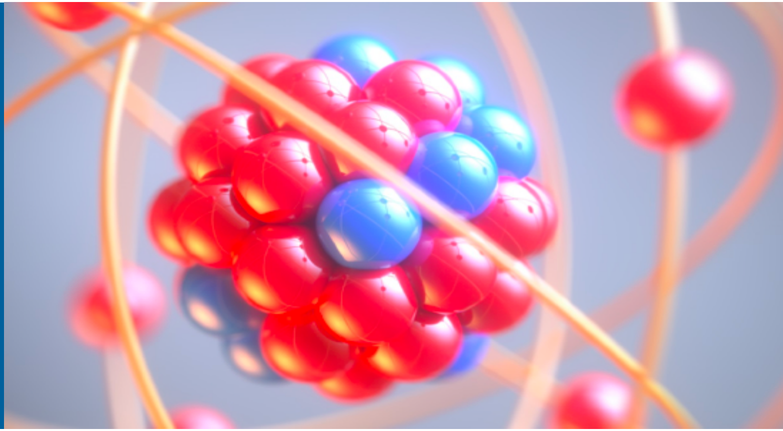
AB-INITIO NUCLEAR STRUCTURE WITH QUANTUM MONTE CARLO TECHNIQUES



ALESSANDRO LOVATO

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Trento Institute for Fundamental Physics and Applications

Argonne NATIONAL LABORATORY

ECT* Workshop

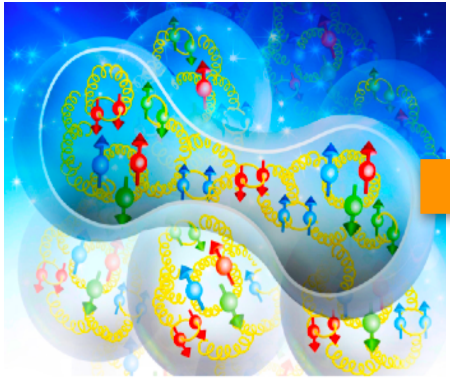
Short-distance nuclear structure and PDFs

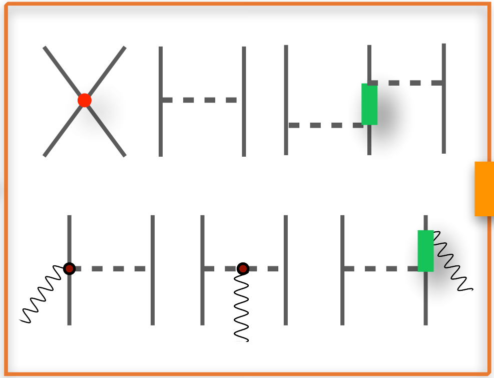
Trento, July 18, 2023

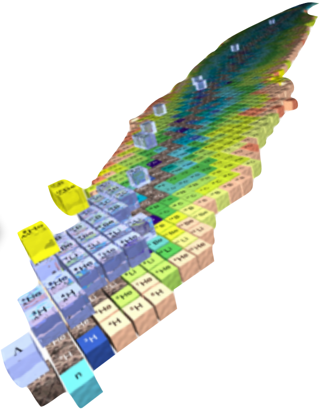
THE NUCLEAR MANY-BODY PROBLEM

In the low-energy regime, quark and gluons are confined within hadrons and the relevant degrees of freedoms are protons, neutrons, and pions

Effective field theories are the link between QCD and nuclear observables.







$$H = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk} \qquad J = \sum_i j_i + \sum_{i<j} j_{ij}$$

THE NUCLEAR MANY-BODY PROBLEM

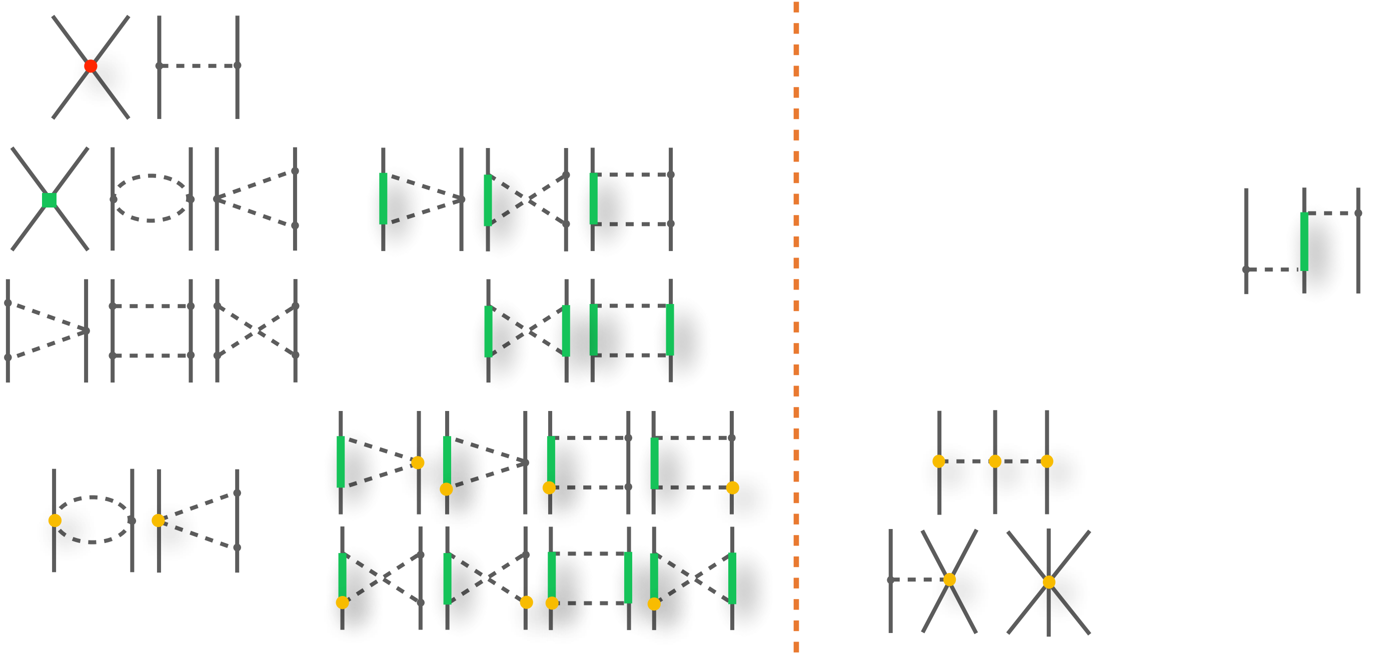
Chiral EFT exploits the broken chiral symmetry of QCD to construct potentials and consistent currents

Δ-less | **Additional Δ-full** | **Δ-less** | **Additional Δ-full**

LO $(p/\Lambda_b)^0$

NLO $(p/\Lambda_b)^2$

N^2LO $(p/\Lambda_b)^3$



*R. Machleidt et al., Phys. Scripta **91**, 083007 (2016)*

*M. Piarulli et al., Front.in Phys. **7**, 245 (2020)*

NUCLEAR MANY-BODY METHODS

Non relativistic many body theory aims at solving the many-body Schrödinger equation

$$H\Psi_0(x_1,\ldots,x_A) = E_0\Psi_0(x_1,\ldots,\ldots,x_A) \quad \longleftrightarrow \quad x_i \equiv \{\mathbf{r}_i, s_i^z, t_i^z\}$$

- Realistic potentials are (typically) non-perturbative and spin-isospin dependent

$$H = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

$$\begin{cases} v_{ij} = \sum_p v^p(r_{ij}) O_{ij}^p \\ O_{ij}^{p=1,8} = (1, \sigma_{ij}, S_{ij}, \mathbf{L}\cdot\mathbf{S}) \times (1, \tau_{ij}) \end{cases}$$

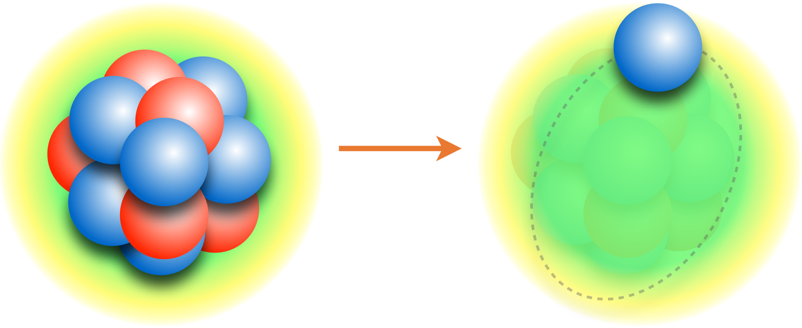
- Nucleons are fermions, so the wave function must be anti-symmetric

$$\Psi_0(x_1,\ldots,x_i,\ldots,x_j,\ldots,x_A) = -\Psi_0(x_1,\ldots,x_j,\ldots,x_i,\ldots,x_A)$$

INTRODUCTION: MEAN-FIELD APPROXIMATION

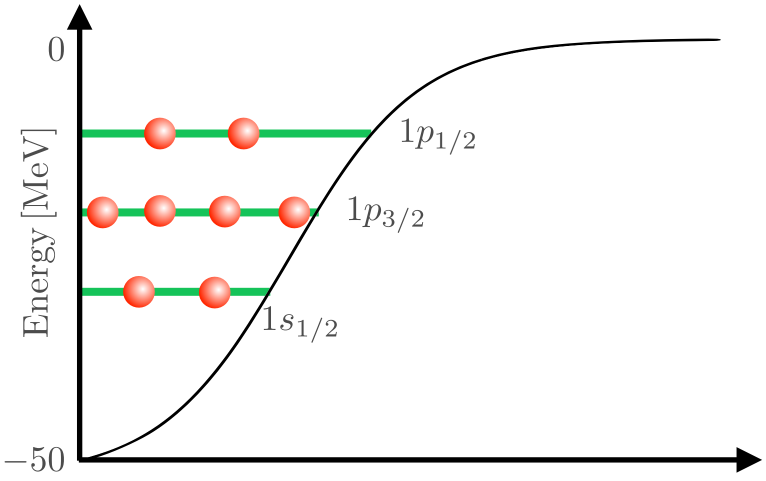
- Nucleons are assumed to be independent particles subject to an average potential

$$\left[\sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}\right] \rightarrow \sum_i U_i$$



