Quantum Monte Carlo calculations of electron-nucleus scattering in the Short-Time Approximation

Short-Distance nuclear structure and PDFs

ECT* Workshop

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Quantum Monte Carlo Group @ WashU

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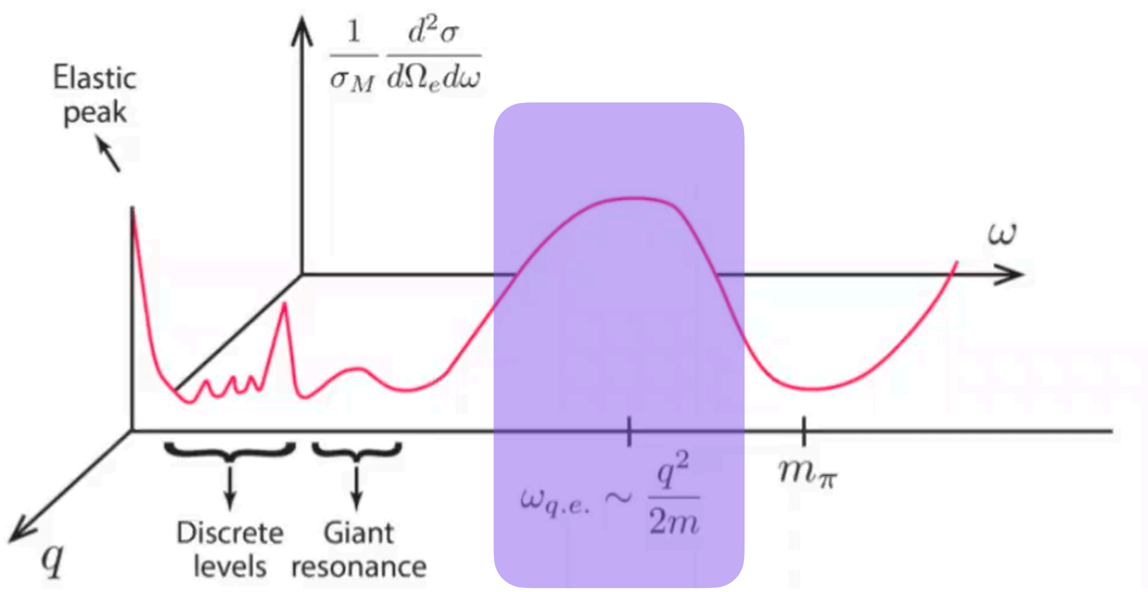
Outline

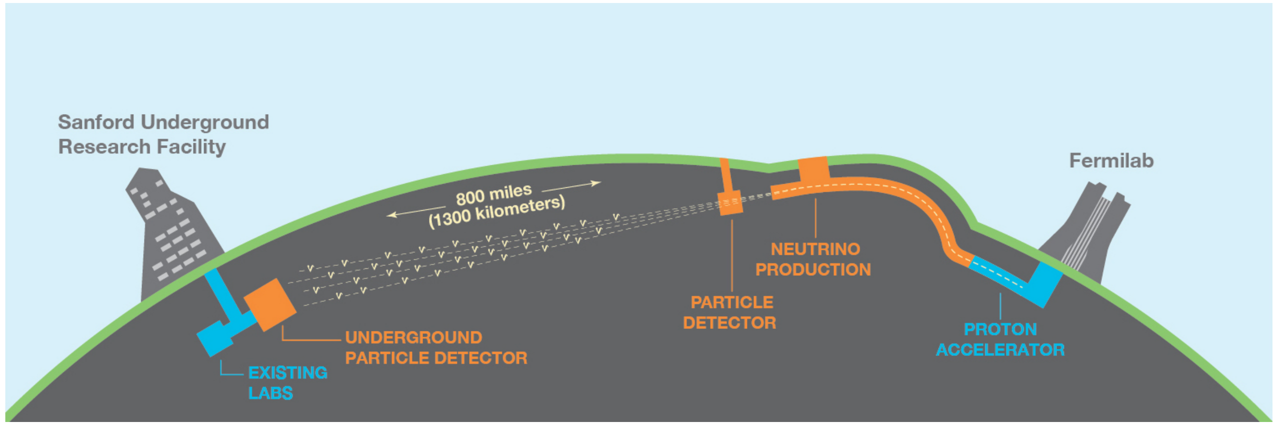
- Quasielastic lepton-nucleus scattering
- Ab initio description of nuclei:
  - Nuclear interaction
  - Electroweak interaction of leptons with nucleons and clusters of correlated nucleons
  - Variational Monte Carlo
- Short-time approximation
- Conclusions and outlook

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)



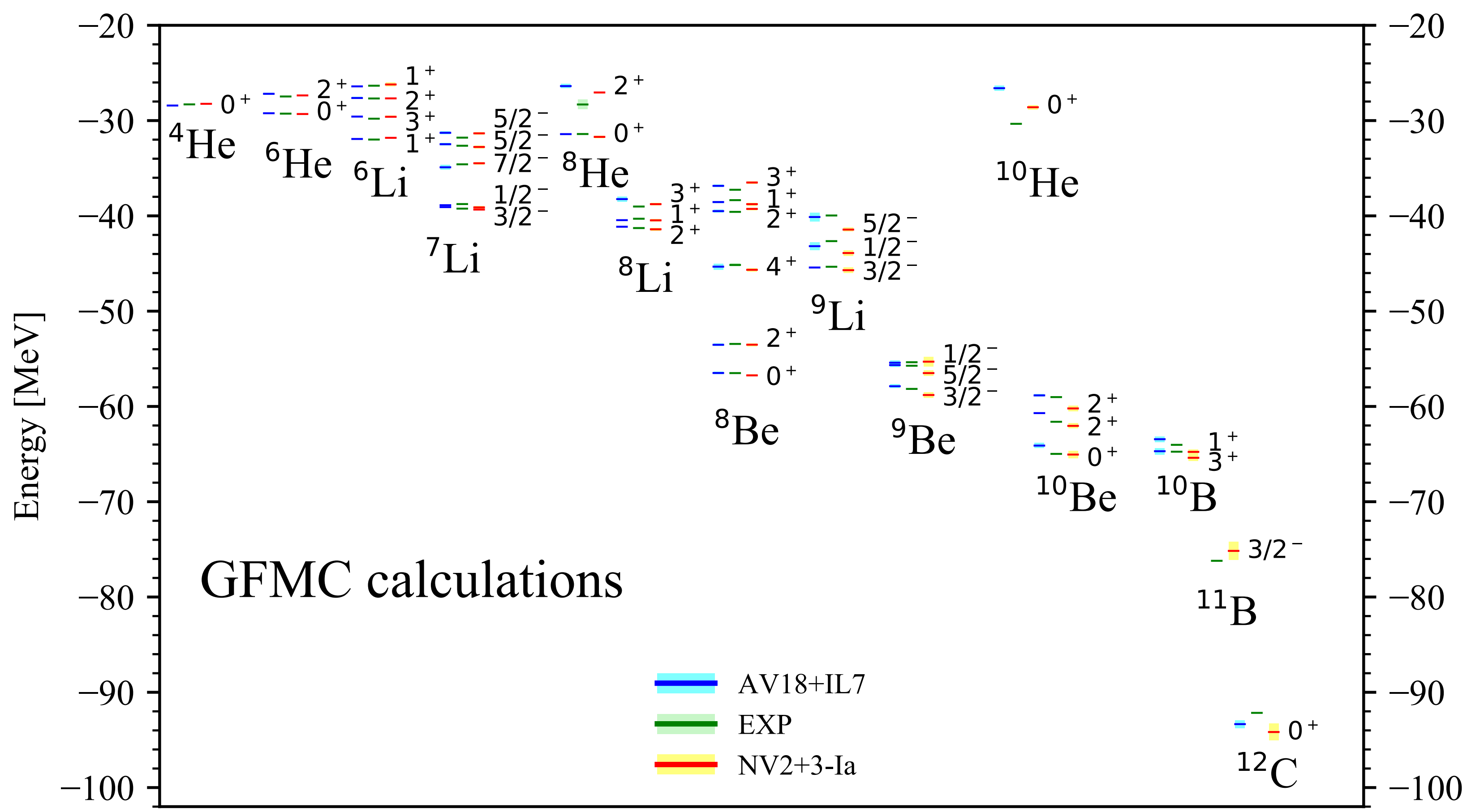


Lepton-nucleus cross sections $\omega \sim 10^2 \text{ MeV}$

Many-body nuclear interaction

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

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



Spectra of light nuclei

Piarulli et al. PRL120(2018)052503

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

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

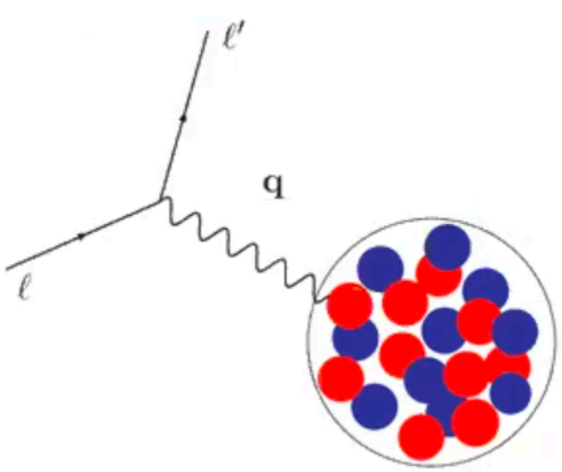
$$O^p_{ij} = [1, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, S_{ij}] \otimes [1, \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j]$$

