# Ab Initio Approach

## NuSTEC 2024 School, São Paulo, Brazil

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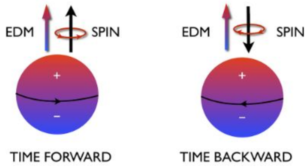
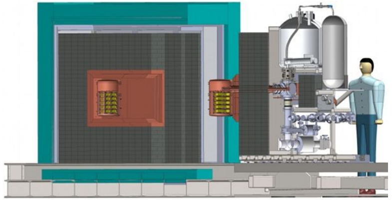
Ground States' Electroweak Moments, Form Factors, Radii




Neutrinoless Double Beta Decay, Muon-Capture



Accelerator Neutrino Experiments, Lepton-Nucleus XSecs

$(\omega, q)$~0 MeV

$\omega$~few MeVs
$q$~0 MeV

$\omega$~few MeVs
$q$~$10^2$ MeV

$\omega$~tens of MeVs

$\omega$~$10^2$ MeV

FRIB

Electromagnetic Decay, Beta Decay, Double Beta Decay & inverse processes

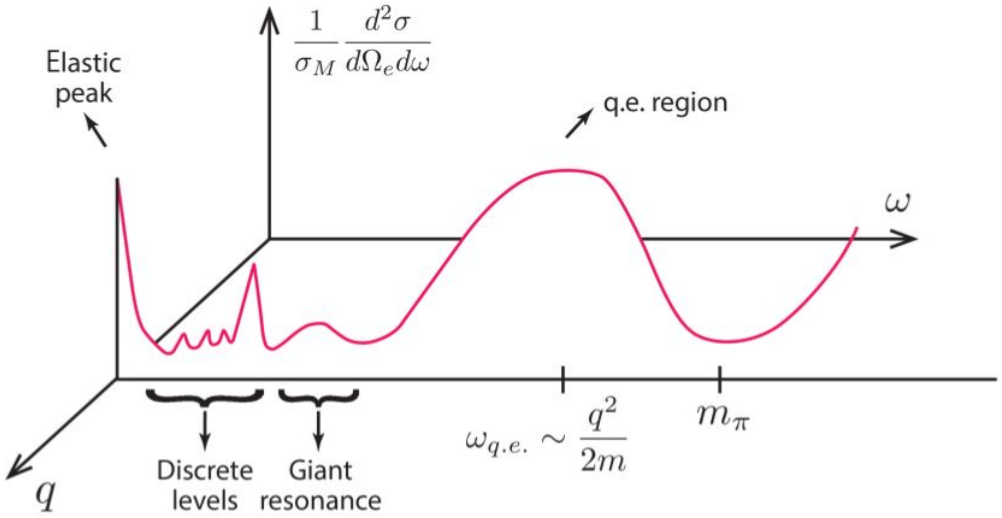
JINA-CEE

Nuclear Rates for Astrophysics

DUNE

Jefferson Lab

# Electron-Nucleus Scattering Cross Section




Energy and momentum transferred (ω,q)

Current and planned experimental programs rely on theoretical calculations at different kinematics

# Outline

**Ab initio description of nuclei:**

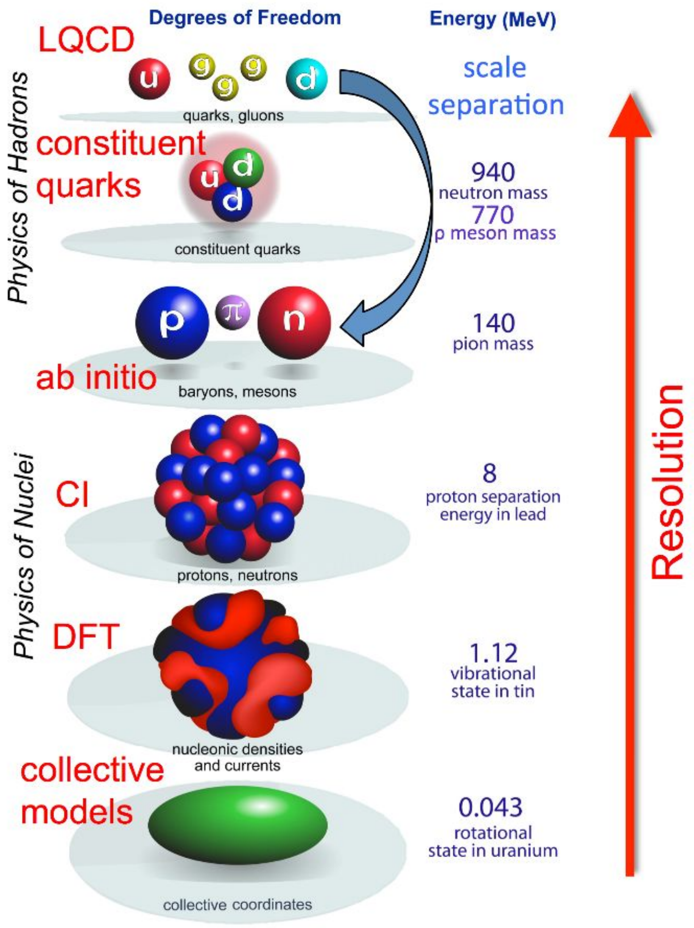
- Many-body nuclear problem
- Nuclear interaction
- Quantum Monte Carlo methods
- Many-body currents

**Lepton nucleus scattering:**

- Inclusive processes
- Beyond inclusive: Short-Time approximation

# From Quarks to Nuclei

- Nuclei are complex systems made of interacting protons and neutrons, which in turns are composite objects made of interacting constituent quarks
- All fundamental forces are at play in nuclei
- **EFTs** low-energy approximations of QCD whose d.o.f. are bound states of QCD (e.g., protons, neutrons, pions, …); used to construct many-nucleon interactions and currents
- Accurate inputs at the single- and few-nucleon level are required (e.g., from **LQCD**)

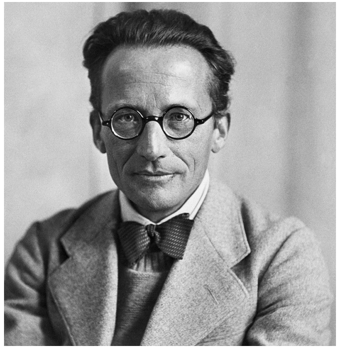


# Microscopic (or *ab initio*) Description of Nuclei

Comprehensive theory that describes quantitatively and predictably nuclear structure and reactions

**Requirements**:

- Accurate understanding of the interactions/correlations between nucleons in **paris**, **triplets**, ... (**two- and three-nucleon forces**)
- Accurate understanding of the electroweak interactions of external probes (electrons, neutrinos, photons) with nucleons, correlated nucleon-pairs, … (**one- and two-body electroweak currents**)
- **Computational methods** to solve the many-body nuclear problem of strongly interacting particles



