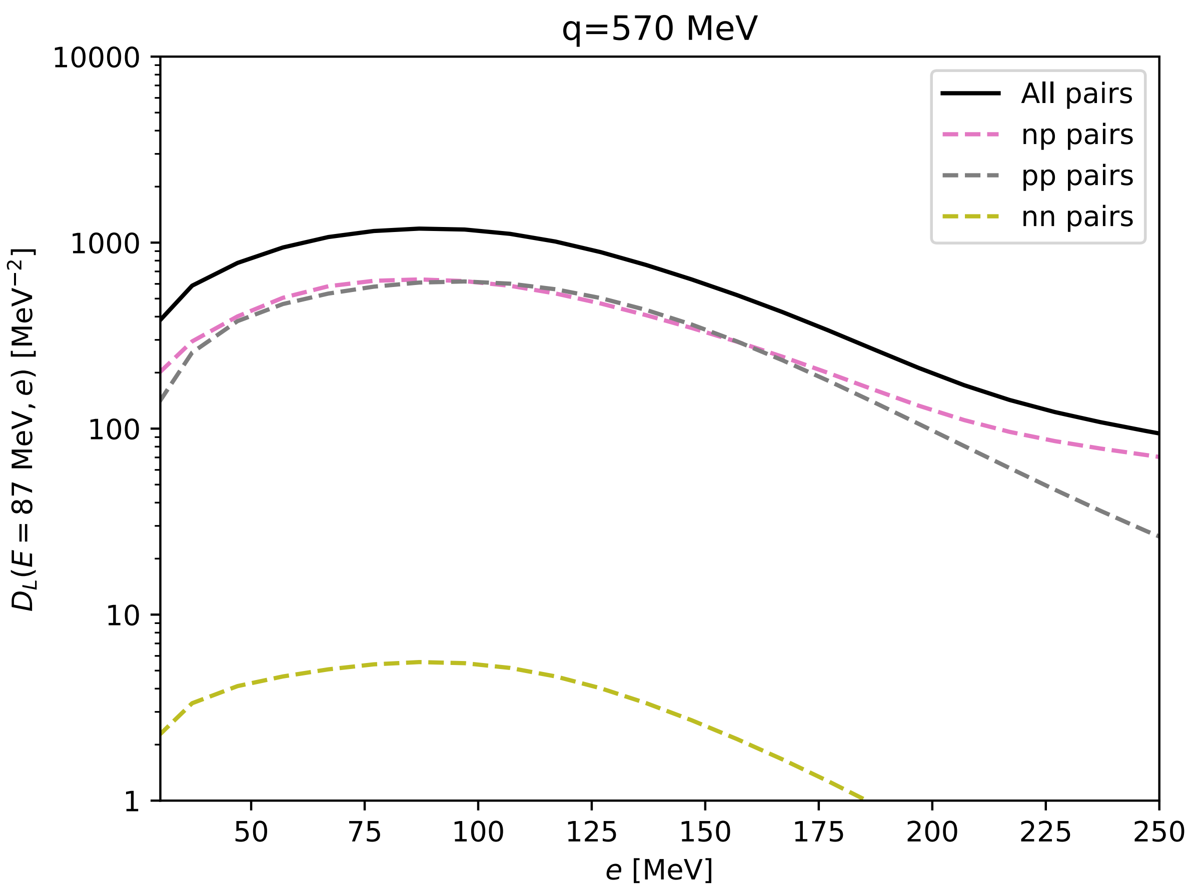
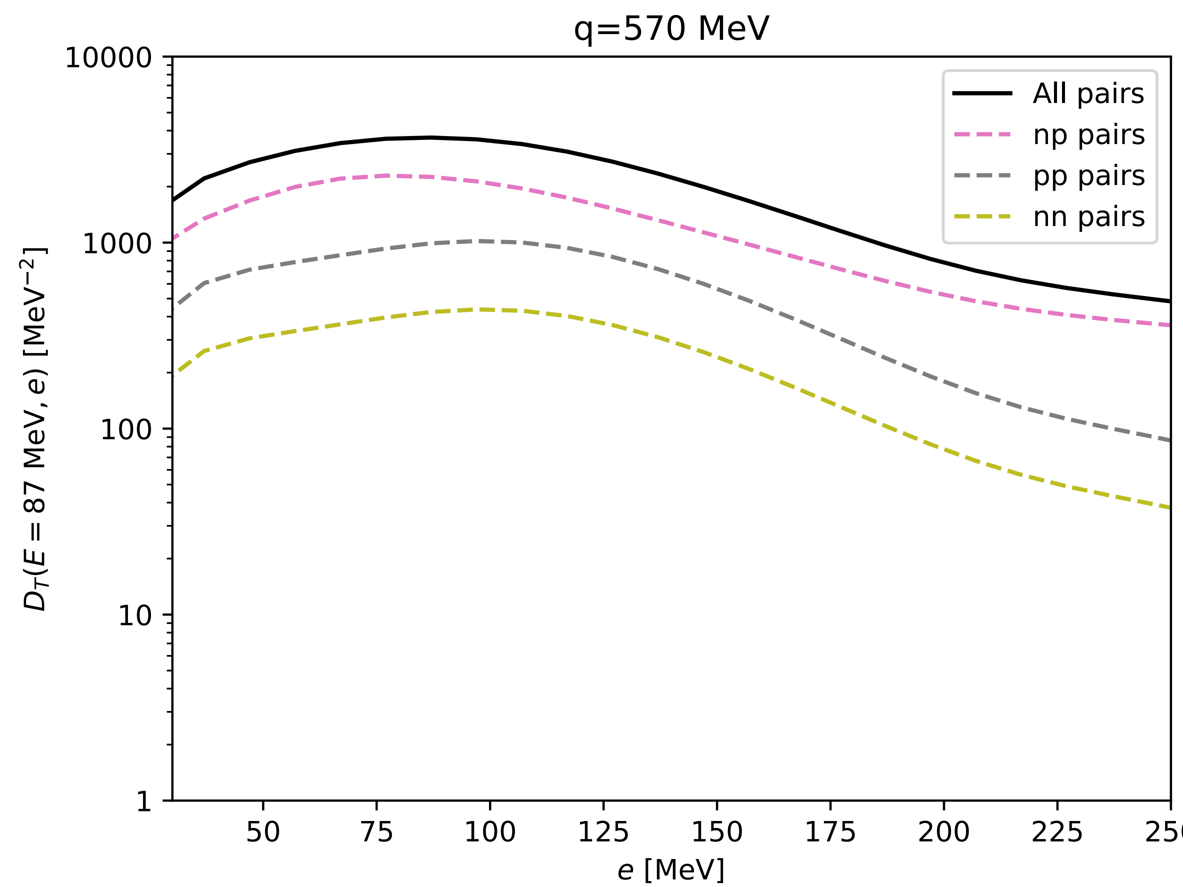
- Give access to particular kinematics for the struck nucleon pair