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

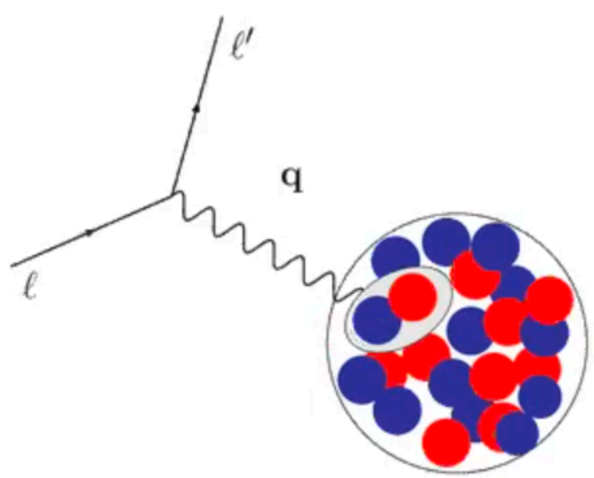
Electromagnetic interactions

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

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

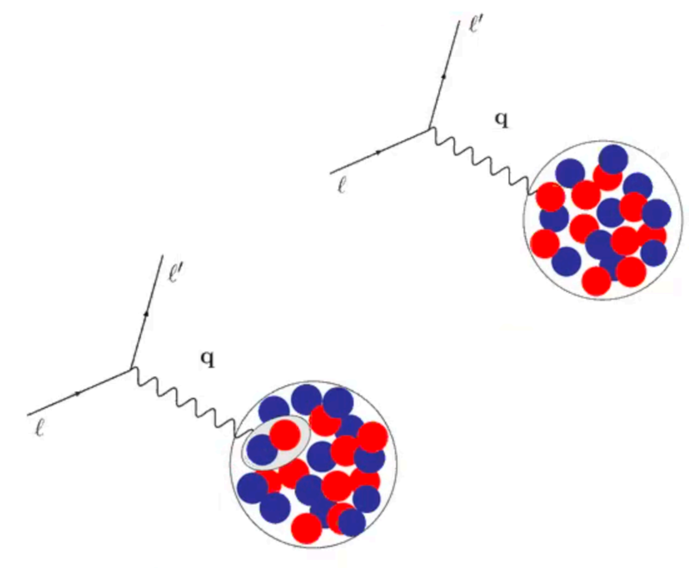
Current operators

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

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

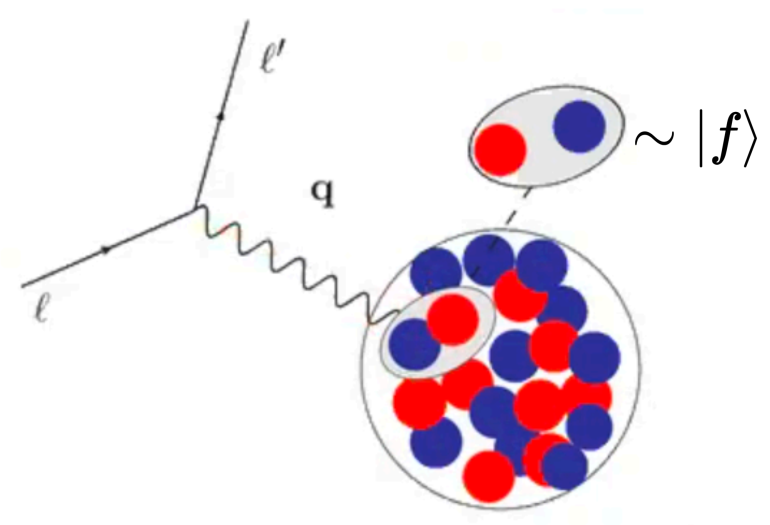


Carlson, Schiavilla 1992. Marcucci et al. 2005

Short-time approximation

Pastore et al. PRC101(2020)044612

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



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

Response functions

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

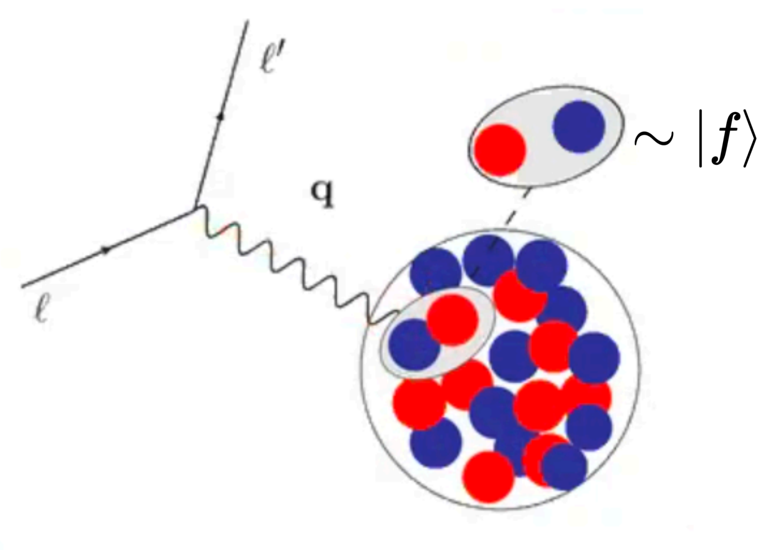
$$R_\alpha(q,\omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i(\omega+E_i)t} \left\langle \Psi_i \middle| O_\alpha^\dagger(\mathbf{q}) e^{-iHt} O_\alpha(\mathbf{q}) \middle| \Psi_i \right\rangle$$

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

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

Validity of the Short Time Approximation

The typical (conservative estimate) energy (time) scale in a nucleus with A correlated nucleons in pairs is:

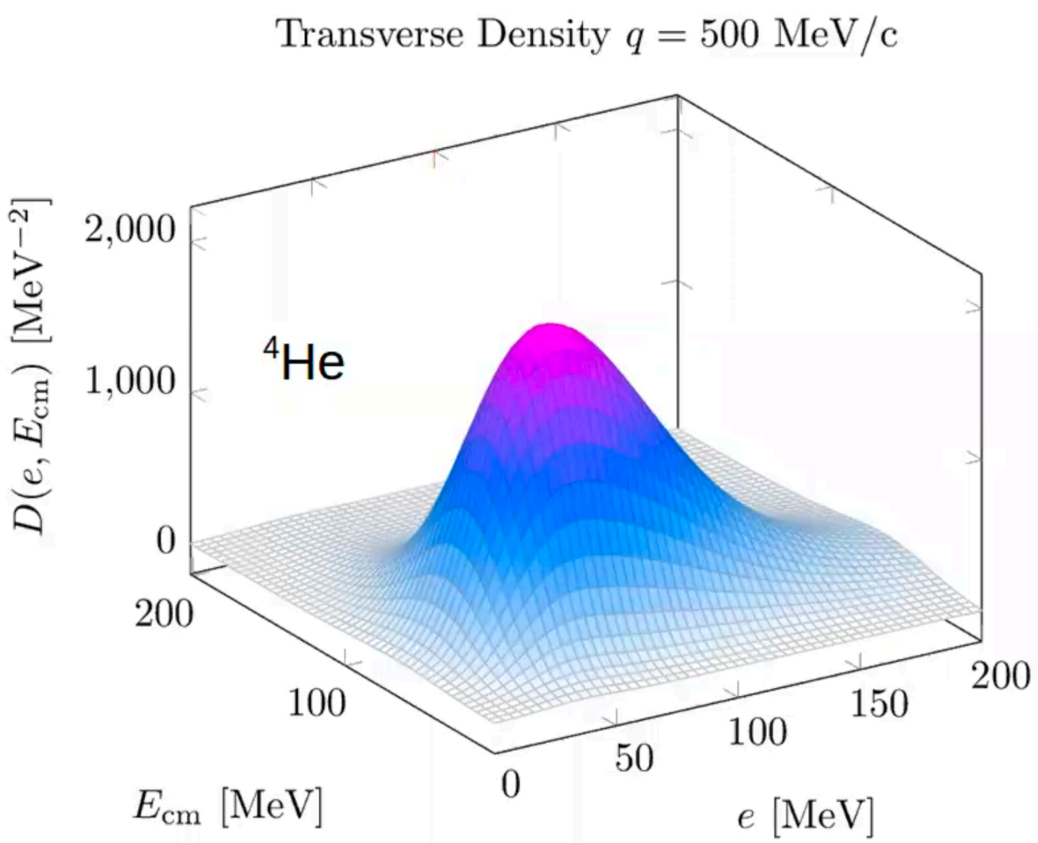
$$\varepsilon_{\text{pair}} \sim 20\text{MeV} \quad (t \sim 1/\varepsilon_{\text{pair}})$$