Erwin Schrödinger

$$H\Psi = E\Psi$$

# Many-body Nuclear Problem

Nuclear Many-body Hamiltonian (in coordinate space)

$$H = T + V = \sum_{i=1}^{A} t_i + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_A, s_1, s_2, \ldots, s_A, t_1, t_2, \ldots, t_A)$$

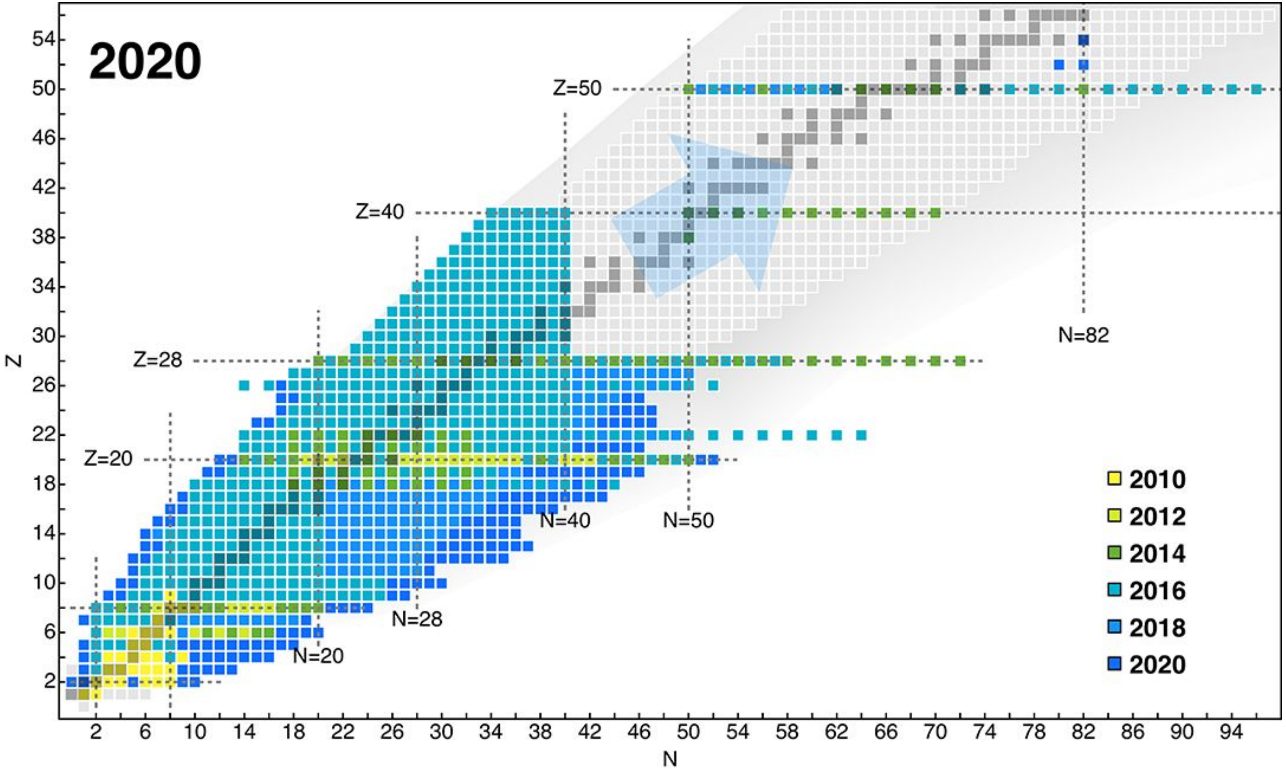

http://exascaleage.org/np/

$\Psi$ are complex spin-isospin vectors in 3A dimensions with components $2^A \times \frac{A!}{Z!(A-Z)!}$

$^4$He : 96
$^6$Li : 1280
$^8$Li : 14336
$^{12}$C : 540572

Develop Computational Methods to solve (numerically) exactly or within approximations that are under control the many-body nuclear problem

# Current Status



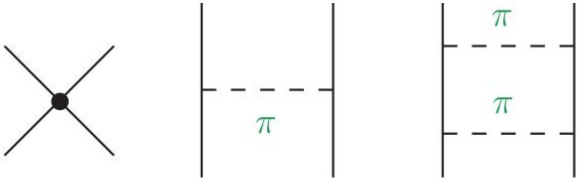

H. Hergert
Front. Phys.
07 October 2020

# Many-body Nuclear Interactions

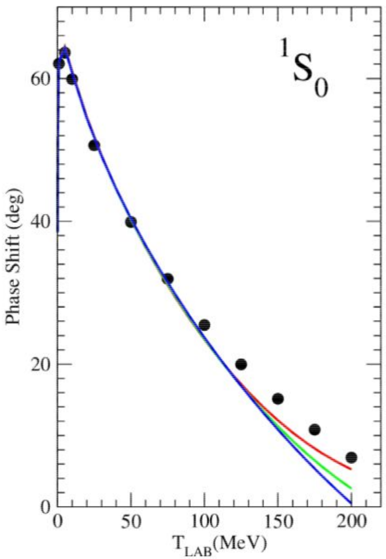
Many-body Nuclear Hamiltonian

$$H = T + V = \sum_{i=1}^{A} t_i + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

$v_{ij}$ and $V_{ijk}$ are two- and three-nucleon operators based on experimental data fitting; fitted parameters subsume underlying QCD dynamics




Contact term: short-range
Two-pion range: intermediate-range $r \propto (2\,m_\pi)^{-1}$
One-pion range: long-range $r \propto m_\pi^{-1}$



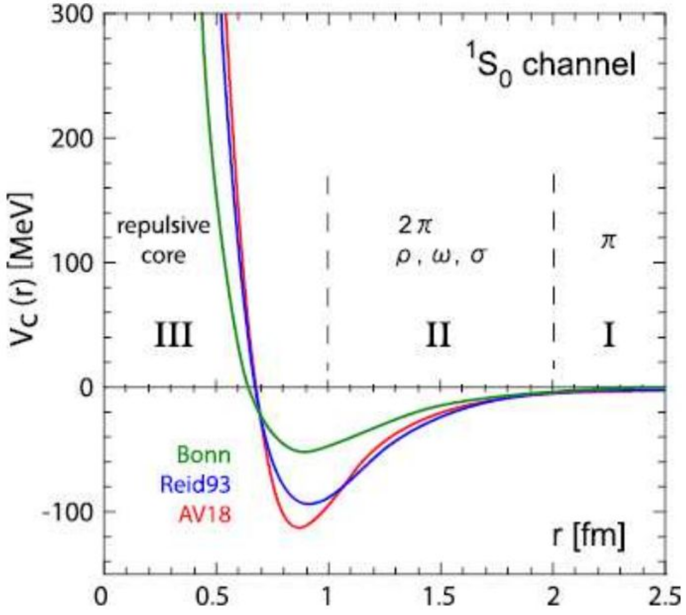

Pastore et al. PRC80(2009)034004

Hideki Yukawa

AV18+UIX; AV18+IL7
Wiringa, Schiavilla, Pieper *et al.*

chiral πNΔ
N3LO+N2LO Piarulli *et al.* **Norfolk Models**

# Nucleon-Nucleon Potential




Aoki *et al.* Comput.Sci.Disc.1(2008)015009

# Quantum Monte Carlo Methods

Stochastic methods that allow to solve the Schrödinger equation with controlled error

