Quantum Monte Carlo calculations of electron Scattering from ^{12}C in the Short-Time Approximation

Fermilab Theory Division seminar

Fermilab Theory Division seminar

Quantum Monte Carlo Group @ WashU
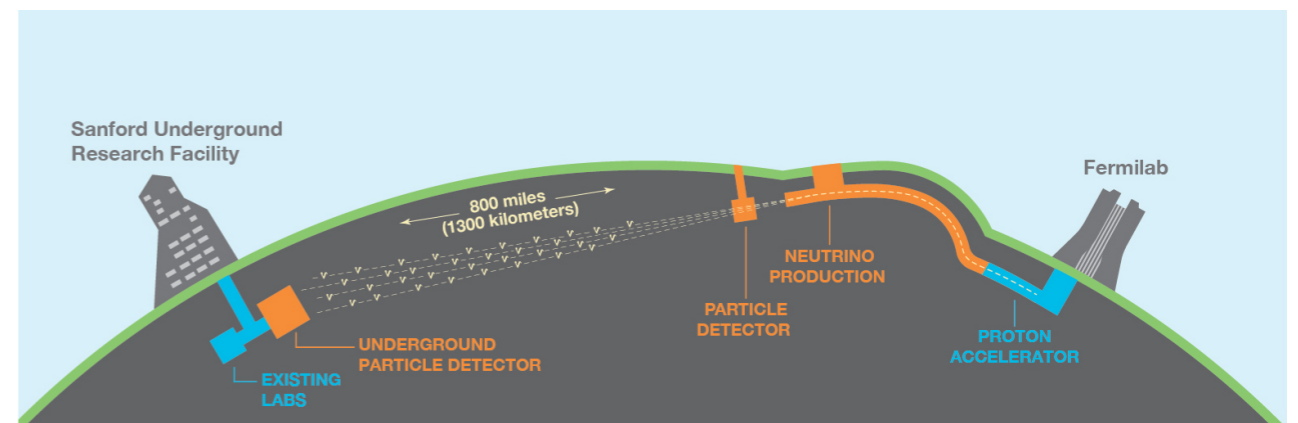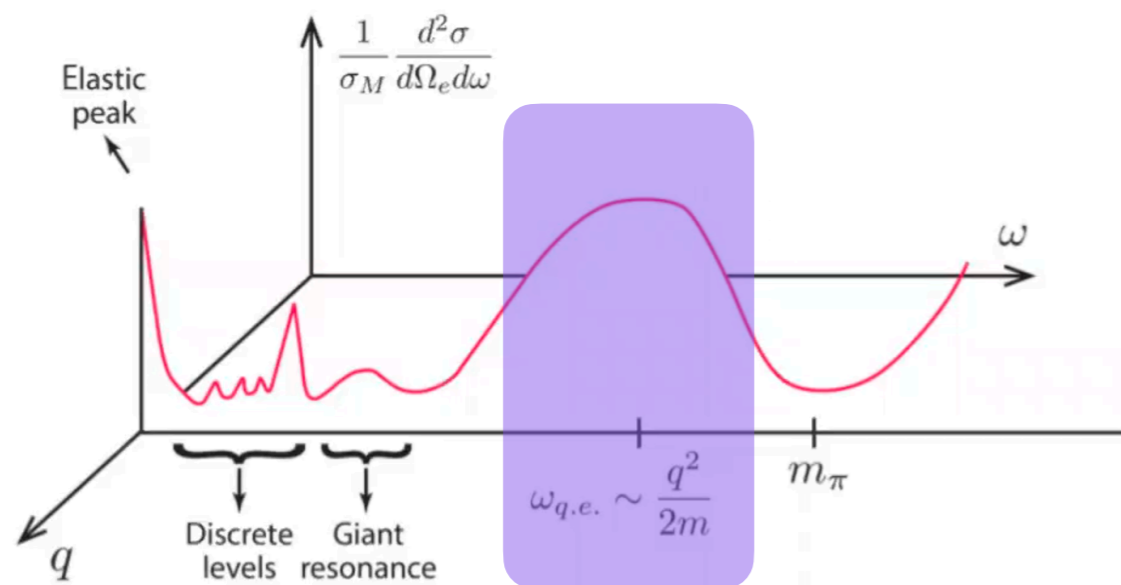
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August 11, 2022

Washington University in St. Louis

Electron-nucleus scattering

Theoretical understanding of nuclear effects is extremely important
for experimental programs

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

Ab-initio description of nuclei

- Nuclear interaction

- Electroweak interaction of leptons with nucleons

- Computational method

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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

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

$$O_{ij}^p = [1, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j, S_{ij}] \otimes [1, \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j]$$
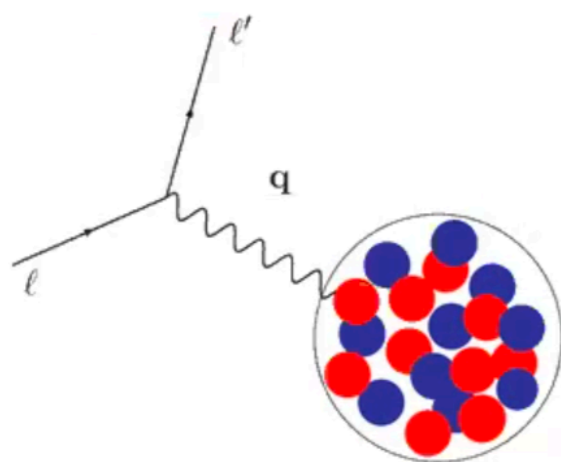
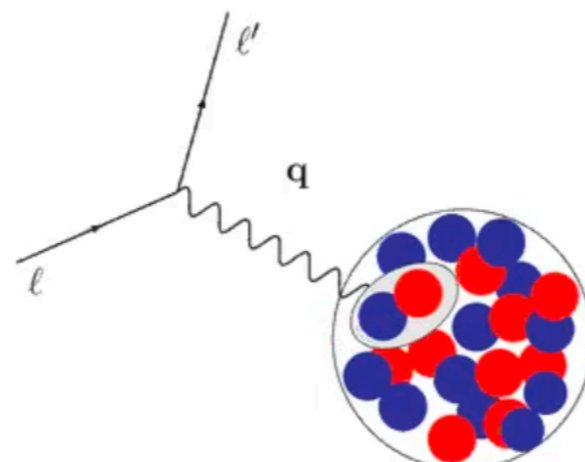$$U_{ijk} = \epsilon v_{ijk}(\bar{r}_{ij}, \bar{r}_{jk}, \bar{r}_{ki})$$

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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

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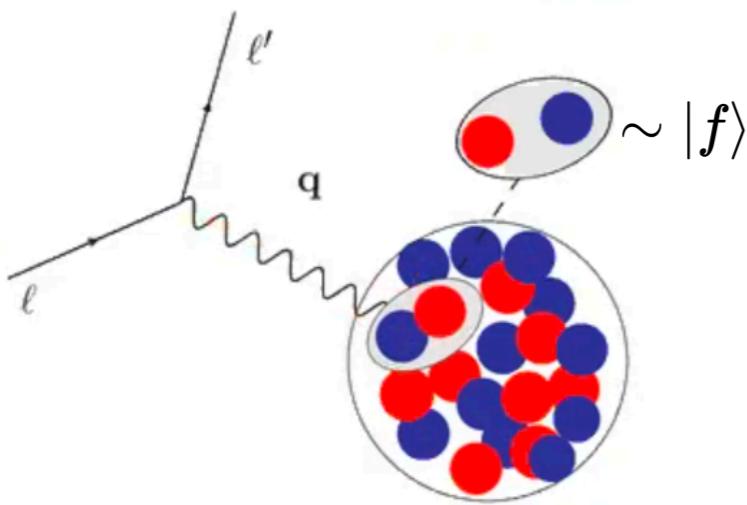
Current operators

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

Short-time approximation

Quasielastic scattering cross sections are expressed in terms of response function