This sets a natural expansion parameter in the QE region characterized by $\varepsilon_{\text{pair}}/\omega_{\text{QE}}$

The STA neglects terms of order

$$O\left((\varepsilon_{\text{pair}}/\omega_{\text{QE}})^2\right)$$

Transverse response density



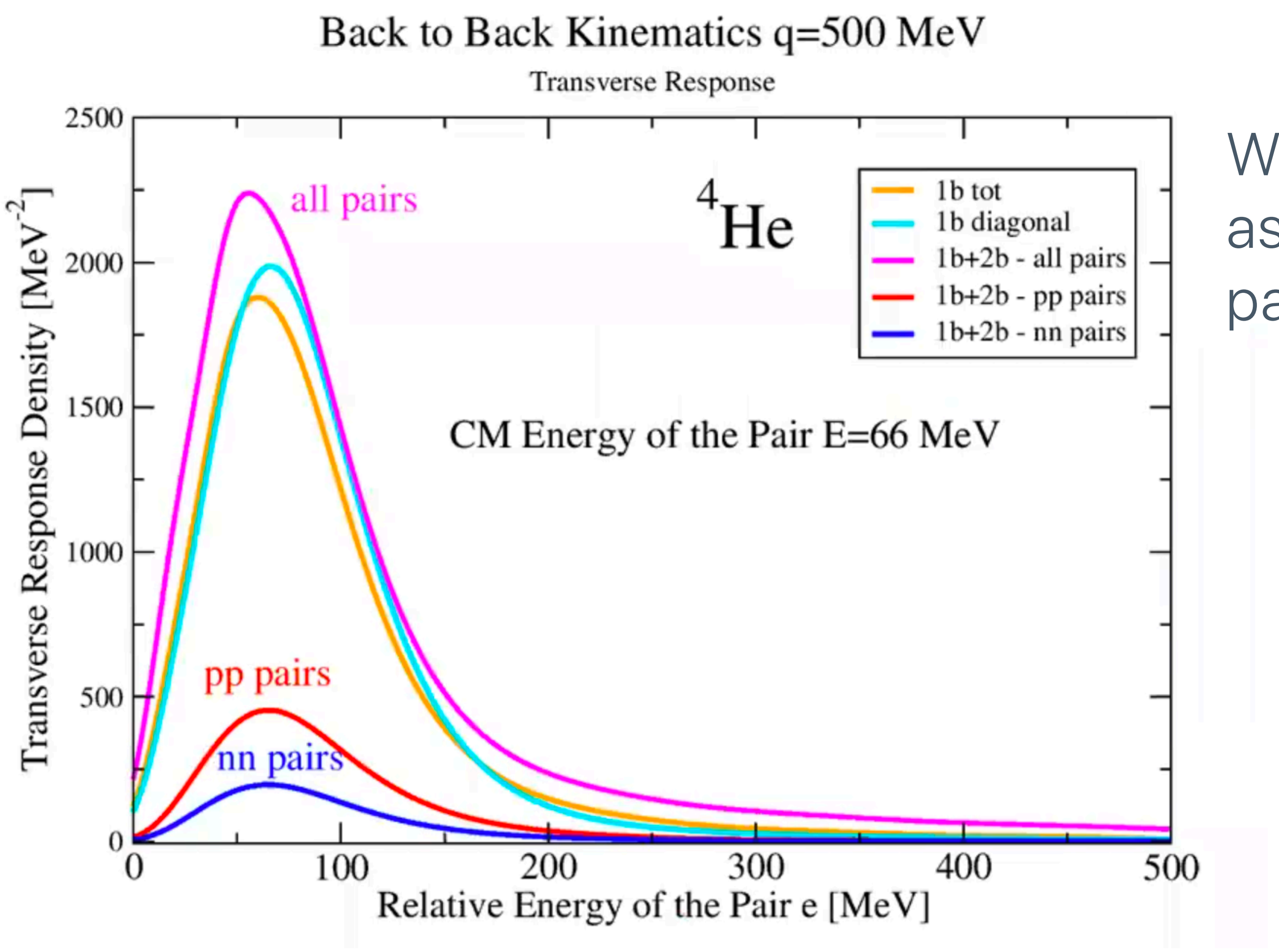
^4He

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



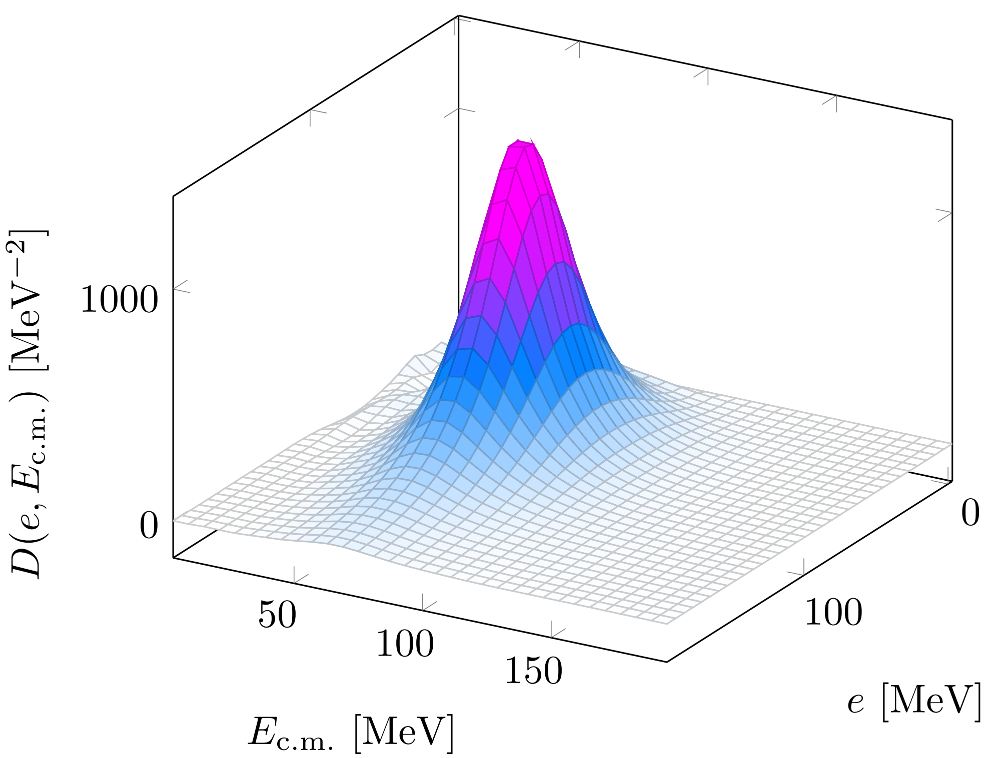
We can select a particular kinematic, and assess the contributions from different particle identities

Pastore et al. PRC101(2020)044612

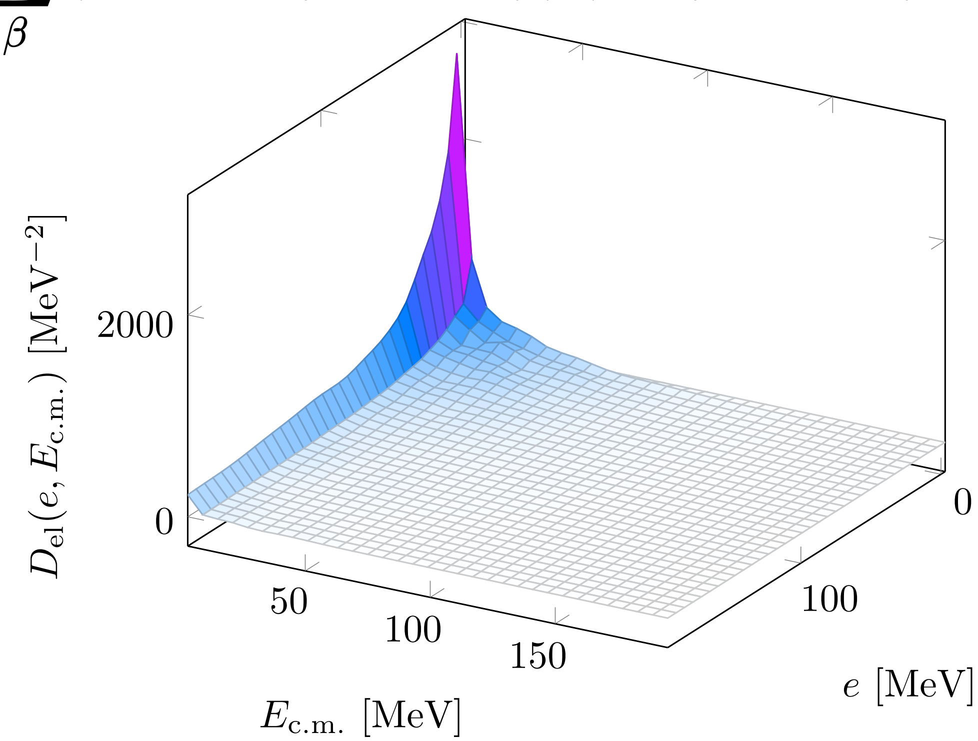
Longitudinal response density: elastic peak removal