Toy example:

$$I = \int_{\Omega} f(\overline{\mathbf{x}}) d\overline{\mathbf{x}} \qquad \overline{\mathbf{x}}_1, \ldots, \overline{\mathbf{x}}_N \in \Omega$$

then

$$I \approx V \frac{1}{N} \sum_{i=1}^{N} f(\overline{\mathbf{x}}_i)$$

And the error on the estimate decreases as $\frac{1}{\sqrt{N}}$

# Quantum Monte Carlo Methods

Minimize the expectation value of the nuclear Hamiltonian: H = T + $v_{ij}$ + $V_{ijk}$

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

using a trial wave function for a nucleus in J state:

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

# Quantum Monte Carlo Methods

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

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

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

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

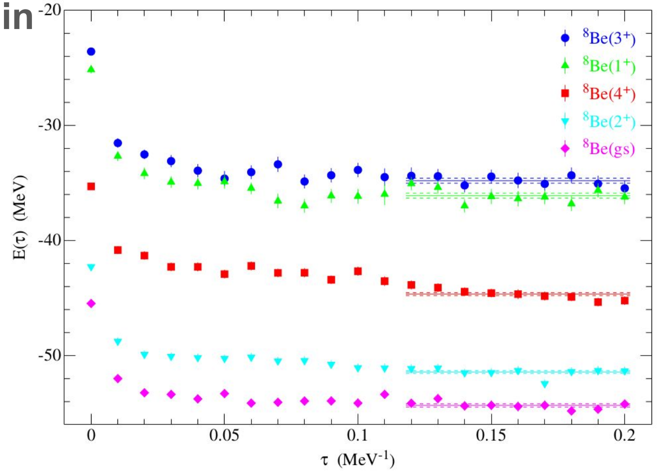
# Quantum Monte Carlo Methods

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

**Further improve the trial wave function by eliminating spurious contaminations via a Green's Function Monte Carlo propagation in imaginary time**

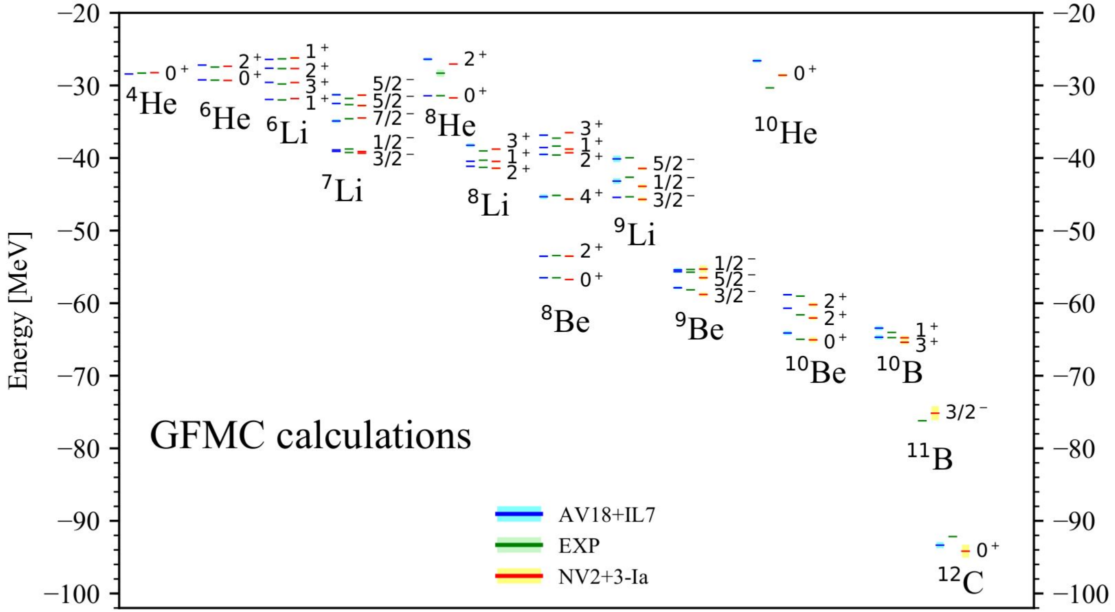
$$\Psi(\tau) = \exp[-(H - E_0)\tau]\Psi_V = \sum_n \exp[-(E_n - E_0)\tau]a_n\psi_n$$

$$\Psi(\tau \to \infty) = a_0\psi_0$$



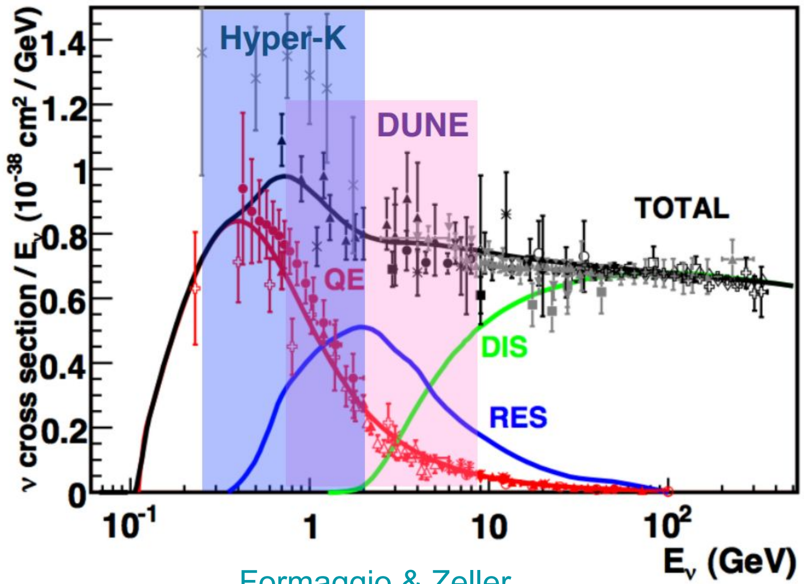

Carlson, Wiringa, Pieper *et al.*

# Energies




Piarulli *et al.* PRL120(2018)052503

# Neutrino cross section anatomy




Formaggio & Zeller

Quasi-elastic: dominated by single-nucleon knockout

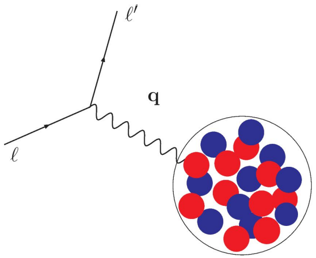
Resonance: excitation to nucleonic resonant states which decay into mesons