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

Response functions

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

$$R_\alpha(q,\omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i(\omega+E_i)t}\langle\Psi_i|O_\alpha^\dagger(\mathbf{q})e^{-iHt}O_\alpha(\mathbf{q})|\Psi_i\rangle$$
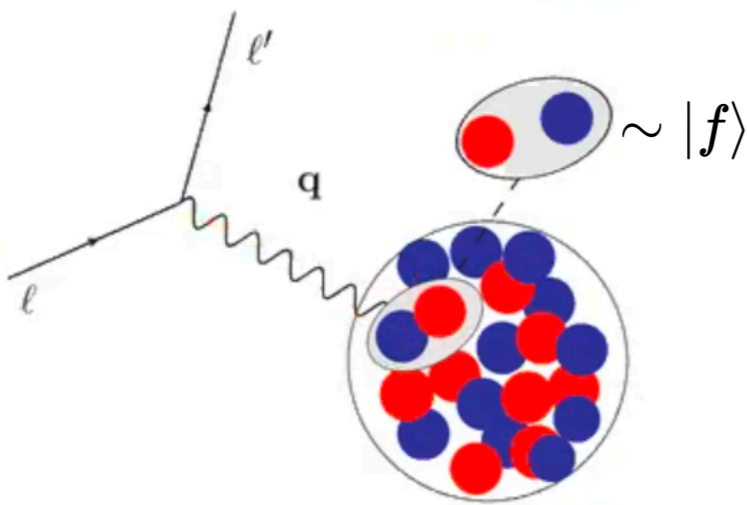
$$O^\dagger e^{-iHt}O = \left(\sum_i O_i^\dagger + \sum_{i<j} O_{ij}^\dagger\right)e^{-iHt}\left(\sum_{i'} O_{i'} + \sum_{i'<j'} O_{i'j'}\right)$$

$$= \sum_i O_i^\dagger e^{-iHt}O_i + \sum_{i\neq j} O_i^\dagger e^{-iHt}O_j$$

$$+ \sum_{i\neq j}\left(O_i^\dagger e^{-iHt}O_{ij} + O_{ij}^\dagger e^{-iHt}O_i\right.$$

$$\left. + O_{ij}^\dagger e^{-iHt}O_{ij}\right) + \dots$$

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Short-time approximation

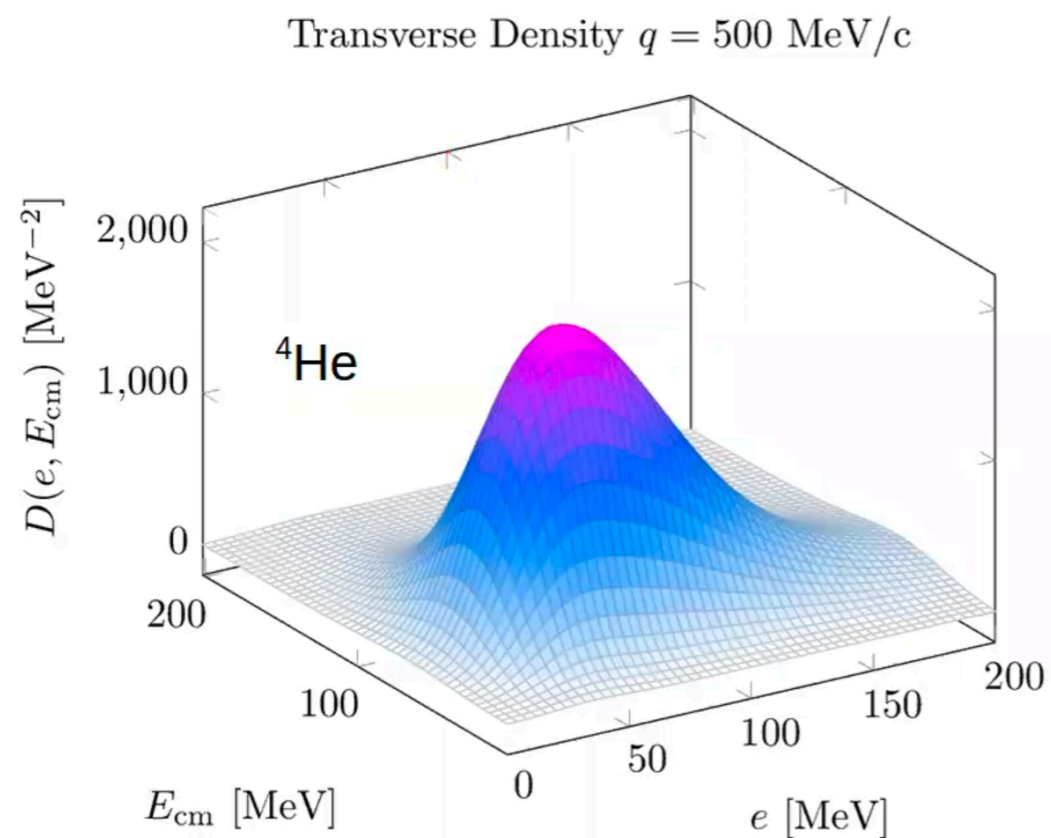Quasielastic scattering cross sections are expressed in terms of response function

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

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

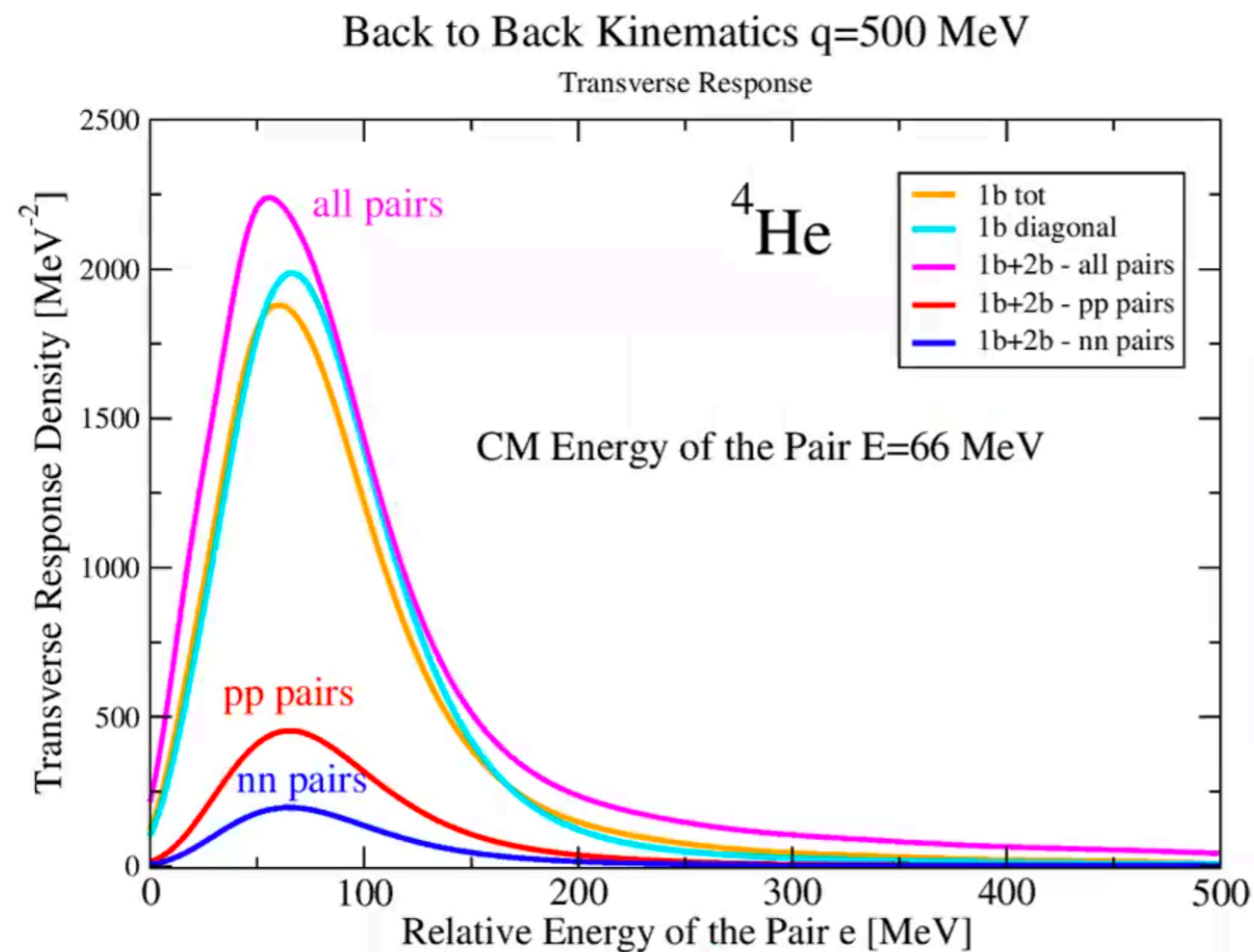STA: scattering of a correlated pair of nucleons inside a nucleus

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Transverse response density

Transverse Density $q = 500$ MeV/c

^{4}He

$D(e, E_{cm})$ [MeV^{-2}]

E_{cm} [MeV]

e [MeV]

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

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Back-to-back kinematic

Back to Back Kinematics q=500 MeV
Transverse Response

^{4}He

CM Energy of the Pair E=66 MeV

Legend:
- 1b tot
- 1b diagonal
- 1b+2b - all pairs
- 1b+2b - pp pairs
- 1b+2b - nn pairs

all pairs

pp pairs

nn pairs

x-axis: Relative Energy of the Pair e [MeV]
y-axis: Transverse Response Density [MeV^{-2}]

