

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

Marciana 2023 - Lepton Interactions with Nucleons and Nuclei

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 Washington University in St. Louis



Outline

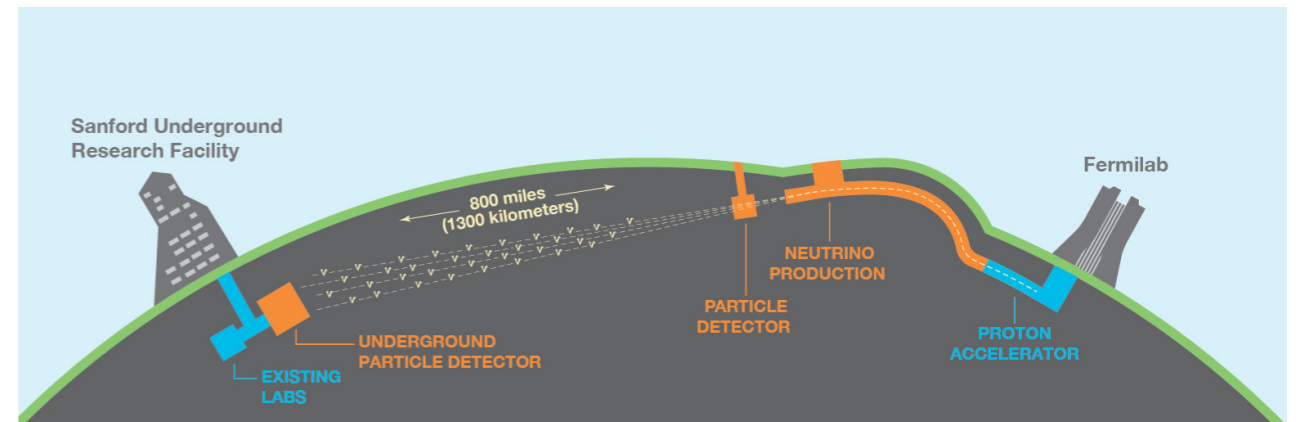
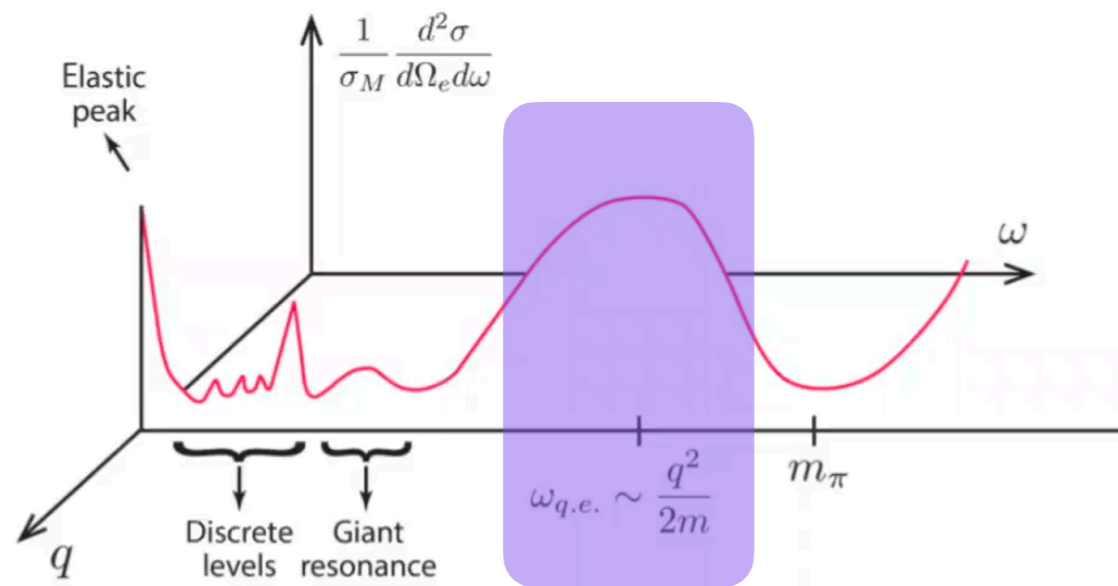
- Quasielastic lepton-nucleus scattering
- Ab initio description of nuclei:
 - Nuclear interaction
 - Electroweak interaction of leptons with nucleons and clusters of correlated nucleons
 - Variational Monte Carlo
- Short-time approximation
- Conclusions and outlook



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

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

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

$$U_{ij} = \sum_p f^p(r_{ij}) O_{ij}^p$$

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

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



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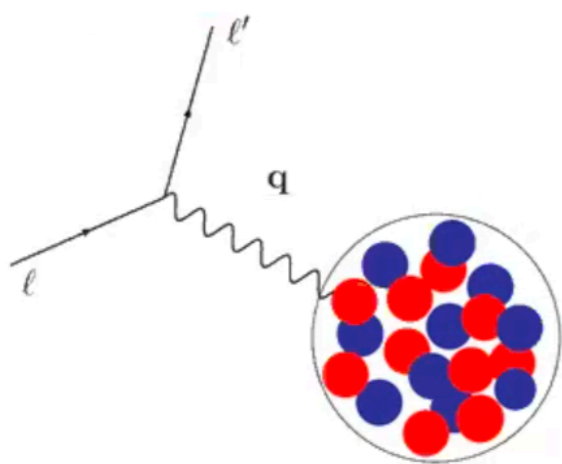
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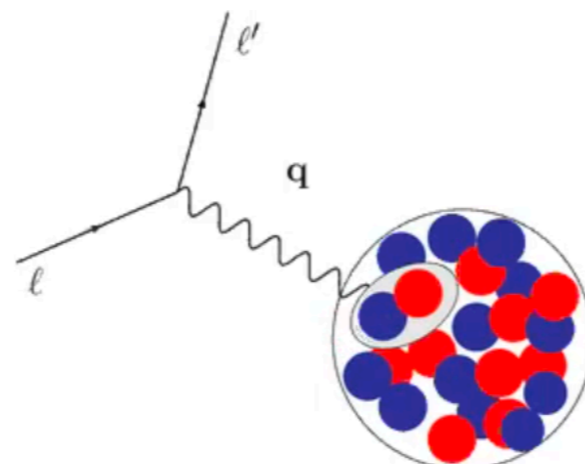
Electromagnetic interactions

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

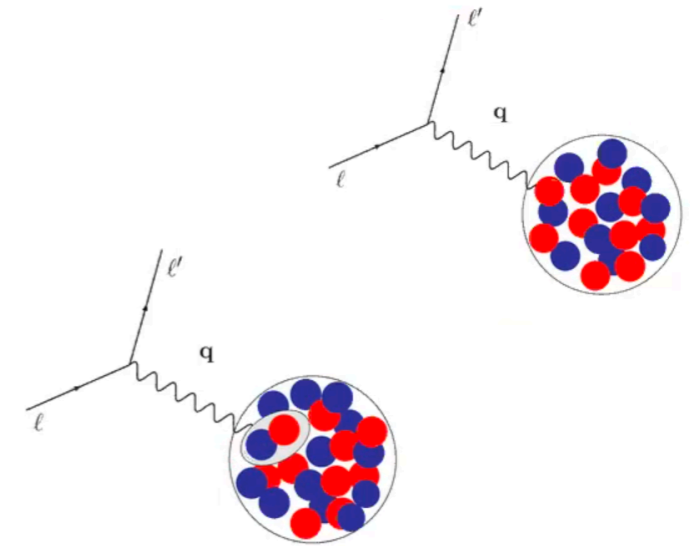
$$\mathbf{j} = \sum_{i=1}^A \mathbf{j}_i + \sum_{i<j} \mathbf{j}_{ij} + \dots$$

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

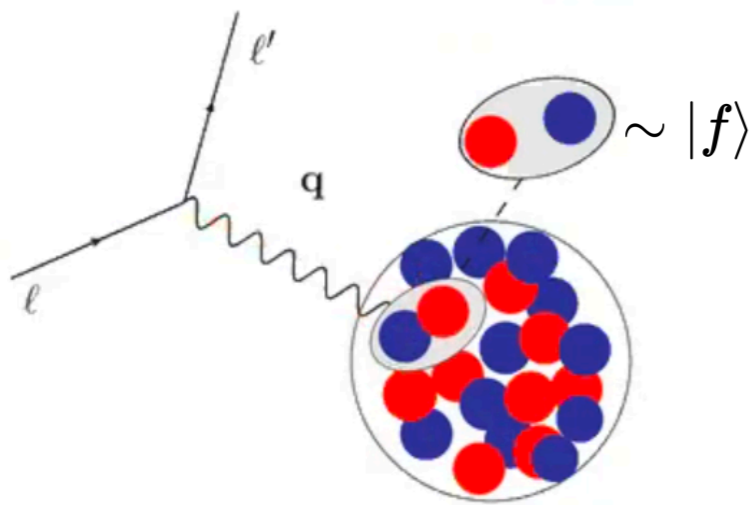




Short-time approximation

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

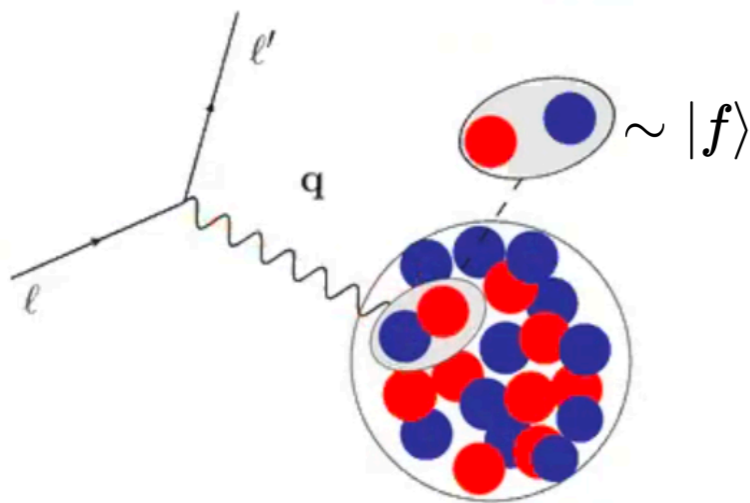
$$R_{\alpha}(q, \omega) = \sum_f \delta(\omega + E_0 - E_f) |\langle f | O_{\alpha}(\mathbf{q}) | 0 \rangle|^2$$



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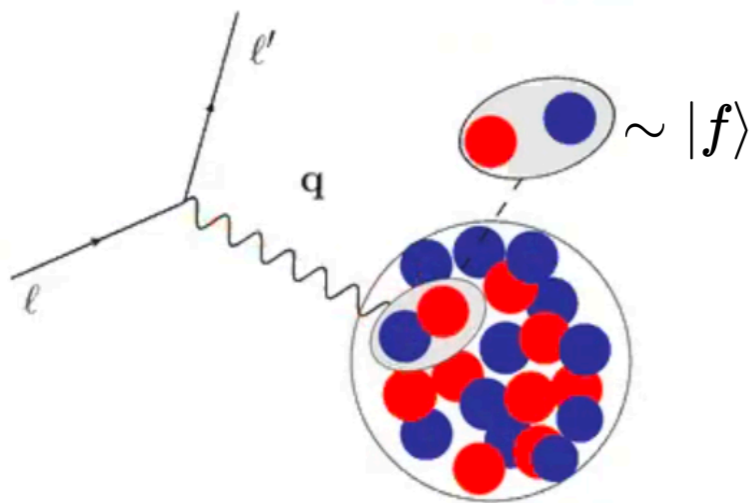
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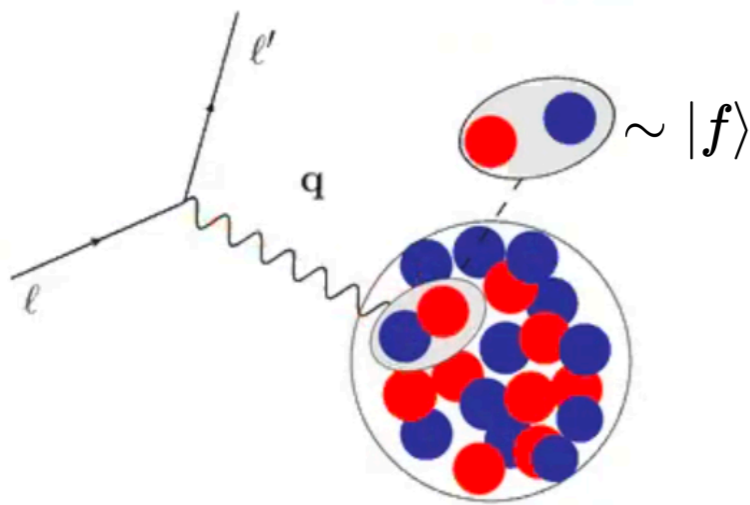
$$\begin{aligned} O^\dagger e^{-iHt} O &= \left(\sum_i O_i^\dagger + \sum_{i<j} O_{ij}^\dagger \right) e^{-iHt} \left(\sum_{i'} O_{i'} + \sum_{i'<j'} O_{i'j'} \right) \\ &= \sum_i O_i^\dagger e^{-iHt} O_i + \sum_{i \neq j} O_i^\dagger e^{-iHt} O_j \\ &\quad + \sum_{i \neq j} \left(O_i^\dagger e^{-iHt}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



Short-time approximation

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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

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

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 $\frac{T}{A} \sim \frac{2|V|}{A(A-1)} \equiv \epsilon_{\text{nuc}}$ 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 $\omega_{qe} = \sqrt{m^2 + q^2} - m$