Deep-inelastic scattering: where the neutrino resolves the nucleonic quark content

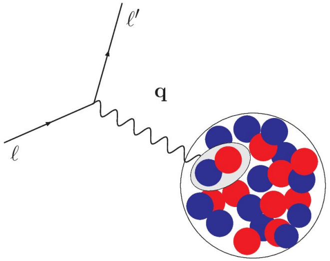
Each of these regimes requires knowledge of both the **nuclear ground state** and the **electroweak coupling** and **propagation of the struck nucleons, hadrons, or partons**

A challenge for achieving precise neutrino-nucleus cross-section is **reliably bridging the transition regions which use different degrees of freedom**

# Many-body Nuclear Electroweak Currents




one-body




two-body

Nuclear Charge Operator

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

Nuclear (Vector) Current Operator

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

- Two-body currents are a manifestation of two-nucleon correlations
- Electromagnetic two-body currents are required to satisfy current conservation
- Currents: phenomenological, or derived within Chiral Effective Field Theory

$$\mathbf{q} \cdot \mathbf{j} = [\, H, \, \rho \,] = [\, t_i + v_{ij} + V_{ijk}, \, \rho \,]$$

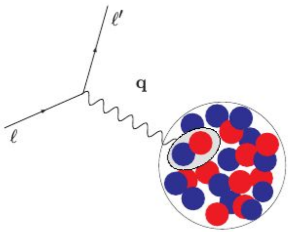
# Lepton-Nucleus scattering: Inclusive Processes

Electromagnetic Nuclear Response Functions

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

Longitudinal response induced by the charge operator $O_L = \rho$
Transverse response induced by the current operator $O_T = \boldsymbol{j}$
5 Responses in neutrino-nucleus scattering

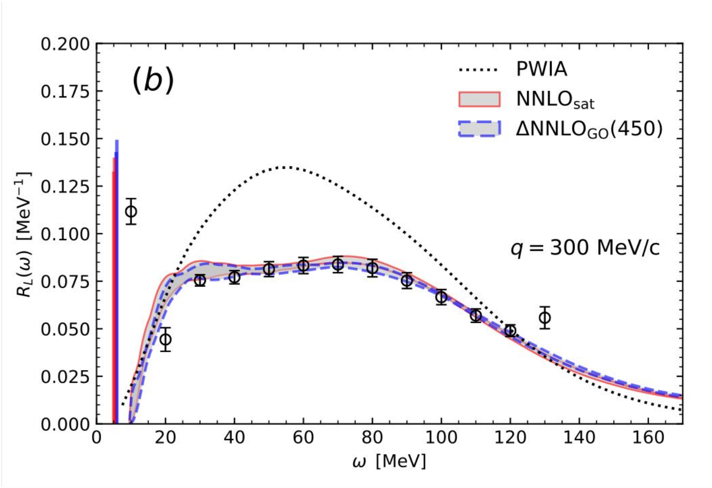
$$\frac{d^2\sigma}{d\omega d\Omega} = \sigma_M \left[v_L R_L(\mathbf{q},\omega) + v_T R_T(\mathbf{q},\omega)\right]$$



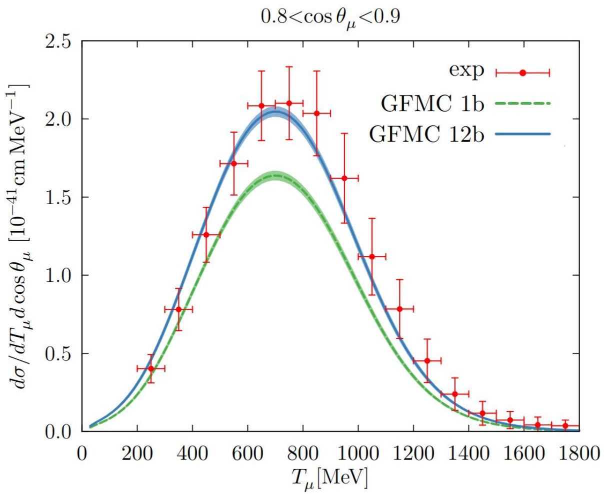
# Inclusive Cross Sections with Integral Transforms

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

Exploit integral properties of the response functions and closure to avoid **explicit calculation of the final states** (Lorentz Integral Transform **LIT**, **Euclidean**, …)




Sobczyk et al, PRL127 (2021)

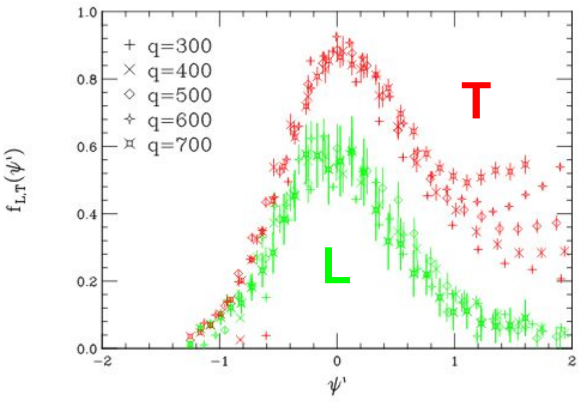



Lovato et al. PRX10 (2020)

# Lepton-Nucleus scattering: Data

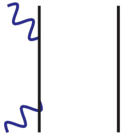
Transverse Sum Rule

$$S_T(q) \propto \langle 0|\mathbf{j}^\dagger\ \mathbf{j}|0\rangle \propto \langle 0|\mathbf{j}_{1b}{}^\dagger\ \mathbf{j}_{1b}|0\rangle + \langle 0|\mathbf{j}_{1b}{}^\dagger\ \mathbf{j}_{2b}|0\rangle + \dots$$



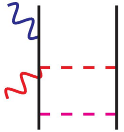

$^4$He Electromagnetic Data
Carlson *et al.* PRC65(2002)024002

Observed transverse enhancement explained by the combined effect of two-body correlations and currents in the interference term