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

Pastore et al. PRC101(2020)044612

Benchmark

L.A., S. Pastore, N. Rocco, et al. arXiv:2108.10824

- 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

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Benchmark

L.A., S. Pastore, N. Rocco, et al. arXiv:2108.10824

Green's function Monte Carlo

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

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

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

Stort-time approximation

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

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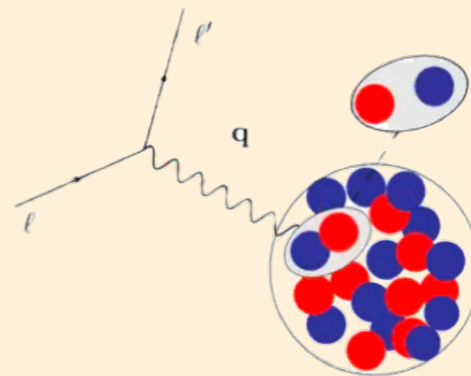
Spectral function

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

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

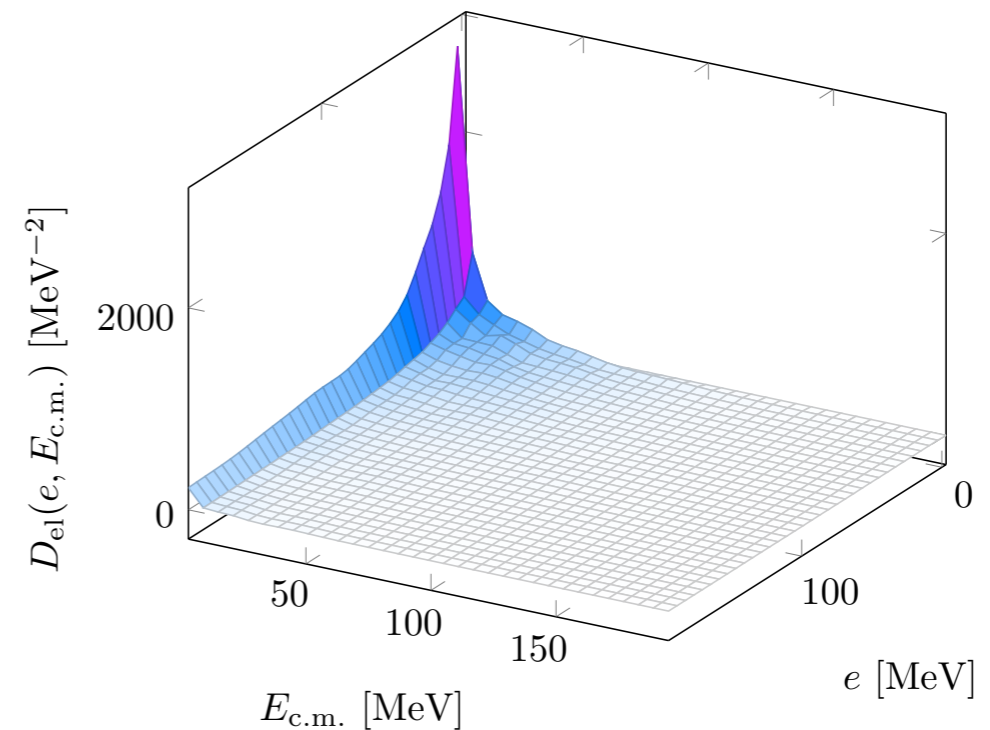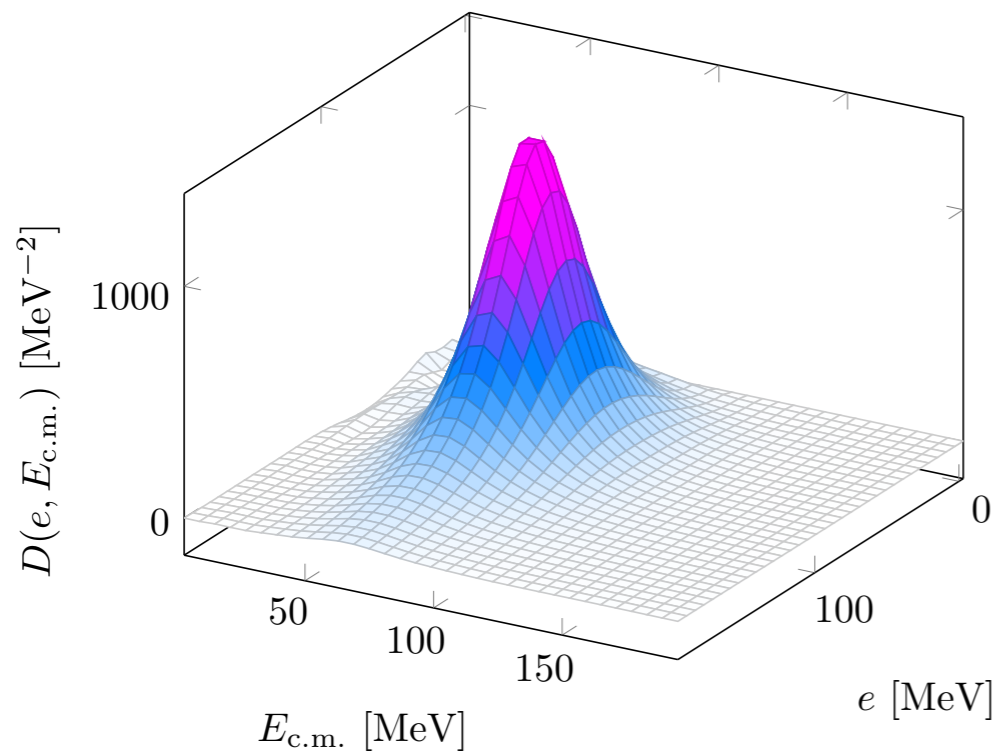Spectral function P, probability distribution of removing a nucleon with momentum k

Elastic contribution

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

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

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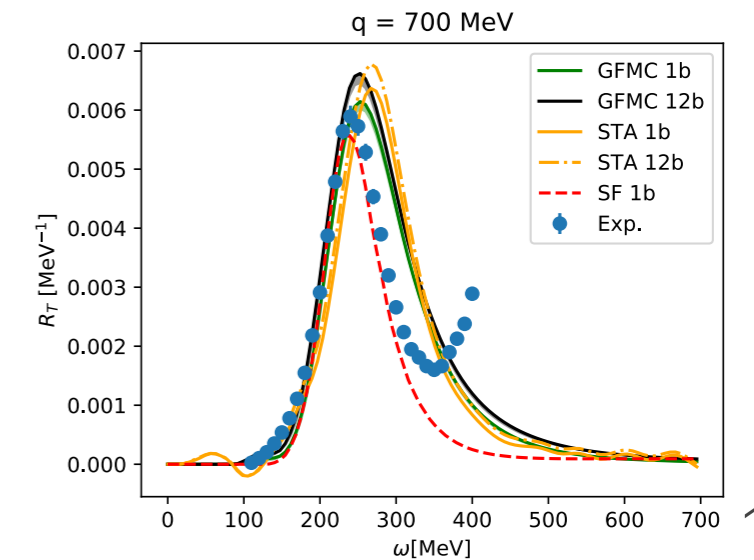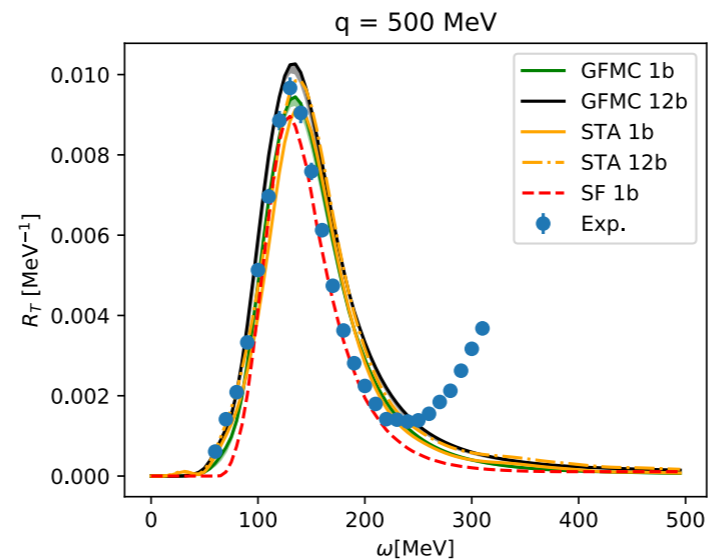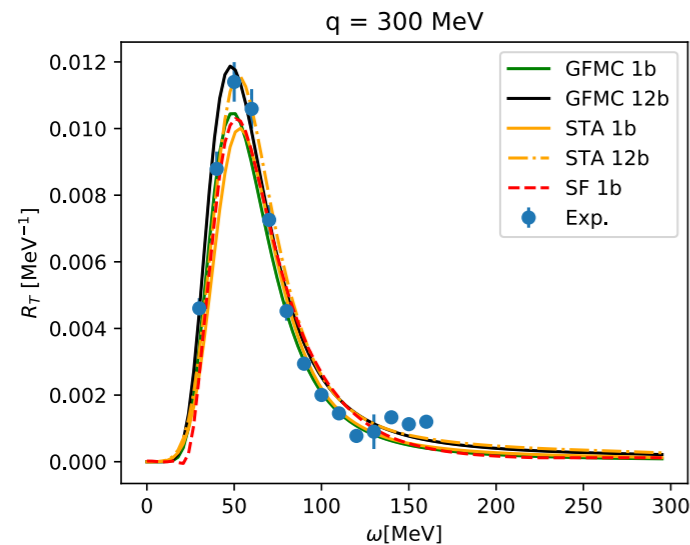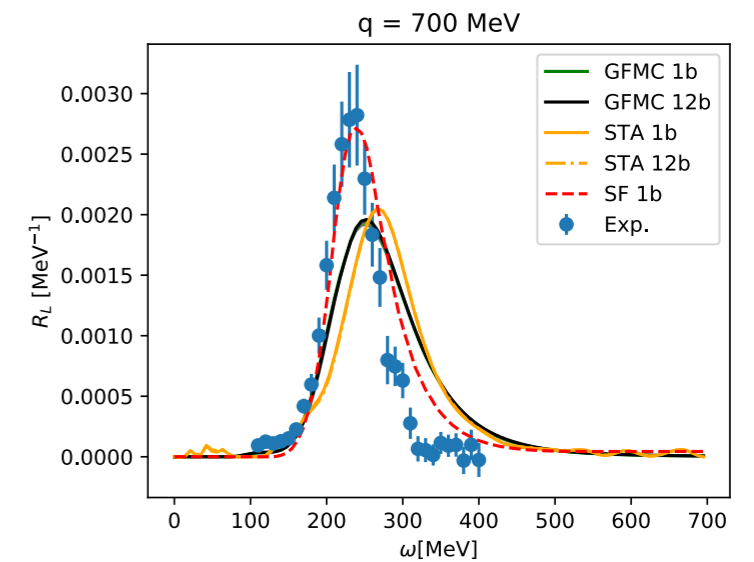