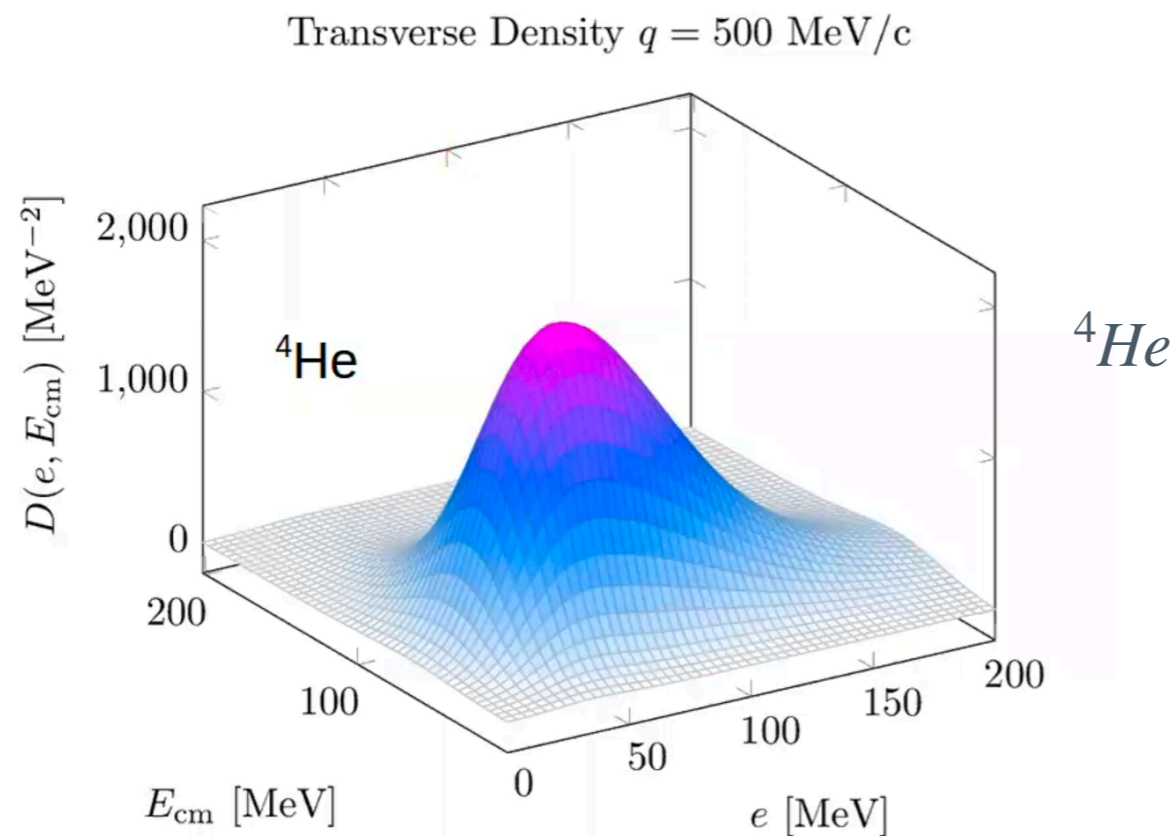
In the STA, one drops terms of order $\mathcal{O} \left(\frac{\epsilon_{\text{nuc}}^2}{\omega_{qe}^2} \right)$ so it is valid at sufficiently high ω and $|\mathbf{q}|$ w.r.t. epsilon nuc

Consistent with the notion that there is a high probability for the correlated pair to absorb the entirety of $|\mathbf{q}|$ when the final state momenta are far from the Fermi surface

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



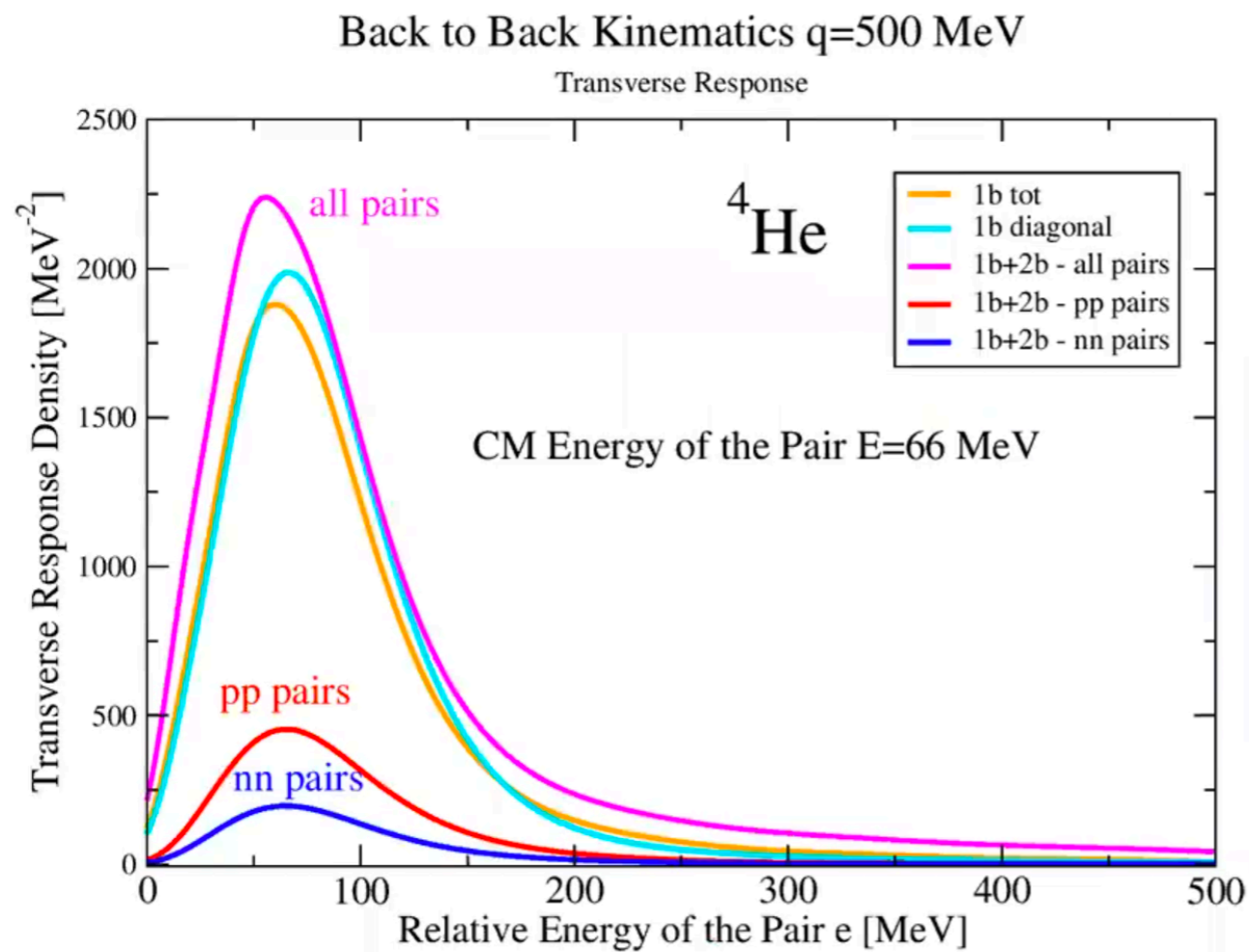
Transverse response density



Electron scattering from ${}^4\text{He}$ 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

Back-to-back kinematic



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

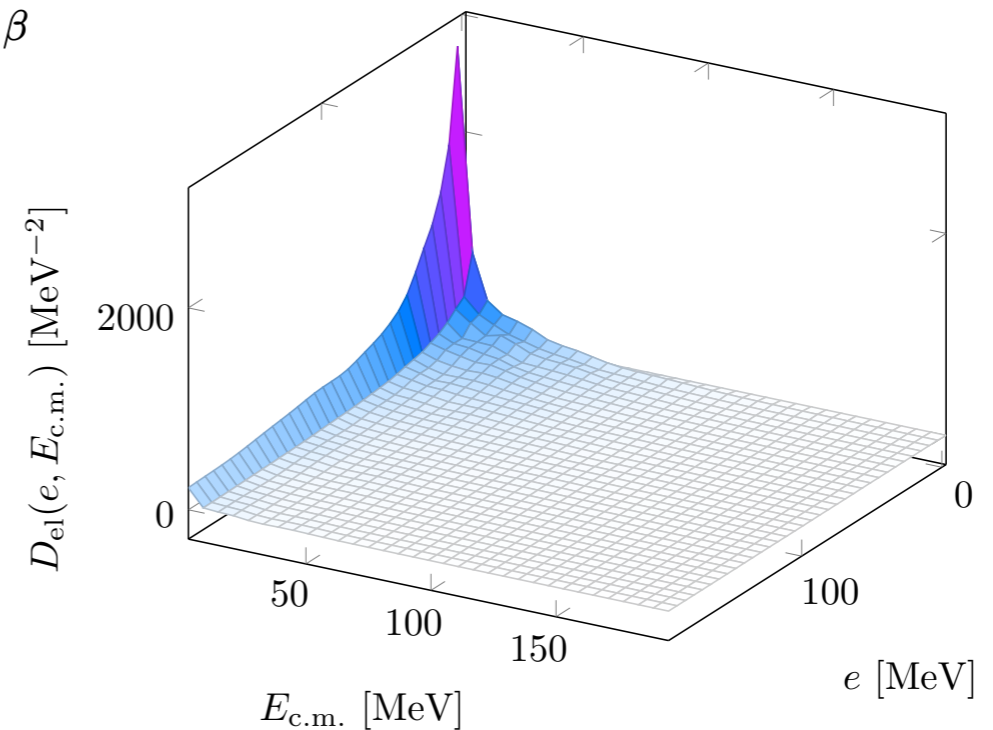
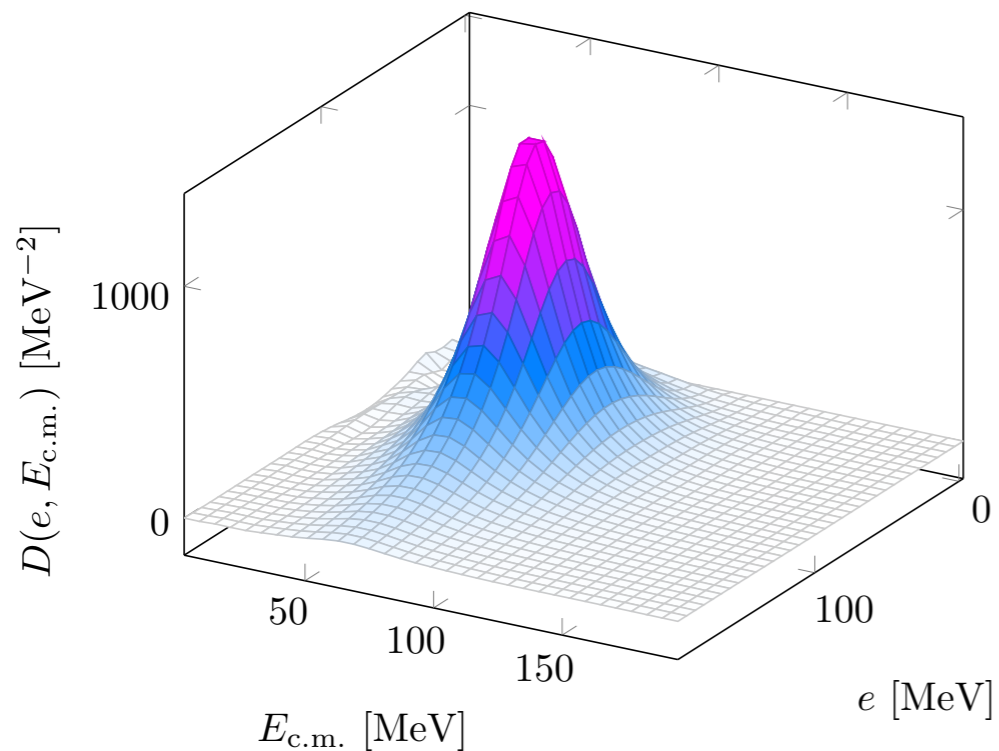


Longitudinal response density: elastic peak removal

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

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

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



³H Longitudinal response at 300 MeV

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 ^3He , and the inclusive cross sections of both ^3He and ^3H
- 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

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

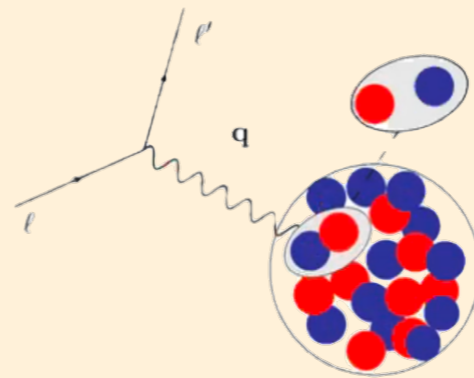
$$E_\alpha(\mathbf{q}, \tau) = \int_{\omega_{\text{th}}}^{\infty} d\omega e^{-\omega\tau} R_\alpha(\mathbf{q}, \omega), \quad \alpha = L, T$$