Back-to-back kinematic





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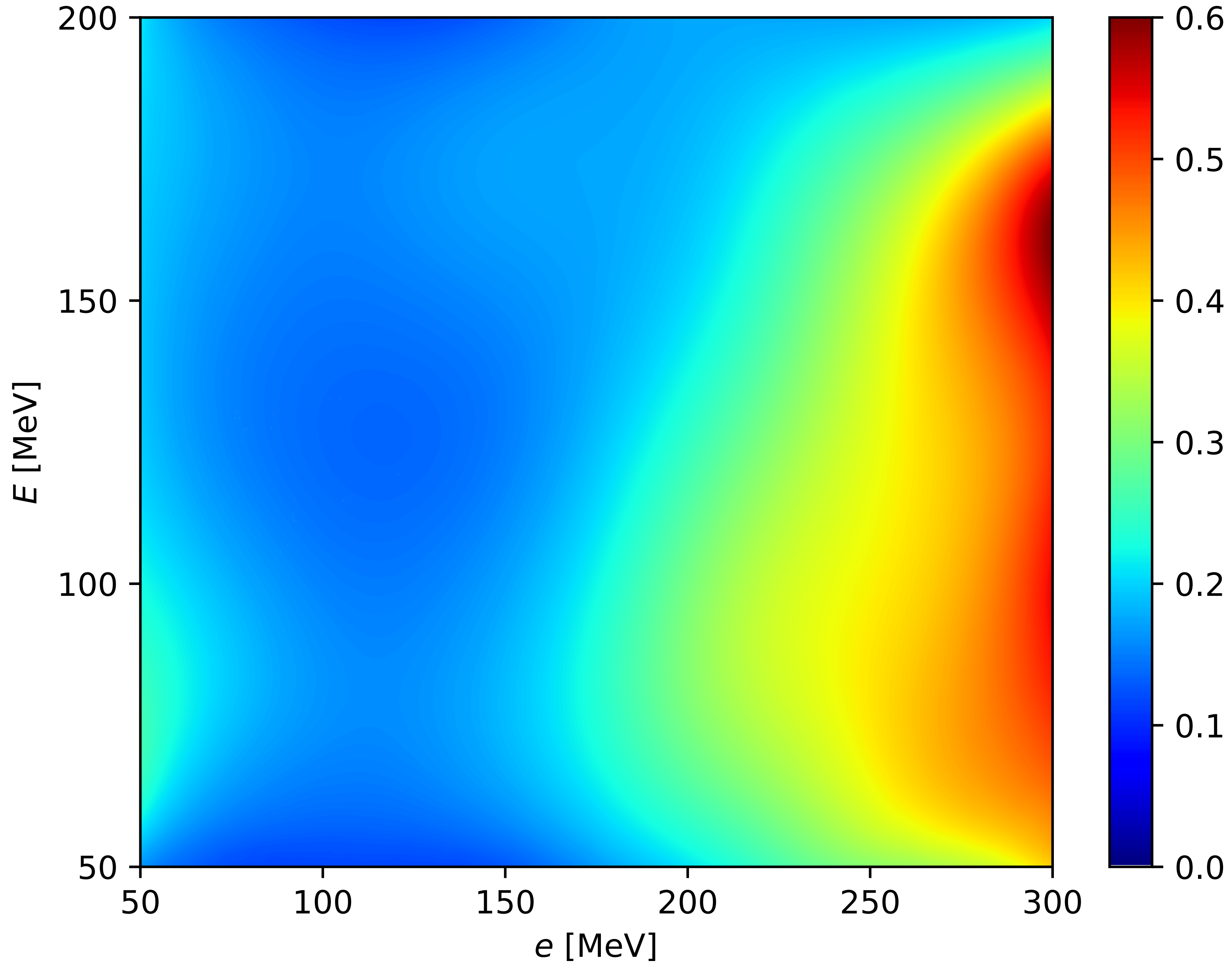
Two-body contributions

Transverse response density at q=570 MeV:



Cross sections: Interpolation schemes

- Given the computational cost of evaluating nuclear responses for heavy nuclei, we can only calculate a limited set. An interpolation scheme is needed.

$$\left(\frac{d^2\sigma}{dE'd\Omega'}\right)_e = \left(\frac{d\sigma}{d\Omega'}\right)_{\mathrm{M}}\left[\left(\frac{q^2}{\mathbf{q}^2}\right)^2 R_L(|\mathbf{q}|,\omega) + \left(\tan^2\frac{\theta}{2} - \frac{1}{2}\frac{q^2}{\mathbf{q}^2}\right)R_T(|\mathbf{q}|,\omega)\right]$$