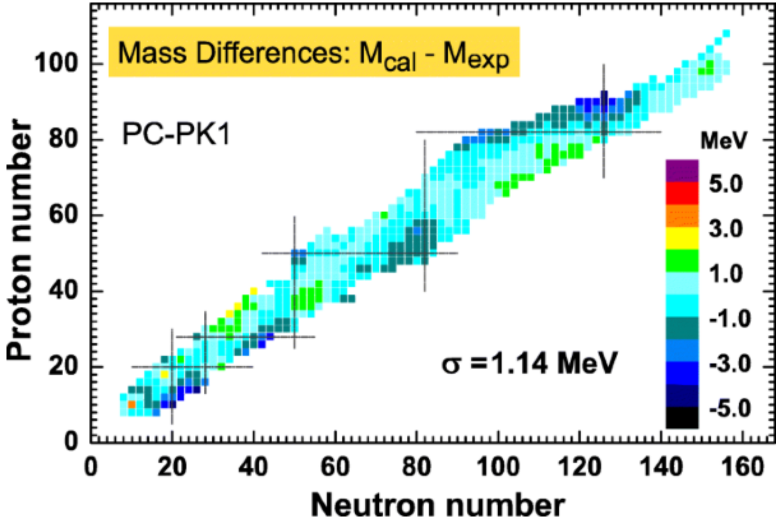
- The ground-state wave function is a Slater determinant of single-particle orbitals

$$\Phi_0(x_1, \ldots, x_A) = \mathcal{A}[\phi_{n_1}(x_1) \ldots \phi_{n_A}(x_A)]$$



INTRODUCTION: MEAN-FIELD APPROXIMATION

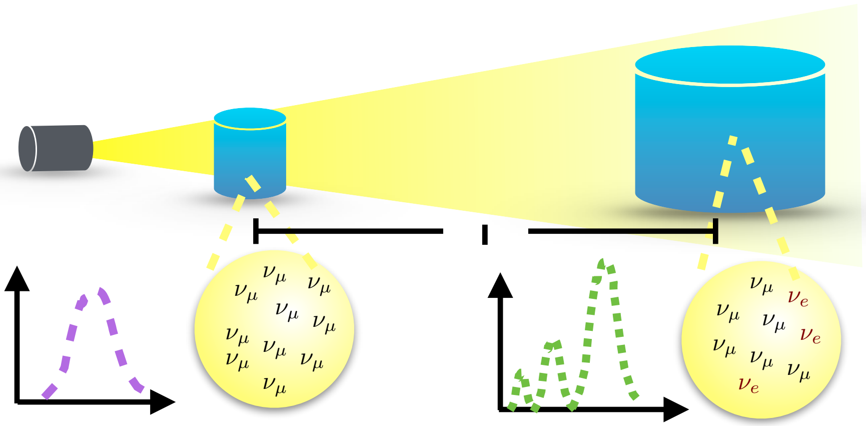
- The interaction is usually fitted on binding energies and charge radii of stable nuclei



- MF is the tool of choice for describing large nuclei, including their real-time dynamics
  - Neglects nucleon-nucleon scattering data and deuteron properties
  - No clear way to derive effective currents

INTRODUCTION

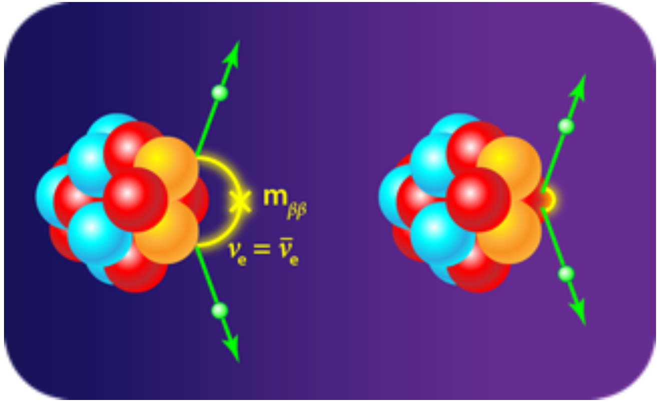
Oscillation parameters are measured by comparing the neutrino flux at near and far detectors



Accurate neutrino-nucleus scattering calculations critical for the success of the experimental program

Credit: N. Rocco

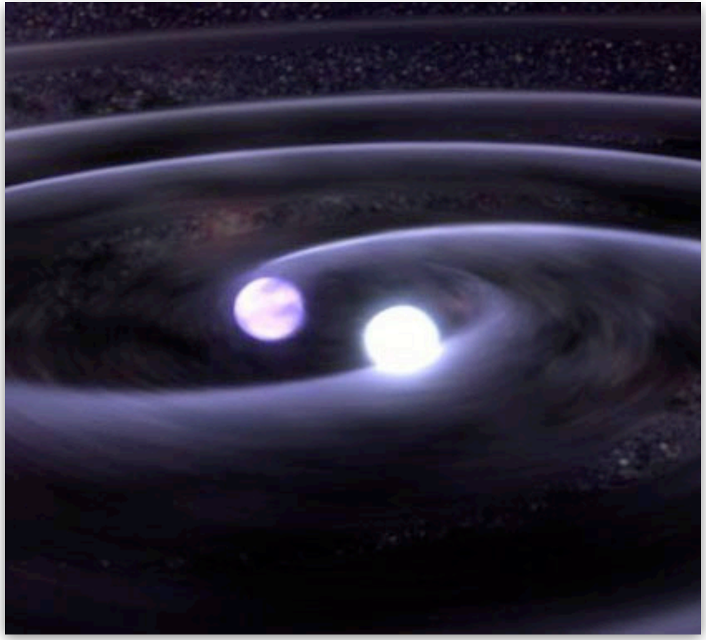
If observed, $0\nu\beta\beta$ would provide key insights into physics beyond the Standard Model

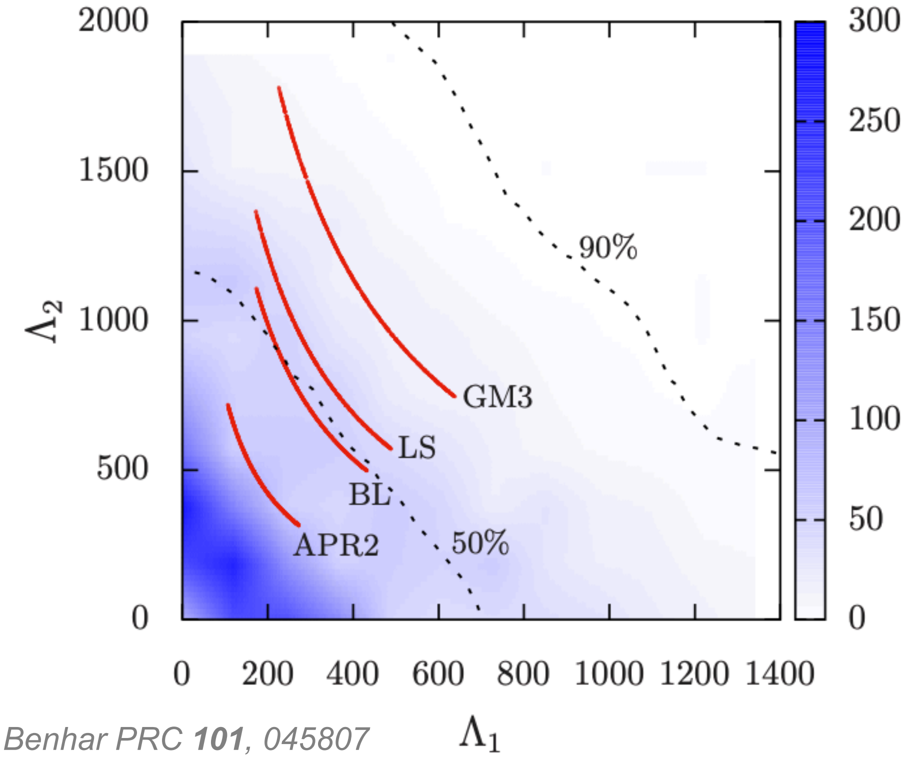


Relating experimental constraints on 0νββ decay rates to the neutrino masses requires quantitative estimates of nuclear matrix elements

INTRODUCTION

An accurate understanding of nuclear dynamics is critical for multi-messenger astronomy





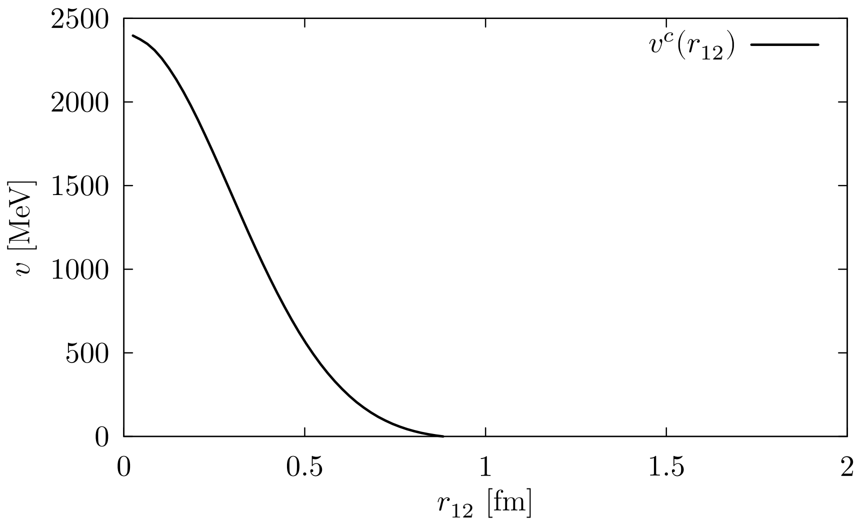
*A. Sabatucci, O. Benhar PRC **101**, 045807*

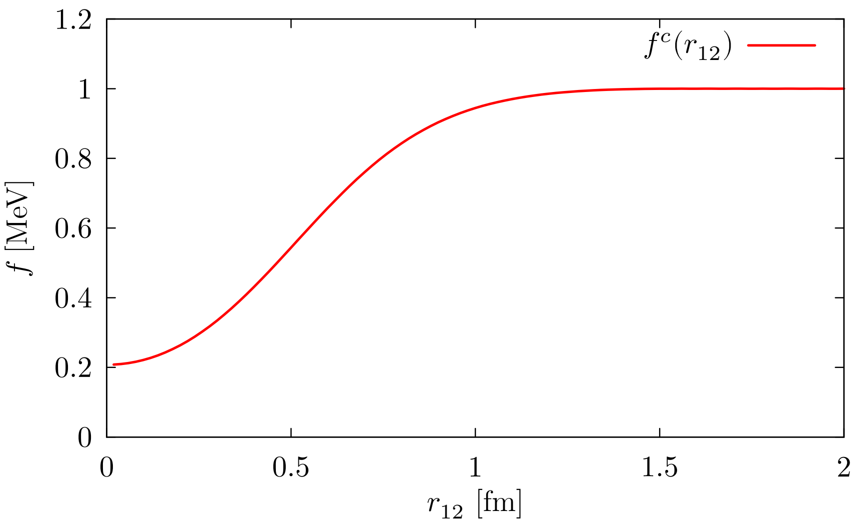
VARIATIONAL MONTE CARLO

In variational Monte Carlo, one assumes a “suitable” ansatz for the trial wave function

$$|\Psi_T\rangle = \Big(1 + \sum_{ijk} F_{ijk}\Big)\Big(\mathcal{S}\prod_{i<j} F_{ij}\Big)|\Phi_{J,T_z}\rangle \quad \longleftrightarrow \quad E_T = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \geq E_0$$