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

Start-time approximation

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

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



Spectral function

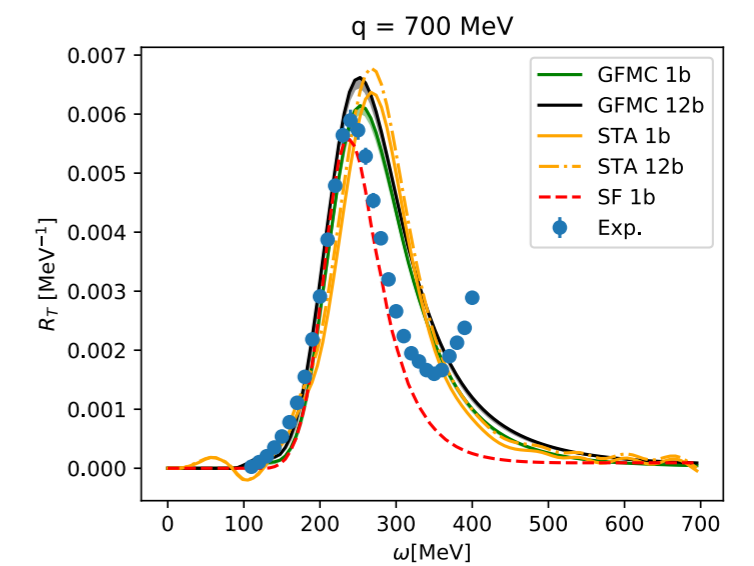
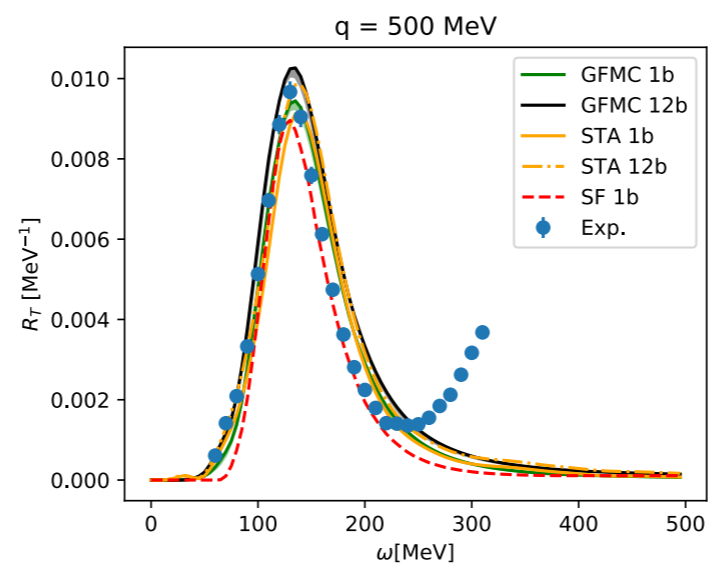
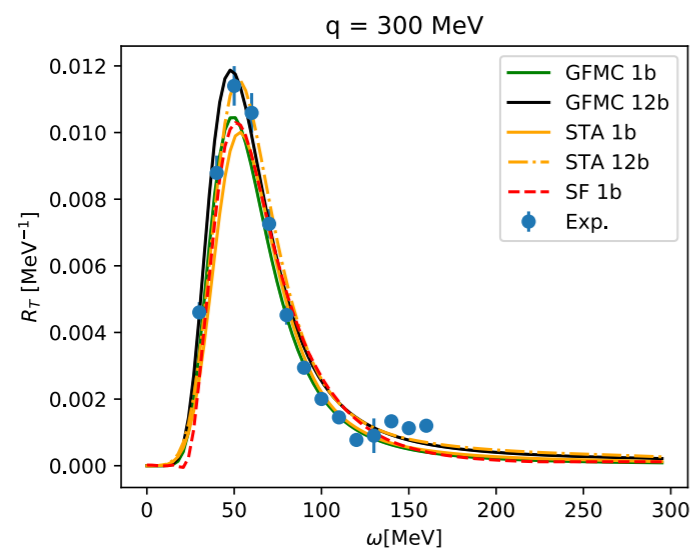
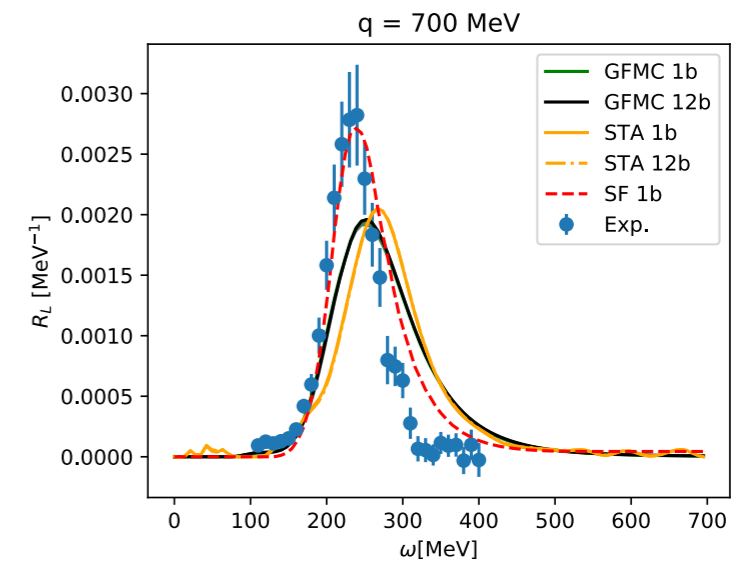
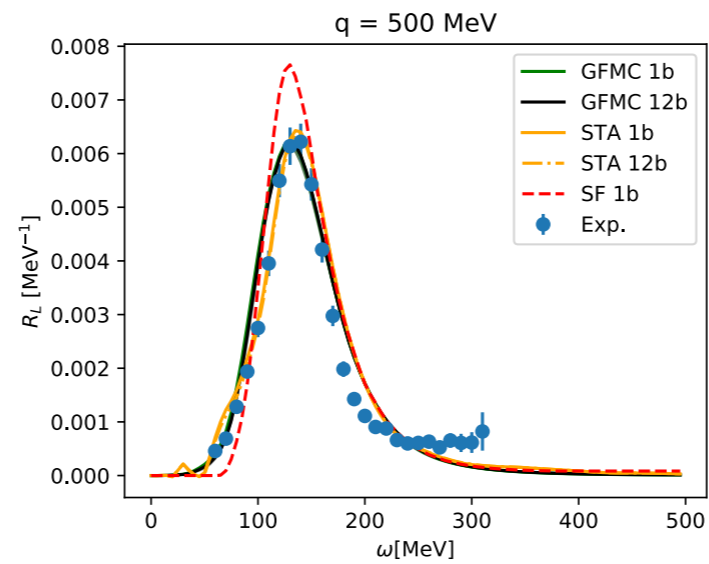
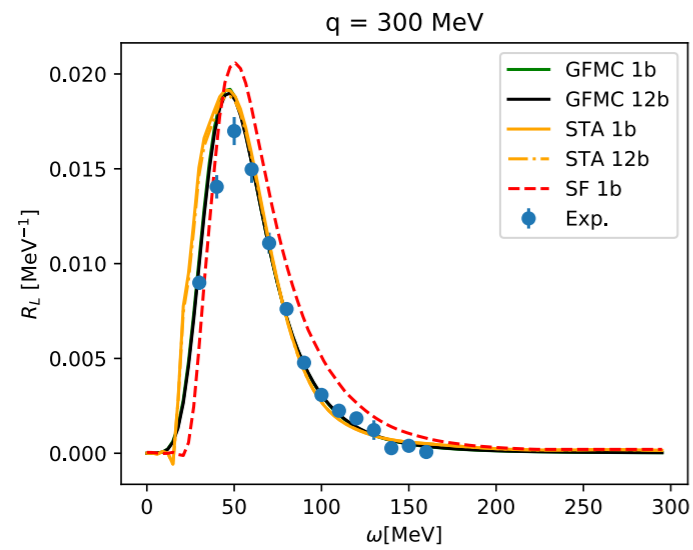
$$|\Psi_f\rangle = |\mathbf{p}\rangle \otimes |\Psi_n^{A-1}\rangle$$

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

Benchmark



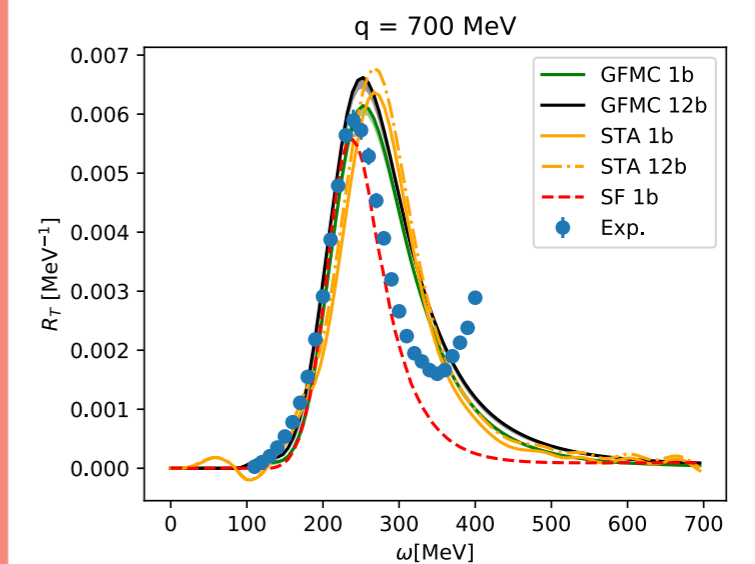
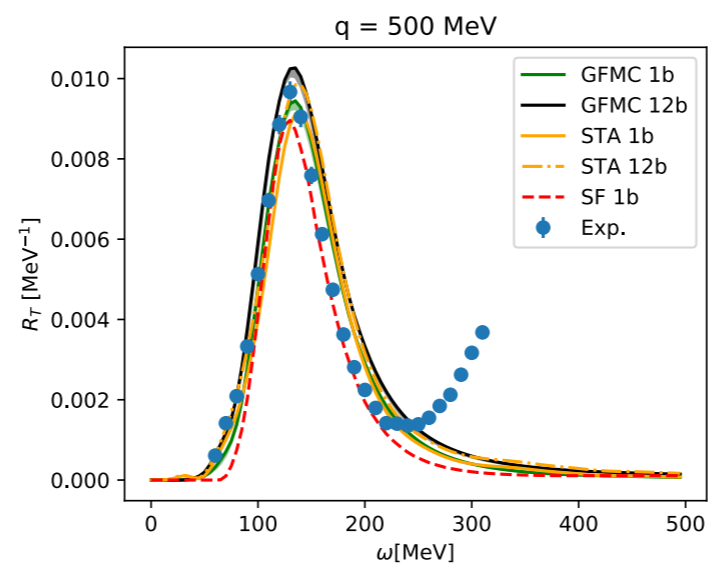
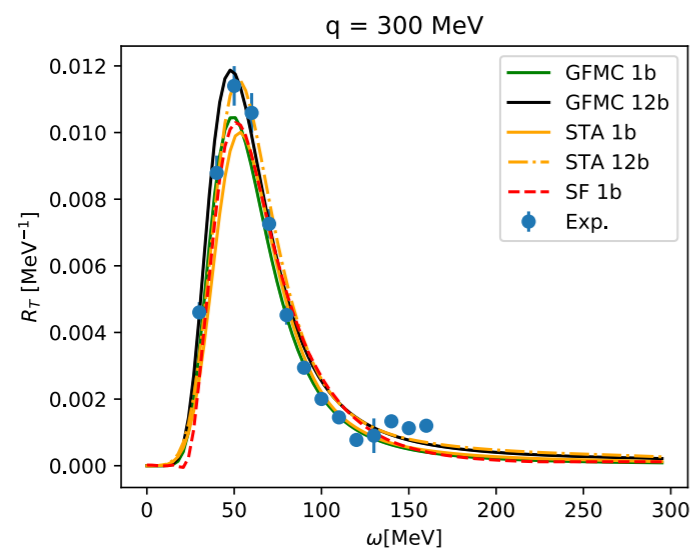
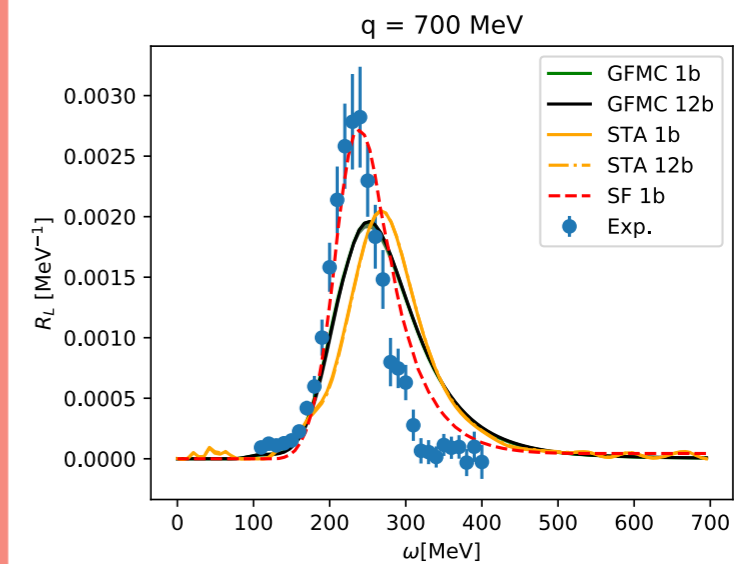
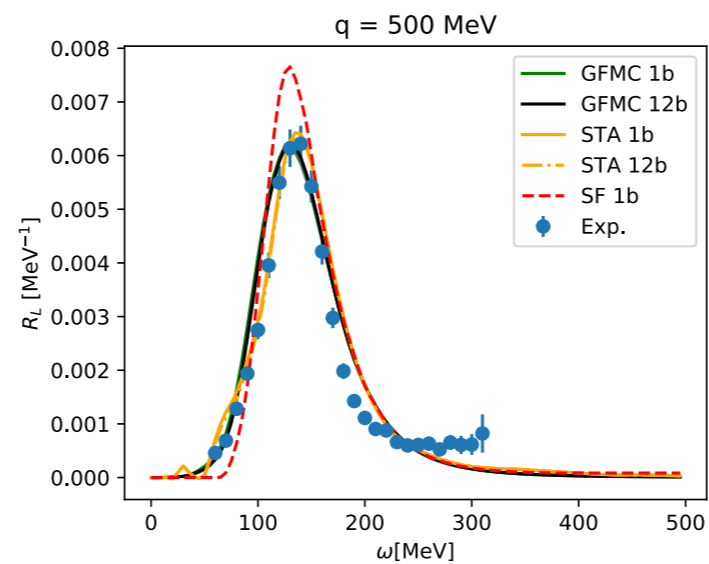
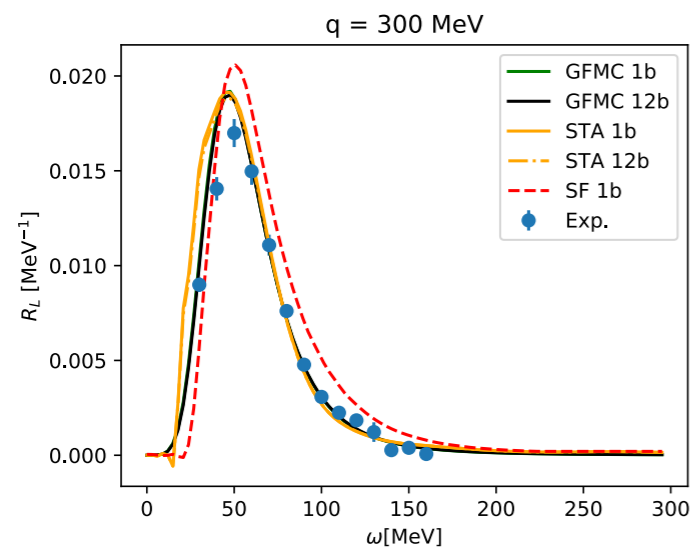
Longitudinal and transverse response function in ^3He