- Cross sections weakly dependent on interpolation scheme in ^4He, but more relevant in ^{12}C
- We tested interpolation schemes on ^4He, where we can evaluate responses for an arbitrary fine grid of values of q: grid with 10 MeV spacing

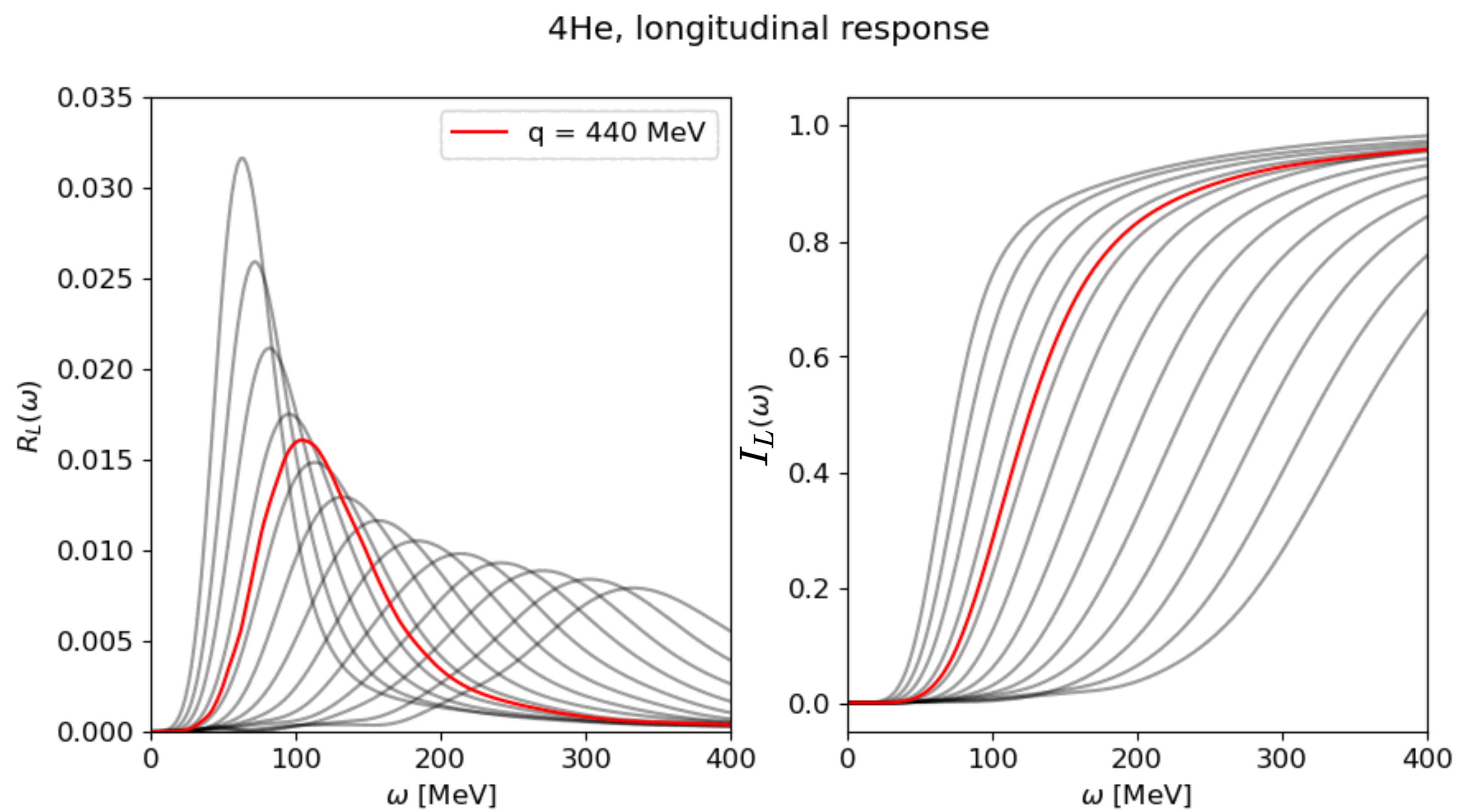
Cross sections: Interpolation schemes

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

$$I_{L/T}(\omega;\mathbf{q}) = \frac{\int_0^\omega R_{L/T}(\omega';\mathbf{q})d\omega'}{\int_0^\infty R_{L/T}(\omega';\mathbf{q})d\omega'}$$