The correlations are consistent with the underlying nuclear interaction





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GREEN'S FUNCTION MONTE CARLO

The trial wave function can be expanded in the set of the Hamiltonian eigenstates

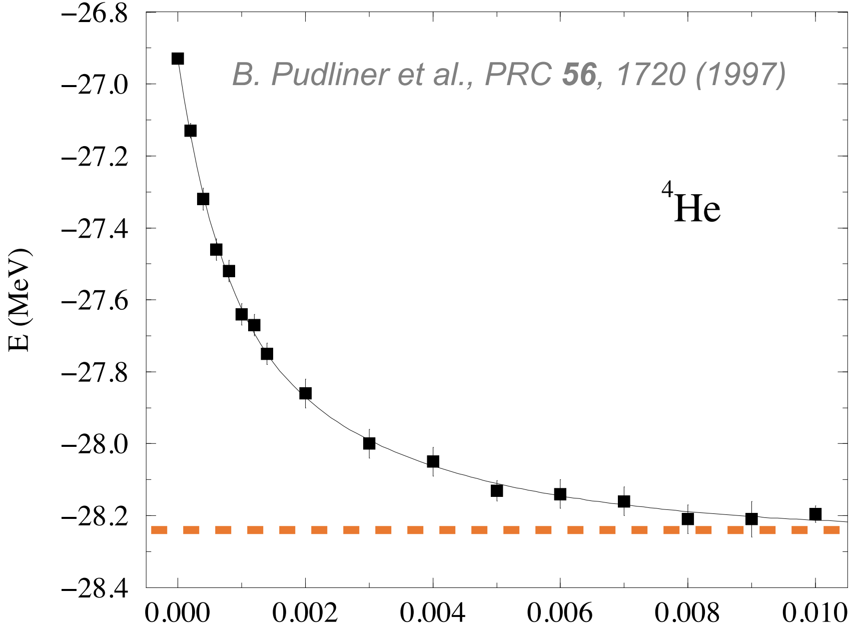
$$|\Psi_T\rangle = \sum_n c_n |\Psi_n\rangle \qquad H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

GFMC projects out the lowest-energy state using an imaginary-time propagation

$$\lim_{\tau\to\infty} e^{-(H-E_0)\tau}|\Psi_T\rangle = c_0|\Psi_0\rangle$$

*J. Carlson Phys. Rev. C **36**, 2026 (1987)*

GFMC suffers from the fermion-sign problem, but it is "virtually exact" for light nuclear systems.



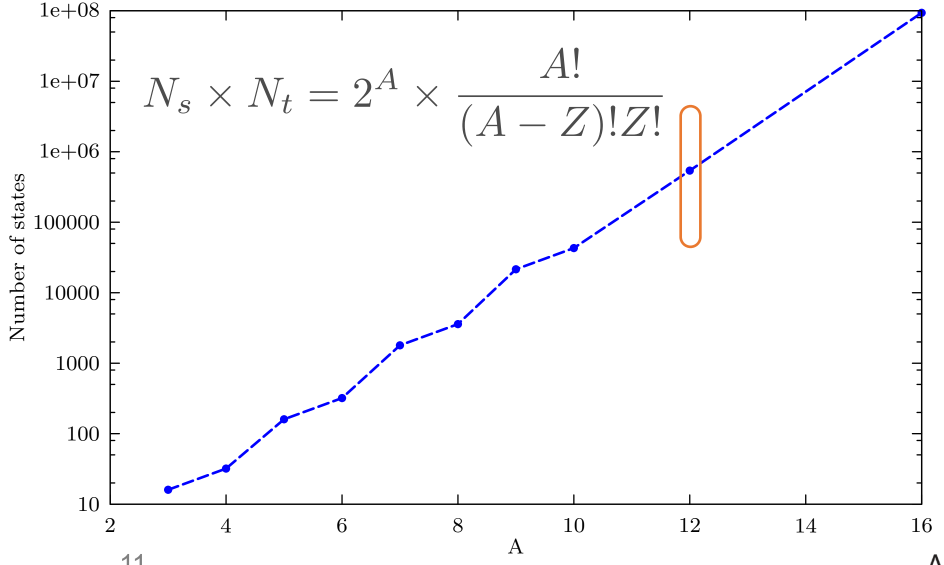
GREEN'S FUNCTION MONTE CARLO

In the GFMC, a sum over all the many-body spin-isospin states is performed

$$\sum_{SS'} \langle S'| e^{-[V-E_0]\delta\tau} |S\rangle \simeq \sum_{SS'} \langle S'| \prod_{i<j} e^{-V_{ij}\delta\tau} |S\rangle e^{E_0 \delta\tau}$$

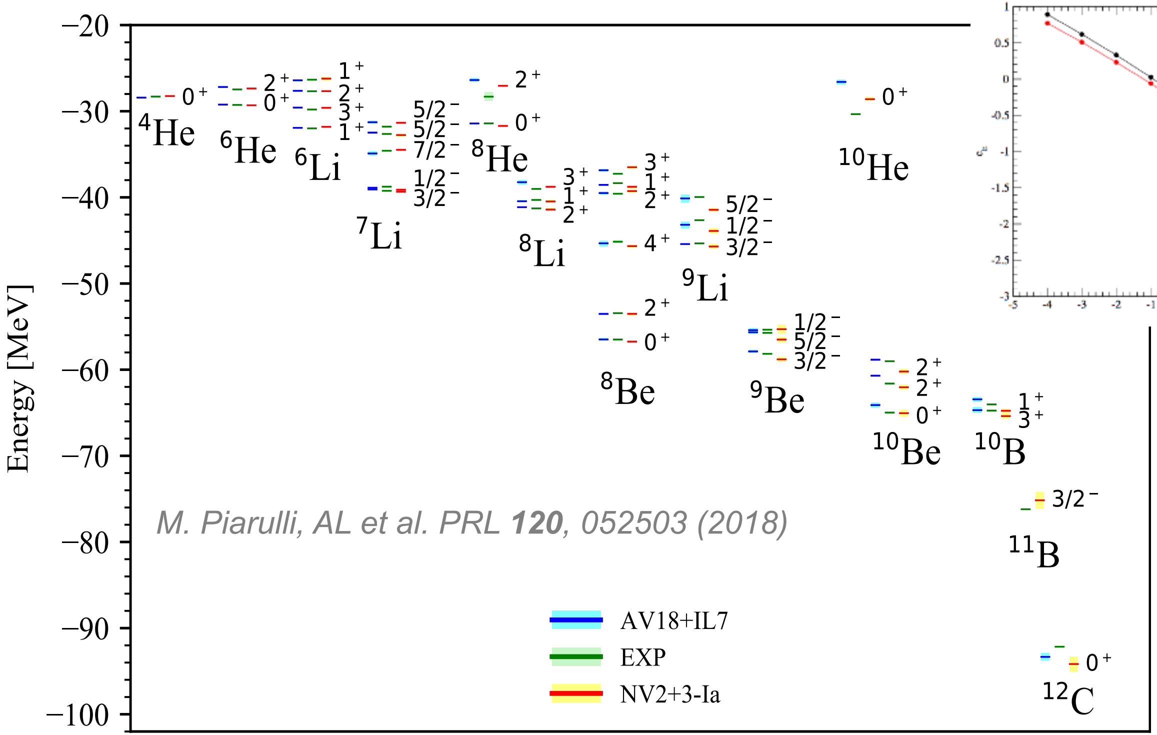
GFMC is extremely accurate but limited to A≲12 nuclei and small (A ≤14) neutron systems

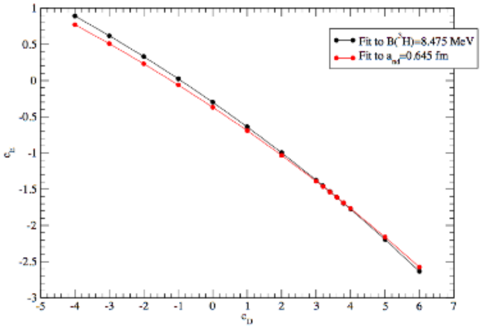
$$|S\rangle = \begin{pmatrix} s_{\uparrow\uparrow\uparrow} \\ s_{\uparrow\uparrow\downarrow} \\ s_{\uparrow\downarrow\uparrow} \\ s_{\uparrow\downarrow\downarrow} \\ s_{\downarrow\uparrow\uparrow} \\ s_{\downarrow\uparrow\downarrow} \\ s_{\downarrow\downarrow\uparrow} \\ s_{\downarrow\downarrow\downarrow} \end{pmatrix}$$



GREEN’S FUNCTION MONTE CARLO

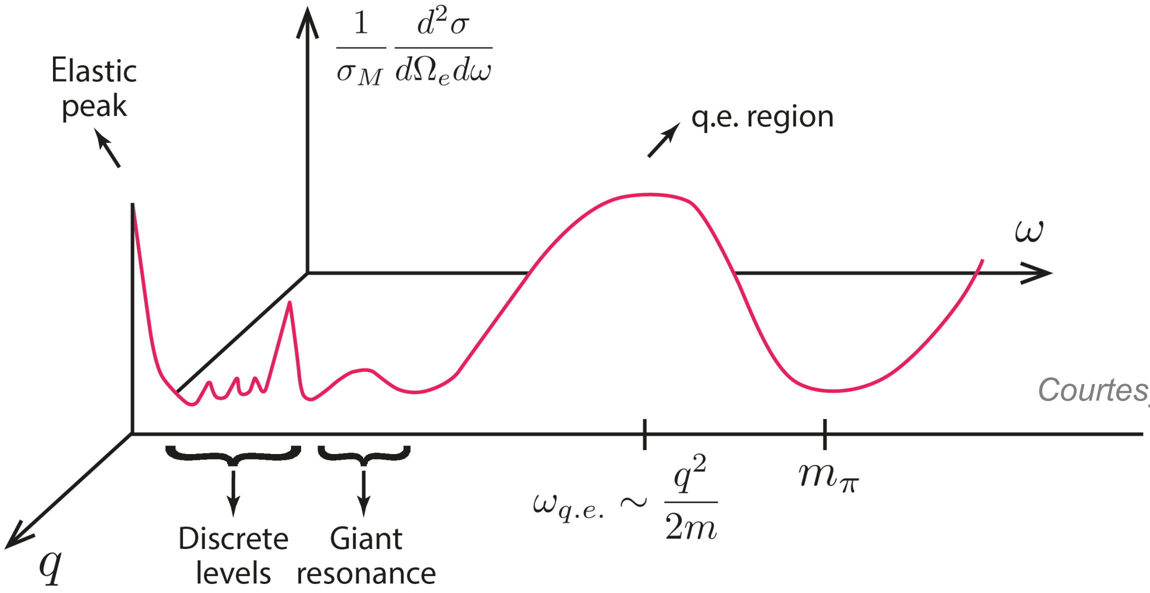
We included the NV2+3 potentials in the GFMC method; same accuracy as AV18 + IL7.