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

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



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



^{3}H Longitudinal response at 300 MeV

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

Benchmark

L.A., N. Rocco, A. Lovato, S. Pastore 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

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

Green's function Monte Carlo

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

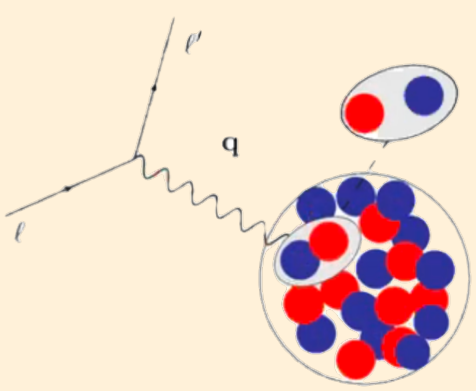
$$E_\alpha(\mathbf{q},\tau) = \int_{\omega_{\rm th}}^{\infty} d\omega e^{-\omega\tau} R_\alpha(\mathbf{q},\omega), \quad \alpha = L, T$$

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

Stort-time approximation

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

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



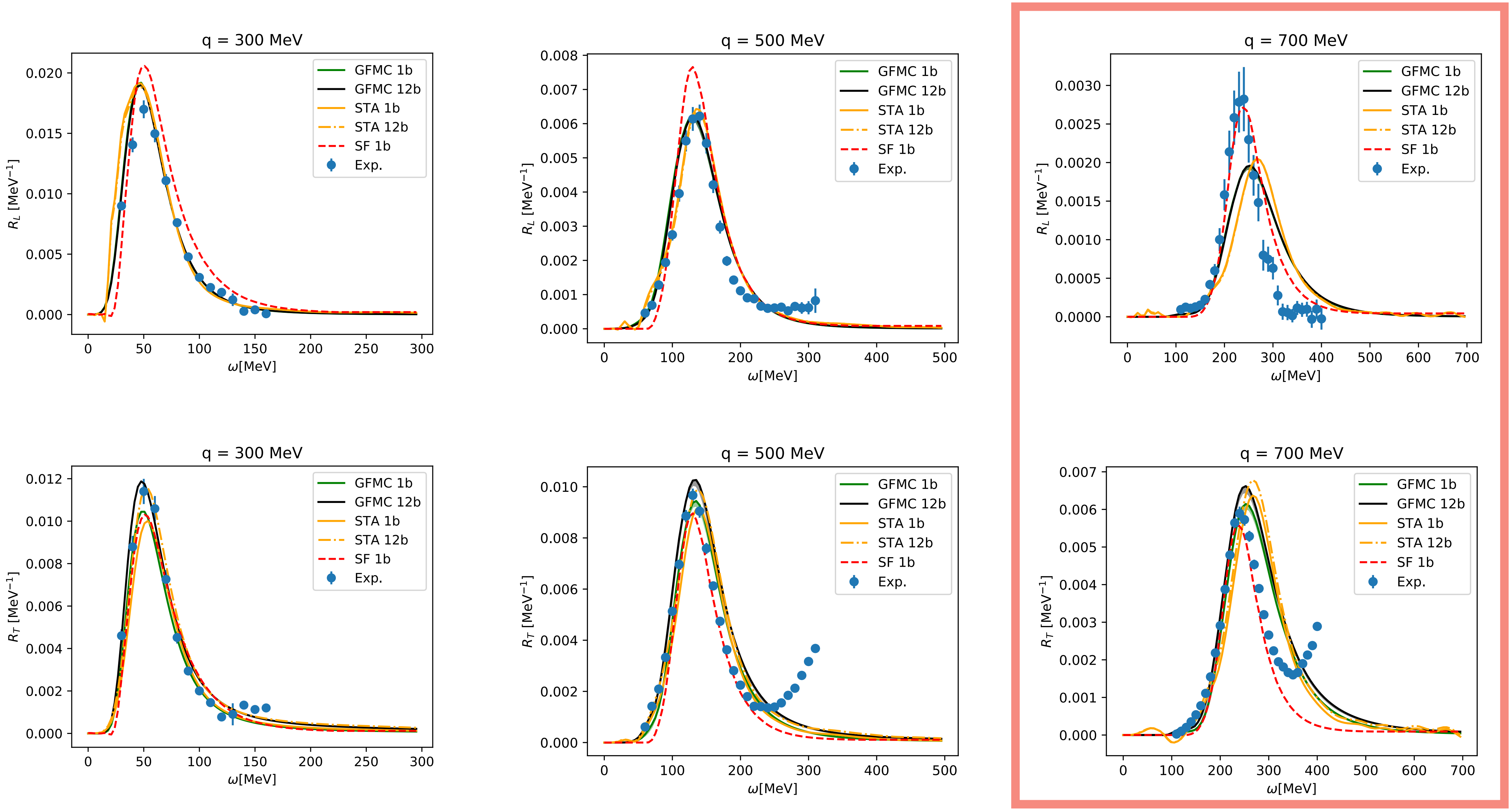
Spectral function

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

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

Benchmark

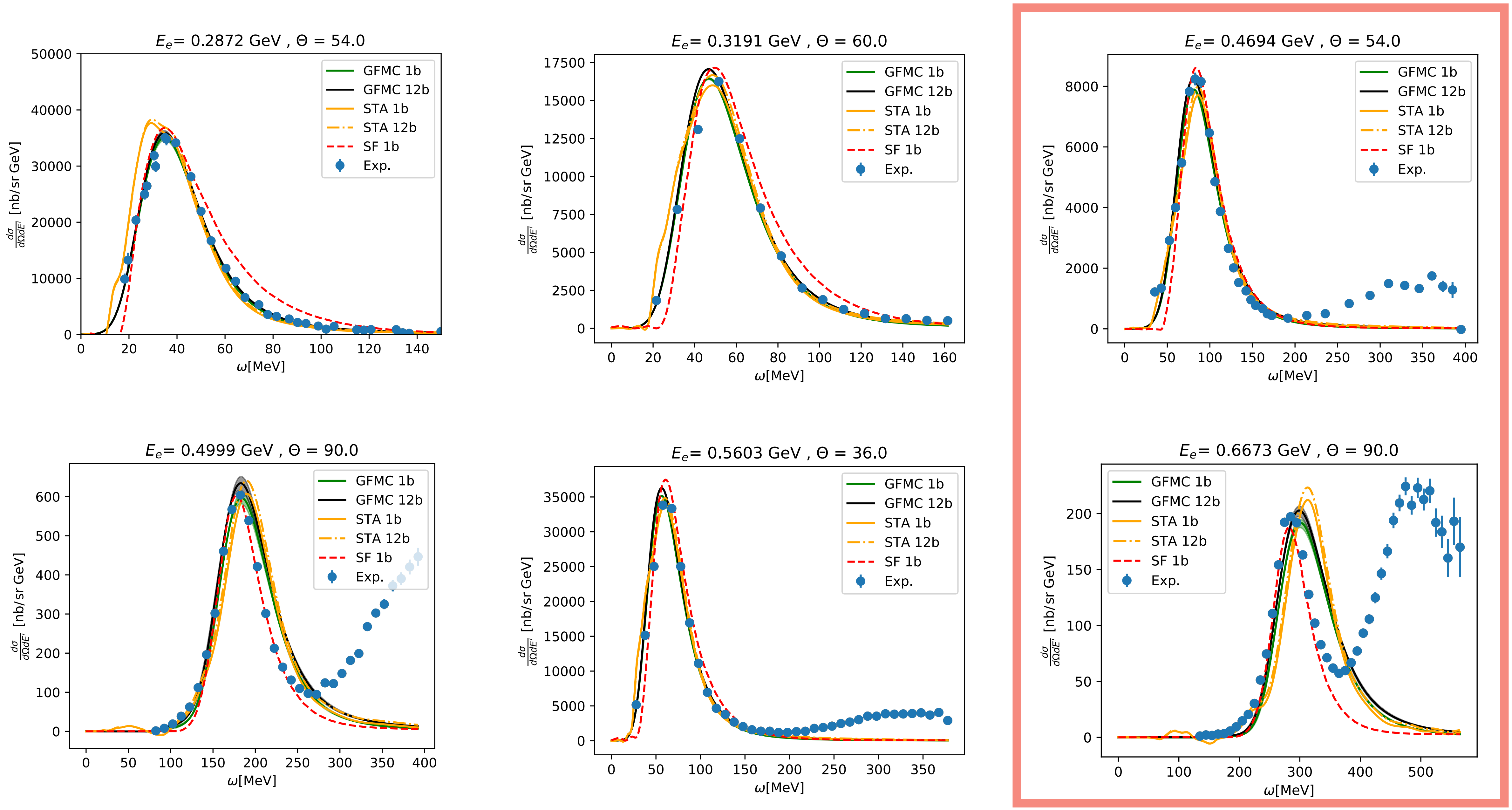
Longitudinal and transverse response function in ^3He