- Outside the range (q < 300 MeV and q > 850 MeV), we use **scaling functions**

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



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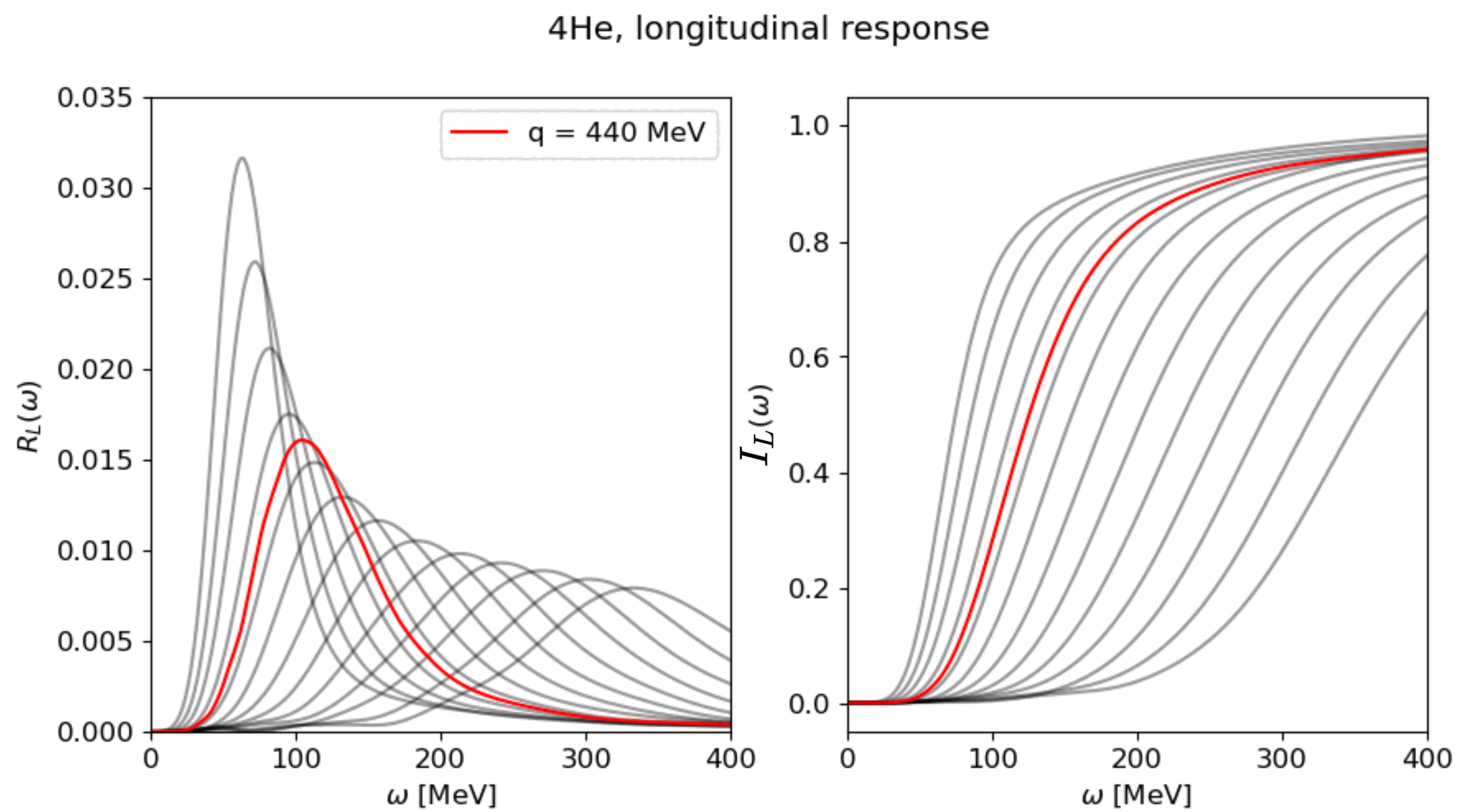