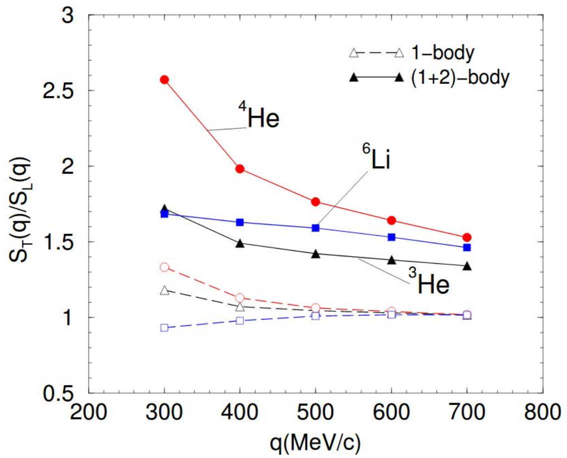
$\langle \mathbf{j}^\dagger_{1b}\ \ \mathbf{j}_{1b}\rangle\ > 0$

Leading one-body term



$\langle \mathbf{j}^\dagger_{1b}\ \mathbf{j}_{2b}\ v_\pi\rangle \propto \langle v_\pi^2\rangle\ > 0$

Interference term

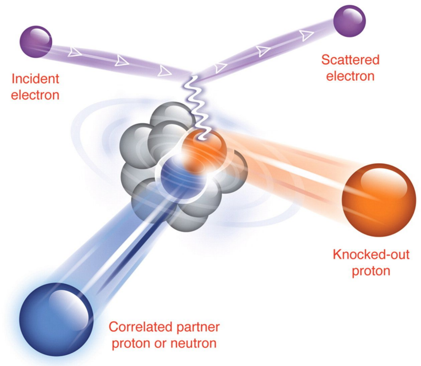



Transverse/Longitudinal Sum Rule
Carlson *et al.* PRC65(2002)024002

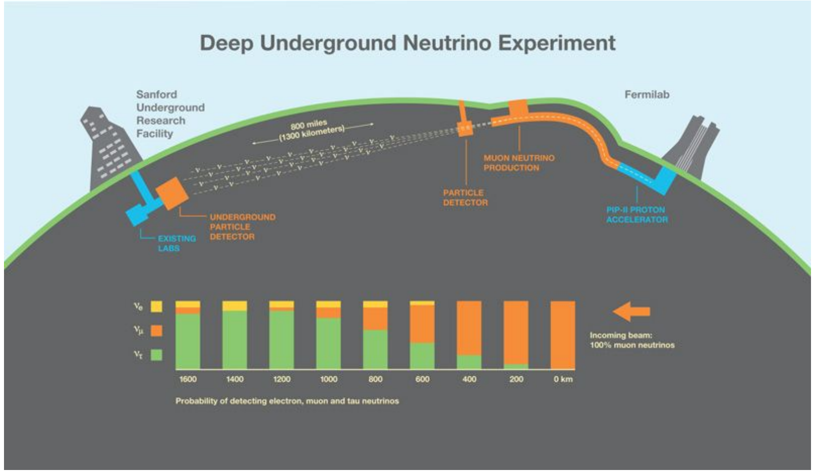
# Beyond Inclusive: Short-Time-Approximation

Short-Time-Approximation Goals:

- Describe electroweak scattering from A > 12 without losing two-body physics
- Account for exclusive processes
- Incorporate relativistic effects



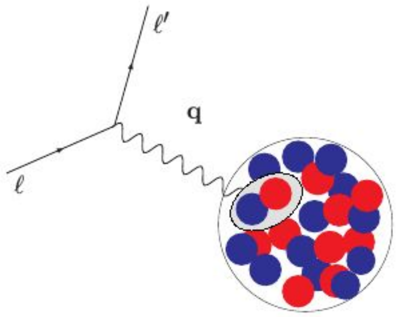

Subedi et al. Science320(2008)1475




Stanford Lab article

e4u collaboration

# Short-Time-Approximation




Short-Time-Approximation:

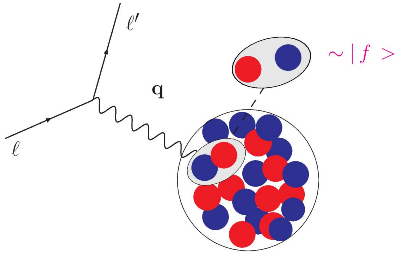
- Based on Factorization
- Retains two-body physics
- Correctly accounts for interference

$$R(q,\omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i(\omega+E_0)t} \langle 0|O^\dagger e^{-iHt} O|0\rangle$$

$$O_i^\dagger e^{-iHt} O_i + O_i^\dagger e^{-iHt} O_j + O_i^\dagger e^{-iHt} O_{ij} + O_{ij}^\dagger e^{-iHt} O_{ij}$$

$$H \sim \sum_i t_i + \sum_{i<j} v_{ij}$$

# Short-Time-Approximation




Short-Time-Approximation:

- Based on Factorization
- **Retains two-body physics**
- Response functions are given by the **scattering from pairs of fully interacting nucleons** that propagate into a correlated pair of nucleons
- Allows to retain both two-body correlations and currents at the vertex
- Provides "more" exclusive information in terms of nucleon-pair kinematics via the Response Densities

Response Functions ∝ Cross Sections

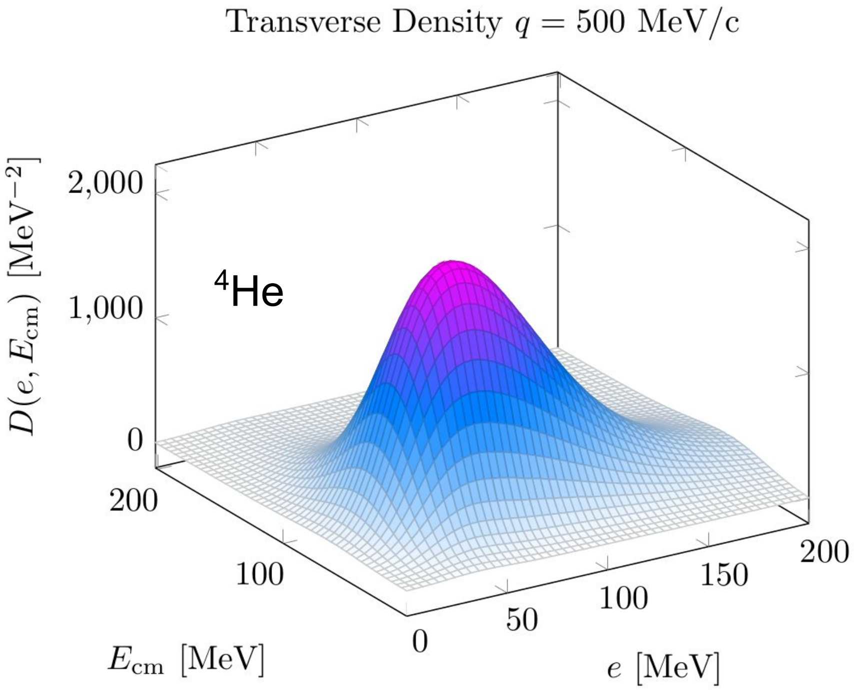
$$R_\alpha(q,\omega) = \sum_f \delta\left(\omega + E_0 - E_f\right) |\langle f|O_\alpha(\mathbf{q})|0\rangle|^2$$