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

Cross sections

^{3}He



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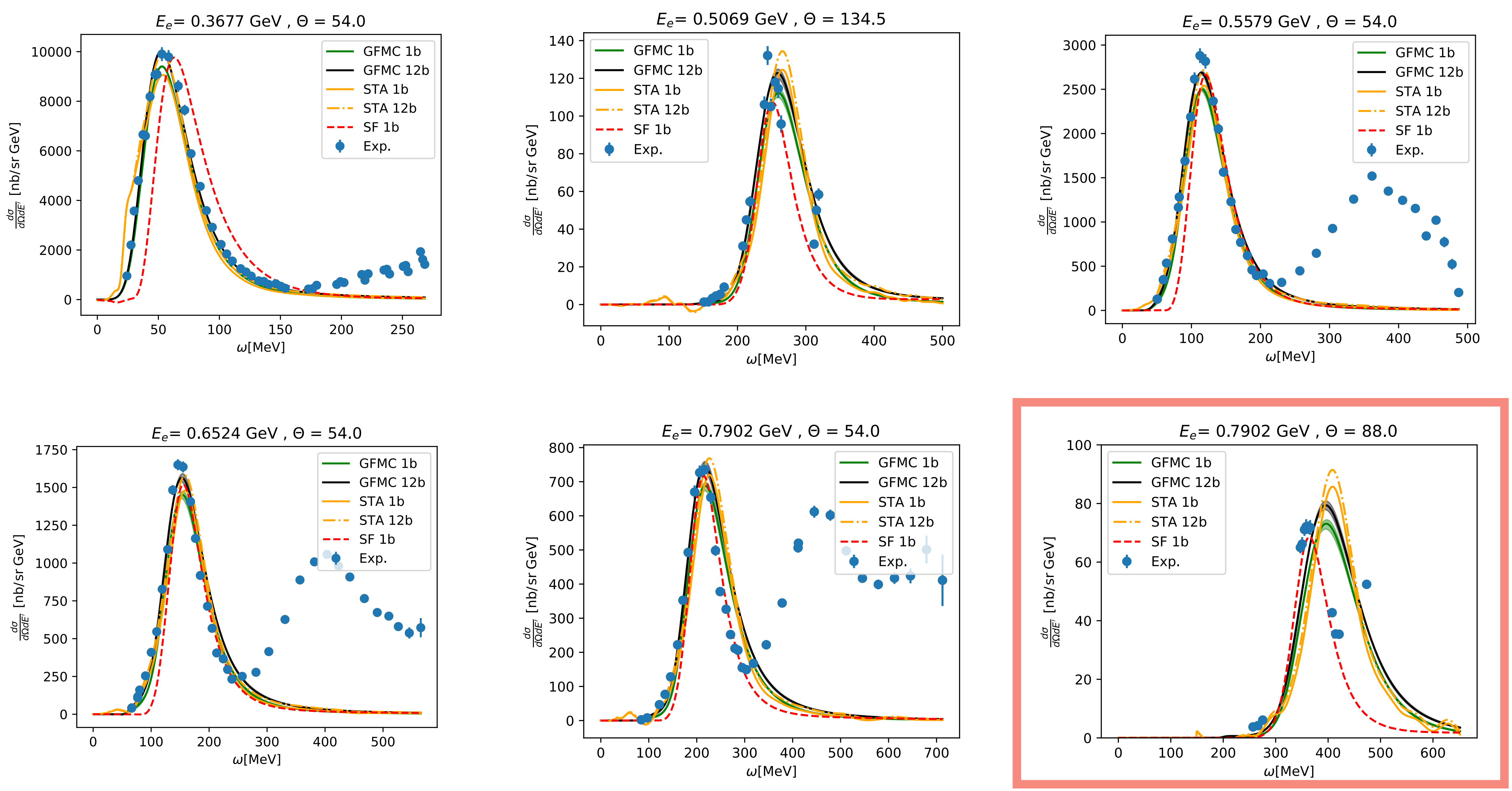
Cross sections

^3H



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Relativistic corrections

Necessary to include relativistic correction at higher momentum q.

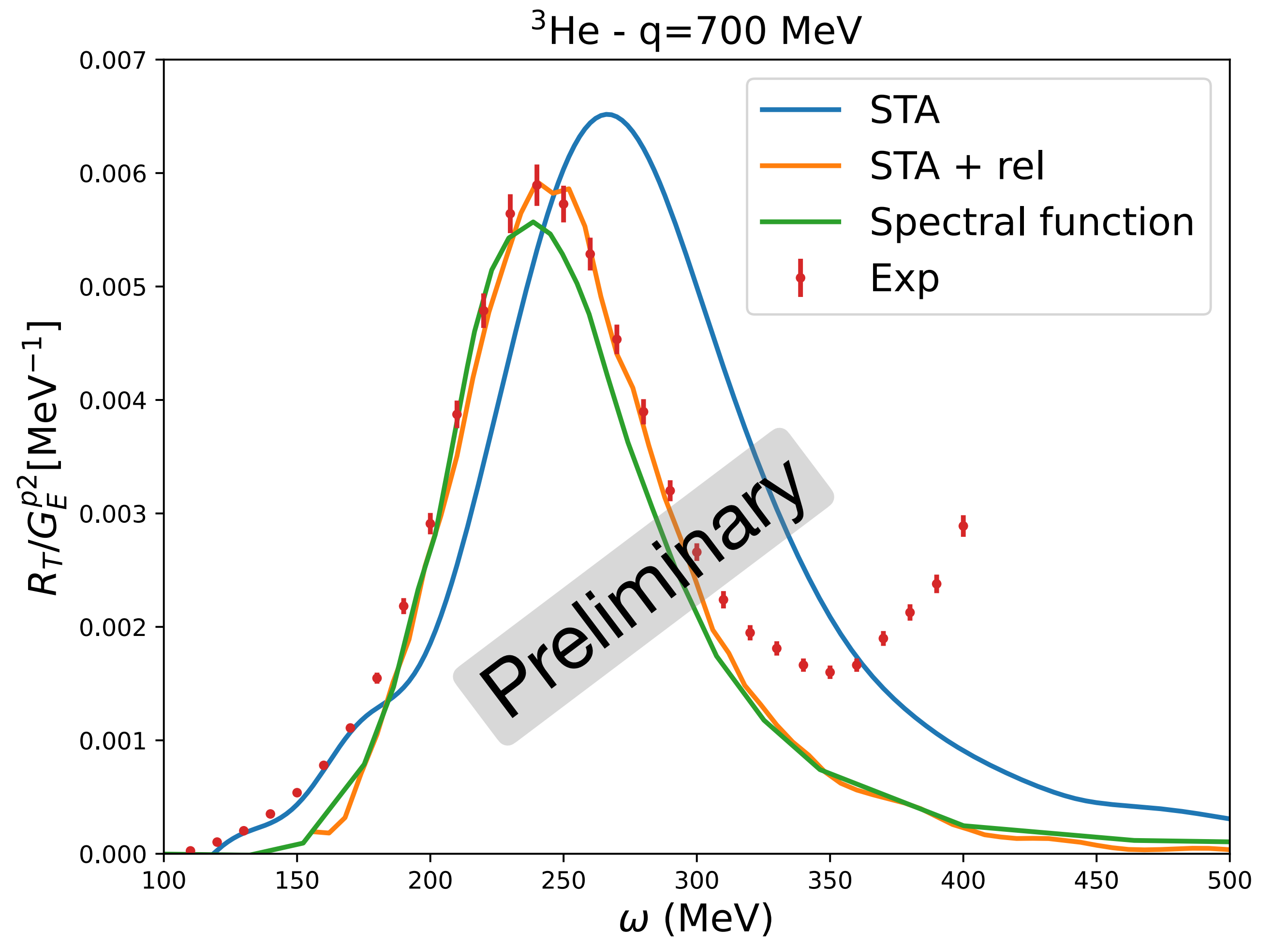
We are currently working on including relativistic corrections within the STA formalism:

R. Weiss (LANL)

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

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

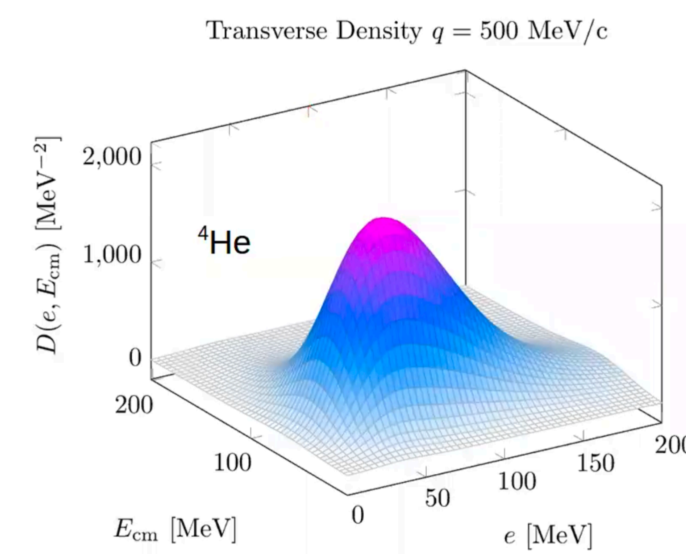
$$\boldsymbol{p}' = \boldsymbol{p} + \boldsymbol{q}$$



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

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

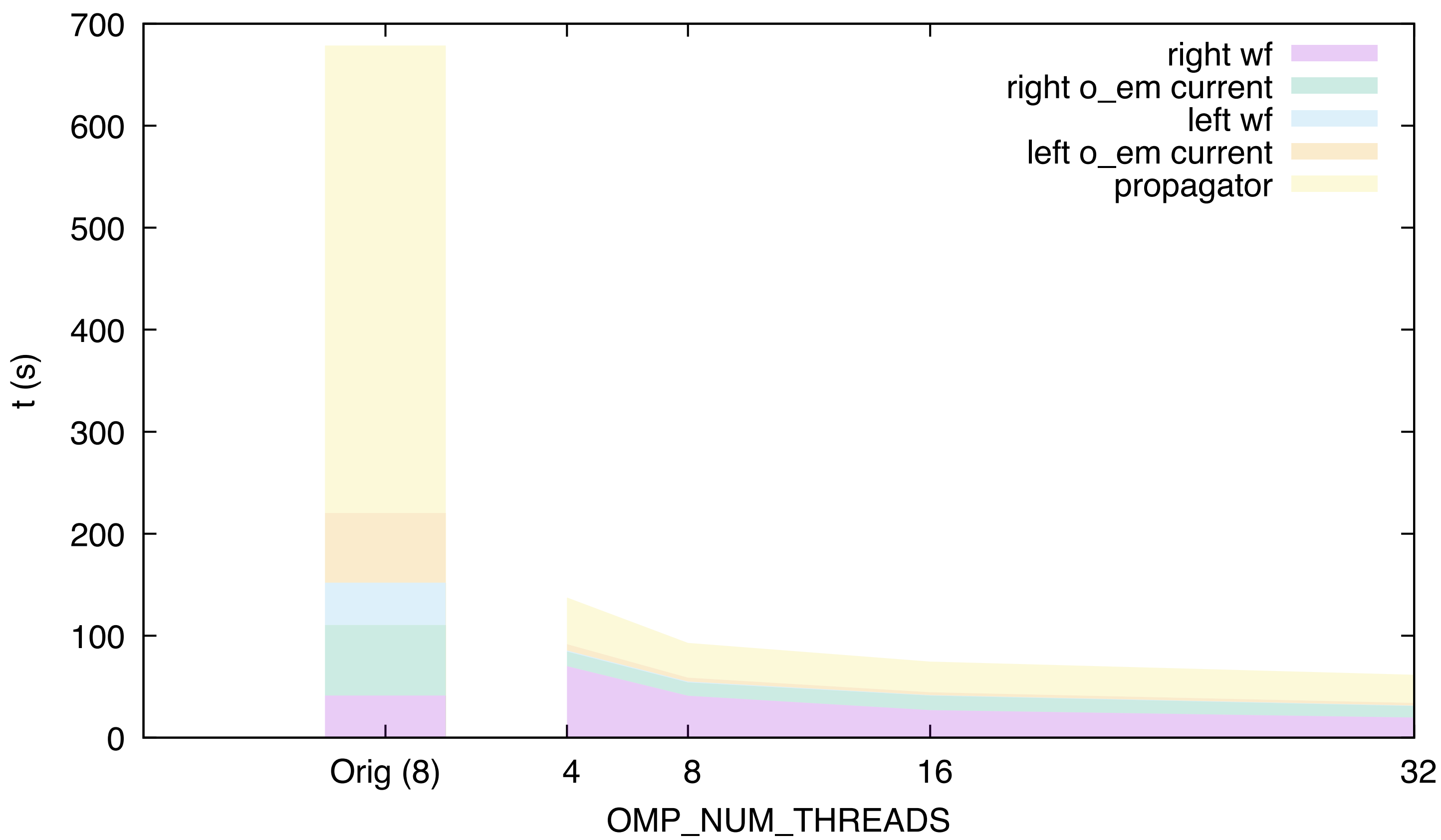
Heavier nuclei

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



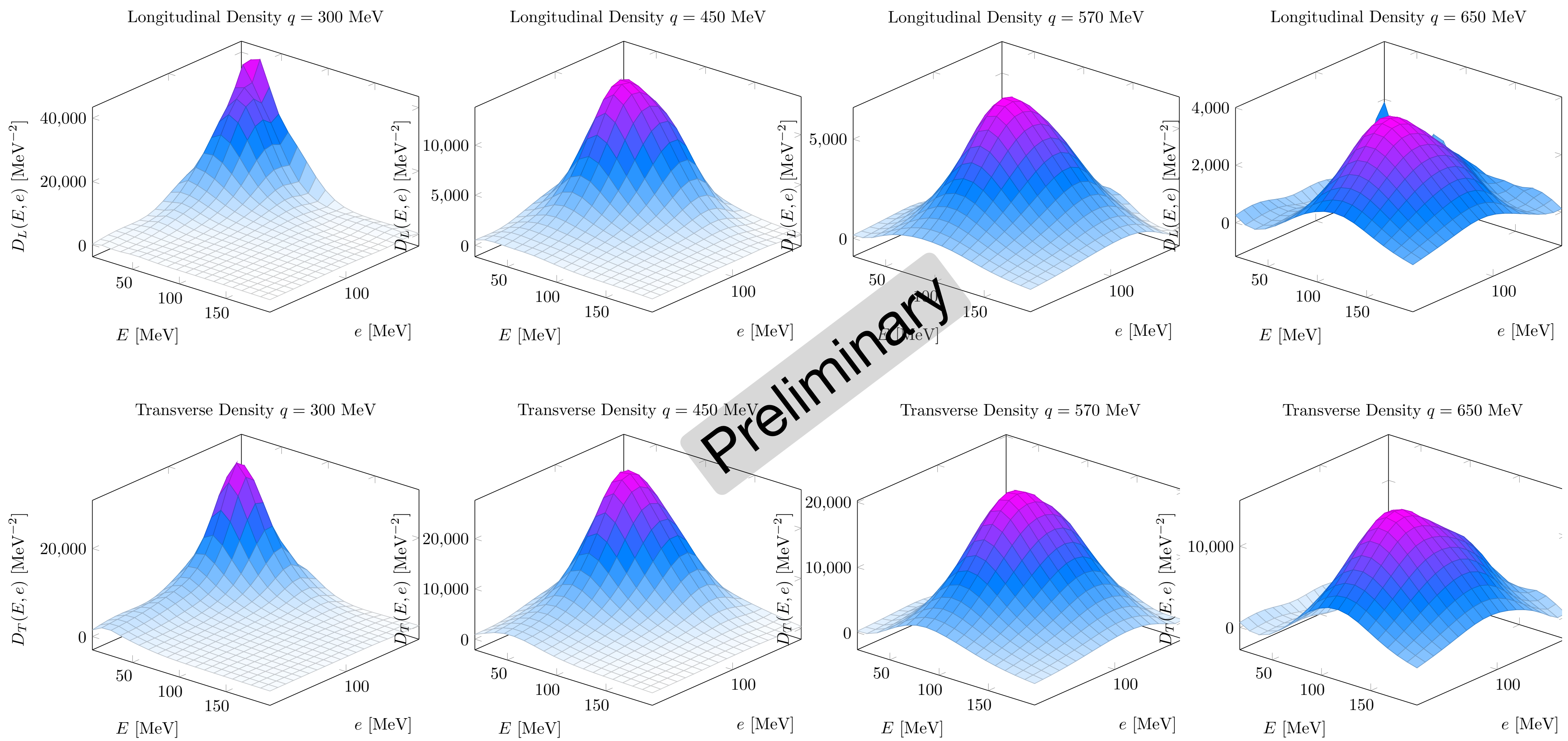
Optimization specific to ^{12}C was needed in oder to perform full response densities calculations:

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

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

Responses for ^{12}C

Longitudinal and transverse response for **300 < q < 850 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

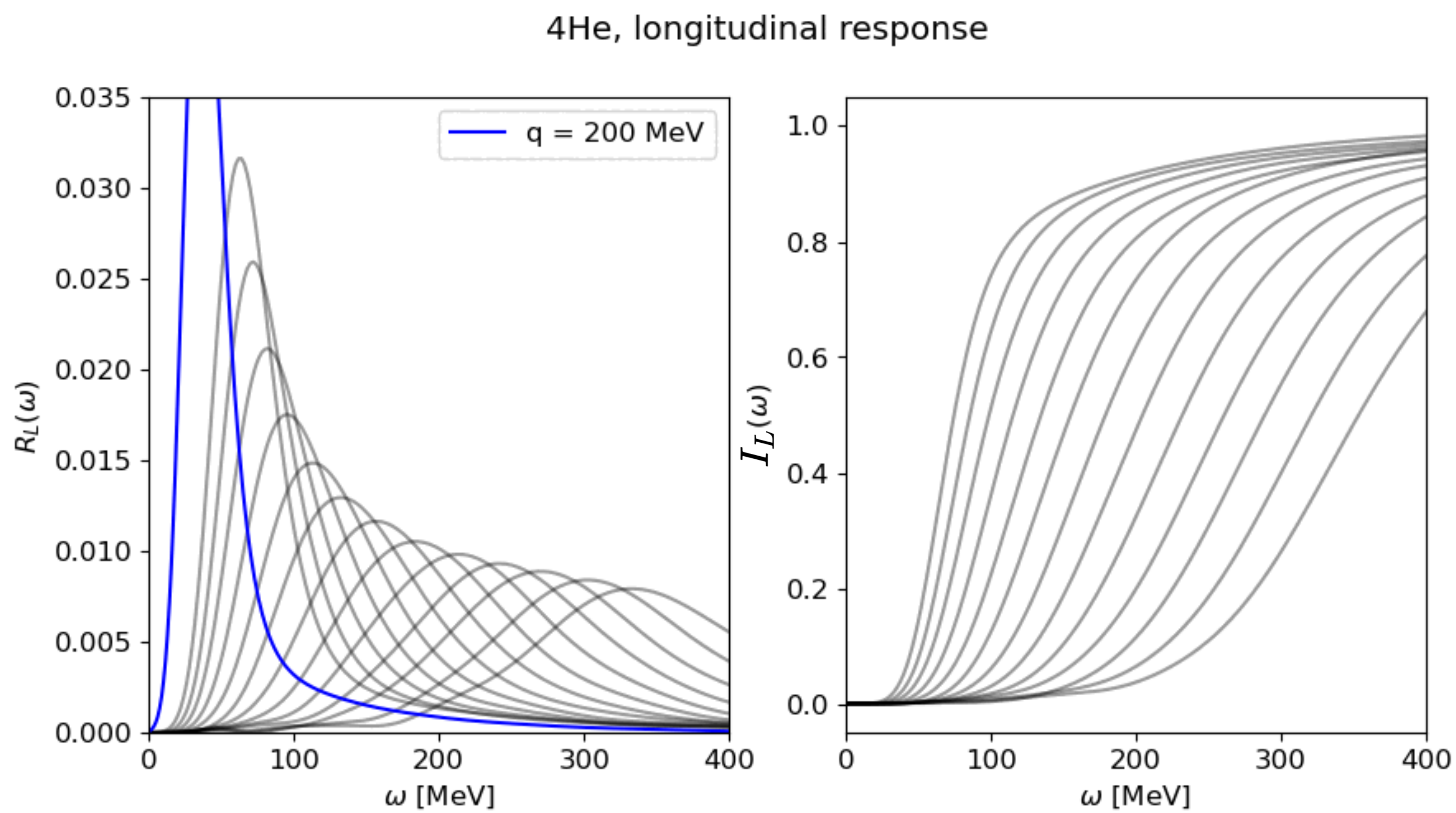
Cross sections: Interpolation schemes

- 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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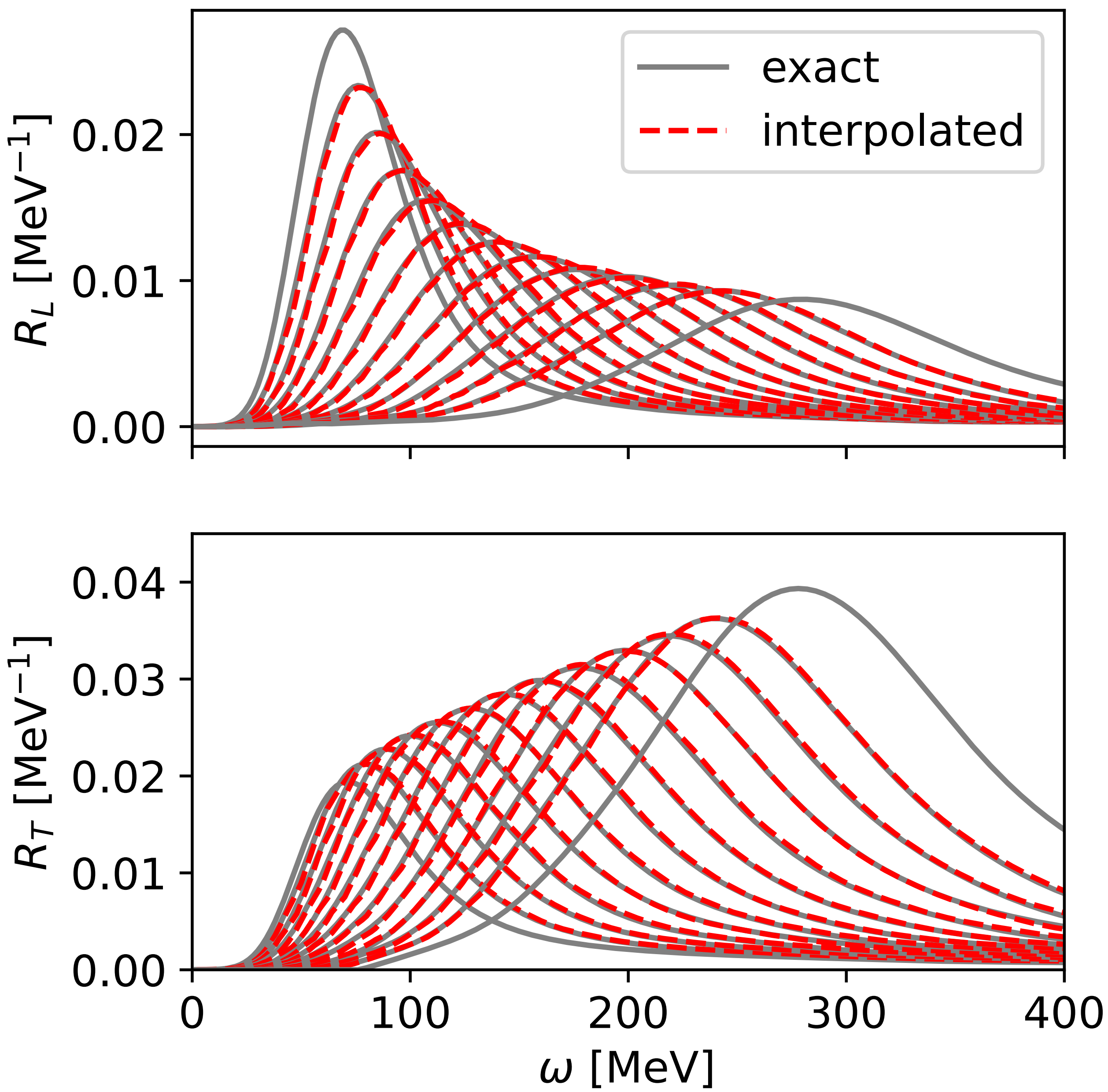
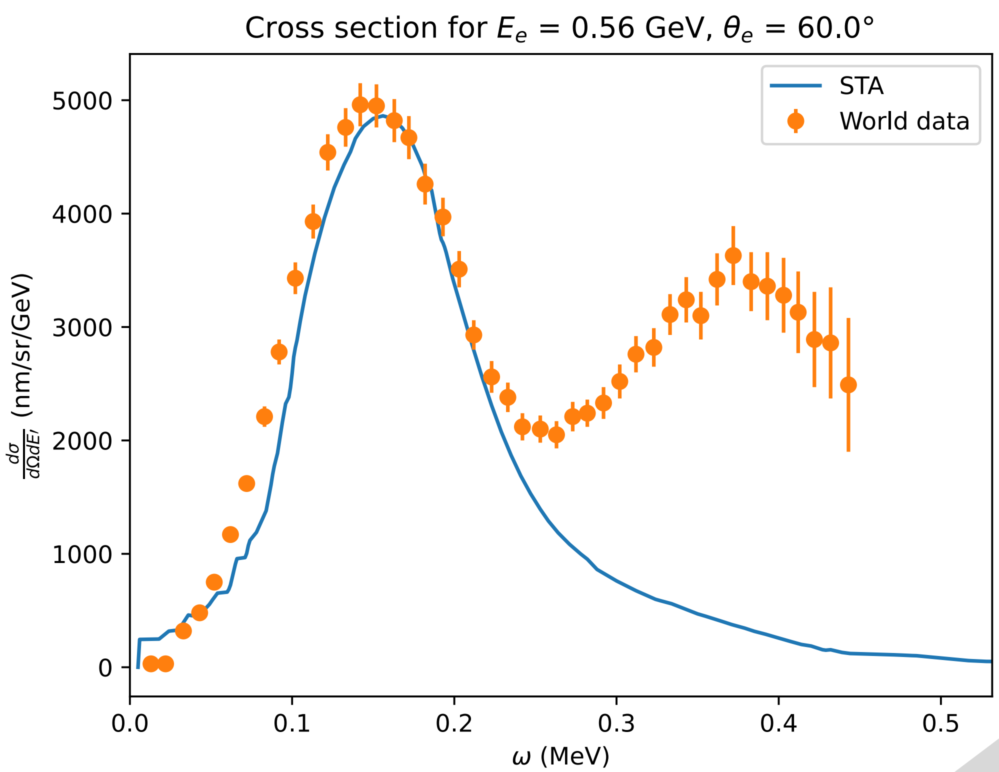
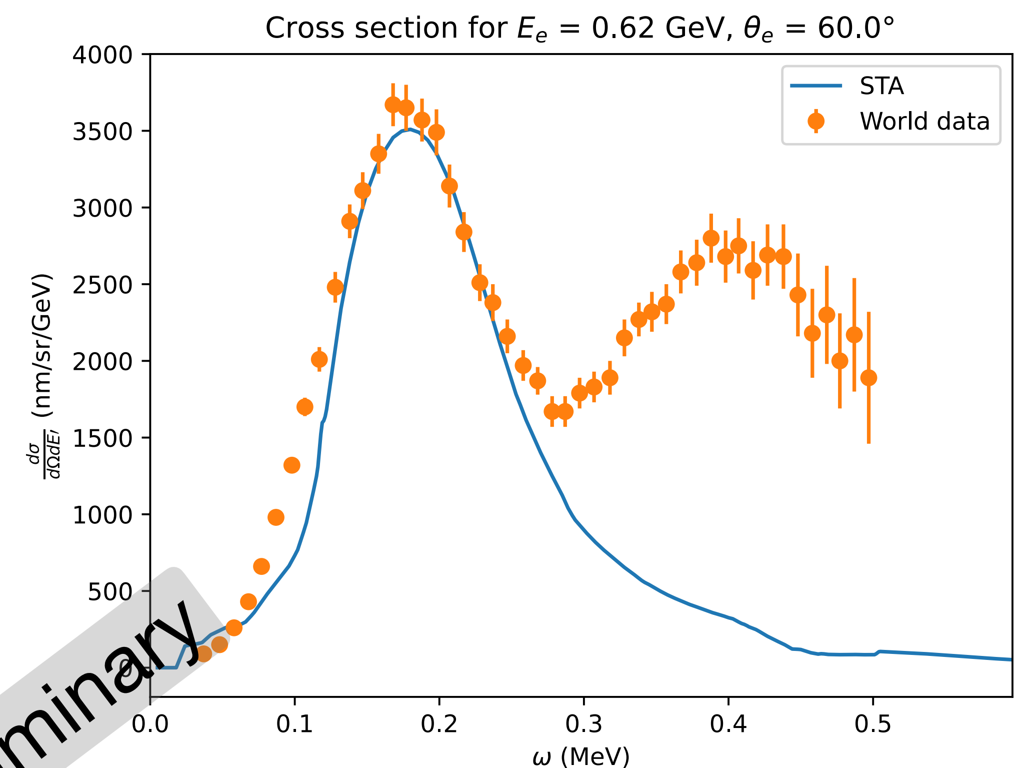
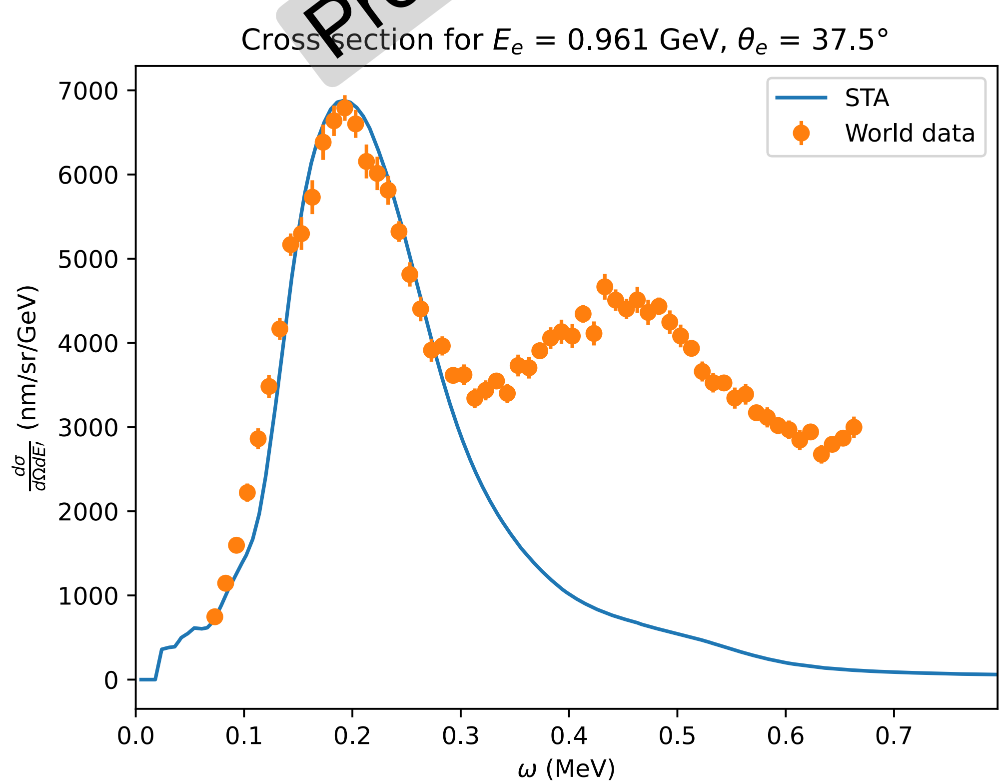


Cross sections results