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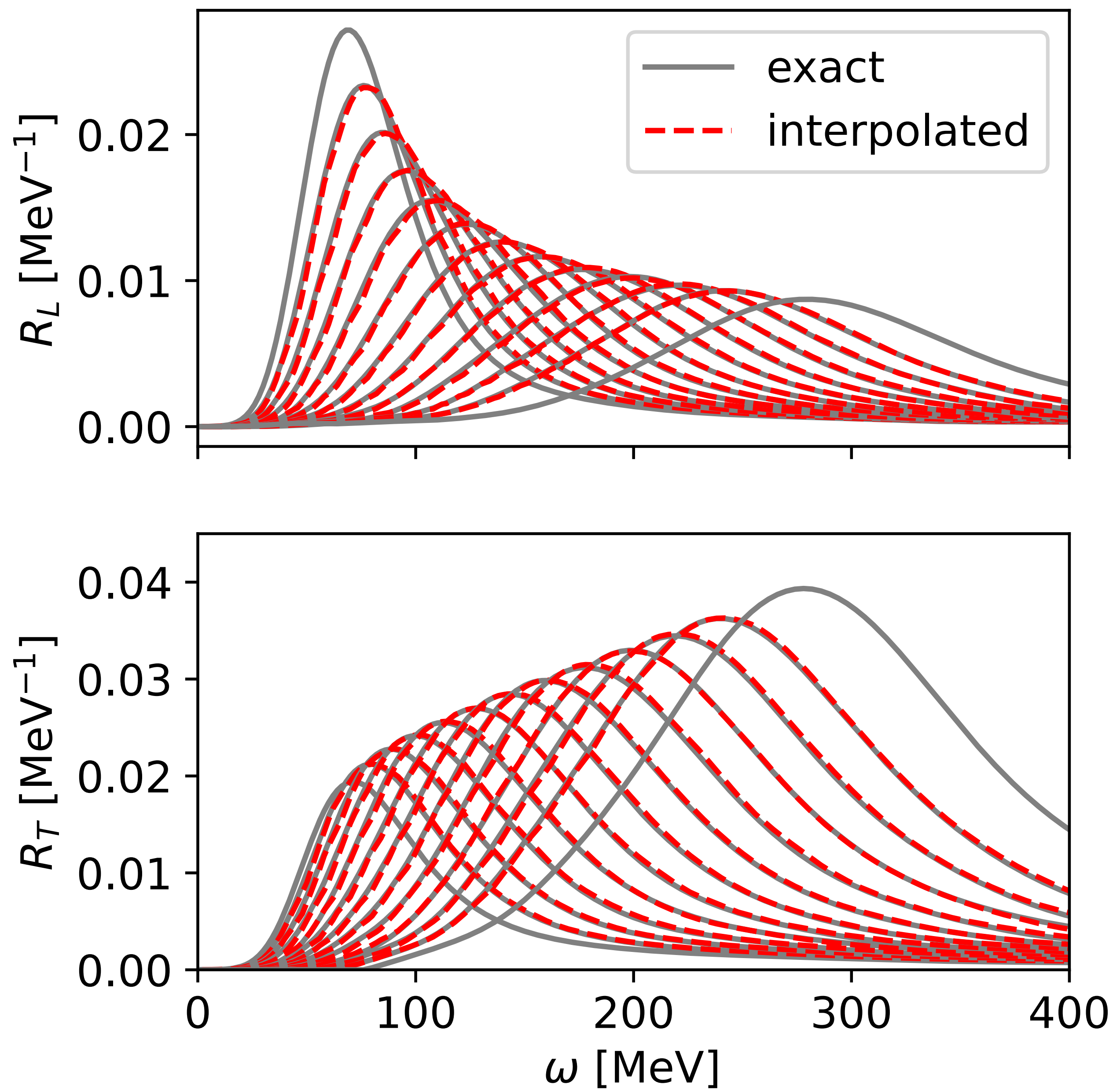
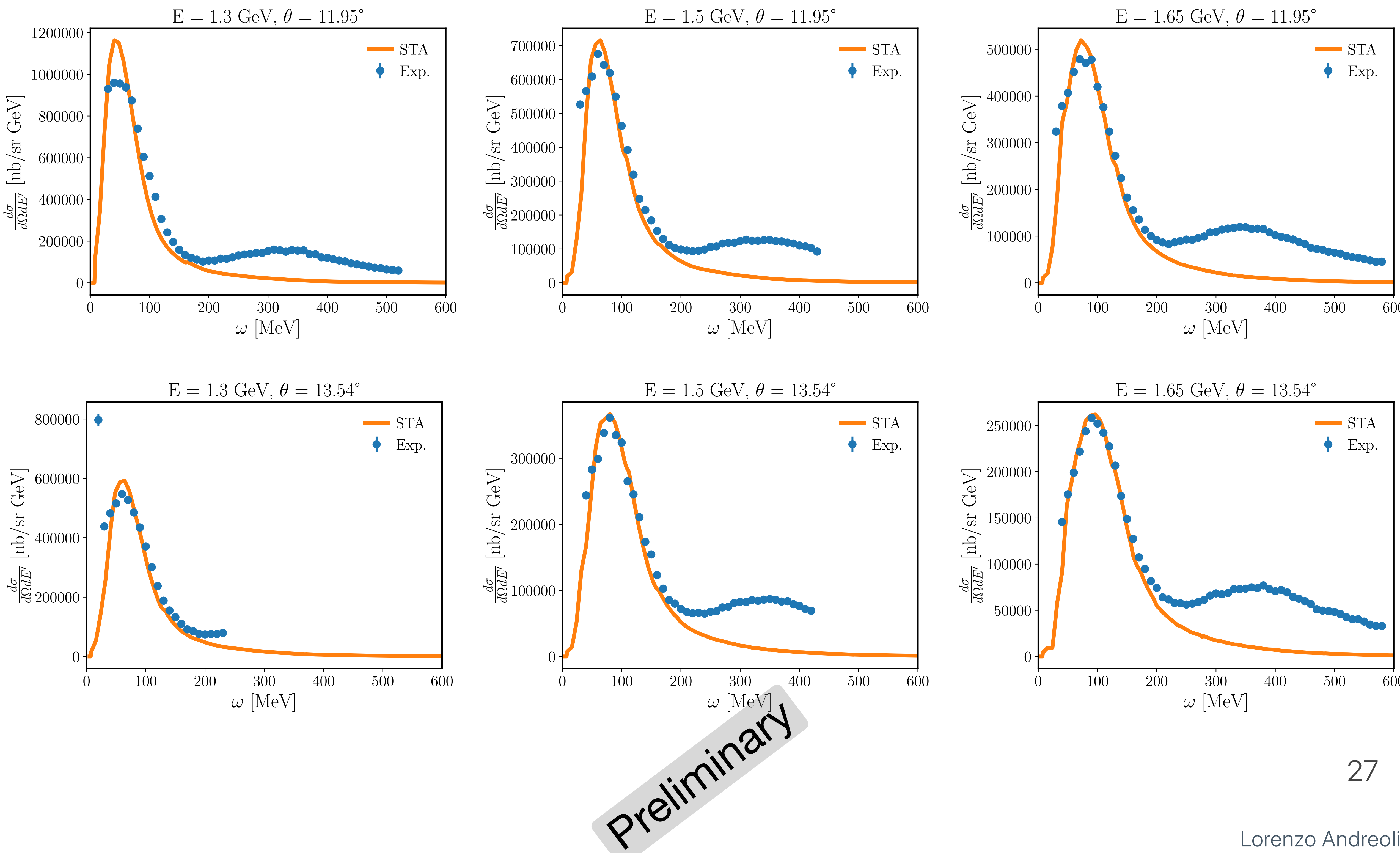
$$I_{L/T}(\omega;\mathbf{q}) = \frac{\int_0^\omega R_{L/T}(\omega';\mathbf{q})d\omega'}{\int_0^\infty R_{L/T}(\omega';\mathbf{q})d\omega'}$$

- Outside the range (q < 300 MeV and q > 850 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 for ^{12}C