LEPTON-NUCLEUS SCATTERING

The inclusive cross section is characterized by a variety of reaction mechanisms



Courtesy of S. Pastore

The response functions contain all nuclear-dynamics information

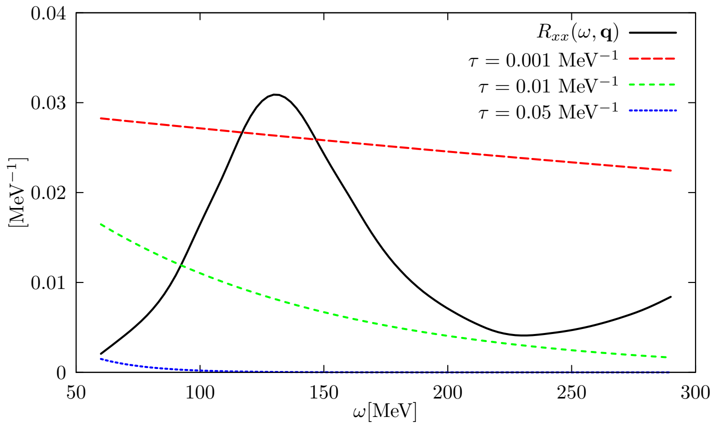
$$R_{\alpha\beta}(\omega, \mathbf{q}) = \sum_f \langle\Psi_0|J^\dagger_\alpha(\mathbf{q})|\Psi_f\rangle\langle\Psi_f|J_\beta(\mathbf{q})|\Psi_0\rangle\delta(\omega - E_f + E_0)$$

EUCLIDEAN RESPONSES

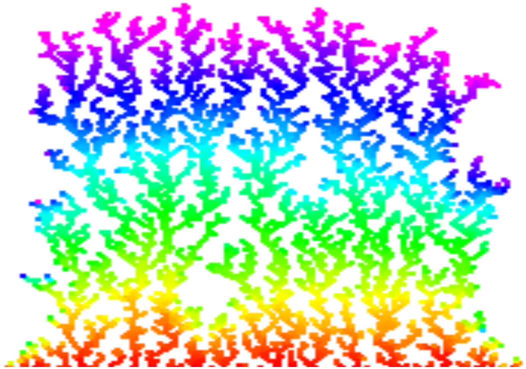
Our GFMC calculations rely on the Laplace kernel

$$E_{\alpha\beta}(\tau, \mathbf{q}) \equiv \int d\omega e^{-\omega\tau} R_{\alpha\beta}(\omega, \mathbf{q})$$

At finite imaginary time the contributions from large energy transfer are quickly suppressed



The system is first heated up by the transition operator. Its cooling determines the Euclidean response of the system



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

$$\sum_f |\Psi_f\rangle\langle\Psi_f|$$

EUCLIDEAN RESPONSES

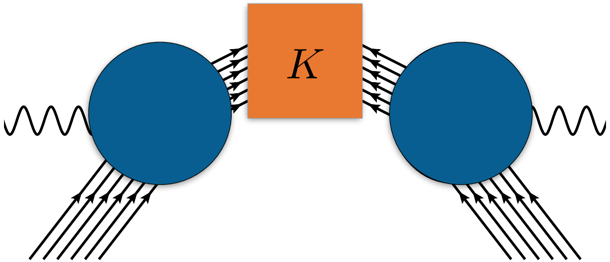
The integral transform of the response function is defined as

$$E_{\alpha\beta}(\sigma, \mathbf{q}) \equiv \int d\omega K(\sigma, \omega) R_{\alpha\beta}(\omega, \mathbf{q})$$

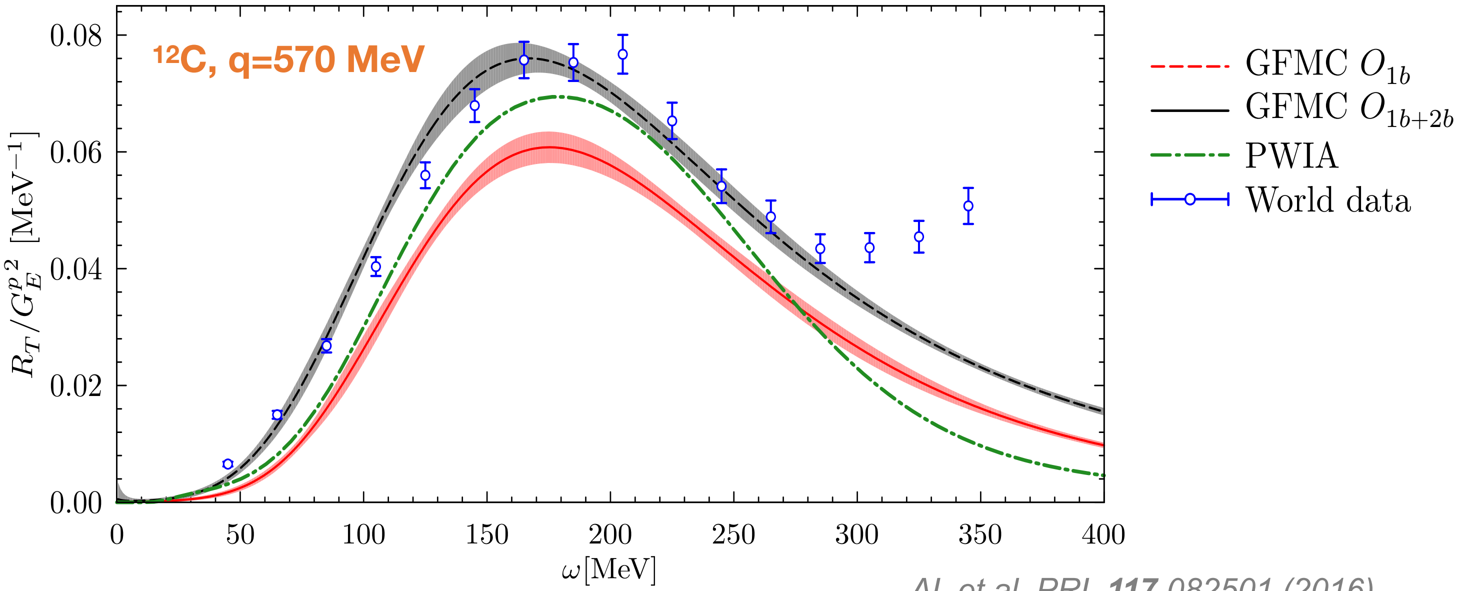
$$= \sum_f \int d\omega K(\sigma, \omega) \langle \Psi_0 | J_\alpha^\dagger(\mathbf{q}) | \Psi_f \rangle \langle \Psi_f | J_\beta(\mathbf{q}) | \Psi_0 \rangle \delta(\omega - E_f + E_0)$$

Using the completeness of the final states, it is expressed as a ground-state expectation value

$$E_{\alpha\beta}(\sigma, \mathbf{q}) = \langle \Psi_0 | J_\alpha^\dagger(\mathbf{q}) K(\sigma, H - E_0) J_\beta(\mathbf{q}) | \Psi_0 \rangle$$



INCLUSIVE ELECTRON SCATTERING



*AL et al. PRL **117** 082501 (2016)*

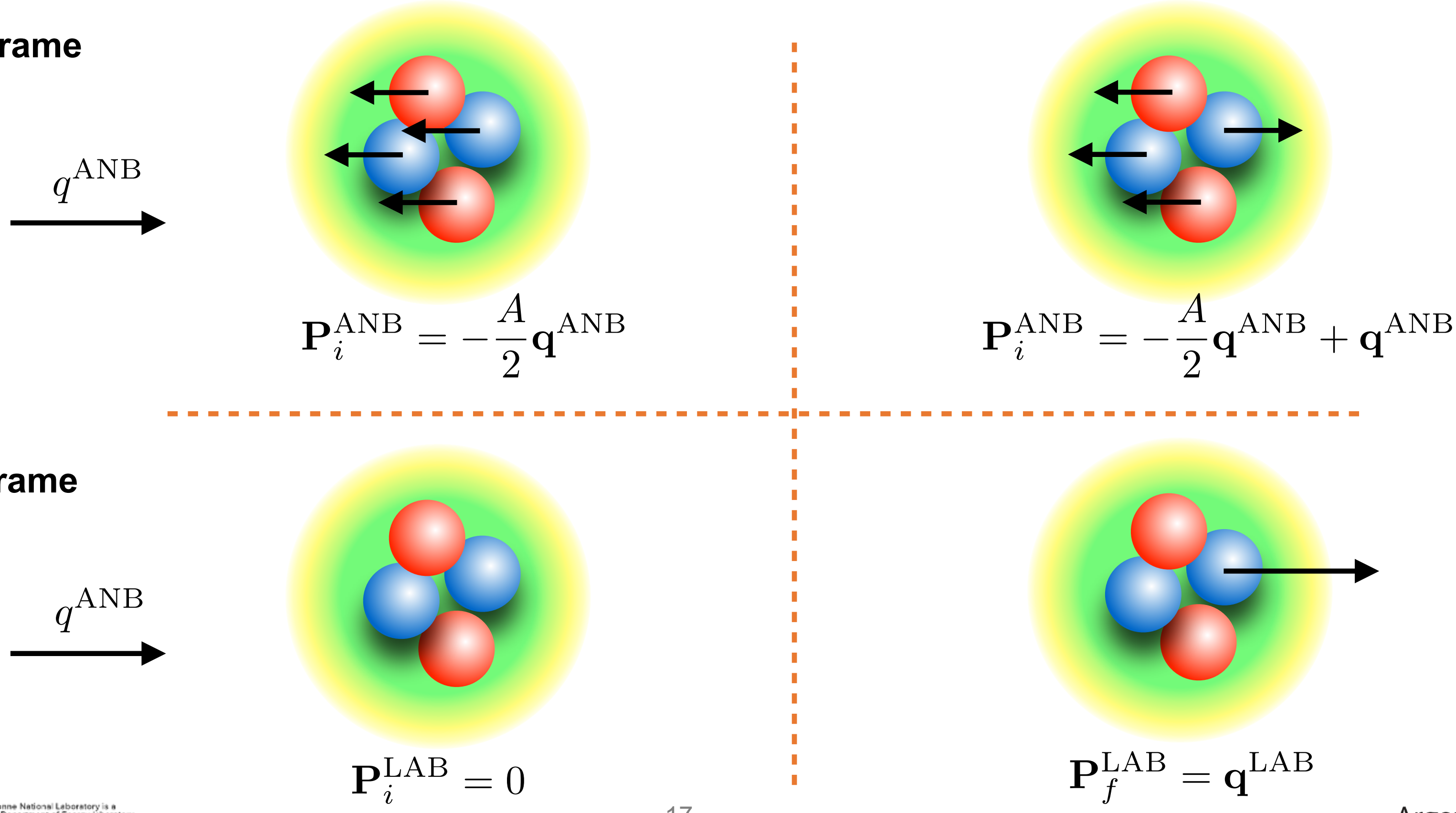
Two-body currents generate additional strength in over the whole quasi-elastic region