Response ***Densities***

$$R(q,\omega) \sim \int \delta\left(\omega + E_0 - E_f\right) \, dP' \, dp' \mathcal{D}(p', P'; q)$$

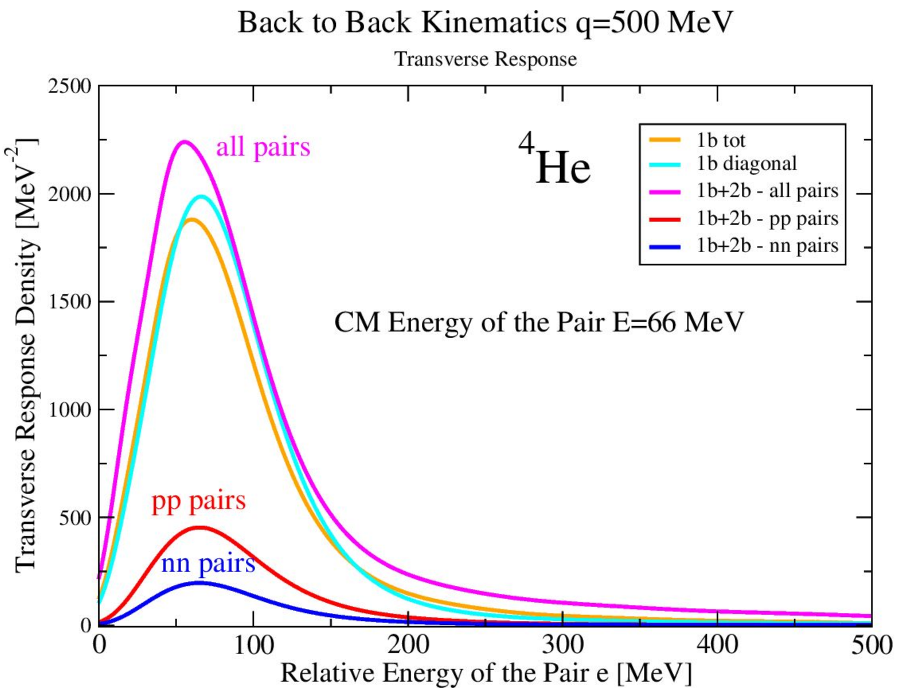
*P'* and *p'* are the CM and relative momenta of the struck nucleon pair

# Transverse Response Density: e-$^4$He scattering



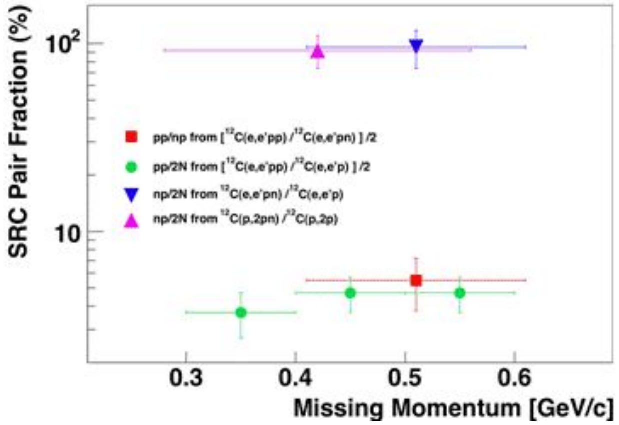

Pastore *et al.* PRC101(2020)044612

# $e$-$^{4}$He scattering in the back-to-back kinematic




Pastore *et al.* PRC101(2020)044612

- pp pairs
- nn pairs
- all pairs 1
- all pairs tot




Subedi et al. Science320(2008)1475

# GFMC SF STA: Benchmark & error estimate

### 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

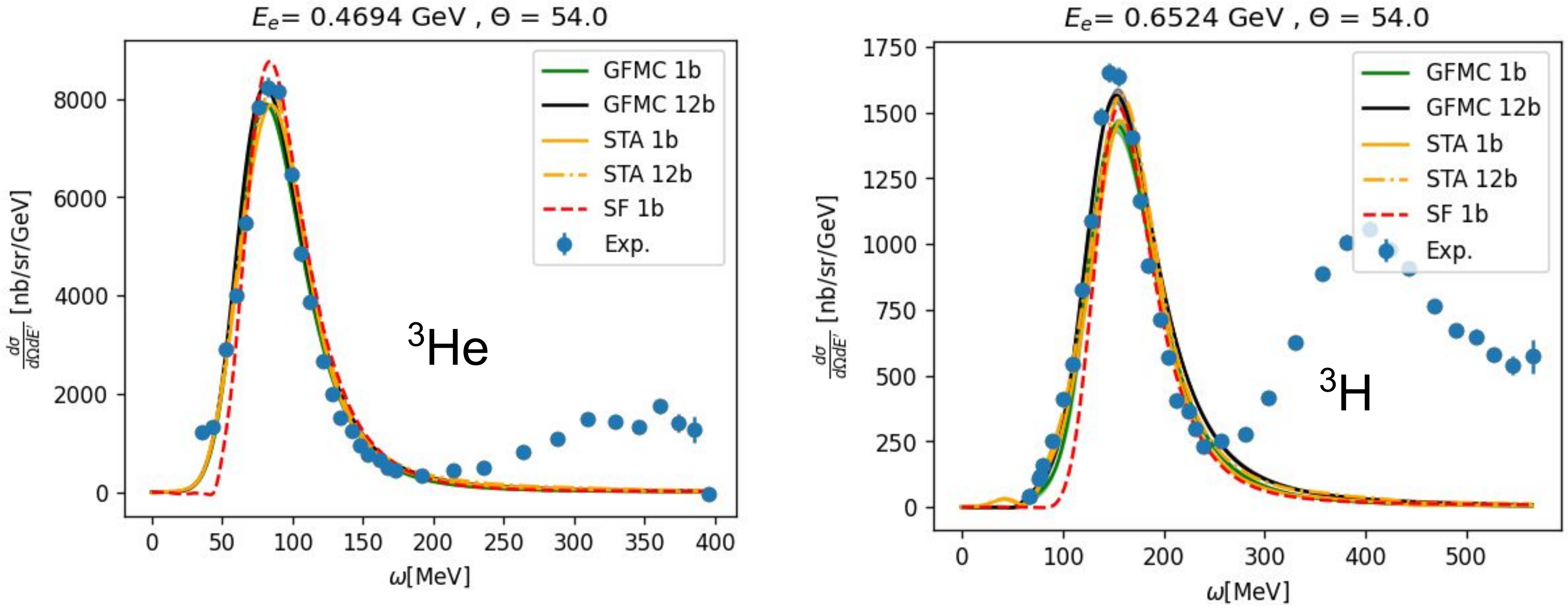
$$|\Psi_f\rangle = |\mathbf{p}\rangle \otimes \left|\Psi_n^{A-1}\right\rangle$$