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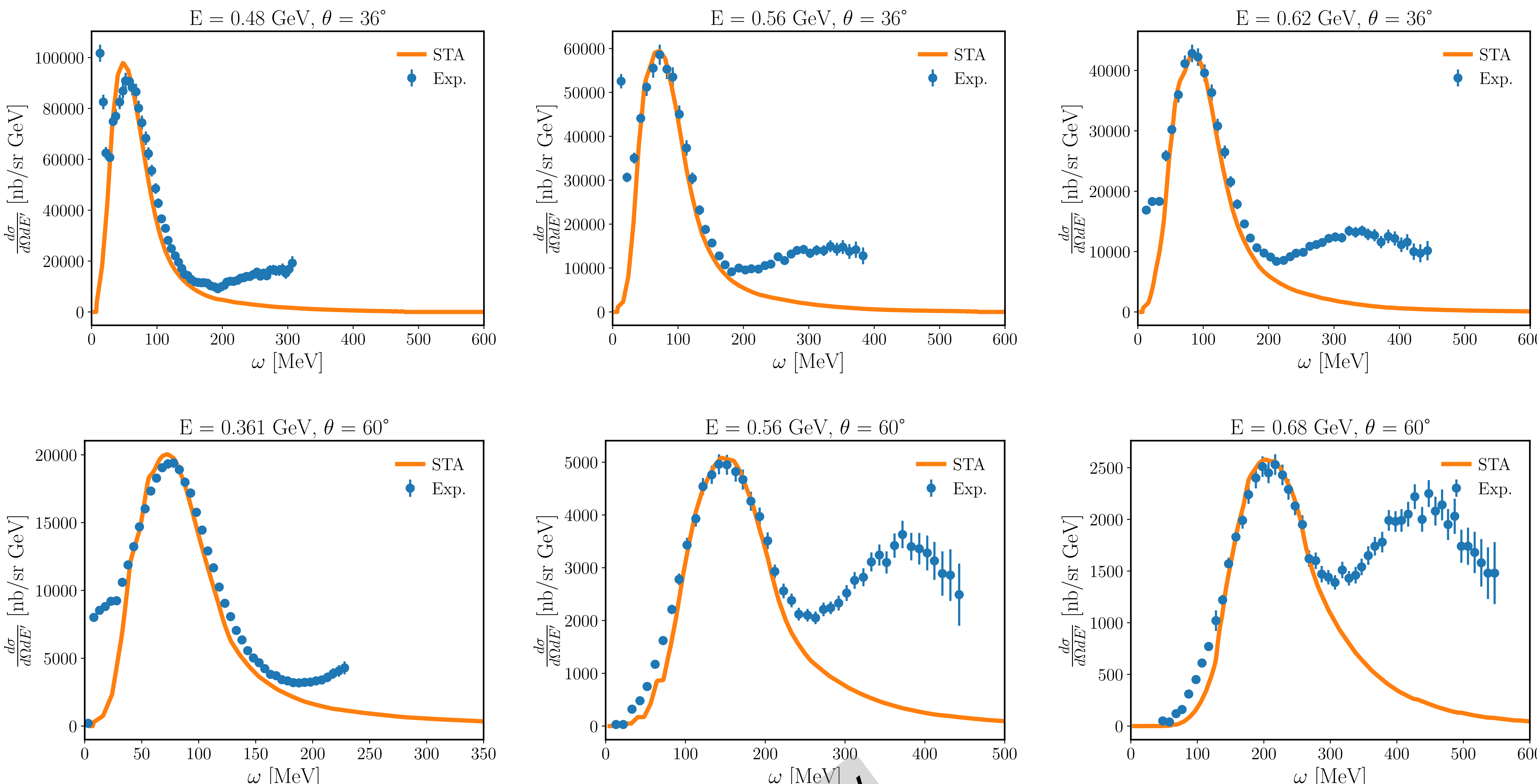
Cross sections results for ^{12}C



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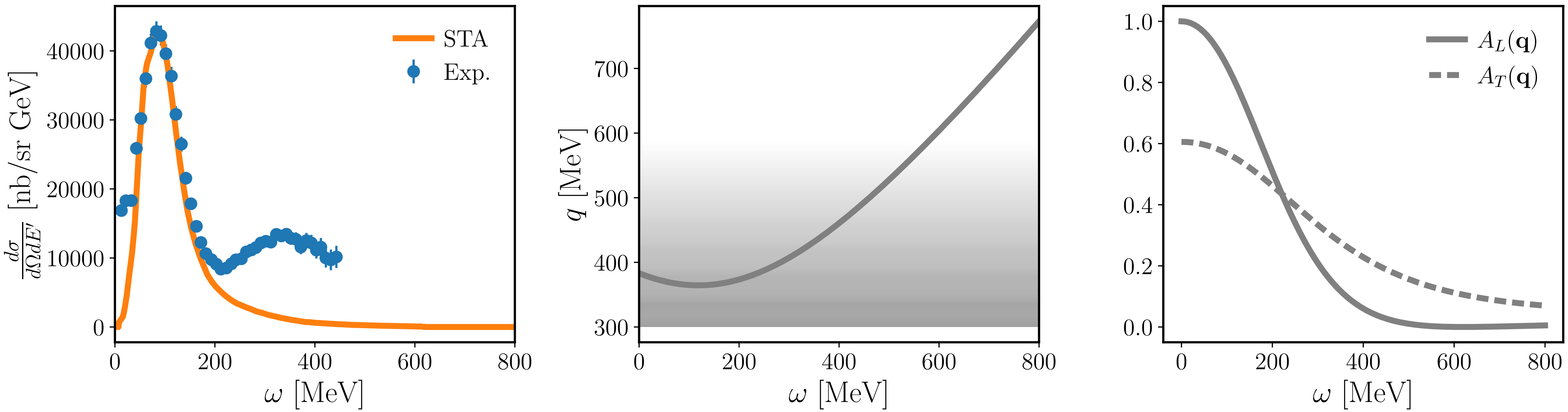
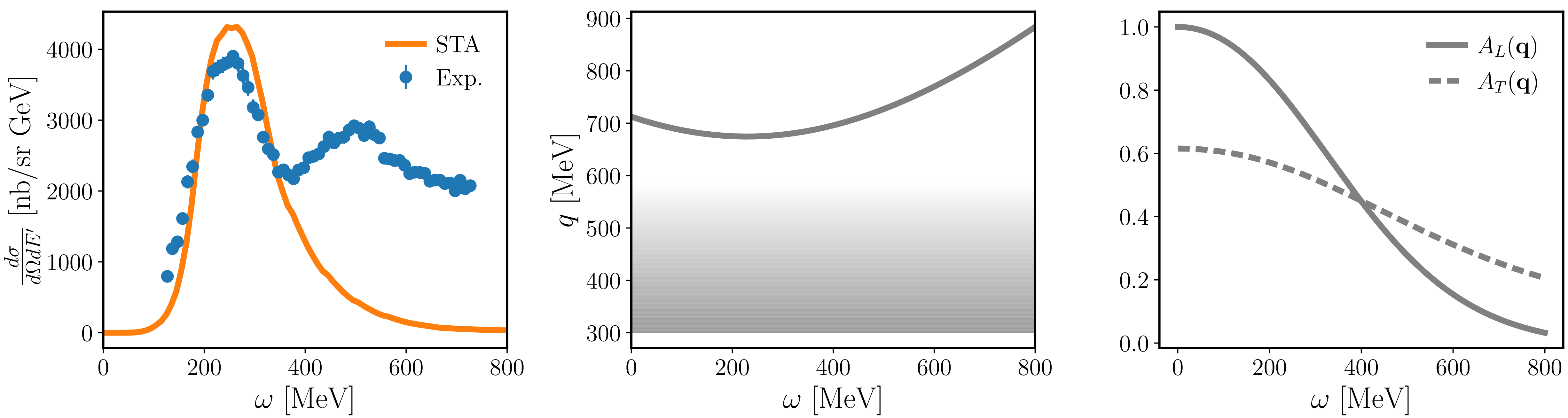
Cross sections results for ^{12}C