^{3}H Longitudinal response at 300 MeV

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

Benchmark

Longitudinal and transverse response function in ³He
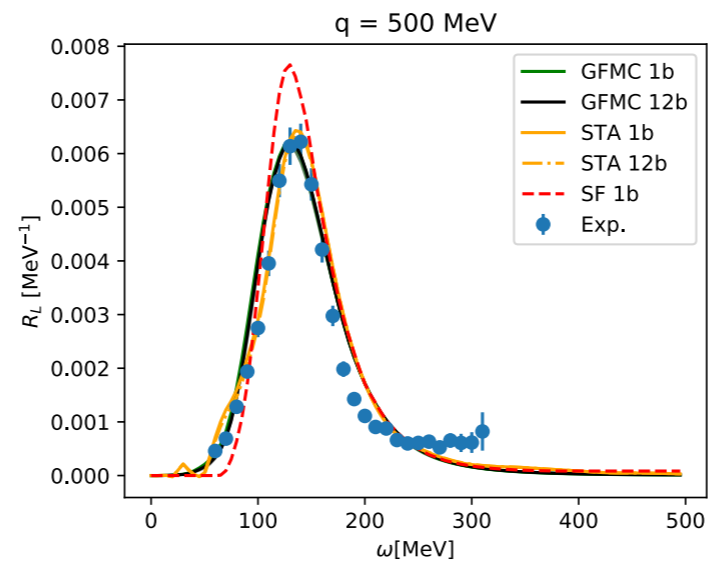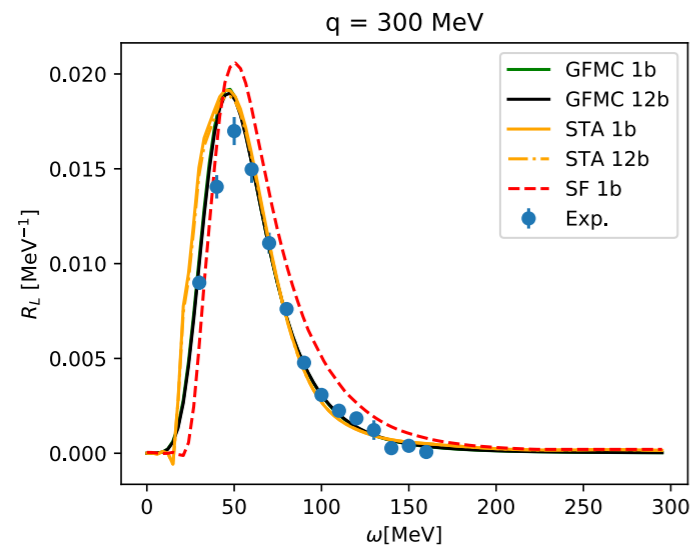
L.A., S. Pastore, N. Rocco, et al. PRC105(2022)014002

Relativistic corrections

Necessary to include relativistic correction at higher momentum q

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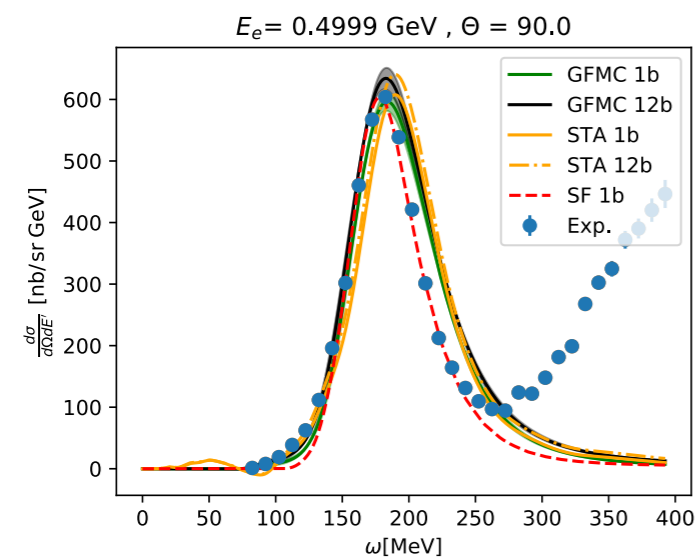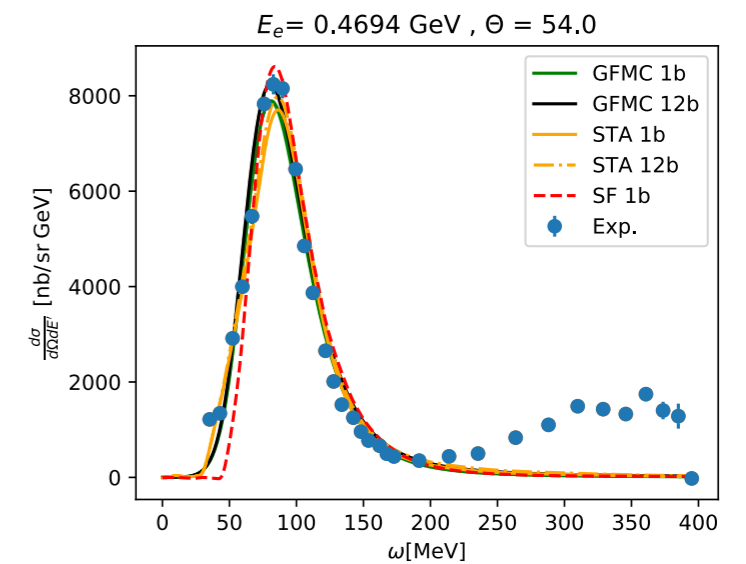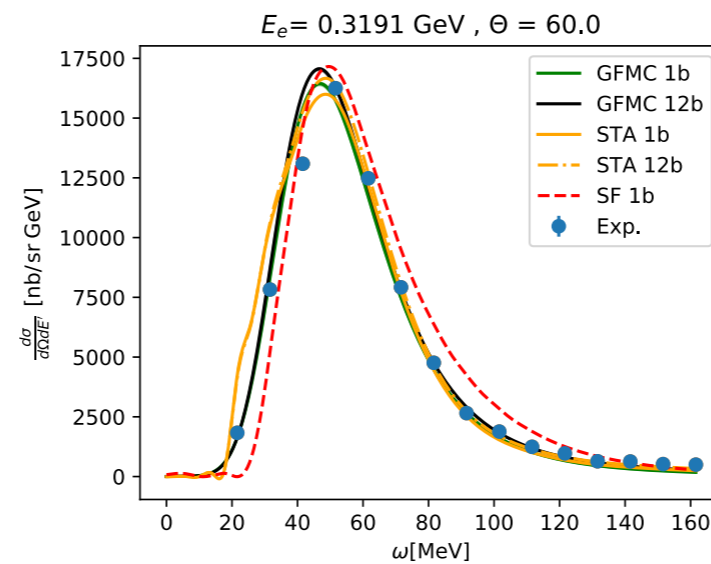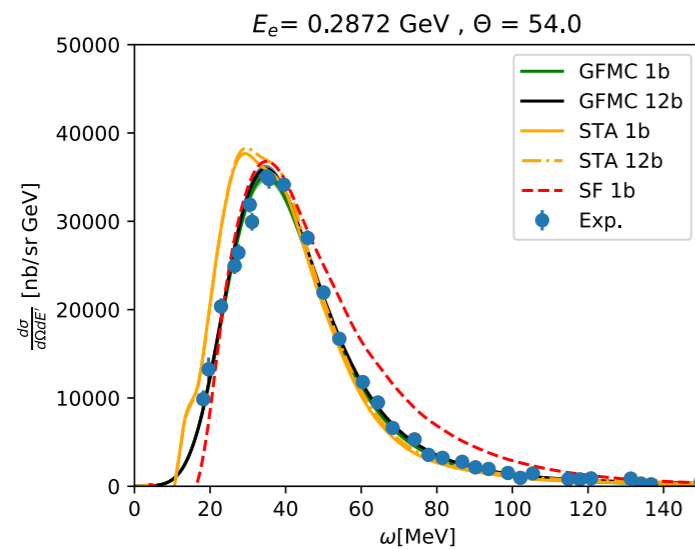
Cross sections