Correlations redistribute strength from the quasi-elastic peak to high-energy transfer regions

TACKLE RELATIVISTIC EFFECTS

ANB Frame

LAB Frame

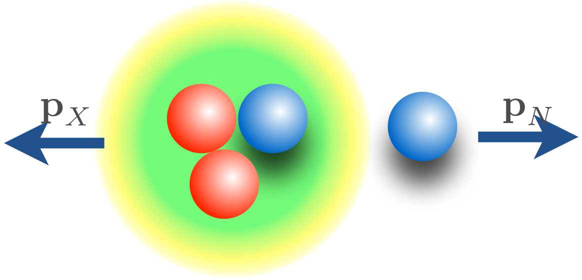


TACKLE RELATIVISTIC EFFECTS

To determine the relativistic corrections in the kinematics, we consider a two-body fragment model

$$\mathbf{p}_f = \mu\left(\frac{\mathbf{p}_N}{m} - \frac{\mathbf{p}_X}{M_X}\right)$$

$$\mathbf{P}_f = \mathbf{p}_N + \mathbf{p}_X$$



The relative momentum is derived in a relativistic fashion

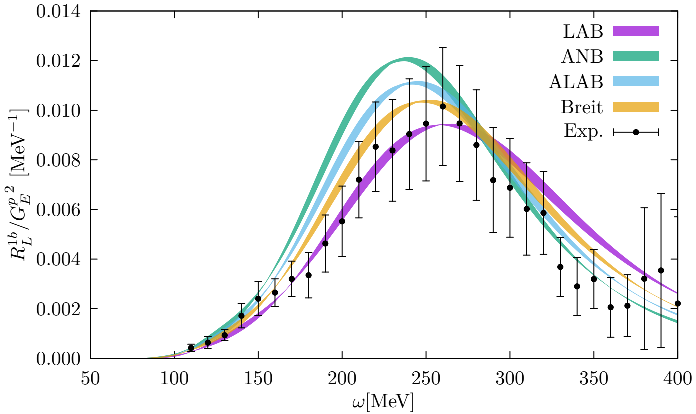
$$E_f = \sqrt{m^2 + [\mathbf{p}_f + (\mu/M_X)\mathbf{P}_f]^2} + \sqrt{M_X^2 + [\mathbf{p}_f - (\mu/m)\mathbf{P}_f]^2} \quad ; \quad E_f = \omega + E_i$$

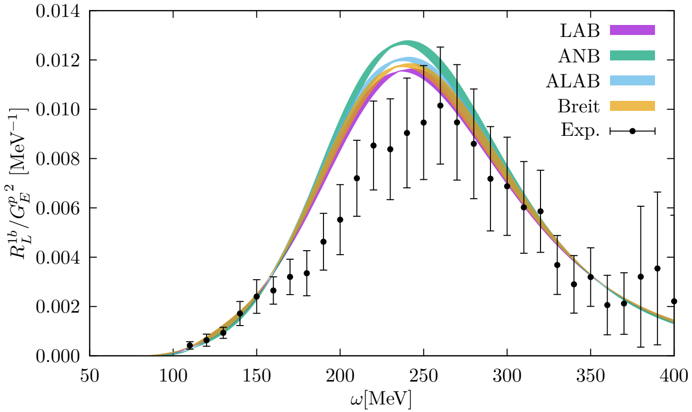
And it is used as input in the non relativistic kinetic energy

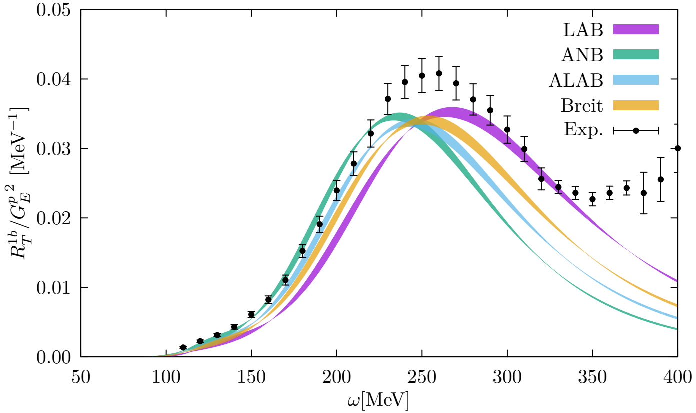
$$\epsilon_f = \frac{\mathbf{p}_f^2}{2\mu} + \epsilon_0^{A-1} \longleftrightarrow \delta(\omega - E_f(\epsilon_f) + E_0) = \left(\frac{\partial E_f(\epsilon_f)}{\partial \epsilon_f}\right)^{-1} \delta\left(\epsilon_f - \frac{\mathbf{p}_f^2}{2\mu} - \epsilon_0^{A-1}\right)$$

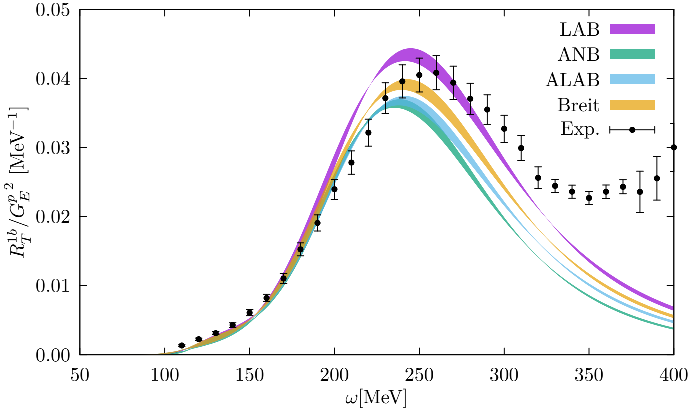
N. Rocco et al. PRC **97** 055501(2018)