Preliminary



Conclusion:

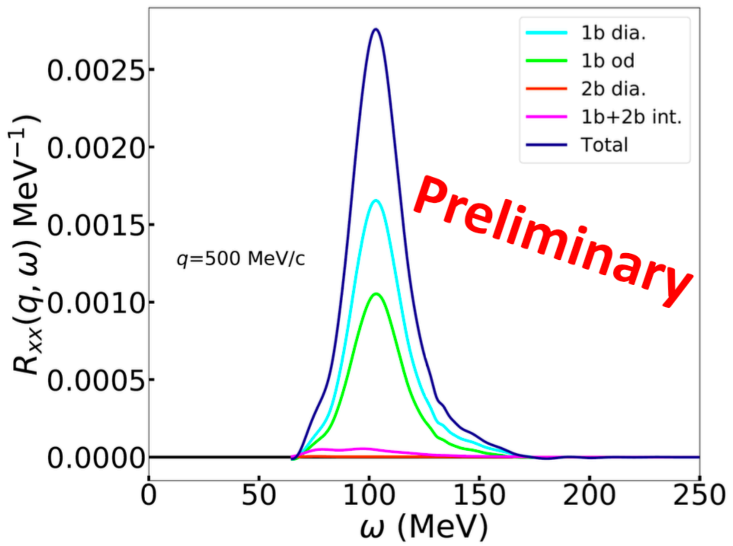
- The STA responses for ^{12}C are in good agreement with the data, and are accurate up to moderate values of q (and consequently to moderate values of incoming electron beam for cross sections calculations)
- Given the computational complexity of evaluating cross sections, an interpolation scheme was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

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



Collaborators:

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R. Weiss, J. Carlson

Thank you!

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