³He

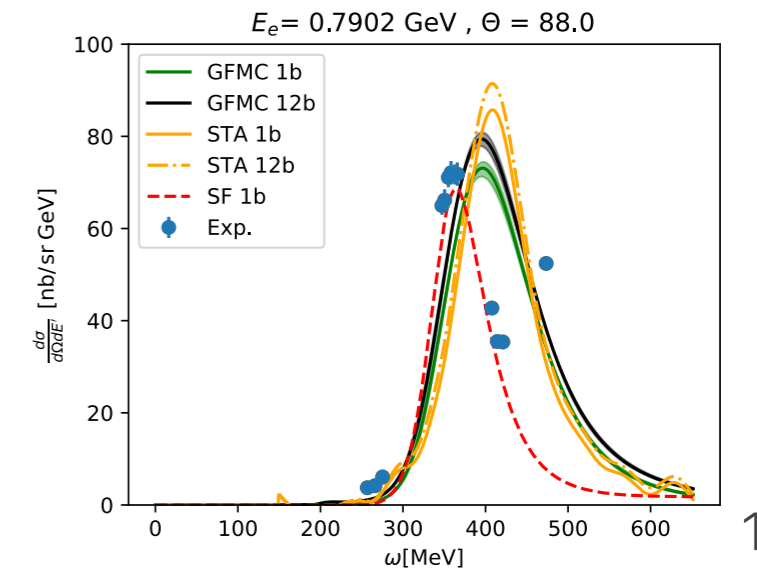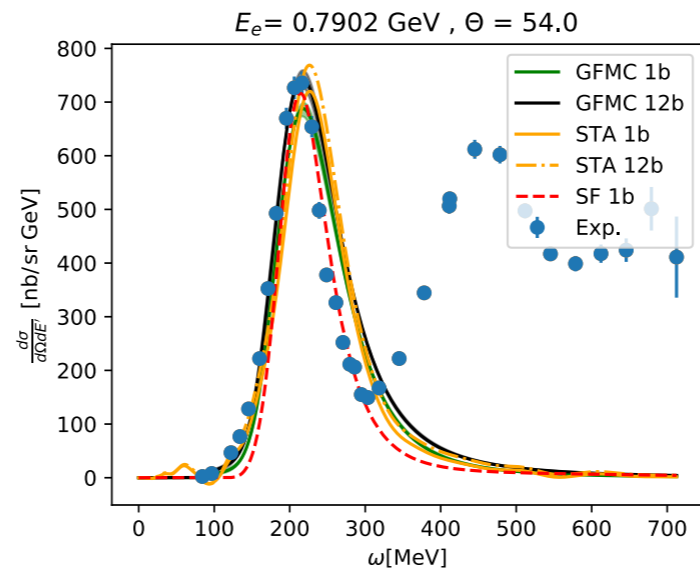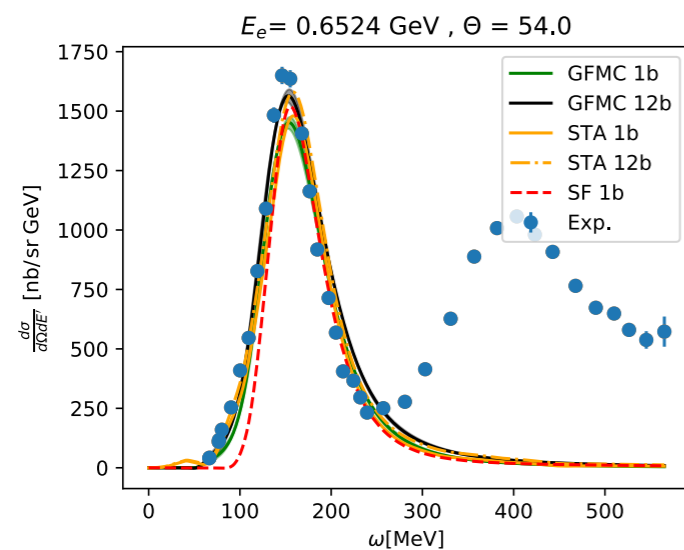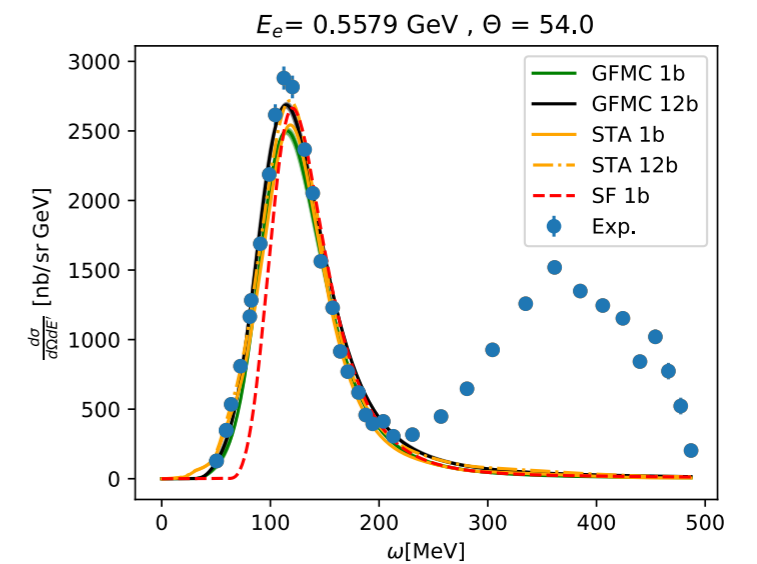L.A., S. Pastore, N. Rocco, et al. PRC105(2022)014002