TACKLE RELATIVISTIC EFFECTS

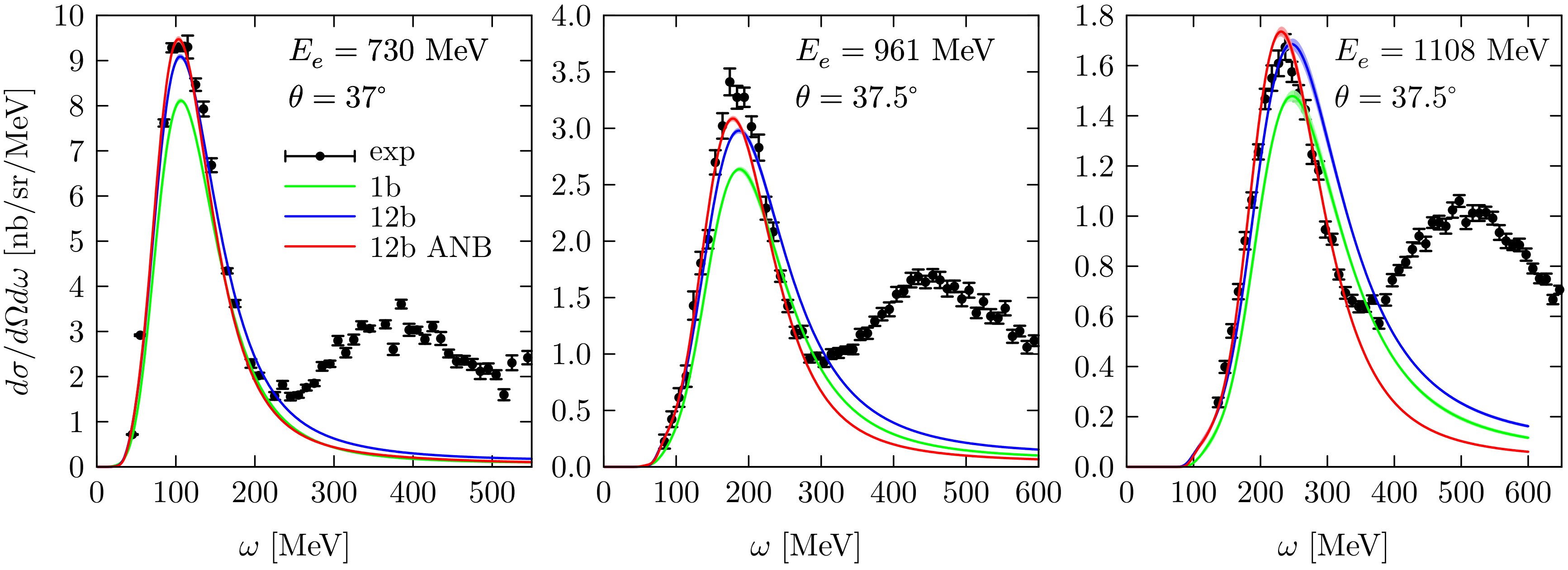






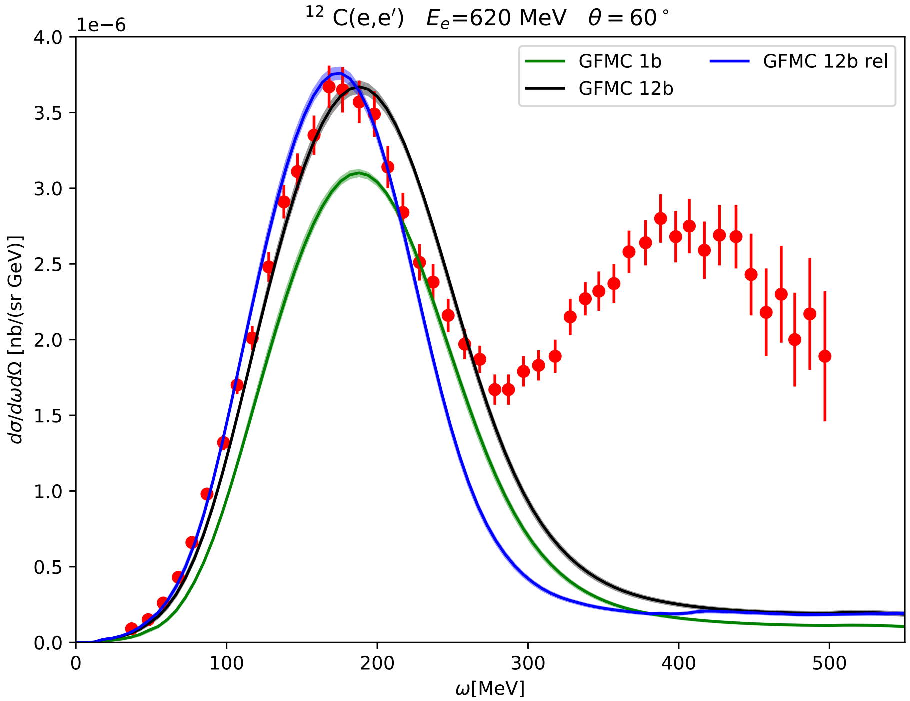


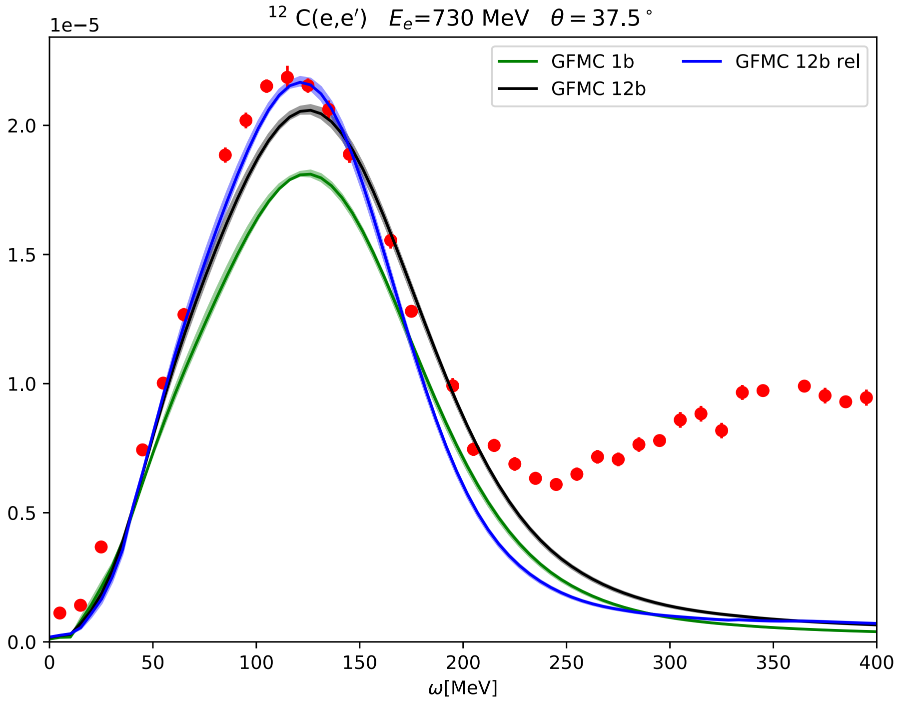
TACKLE RELATIVISTIC EFFECTS



*N. Rocco et al. PRC **97** 055501(2018)*

TACKLE RELATIVISTIC EFFECTS



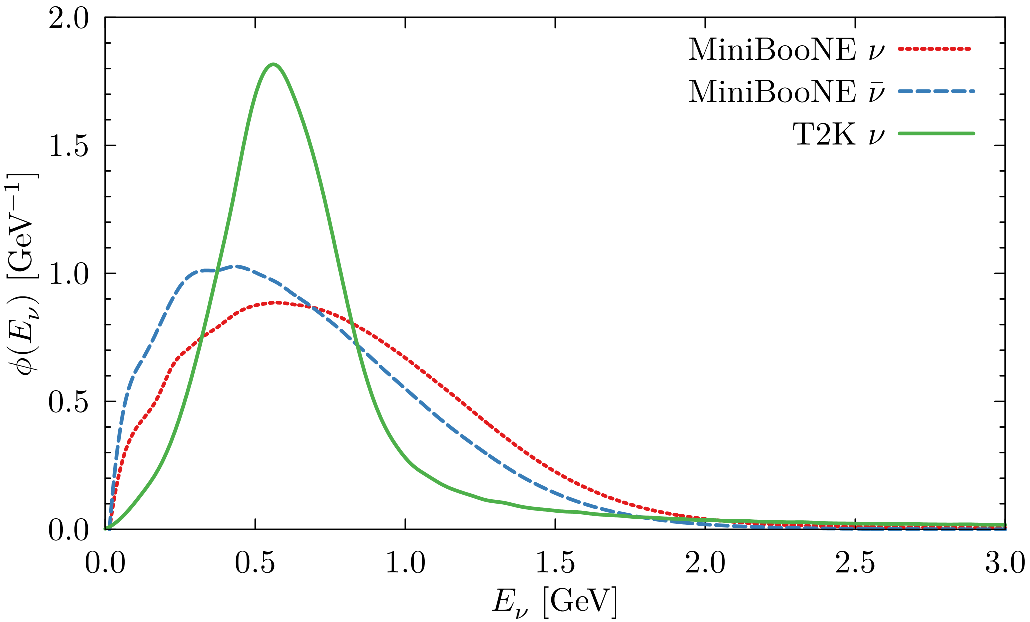


N. Rocco et al., submitted to Universe

^{12}C CHARGED-CURRENT CROSS SECTIONS

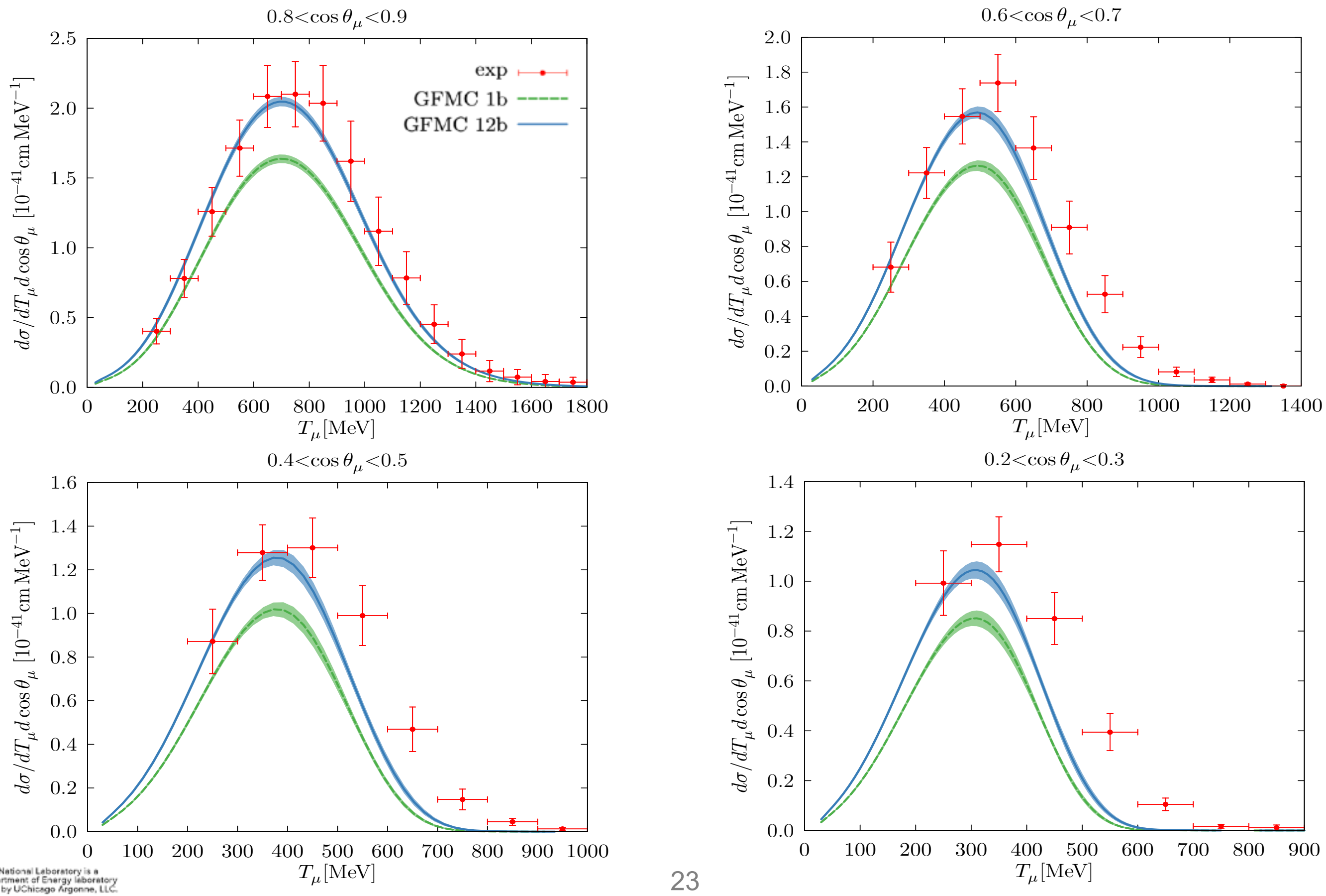
To obtain the inclusive cross section, we fold the MiniBooNE and T2K fluxes

$$\left\langle \frac{d\sigma}{dT_\mu\, d\cos\theta_\mu} \right\rangle = \int dE_\nu\, \phi(E_\nu)\, \frac{d\sigma(E_\nu)}{dT_\mu\, d\cos\theta_\mu} \ ,$$