Benchmark



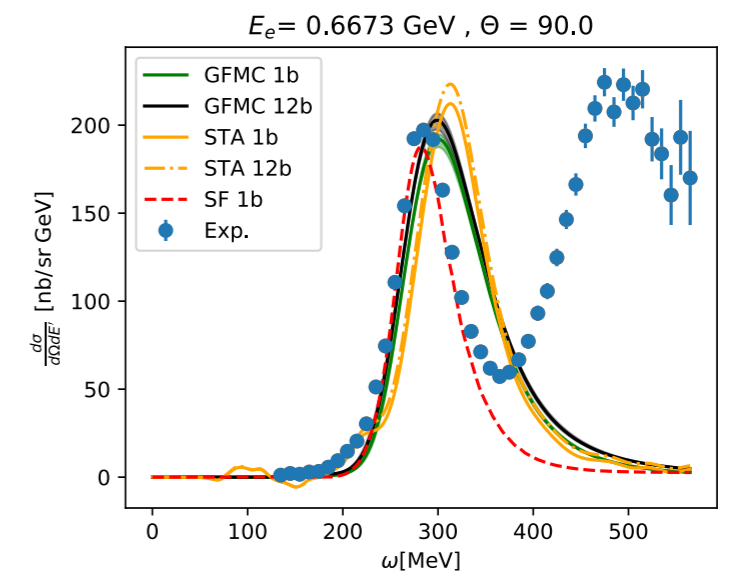
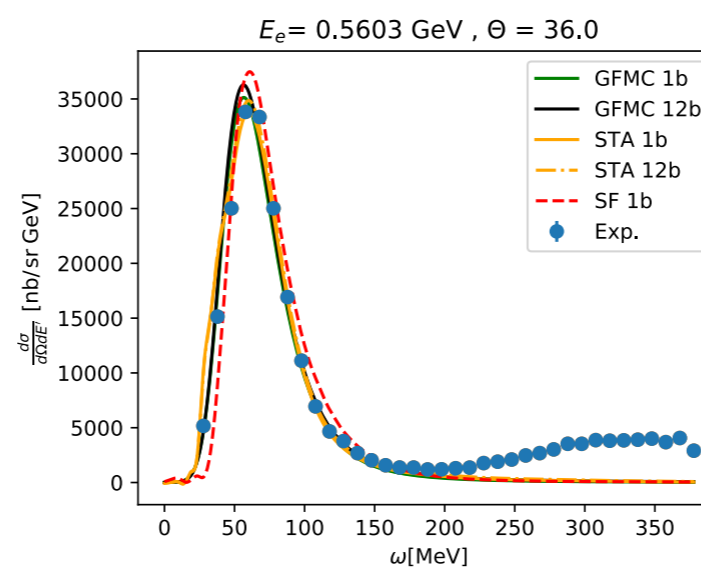
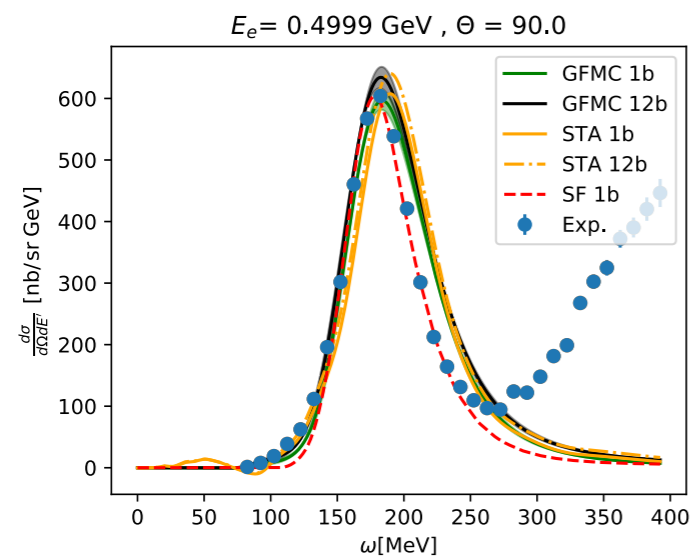
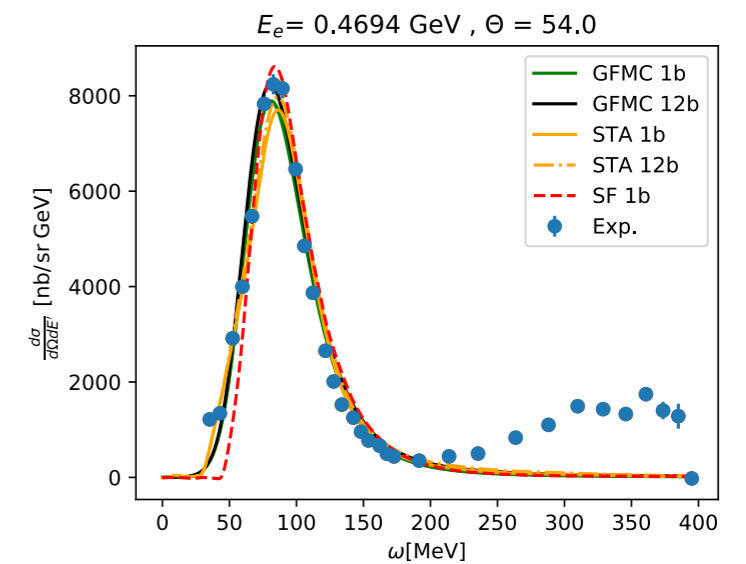
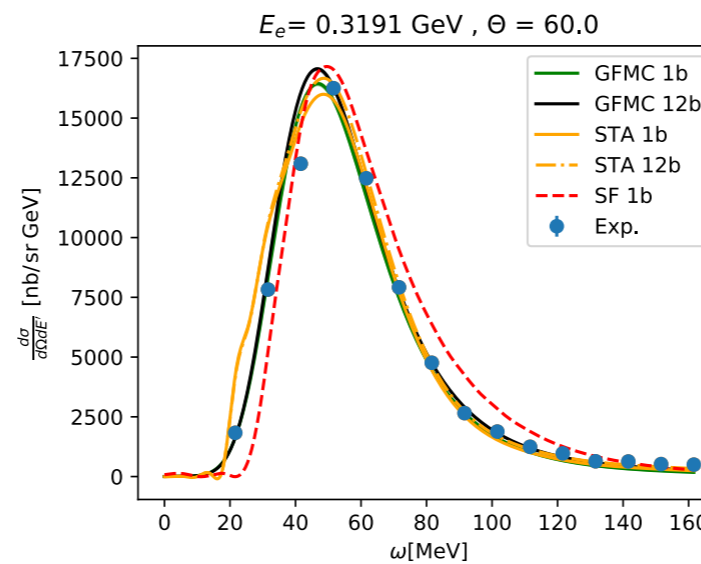
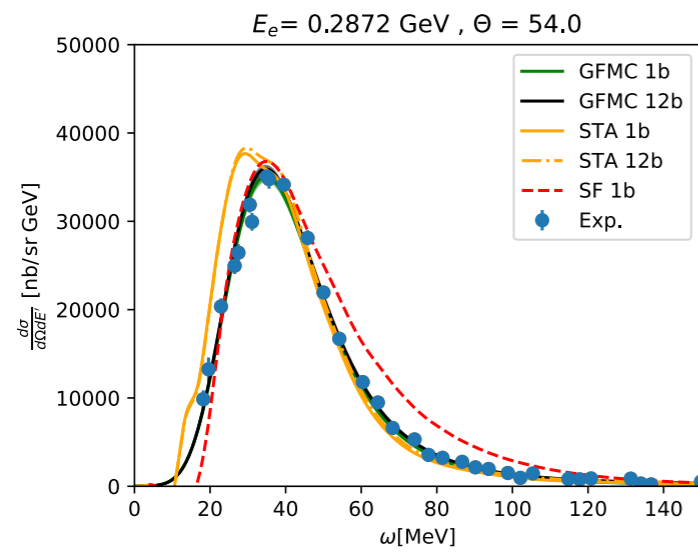
Longitudinal and transverse response function in ^3He



Cross sections



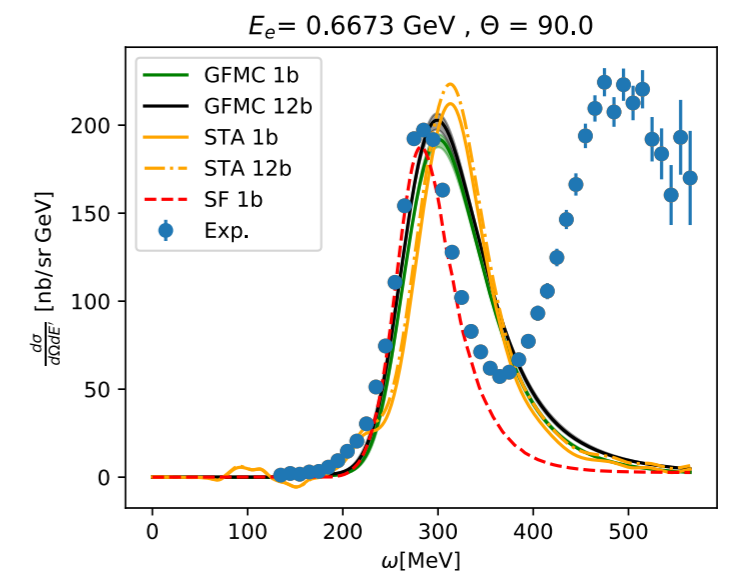
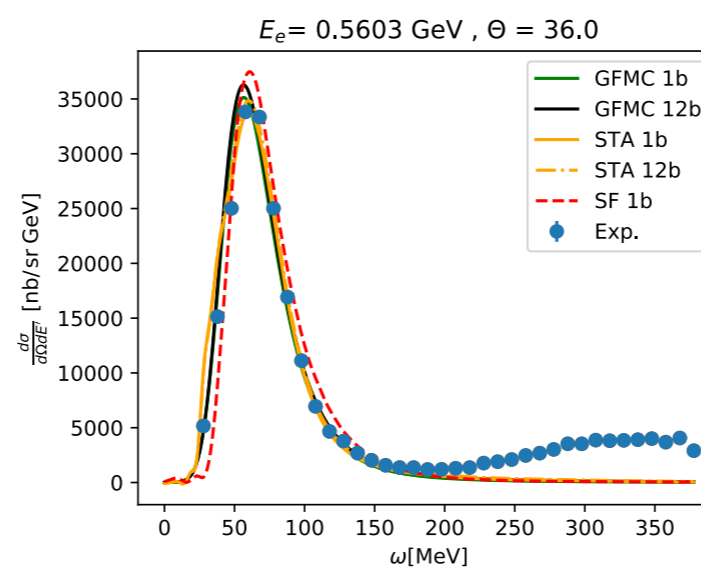
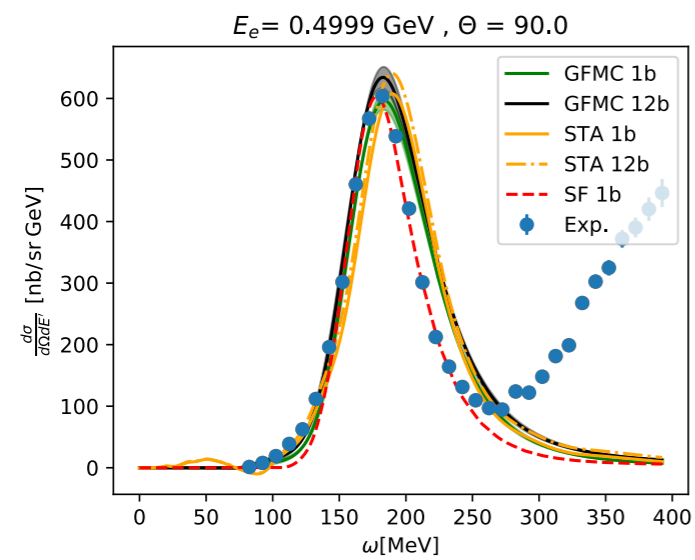
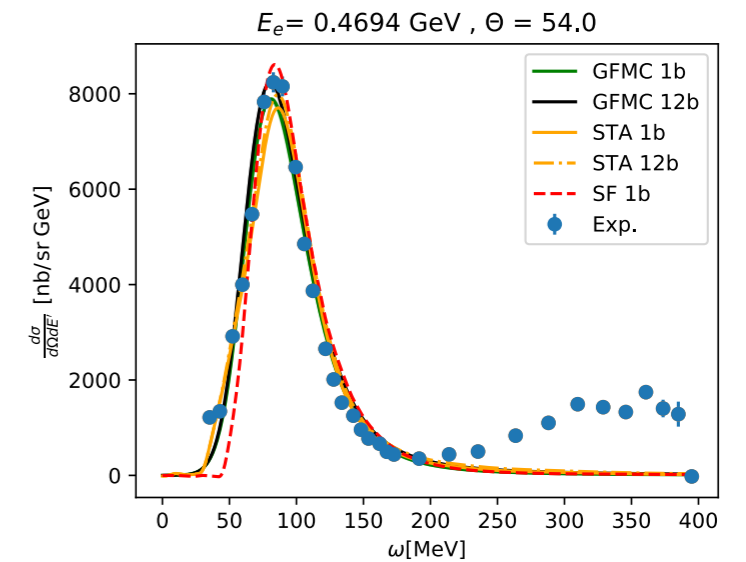
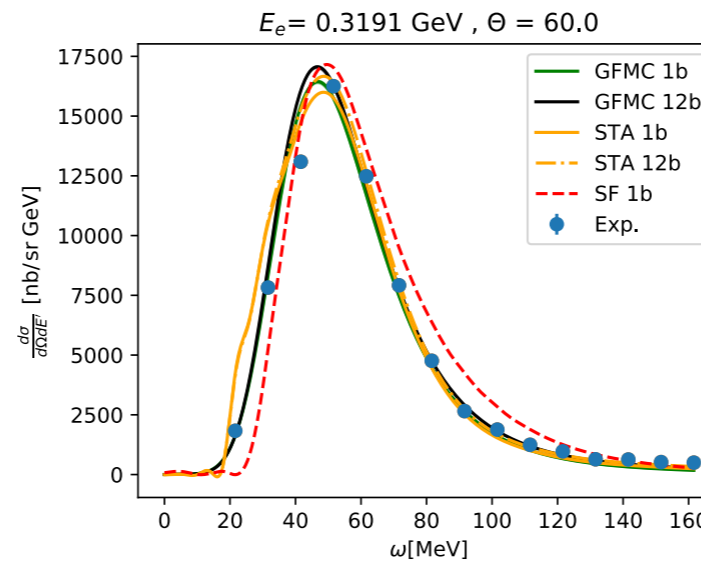
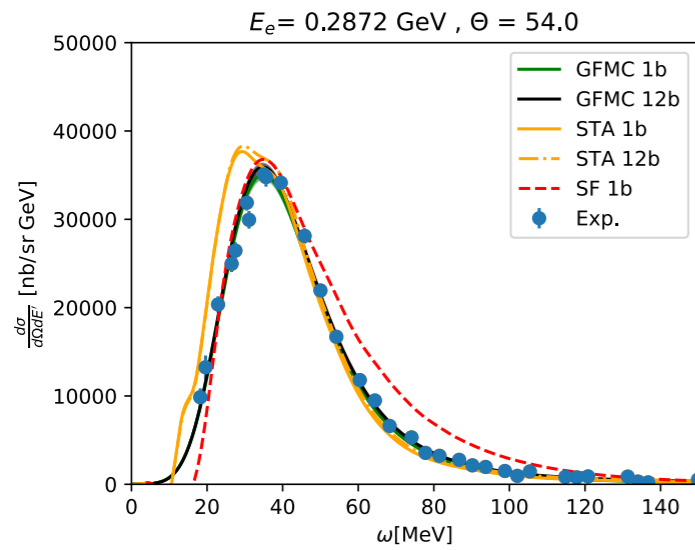
^3He