$E_e = 0.62$ GeV, θ=36°

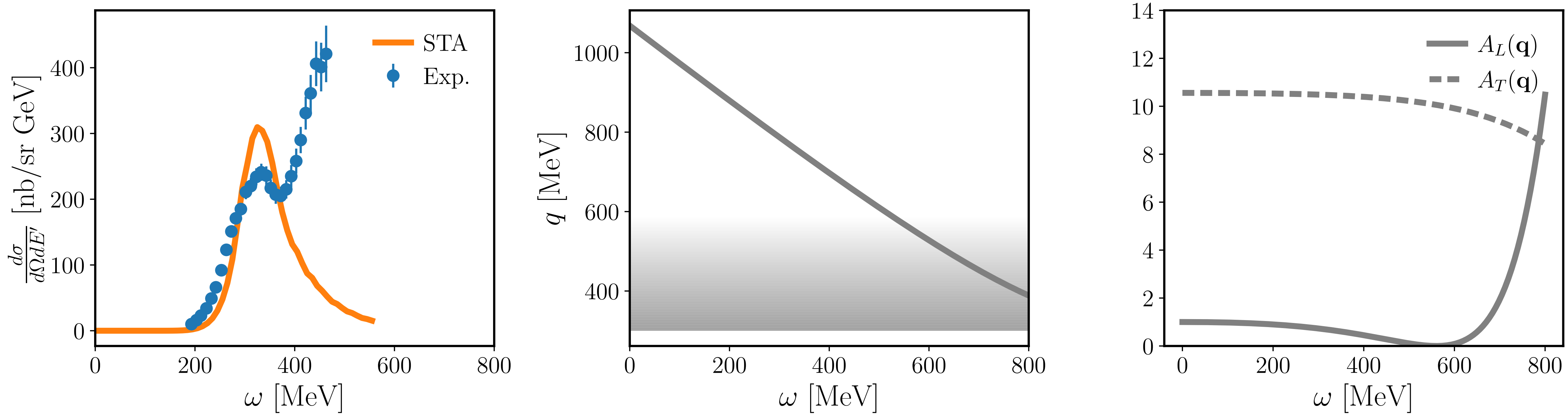


$E_e = 1.108$ GeV, θ=37.5°



Cross sections results for ^{12}C

$E_e = 0.56$ GeV, θ=145°



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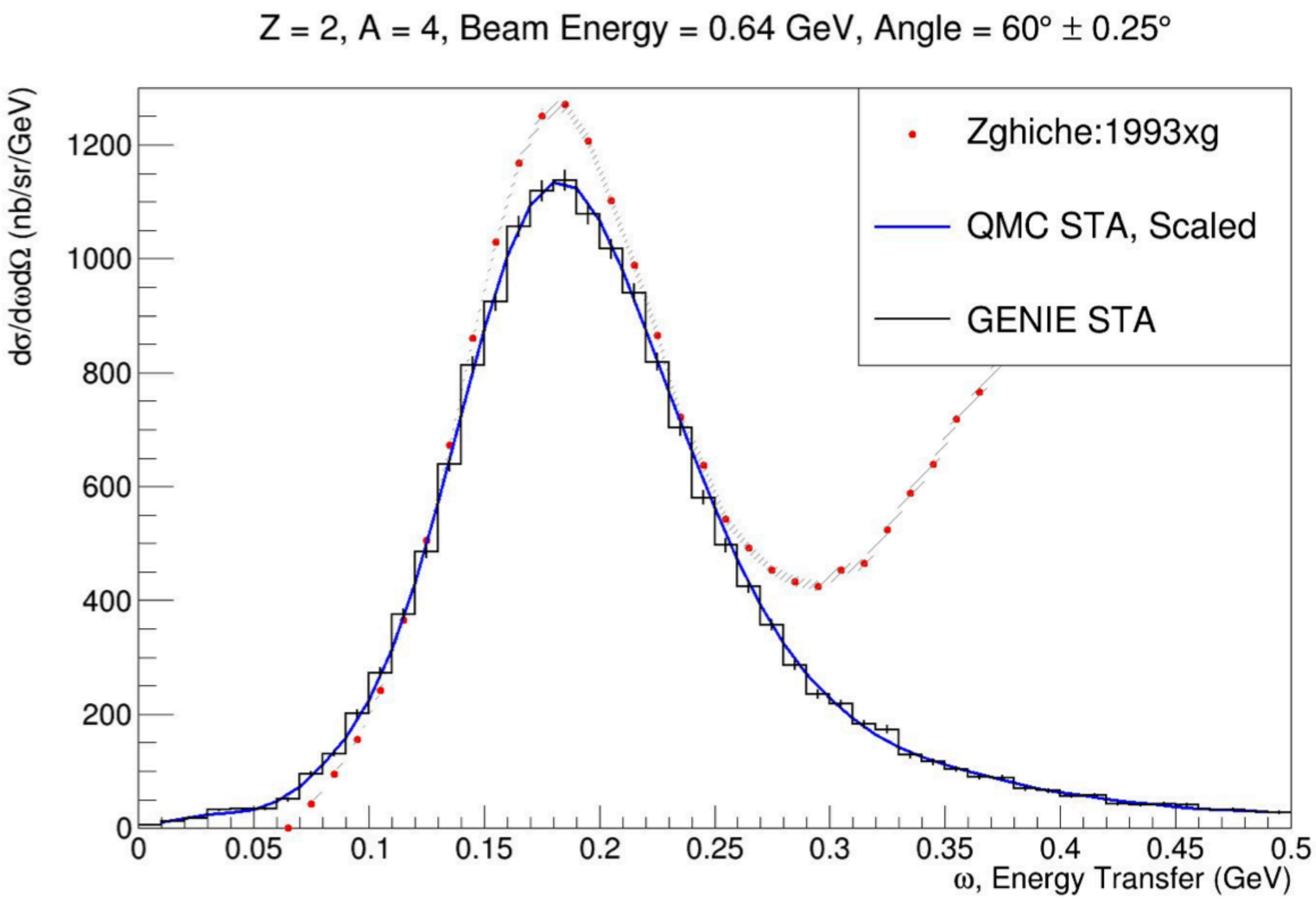
GENIE validation using e-scattering



- STA responses used to build the cross sections
- Cross sections are used to generate events in GENIE
- Electromagnetic processes (for which data are available) are used to validate the generator
- Next step: use response densities

$$\frac{d^2\sigma}{d\omega d\Omega} = \sigma_M \left[v_L R_L(\mathbf{q},\omega) + v_T R_T(\mathbf{q},\omega) \right]$$

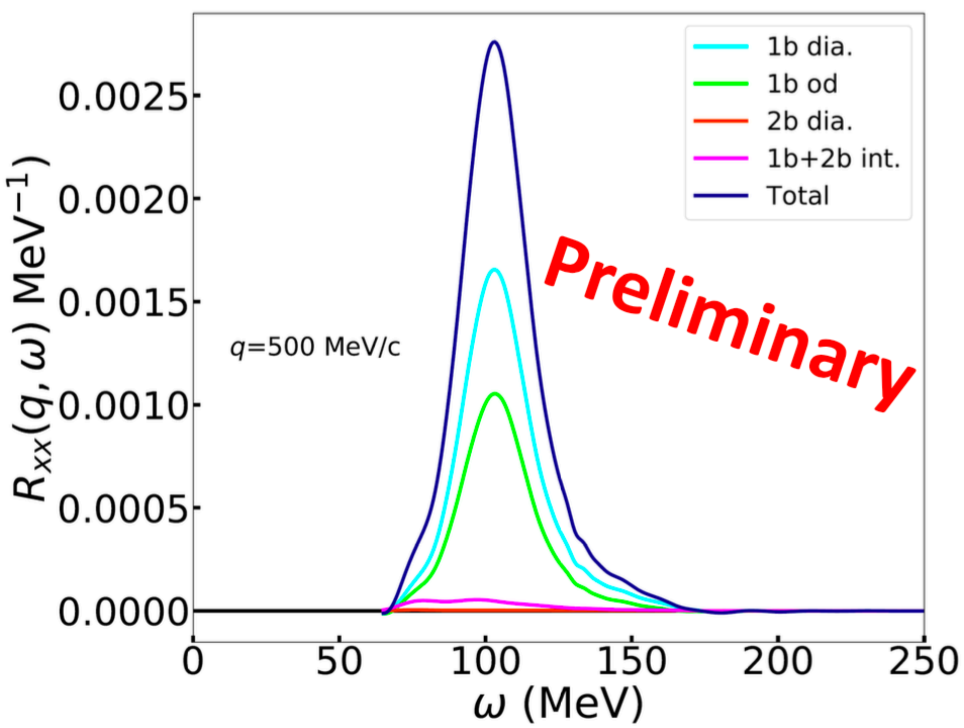
Barrow, Gardiner, Pastore et al. PRD 103 (2021) 5, 052001

GENIE HadronTensorModelI Class: https://internal.dunescience.org/doxygen/classgenie_1_1HadronTensorModelI.html

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

- **G. King**: neutral weak currents quasi-elastic responses evaluated for ^{2}H



Conclusion:

- The STA responses for ^{12}C are in good agreement with the data, and are accurate up to moderate values of q (and consequently to moderate values of incoming electron beam for cross sections calculations)
- Given the computational complexity of evaluating cross sections, an interpolation scheme was adopted

- Describe electroweak scattering from A > 12 without losing two-body physics, the STA is exportable to other QMC methods to address larger nuclei, e.g. AFDMC
- Incorporate relativistic effects
- Use of information from response densities in event generators: collaboration with GENIE Monte Carlo event generator (S. Gardiner, J. Barrow)

Collaborators:

G. King, S. Pastore, M. Piarulli

R. Weiss, J. Carlson

J. Barrow, S. Gardiner

Thank you!

Washington University in St. Louis

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