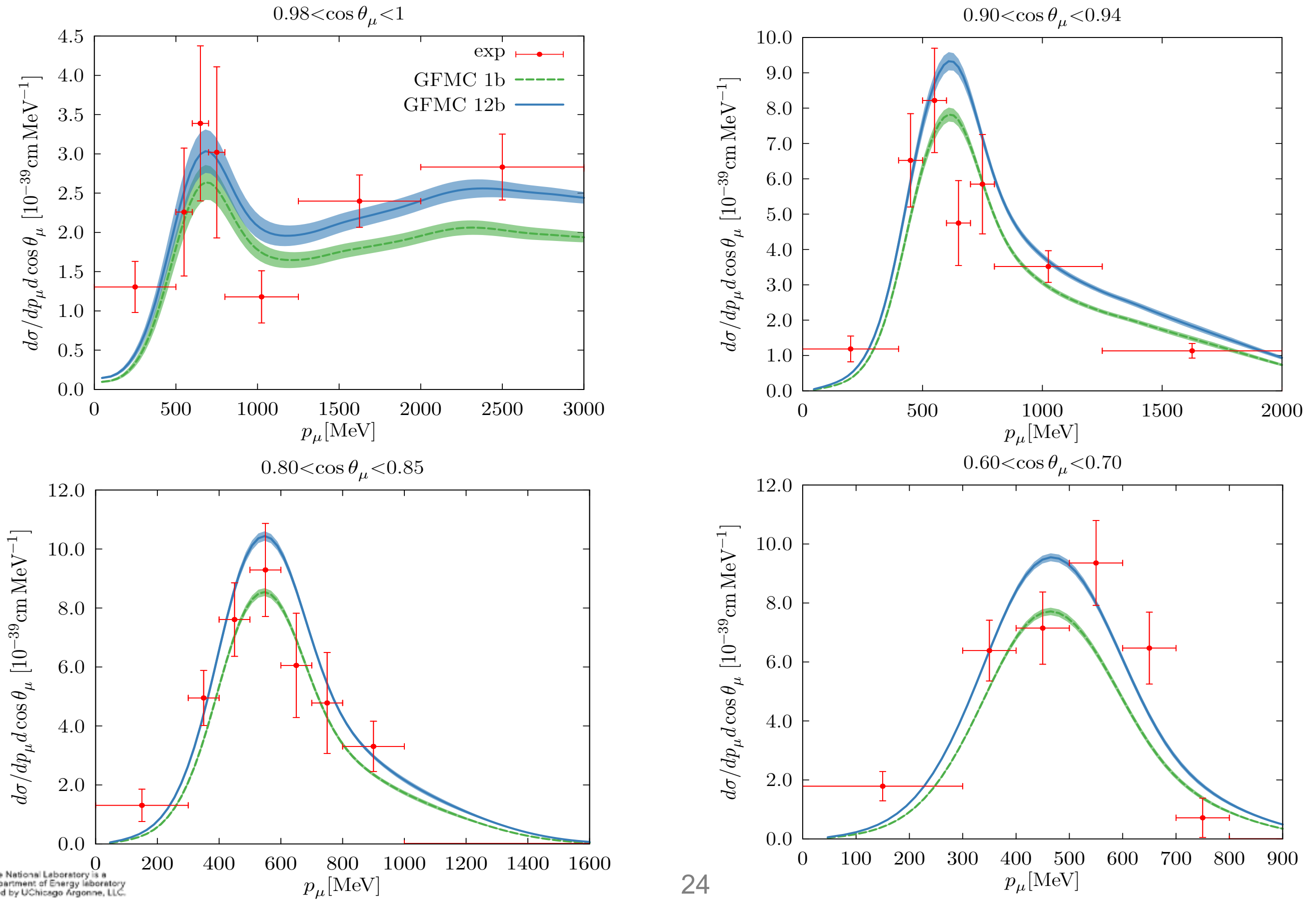
MINIBOONE CROSS SECTIONS

*AL et al., PRX **10**, 031068 (2020)*



T2K CROSS SECTIONS

*AL et al., PRX **10**, 031068 (2020)*



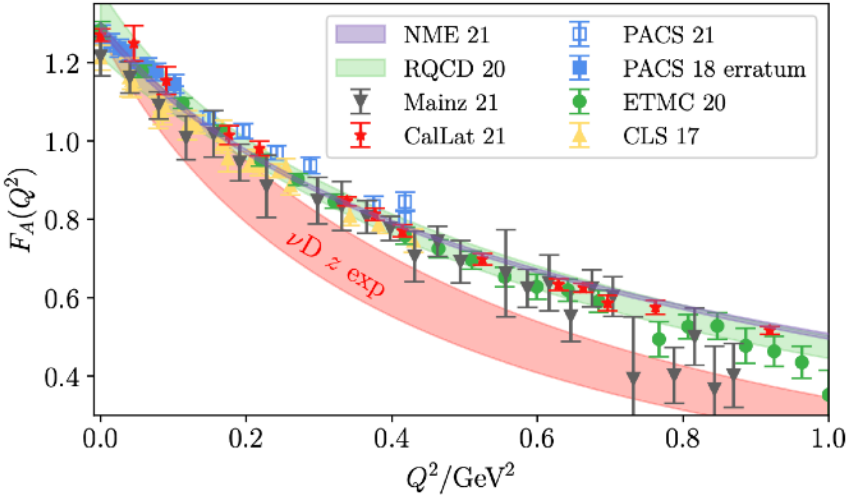
AXIAL FORM FACTOR

A precise knowledge of the **nucleon's axial-current form factors** is crucial for modeling neutrino-nucleus interactions;

Scarce (old) experimental data available

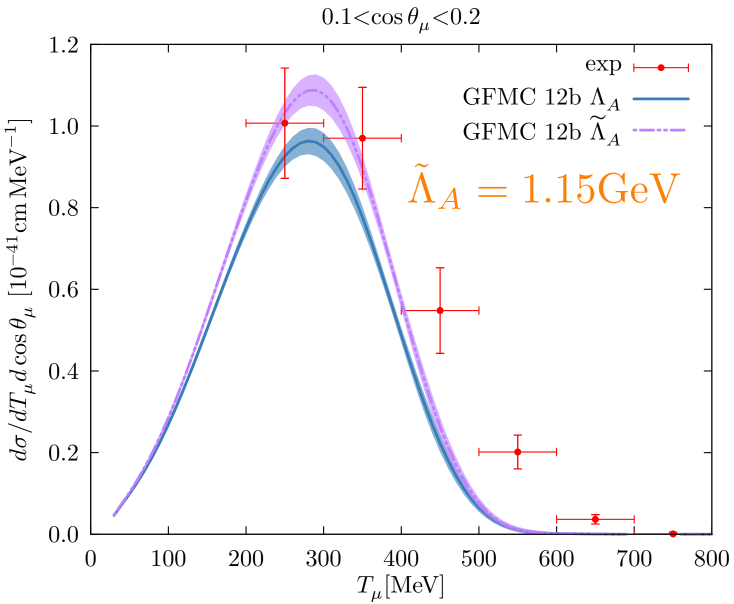
↕

Lattice-QCD calculations are essential



A. Meyer et al., arXiv:2201.01839

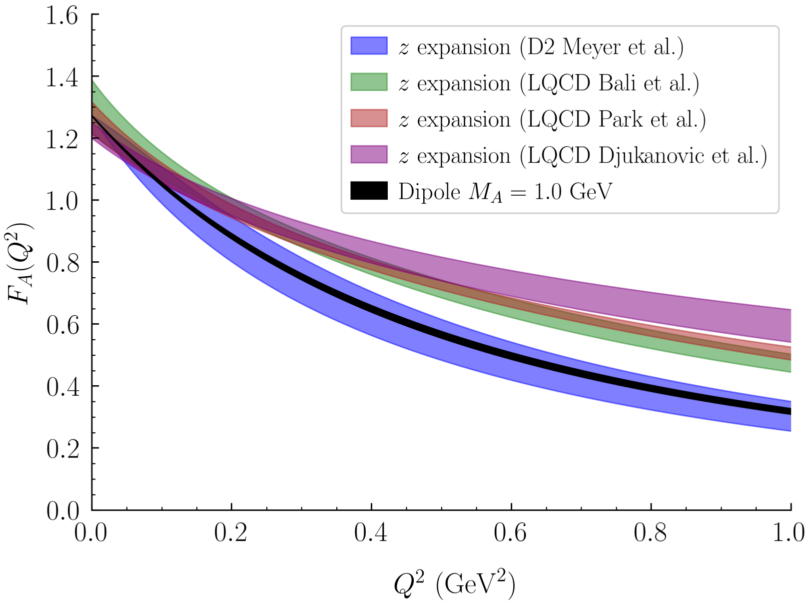
We have considered a value of the axial mass more in line with recent LQCD determinations



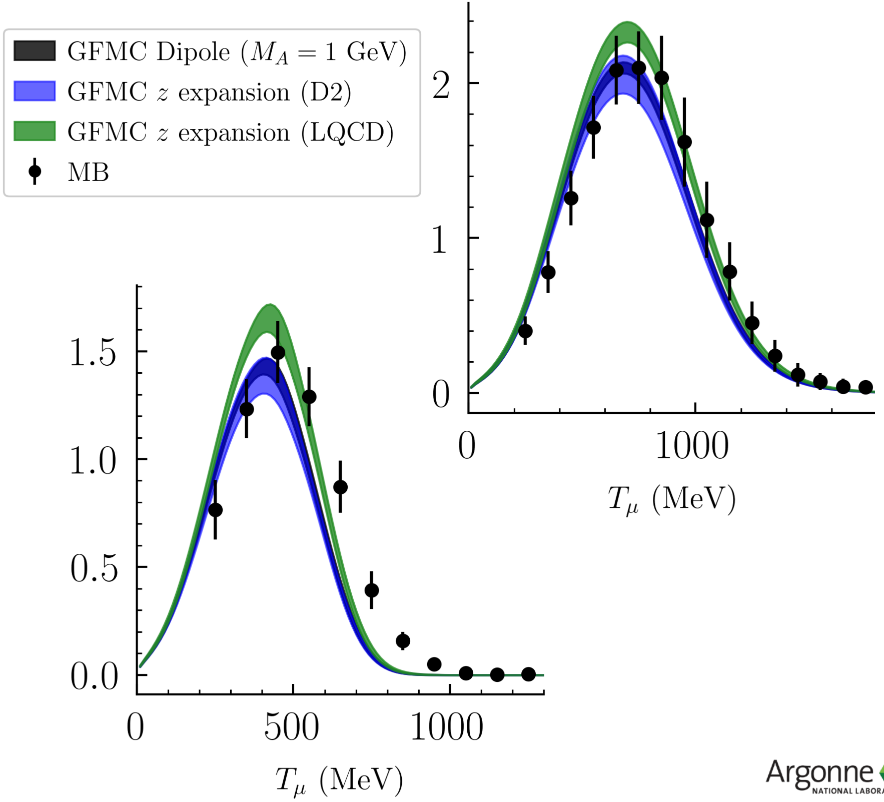
*AL et al., PRX **10**, 031068 (2020)*

AXIAL FORM FACTOR, CAREFUL ANALYSIS

We employed z-expansion parameterizations of axial form factors, consistent with experimental or LQCD data