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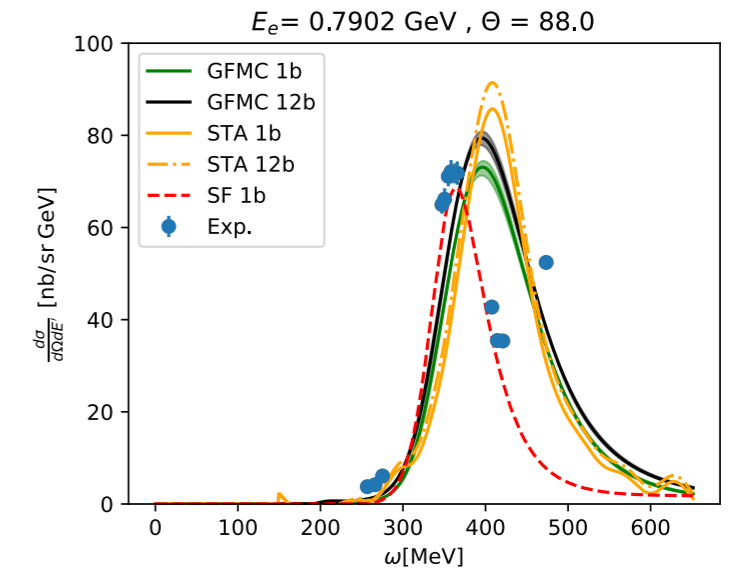
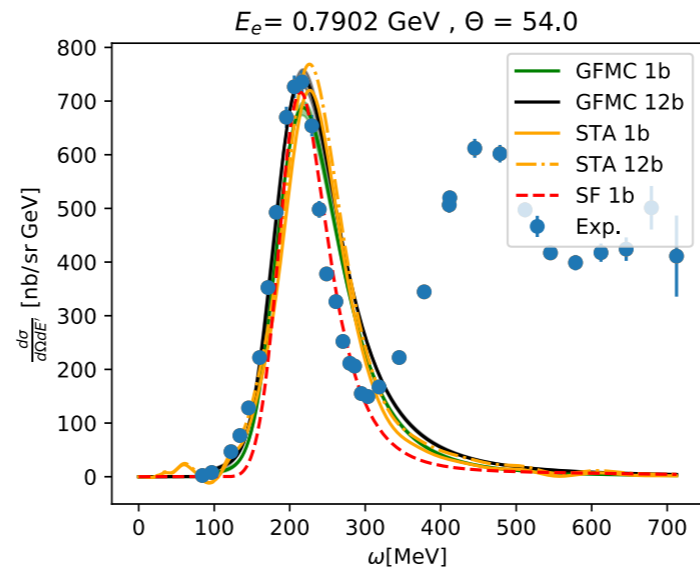
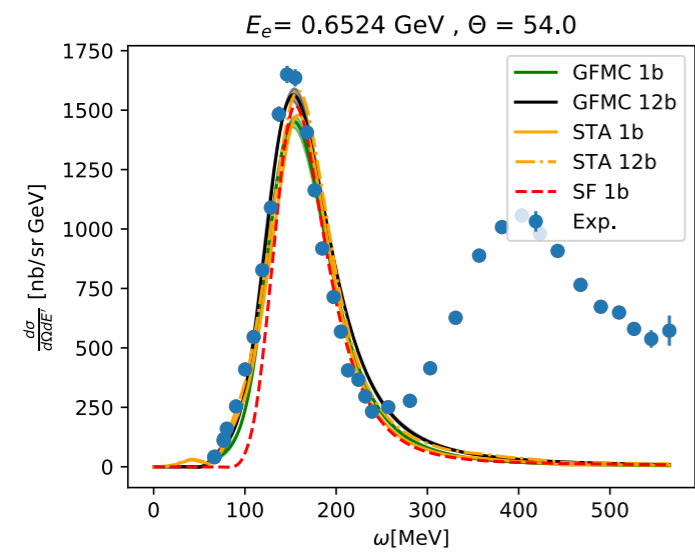
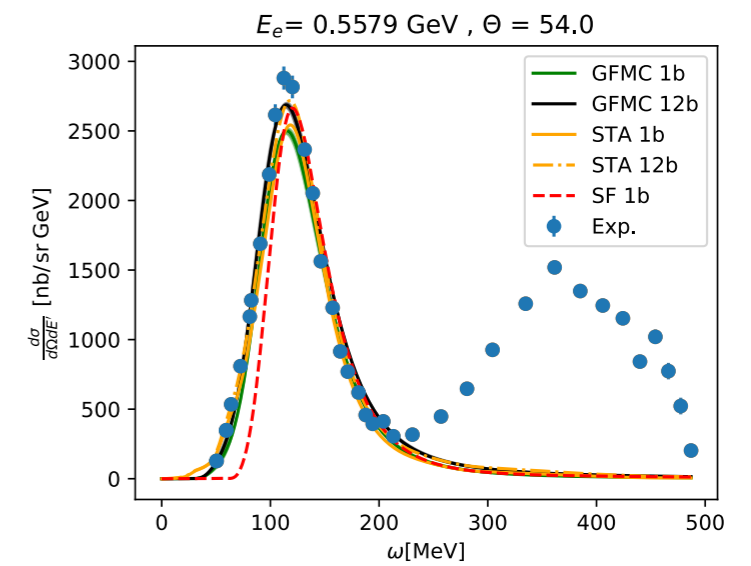
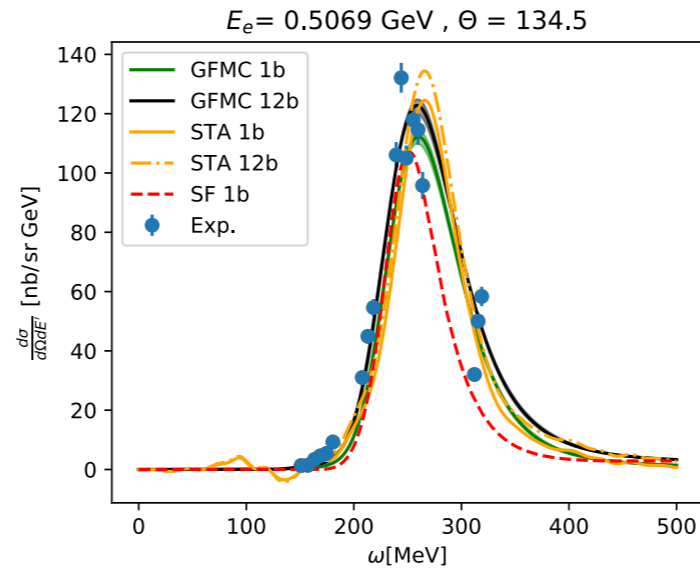
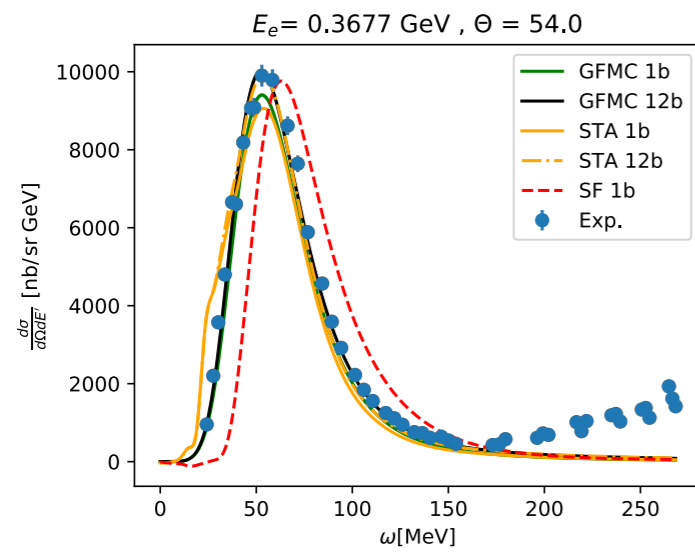
^3He



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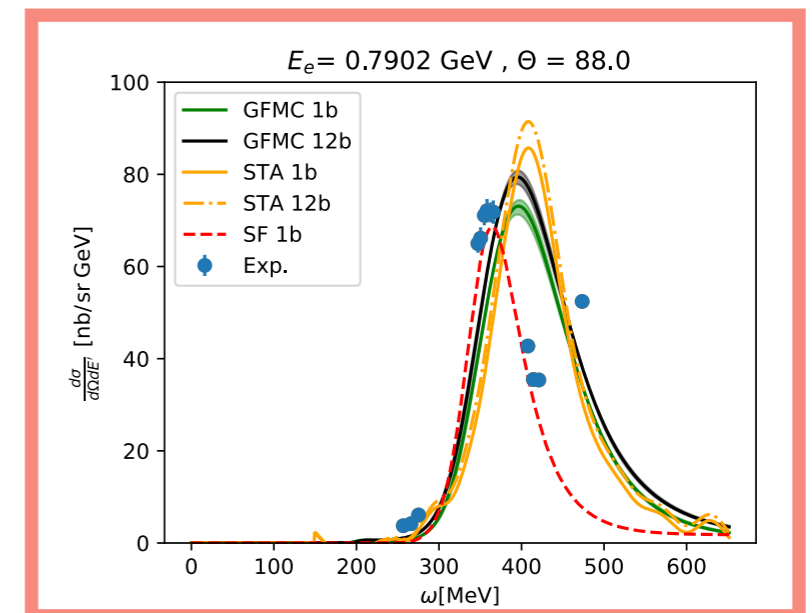
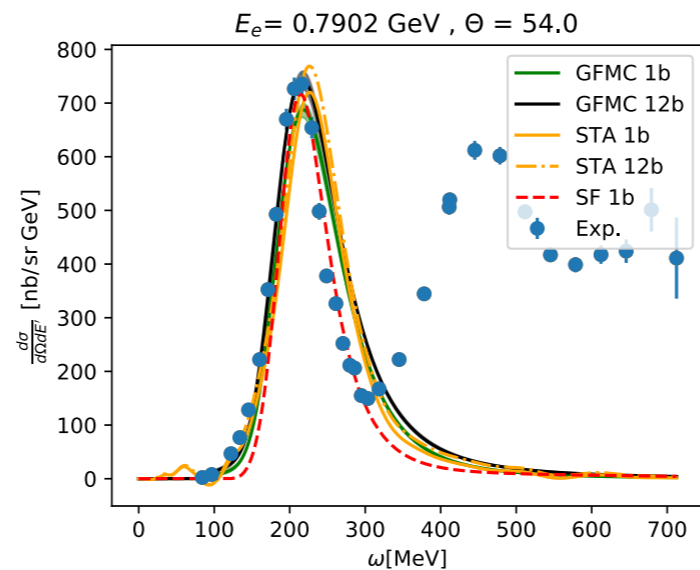
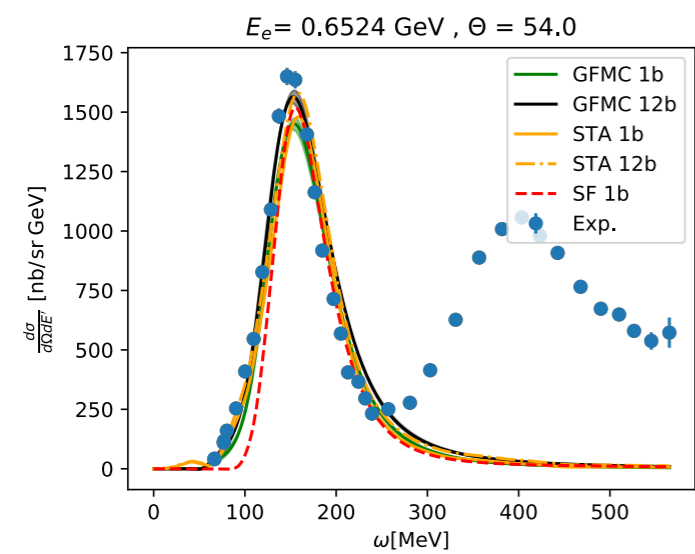
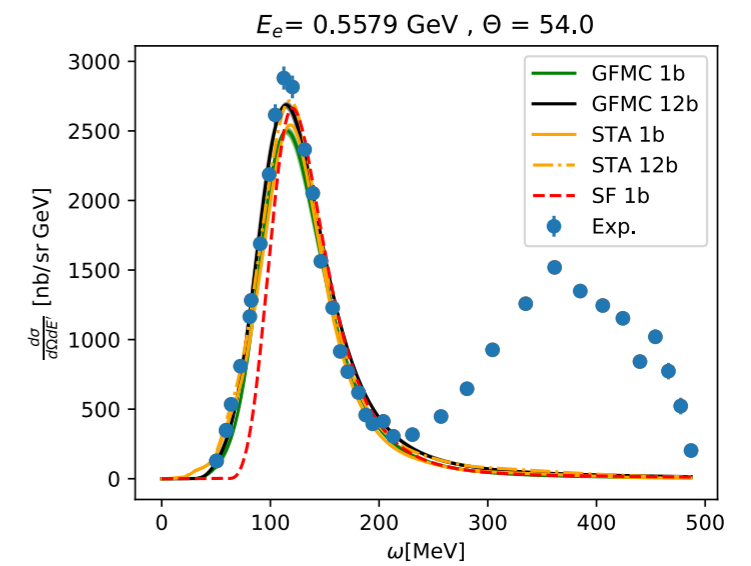
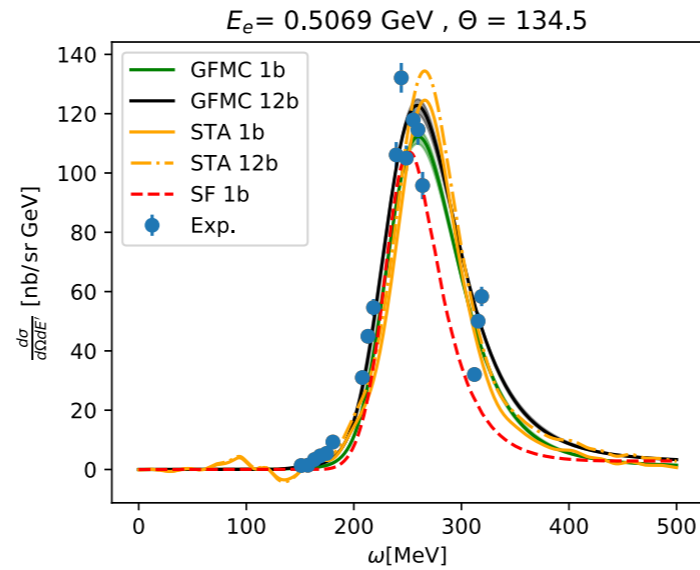
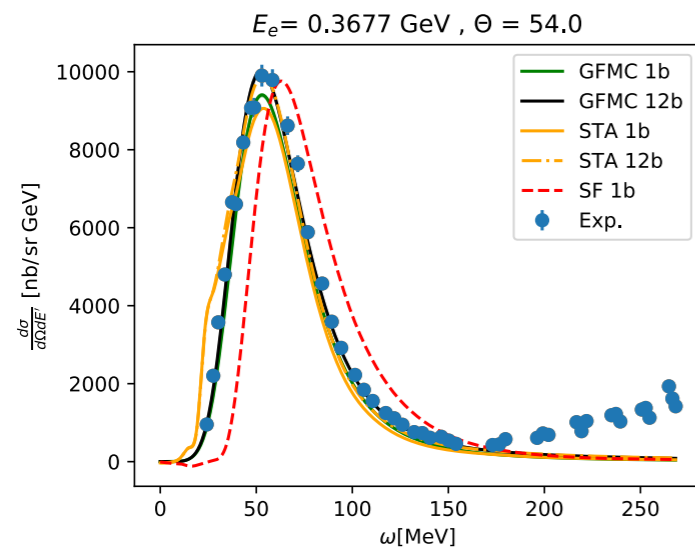
^3H



Cross sections



^3H





Relativistic corrections

Necessary to include relativistic correction at higher momentum q .