Cross sections

³H
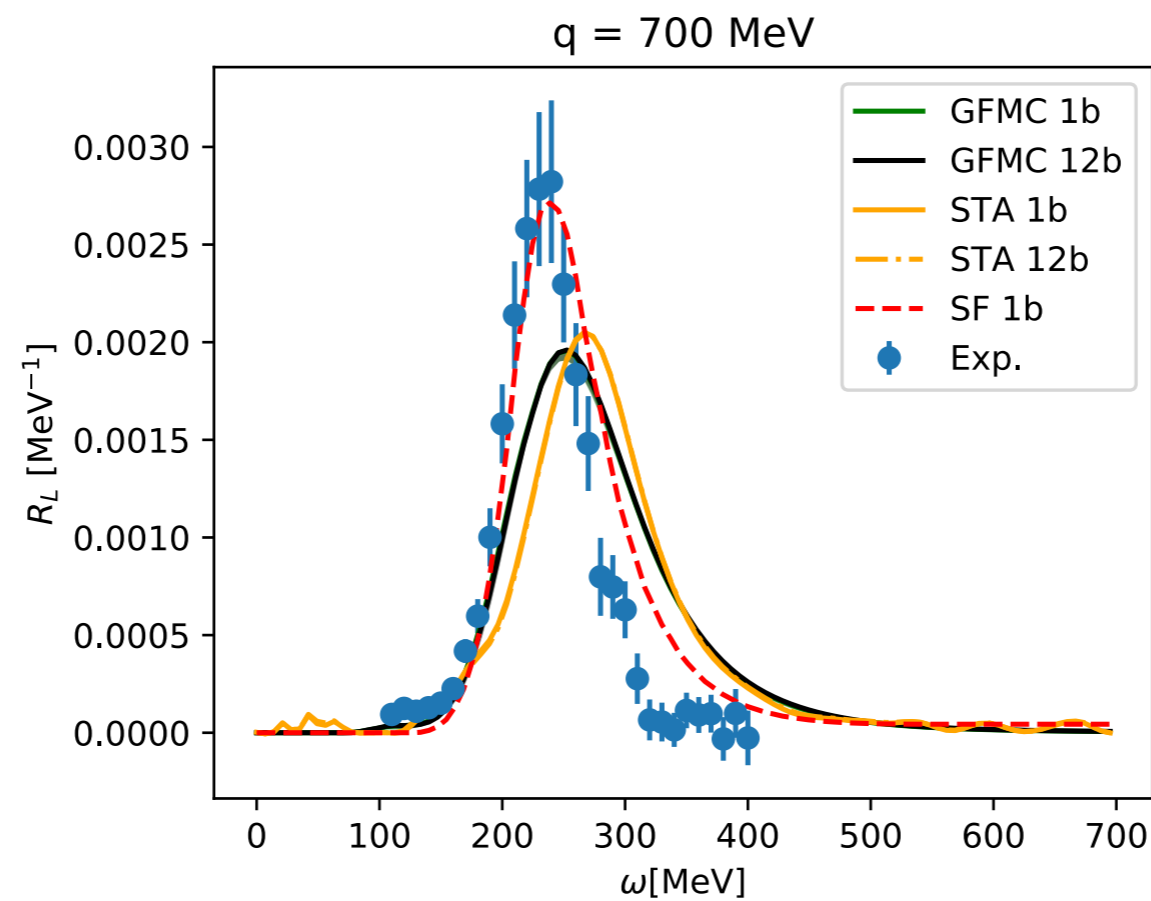
L.A., S. Pastore, N. Rocco, et al. PRC105(2022)014002
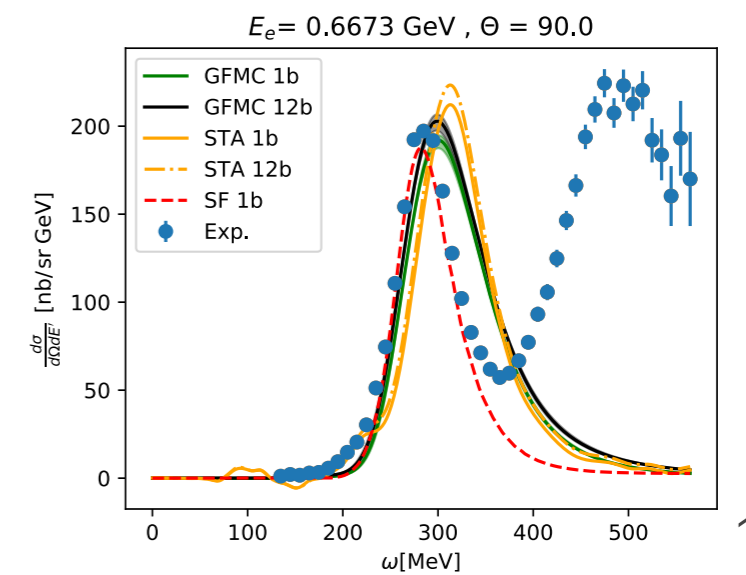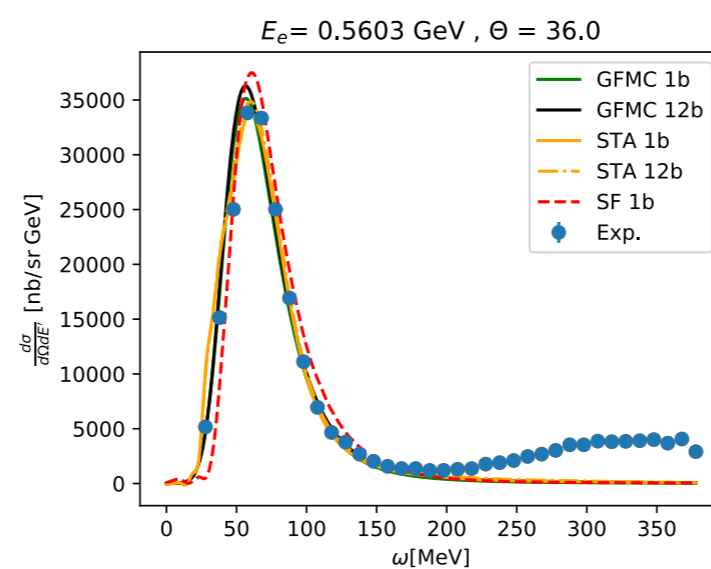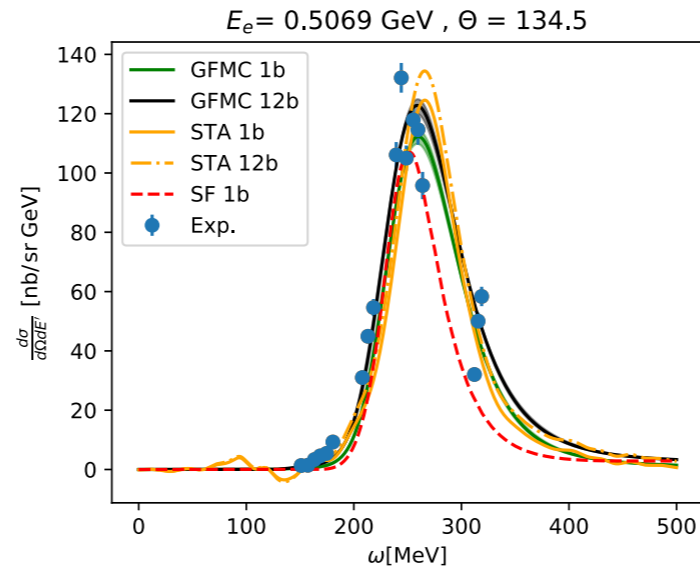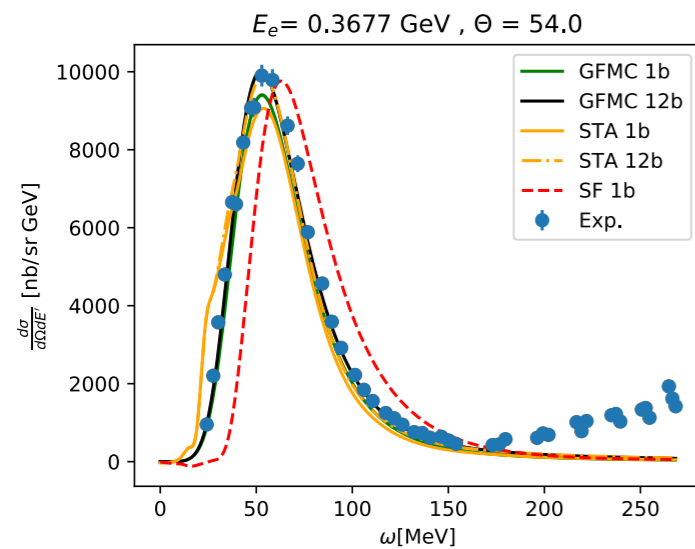
Heavier nuclei

Computational complexity of response functions and densities:

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

Response densities: E, e grid

Transverse Density $q = 500$ MeV/c

^{4}He

$D(e, E_{cm})$ [MeV^{-2}]

E_{cm} [MeV]

e [MeV]

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

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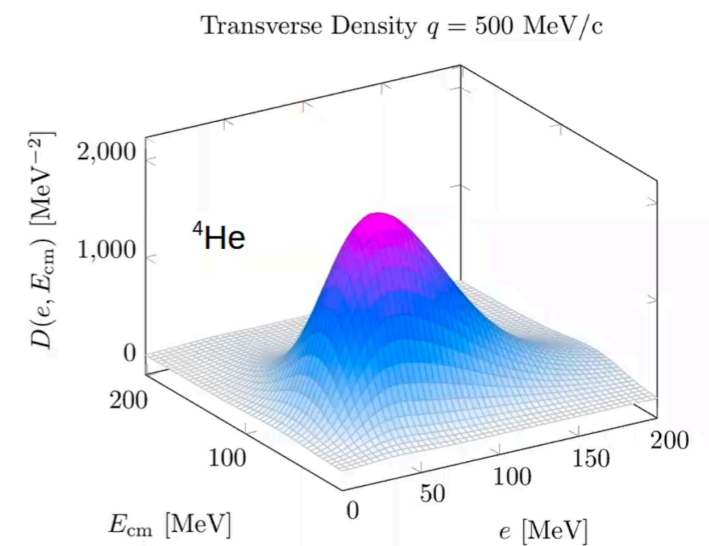
Heavier nuclei

Optimization was necessary to tackle heavier nuclei

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

- 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

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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