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

See

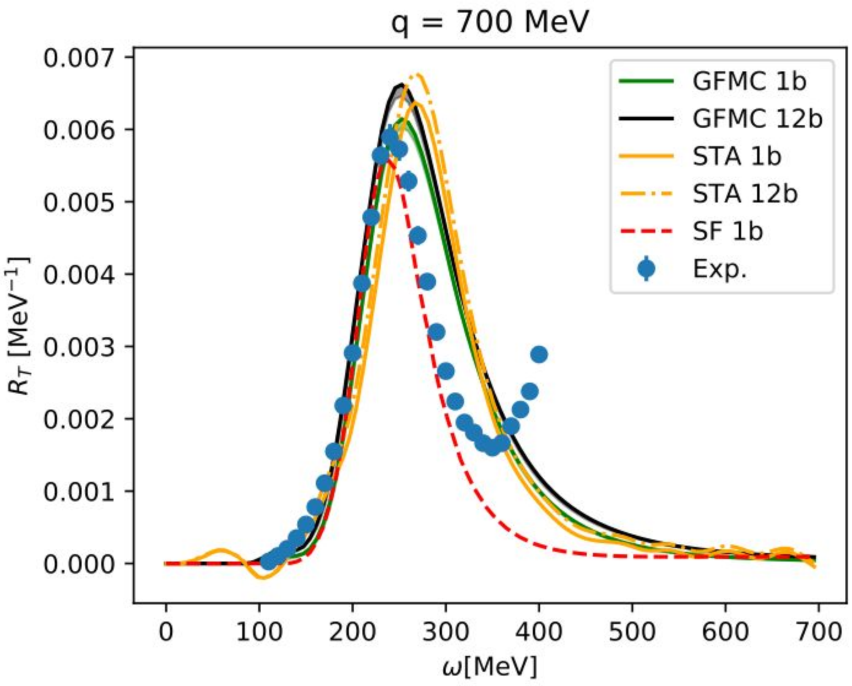
LA et al. PRC105(2022)014002

# GFMC SF STA: Benchmark & error estimate




LA et al. PRC105(2022)014002

# Importance of relativistic corrections

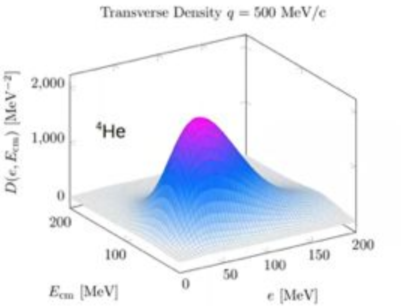



LA et al. PRC105(2022)014002

# Response Densities in heavier systems: $^{12}$C

| 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 |

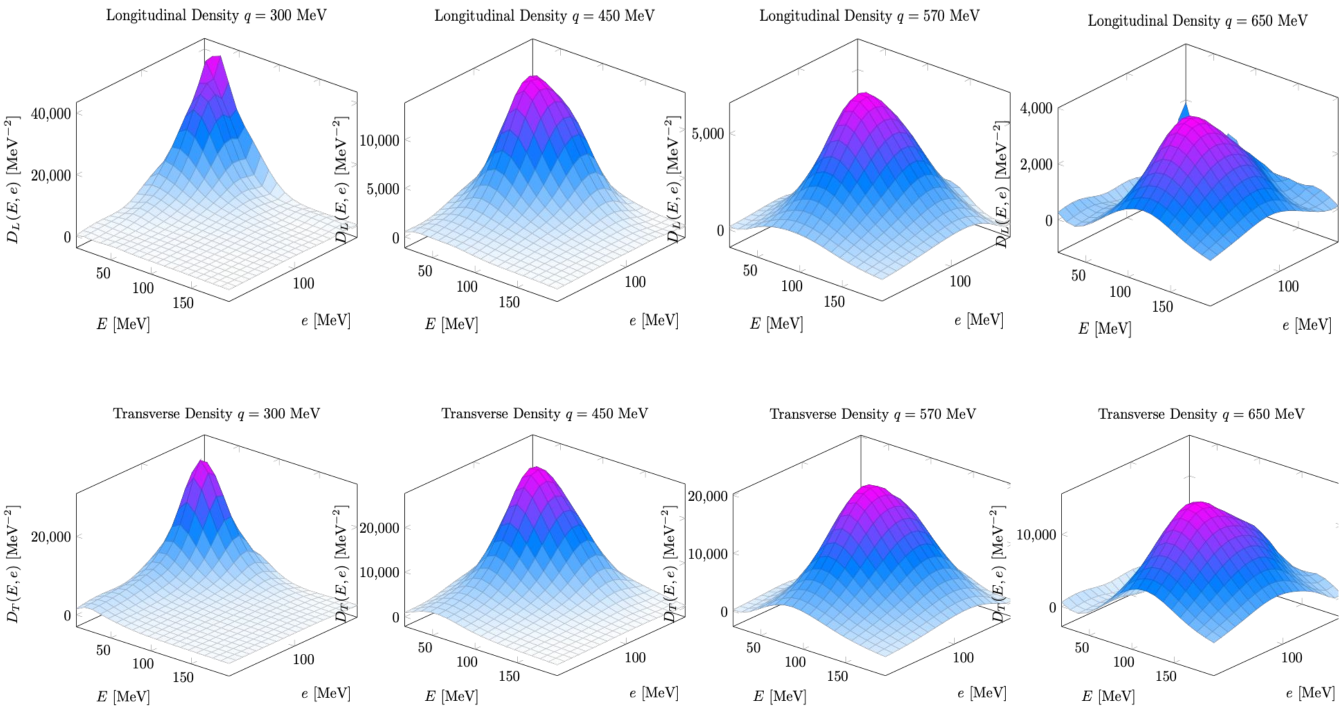

Response densities: E, e grid




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

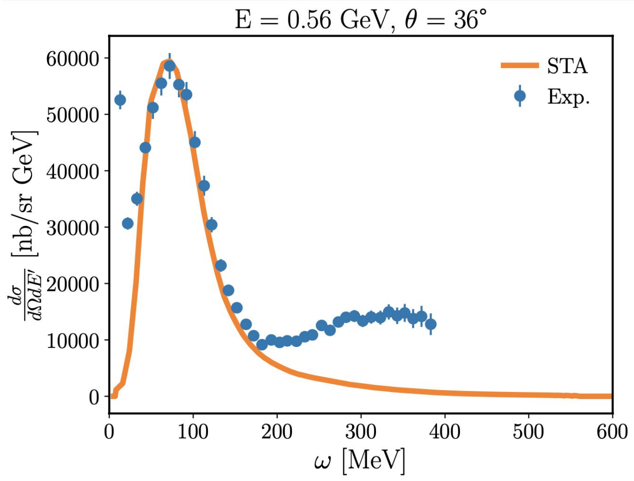
X

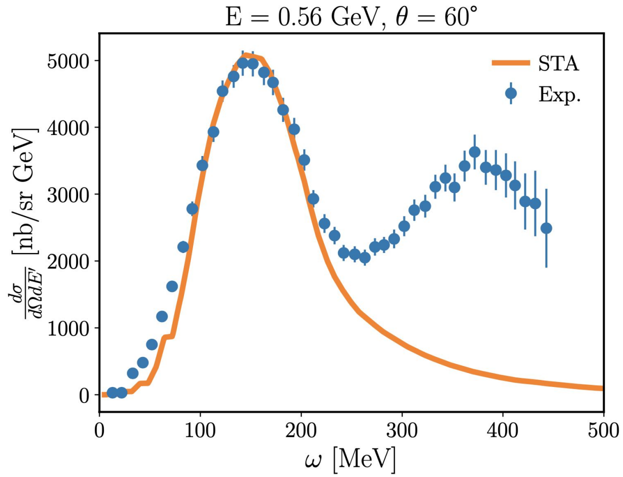
# Response Densities in heavier systems: $^{12}C$

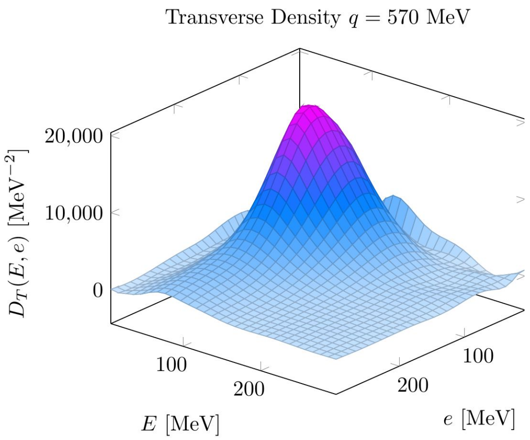



**LA et al. in preparation**

# STA for $^{12}$C: cross sections



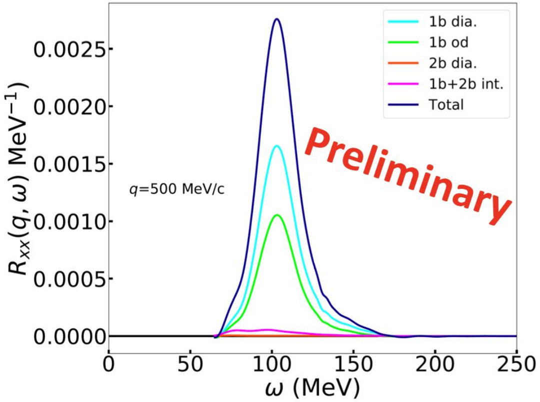




**LA et al. in preparation**

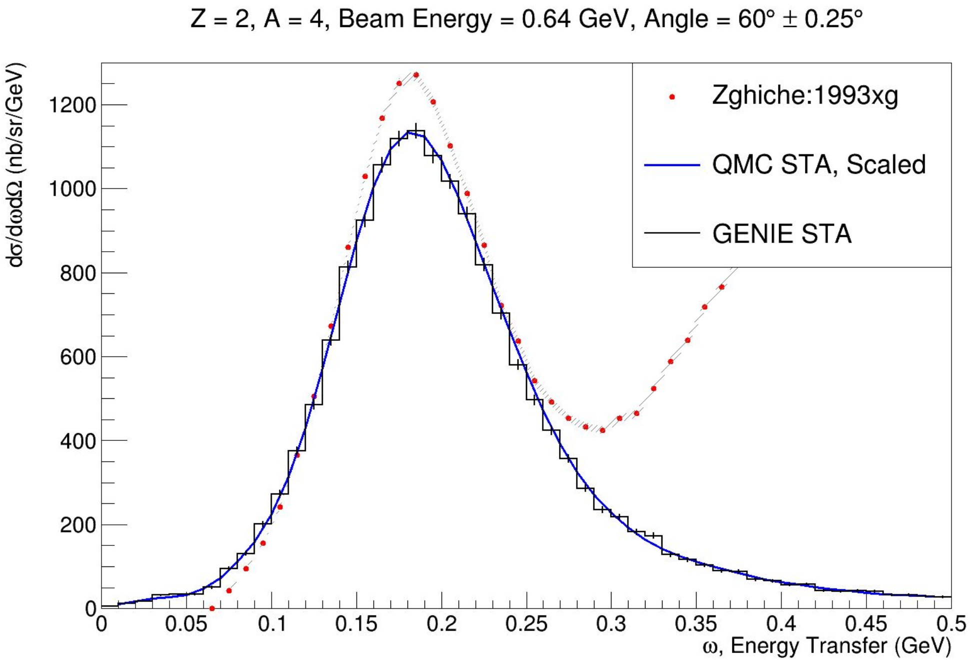
# EW interactions

- Calculations of EM interactions allows for a thorough evaluation of our methods and a comparison with the abundant experimental data for electron-nucleus scattering
- **G. King:** neutral weak currents quasi-elastic responses evaluated for 2H




- Event generator are necessary: interface between ab initio nuclear calculations and EG

# 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

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

Barrow, Gardiner, SP *et al.* PRD 103 (2021) 5, 052001
GENIE HadronTensorModell Class

# Conclusions

- Ab initio calculations of light nuclei yield a picture of nuclear structure and dynamics where many-body effects play an essential role in explaining available data

- Nuclear theory input will be fundamental for the success of the neutrino experimental program

- Factorization schemes like the STA can extend the reach of ab initio calculations to heavier nuclei  (for example using Auxiliary Field Diffusion Monte Carlo, based on imaginary time propagation)