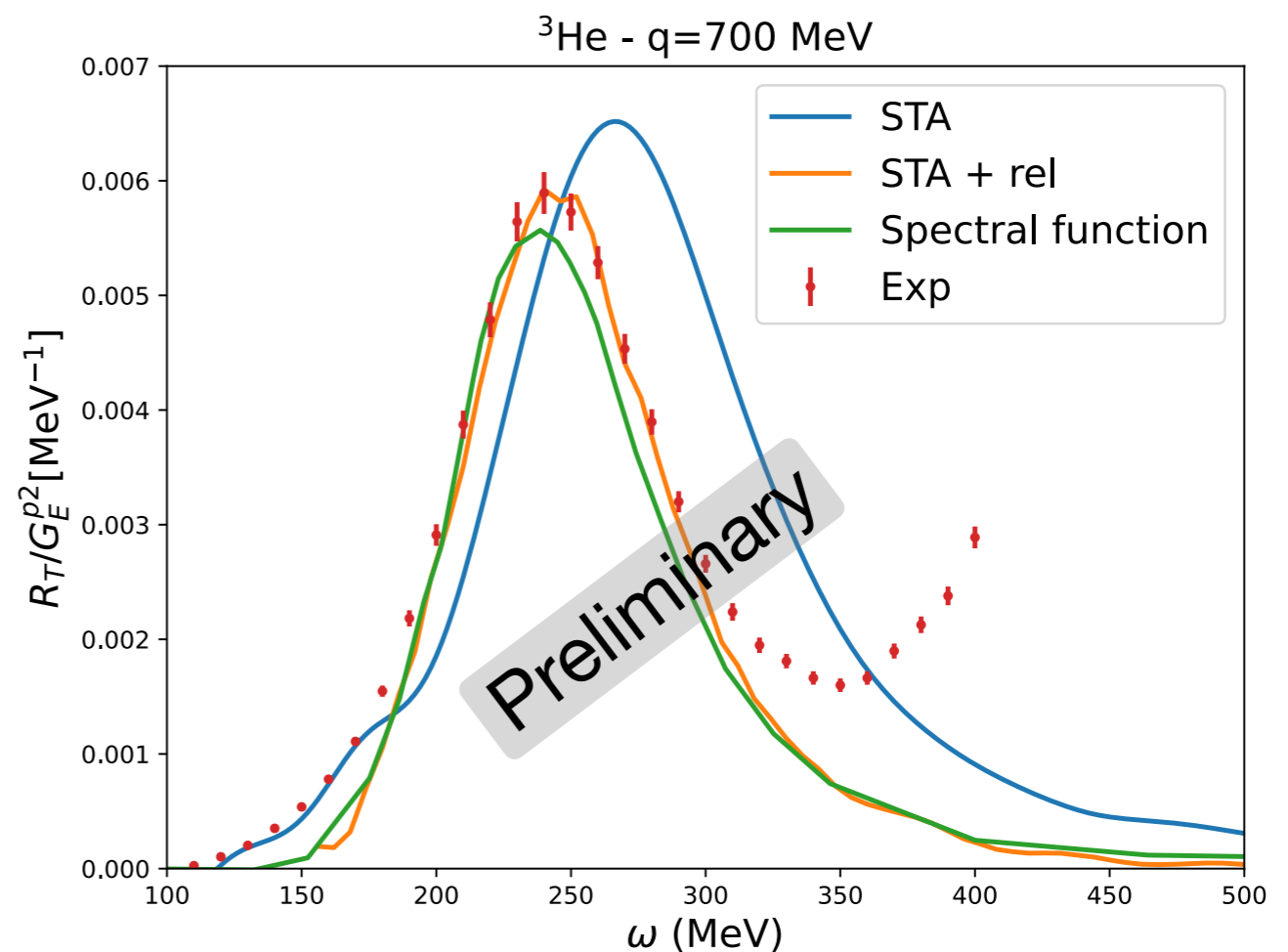
We are currently working on including relativistic corrections within the STA formalism:

R. Weiss, J. Carlson (LANL)

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

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

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



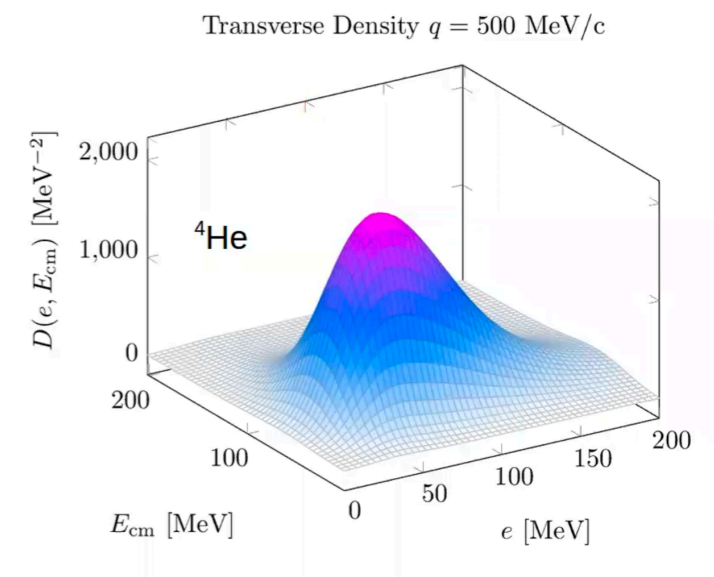
Heavier nuclei



Computational complexity of response functions and densities:

		${}^4\text{He}$	${}^{12}\text{C}$
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



Heavier nuclei

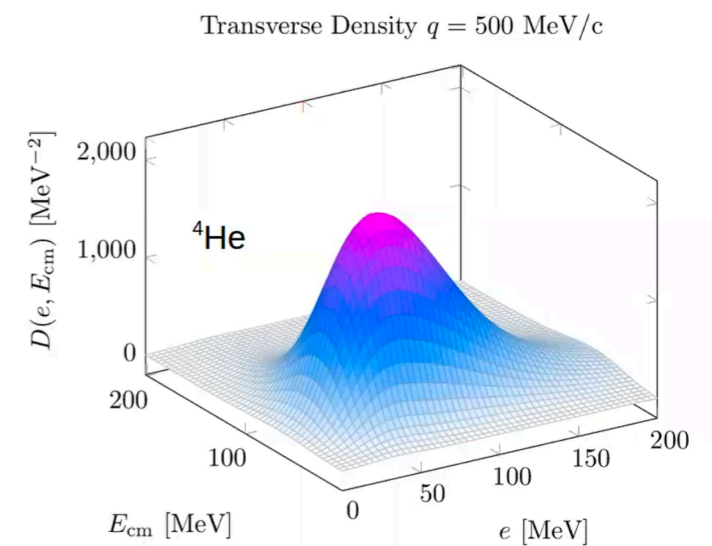


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Response densities: E, e grid