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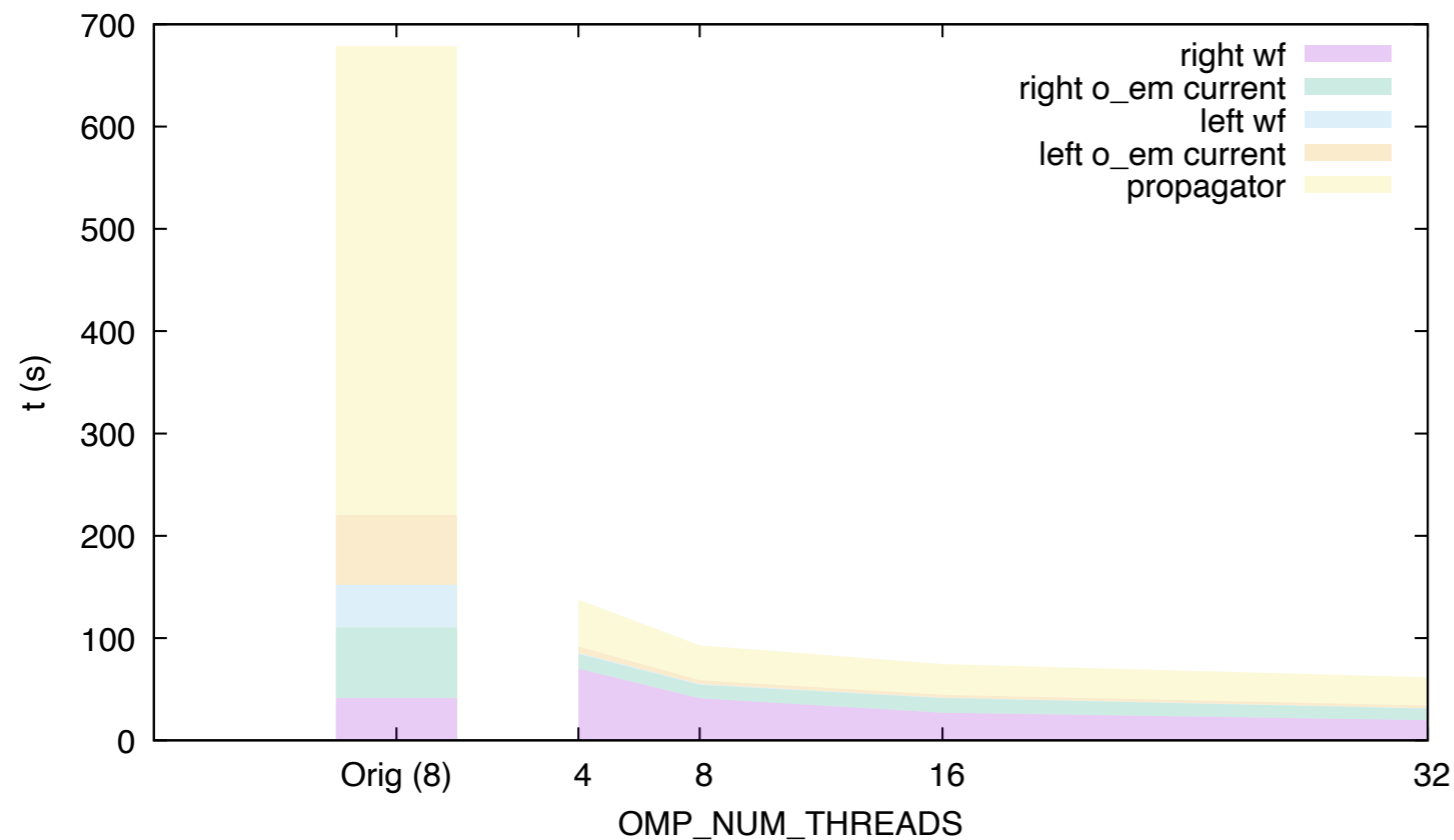
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Heavier nuclei

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

Original:

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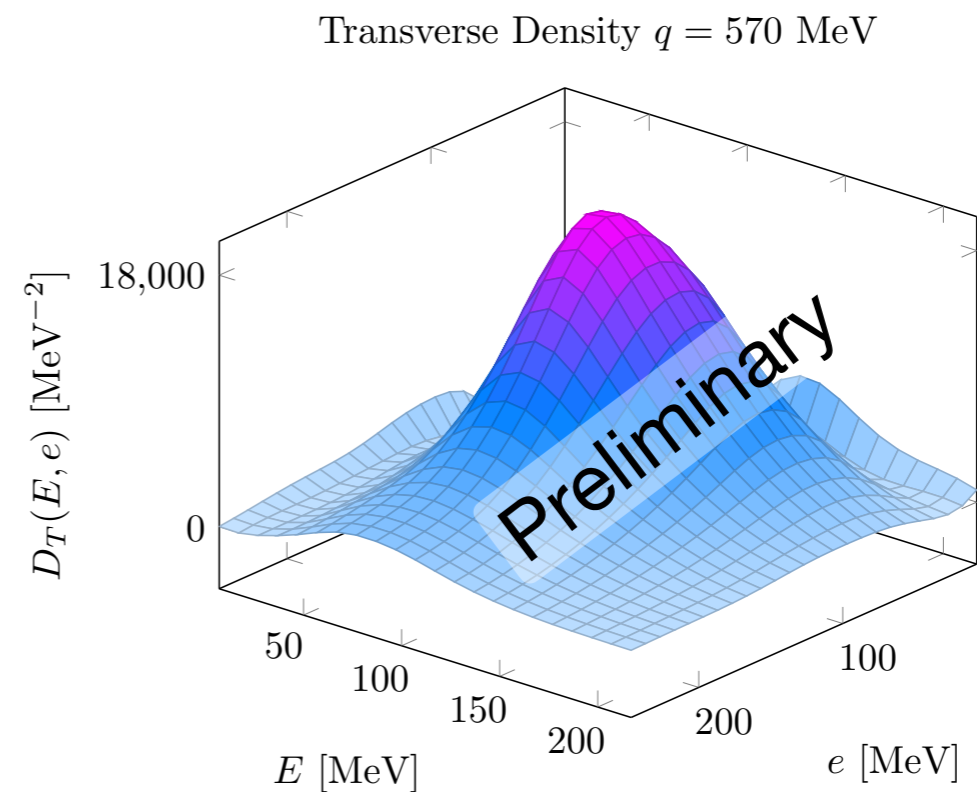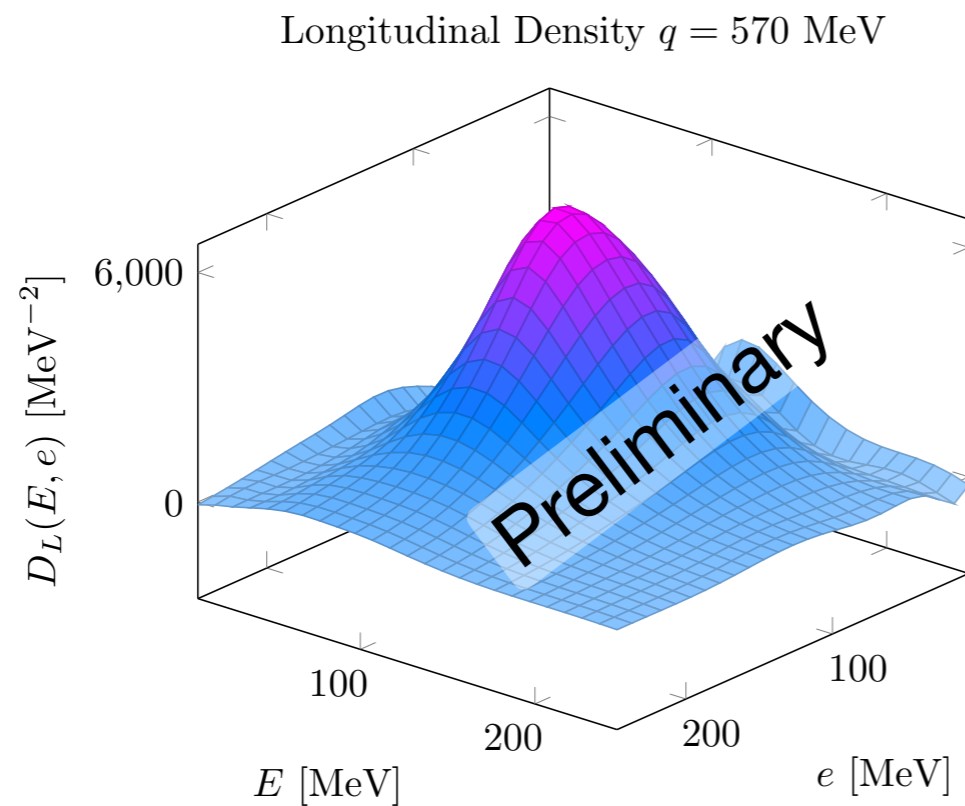 (LA et al arXiv:2108.10824)