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



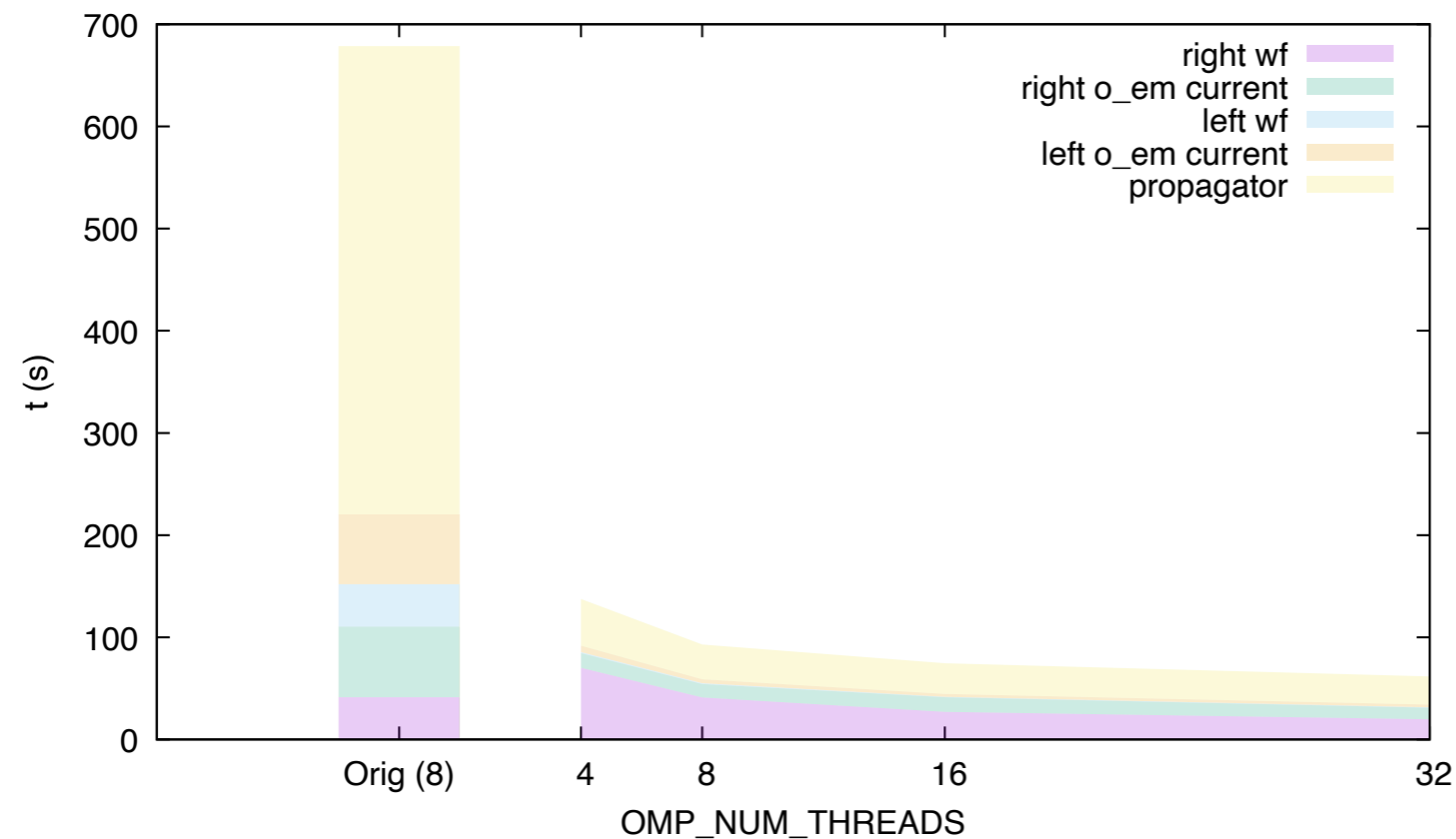
Heavier nuclei

Optimization was necessary to tackle heavier nuclei

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

- 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

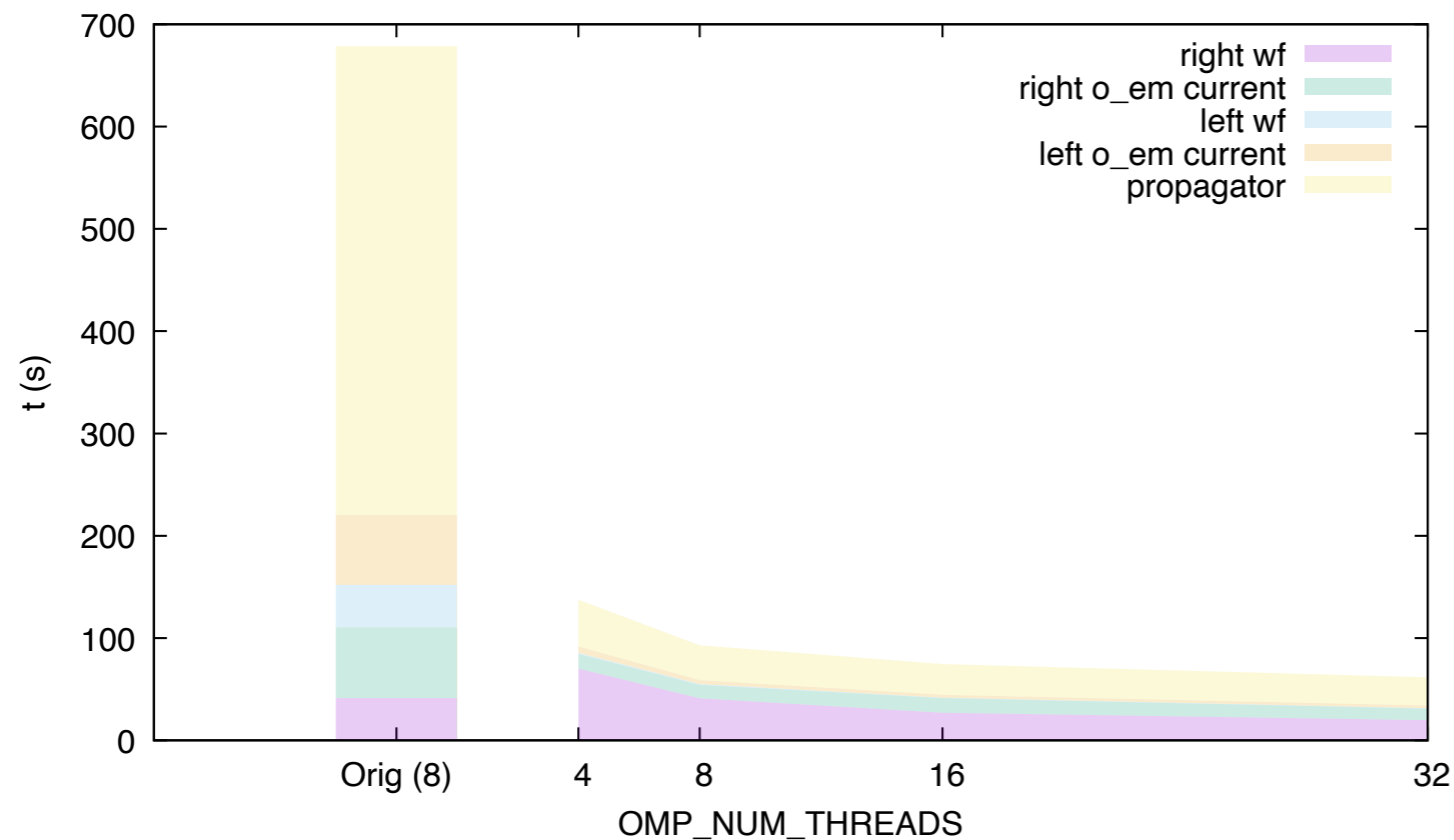
Heavier nuclei: ^{12}C



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

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

Heavier nuclei: ^{12}C



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

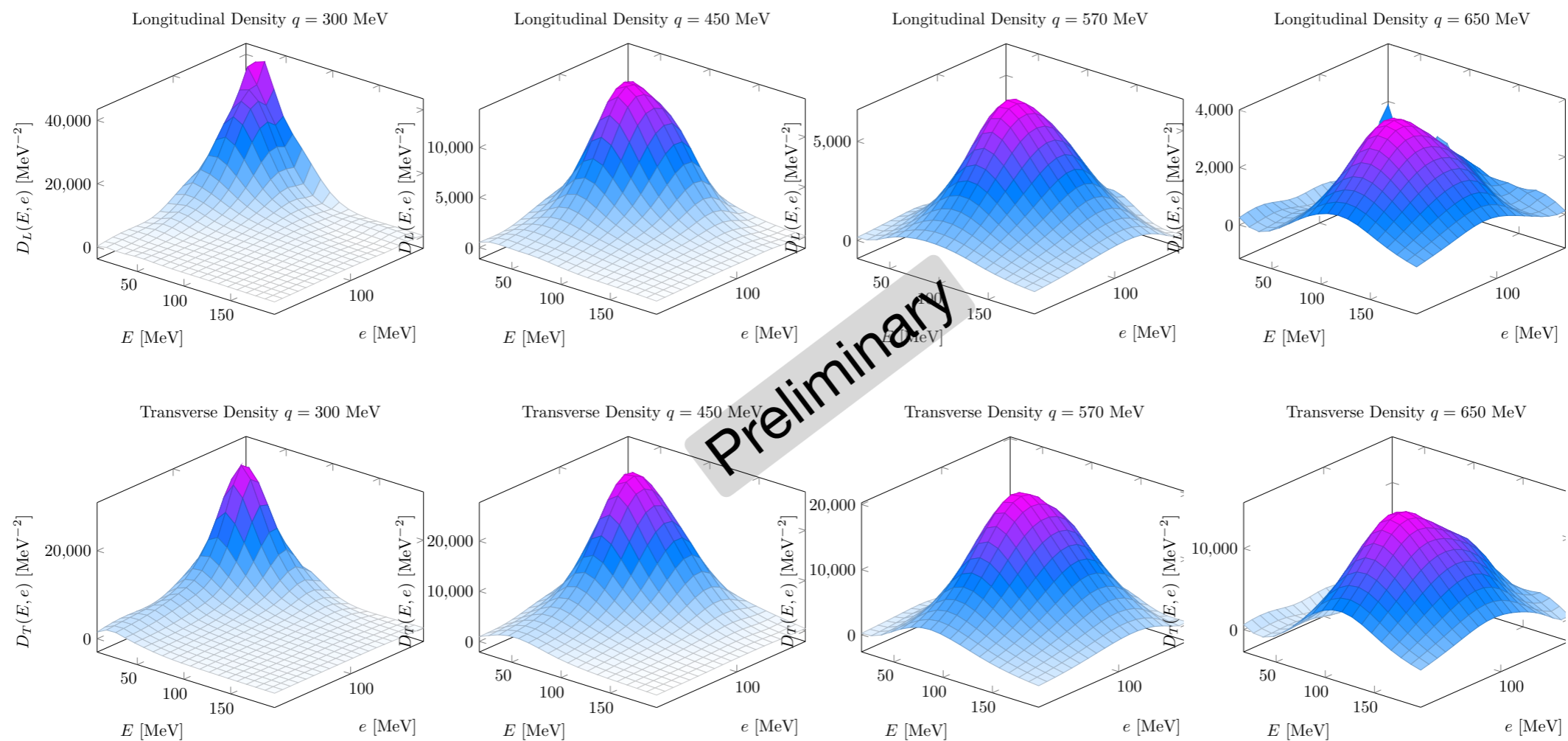
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Responses for ^{12}C



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.

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

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



Cross sections: Interpolation schemes

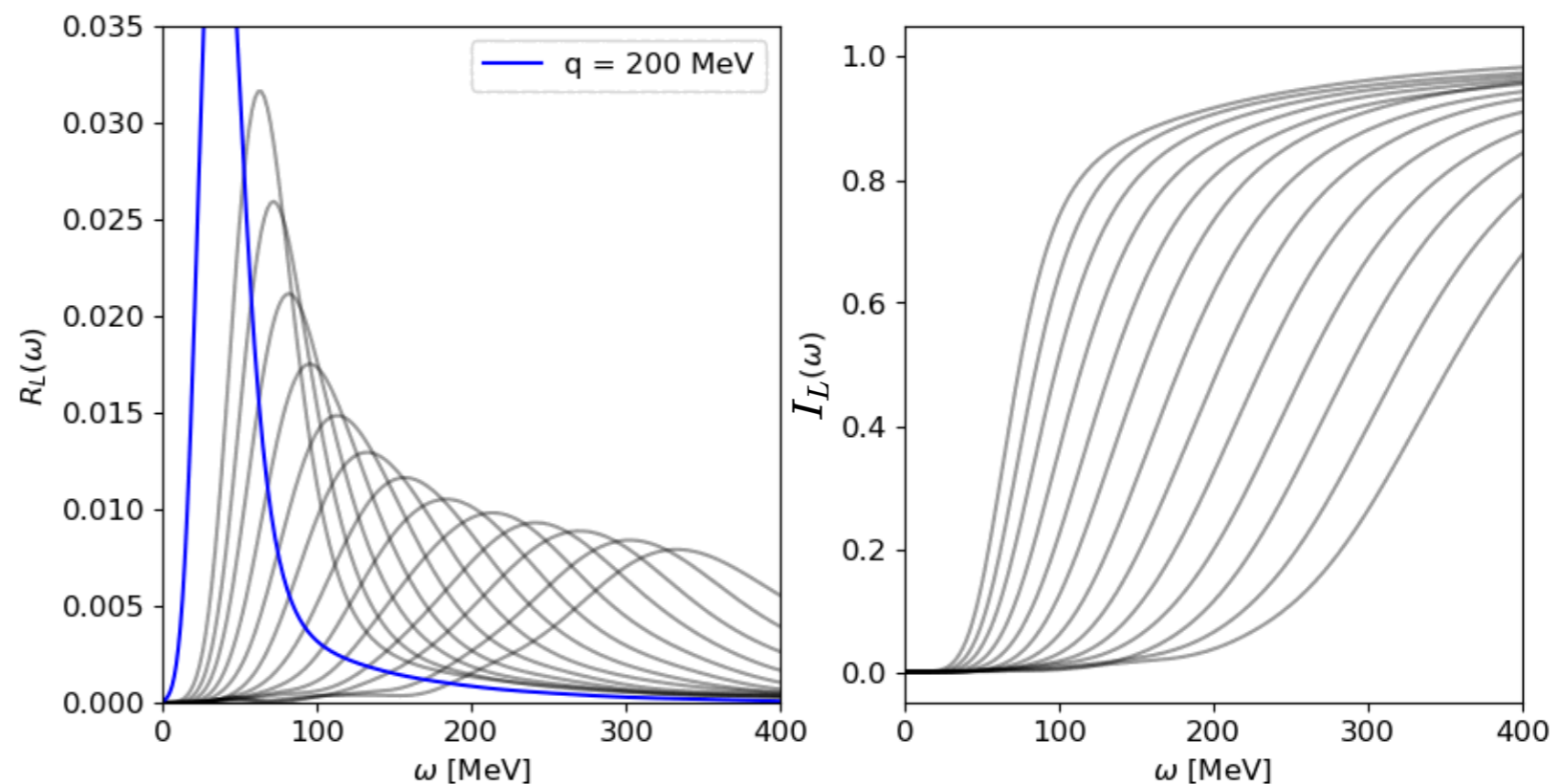
- We **interpolate** in between cumulative integrals of responses, using information from the sum rules

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

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

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

4He, longitudinal response





Cross sections: Interpolation schemes

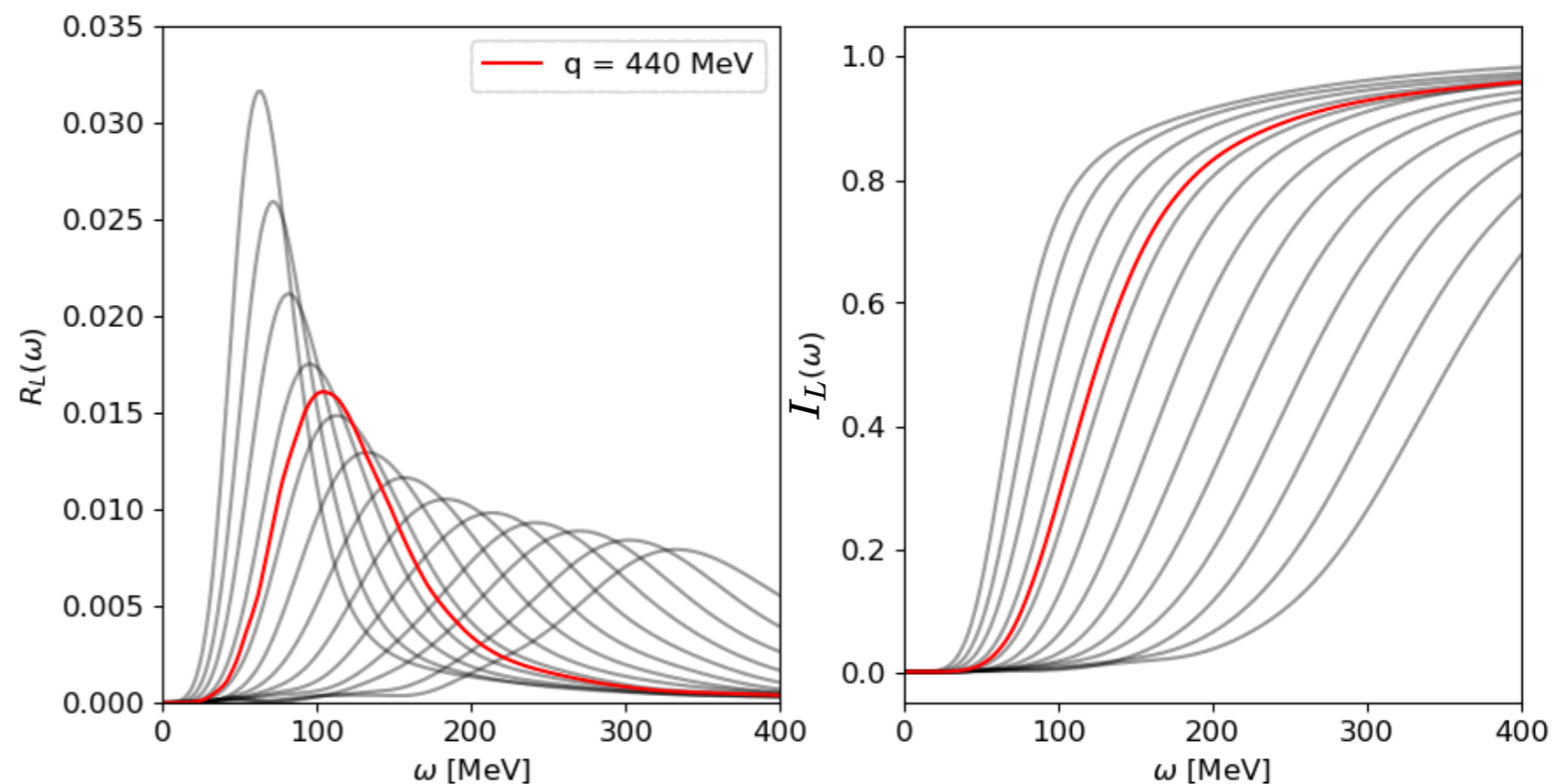
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Cross sections: Interpolation schemes

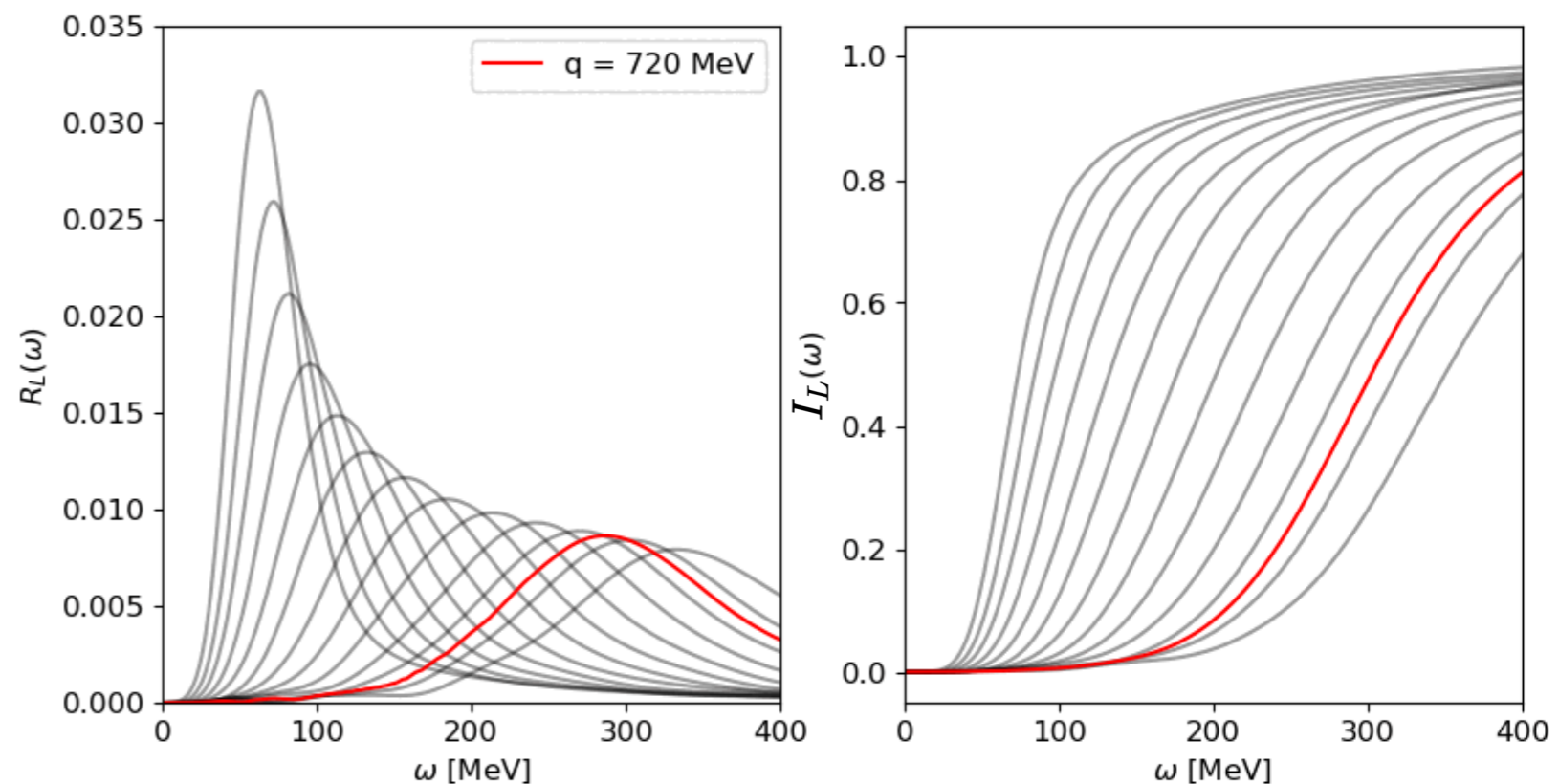
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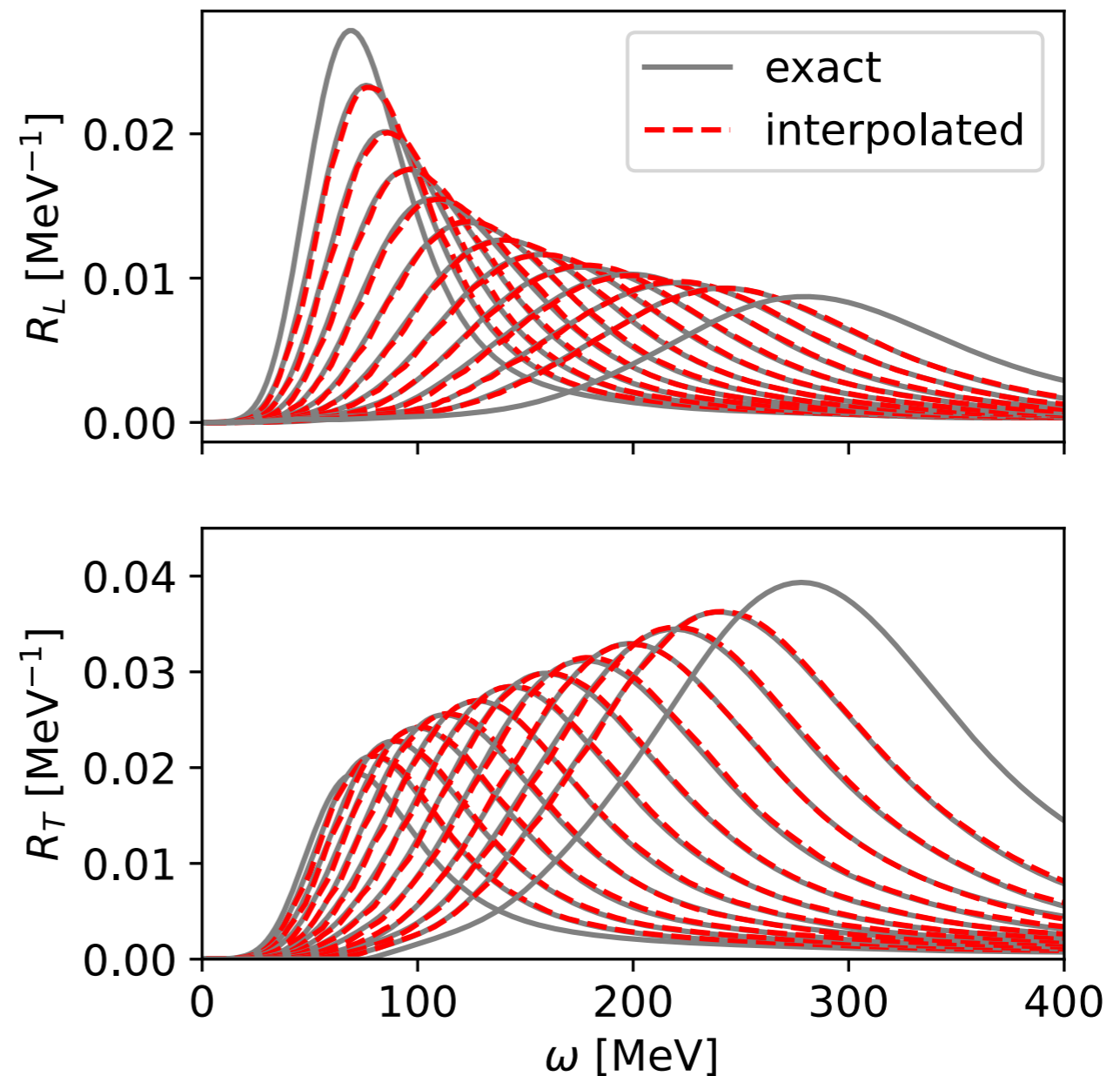
Cross sections: Interpolation schemes

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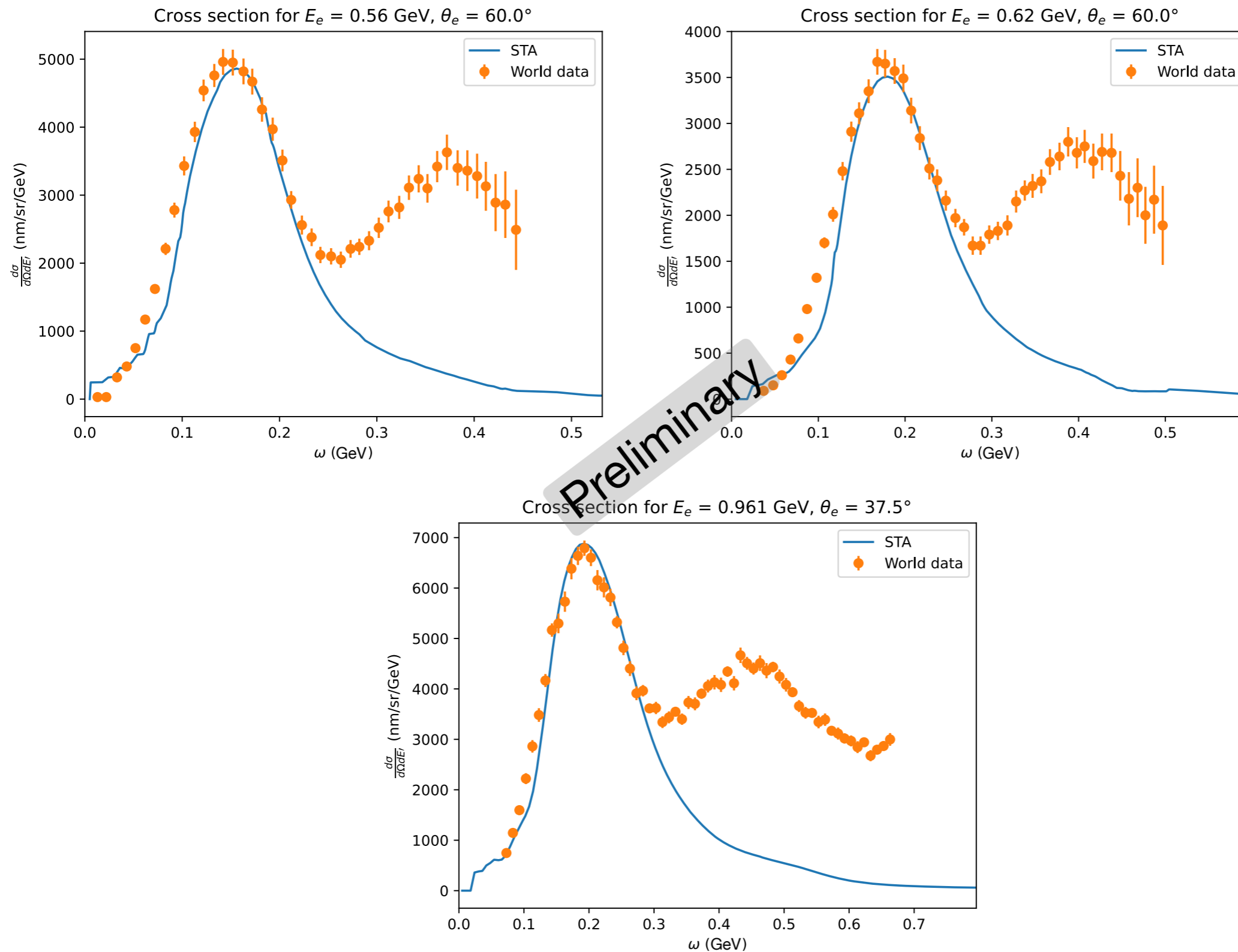
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- Outside the range ($q < 300$ MeV and $q > 850$ MeV), we use **scaling functions**

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



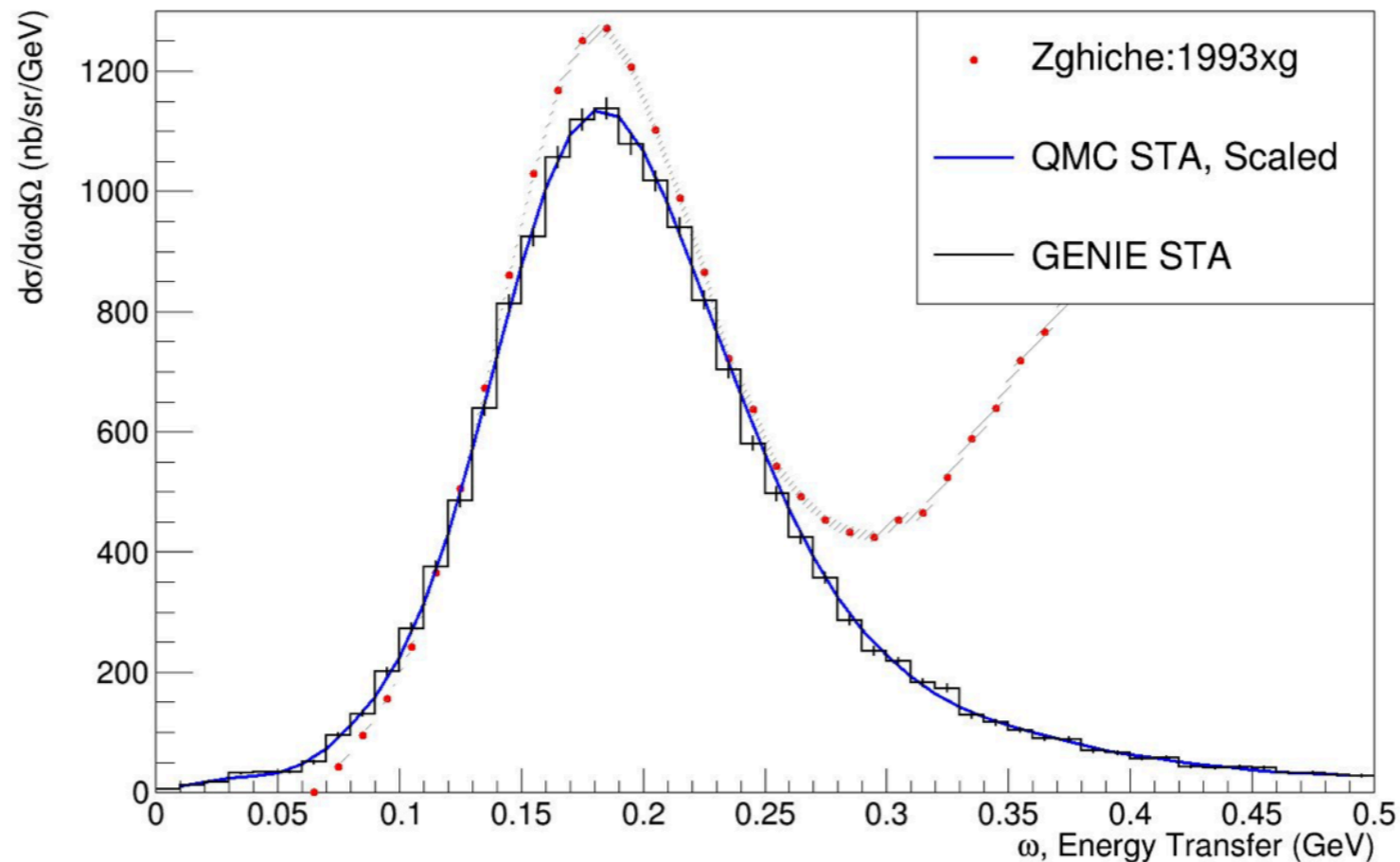
Cross sections results





GENIE validation using e-scattering

Z = 2, A = 4, Beam Energy = 0.64 GeV, Angle = 60° ± 0.25°



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

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

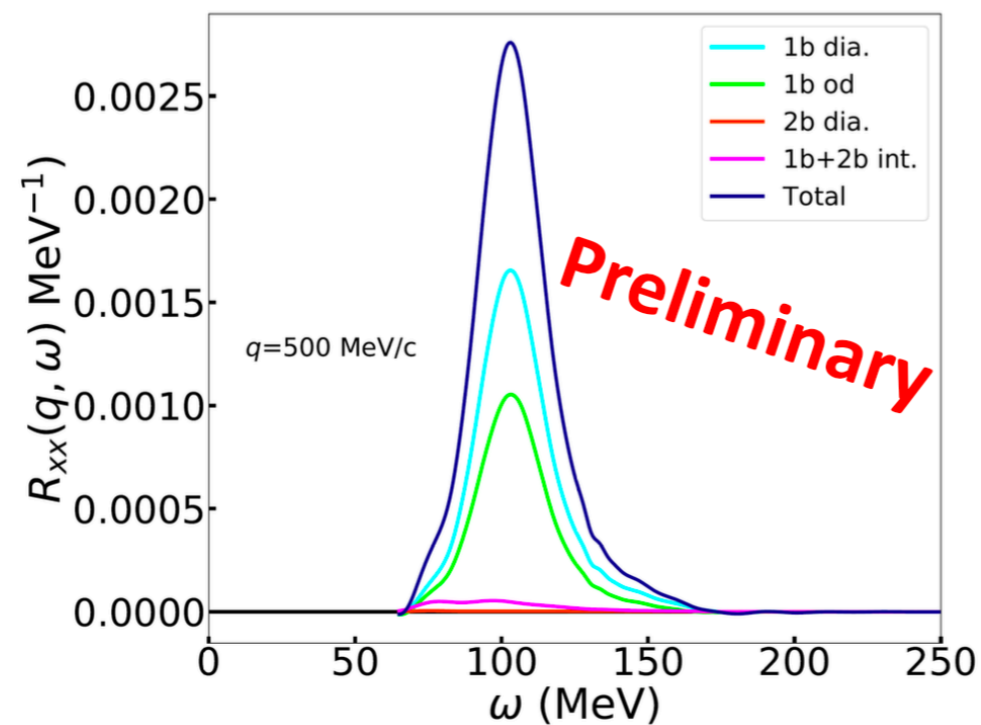
Barrow, Gardiner, Pastore et al. PRD 103 (2021) 5, 052001

GENIE HadronTensorModell Class: https://internal.dunescience.org/doxygen/classgenie_1_1HadronTensorModell.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 ^2H





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

Thank you!

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Lorenzo Andreoli (PD)

Maria Piarulli and Saori Pastore

 Washington University in St. Louis