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*

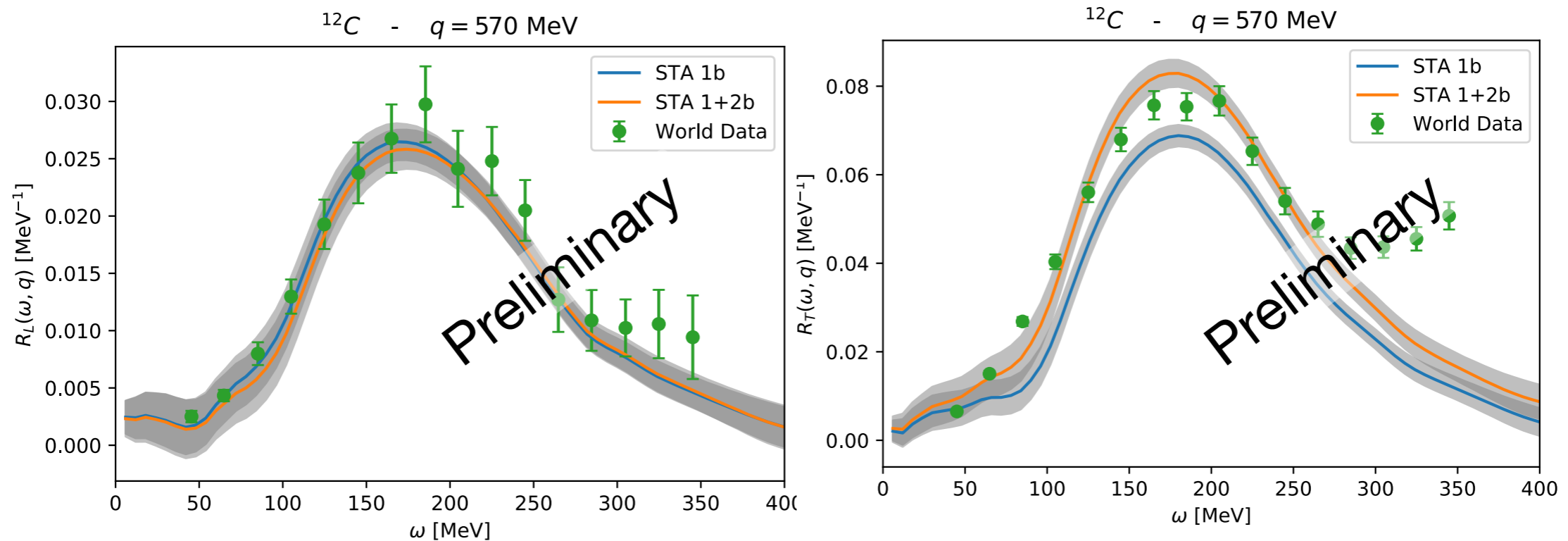# Response densities for ^{12}C

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
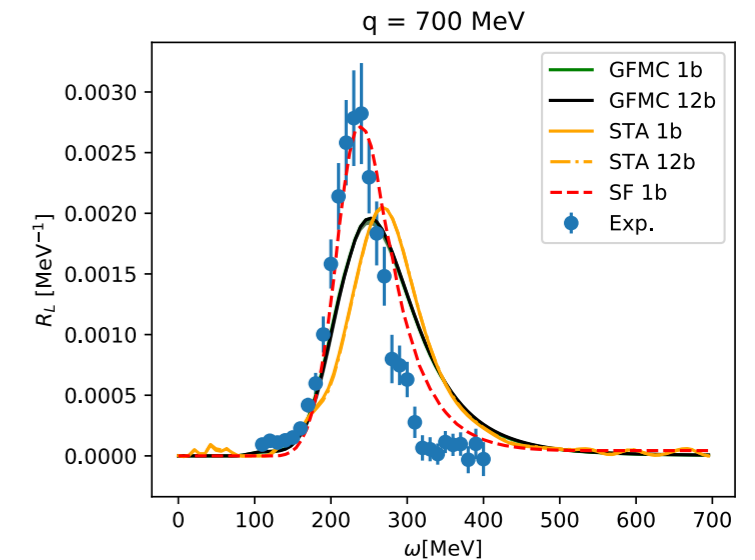
q = 570 MeV

Current and future projects

- Elastic contribution

- Relativistic corrections

- Collaboration with GENIE to include response **densities** in event generator

Relativistic corrections

Necessary to include relativistic correction at higher momentum q

- Include kinematics

- Full relativistic treatment of final states

$q = 700$ MeV
Legend: GFMC 1b, GFMC 12b, STA 1b, STA 12b, SF 1b, Exp.
Axes: R_L [MeV^{-1}] vs ω[MeV]

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

$$R_\alpha(\boldsymbol{q}, \omega) =$$
$$\cdots$$
$$\cdots$$
$$\cdots$$

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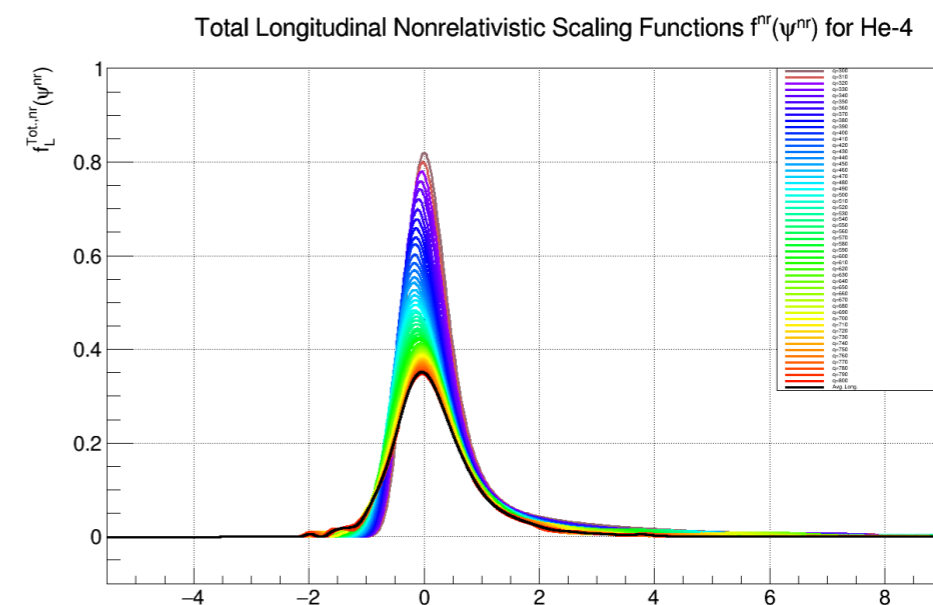
GENIE event generator

URA Visiting Scholars Program funding, collaboration with GENIE experts at Fermilab

Light systems:

- Responses and response densities w/o the elastic peak

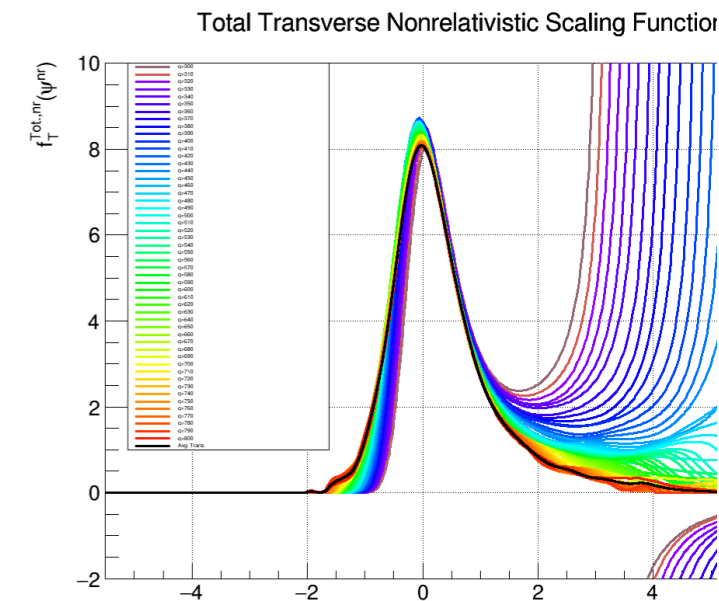- Finer grid and study of interpolation methods

GENIE event generator

URA Visiting Scholars Program funding, collaboration with GENIE experts at Fermilab

Light systems:

- Responses and response densities w/o the elastic peak

- Finer grid and study of interpolation methods

- Implement **densities** into GENIE:
    - currently responses have been implemented
      (J. Barrow, S. Gardiner, S. Pastore, M. Betancourt, and J. Carlson. Phys. Rev. D 103, 052001)
    - at the moment GENIE has a way of "making up" that information rather than a direct theoretical prediction
    - test interpolation and morphing scheme

- More momenta for ^{12}C

- EW currents

Collaborators:

S. Pastore, M. Piarulli

J. Carlson, S. Gandolfi, A. Lovato, N. Rocco, R. Wiringa

S. Gardiner, J. Barrow, M. Betancourt

Thank you!

Washington University in St.Louis