D. Simons, et al, arXiv:2210.02455



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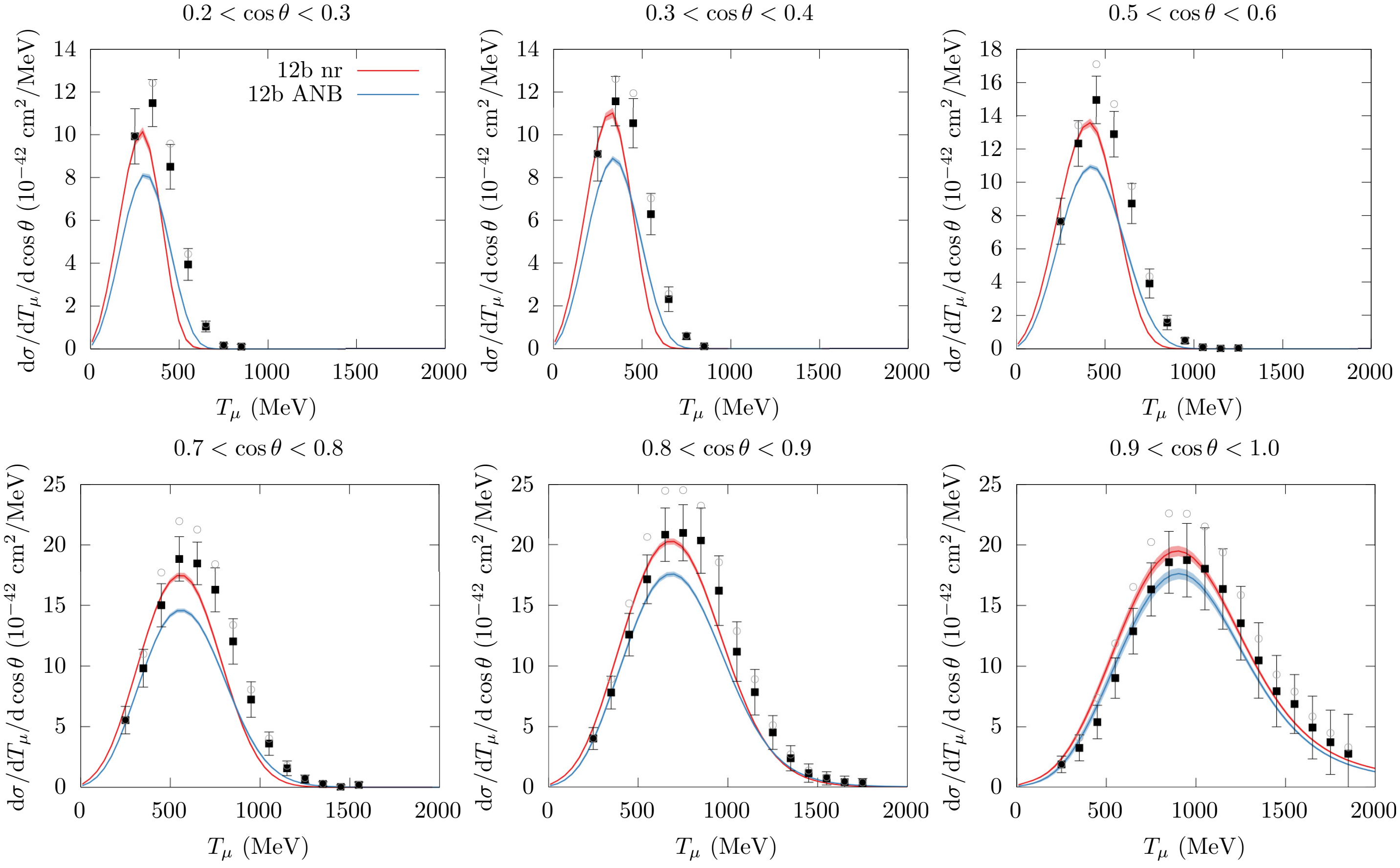
RELATIVISTIC EFFECTS

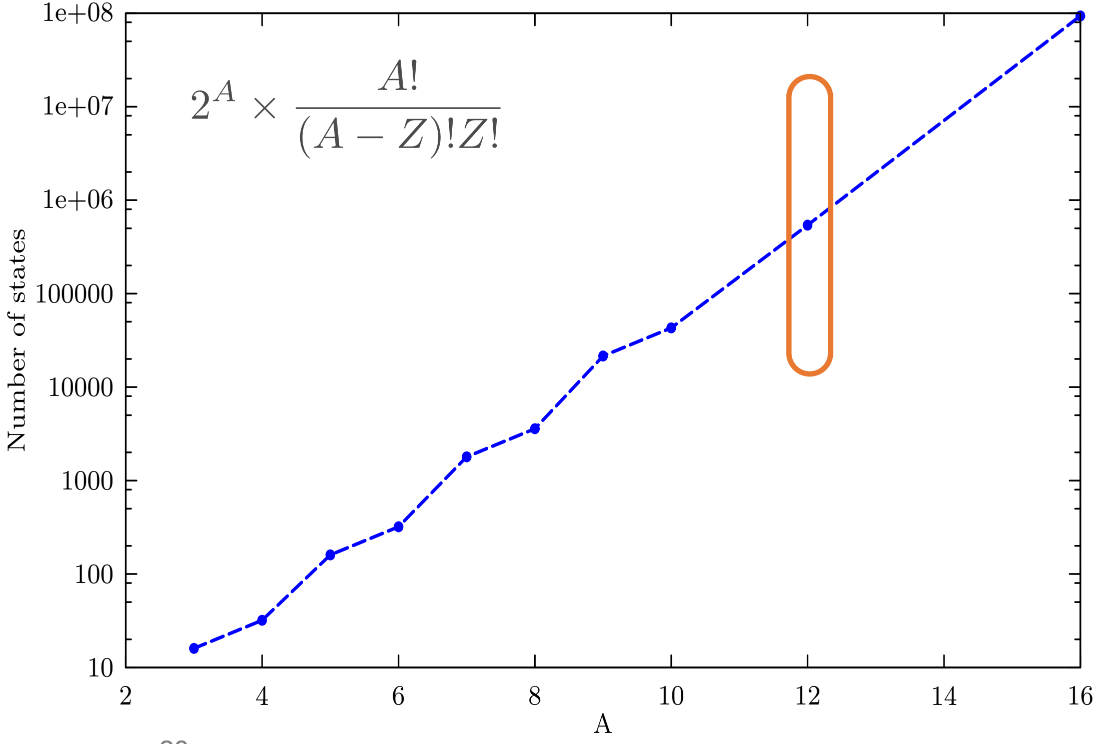
A. Nikolakopoulos, AL, N. Rocco, arXiv:2304.11772



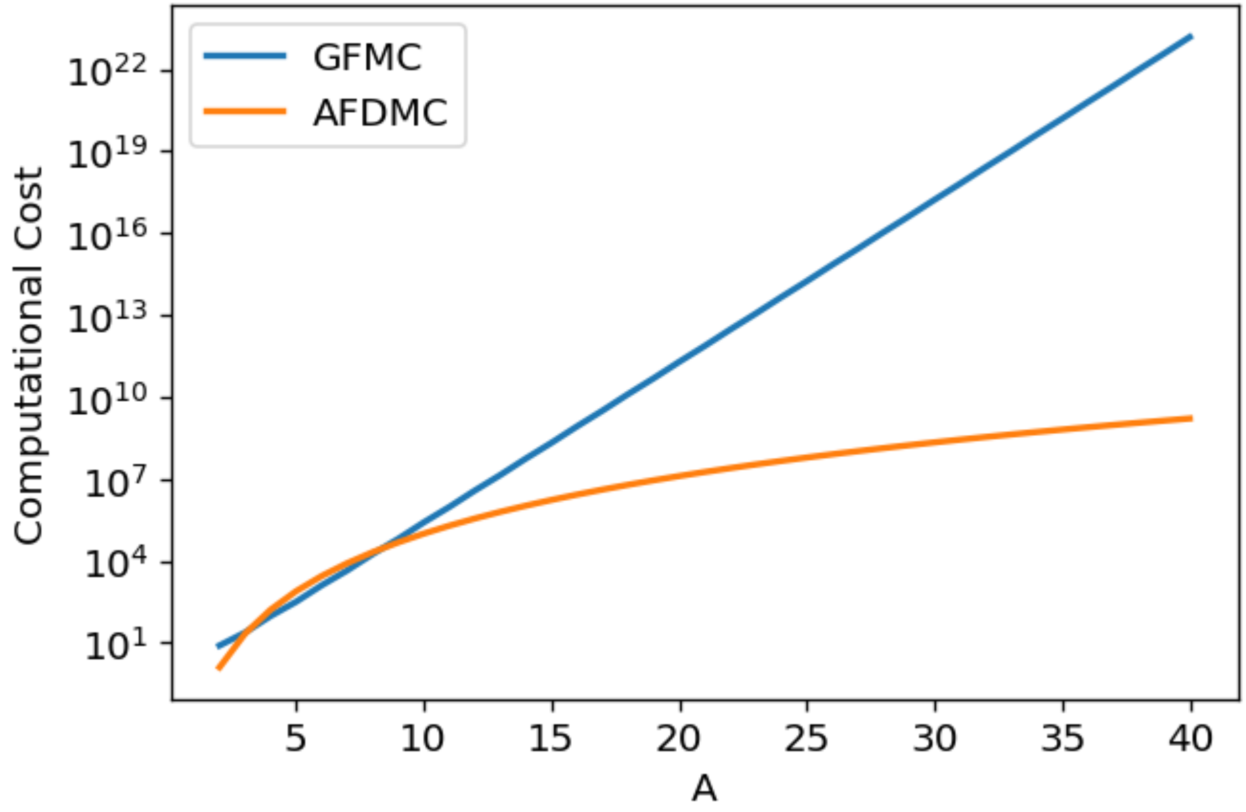
EXPONENTIAL SCALING

Green's function Monte Carlo uses all spin-isospin components of the wave function

$$|S\rangle = \begin{pmatrix} s_{\uparrow\uparrow\uparrow} \\ s_{\uparrow\uparrow\downarrow} \\ s_{\uparrow\downarrow\uparrow} \\ s_{\uparrow\downarrow\downarrow} \\ s_{\downarrow\uparrow\uparrow} \\ s_{\downarrow\uparrow\downarrow} \\ s_{\downarrow\downarrow\uparrow} \\ s_{\downarrow\downarrow\downarrow} \end{pmatrix}$$



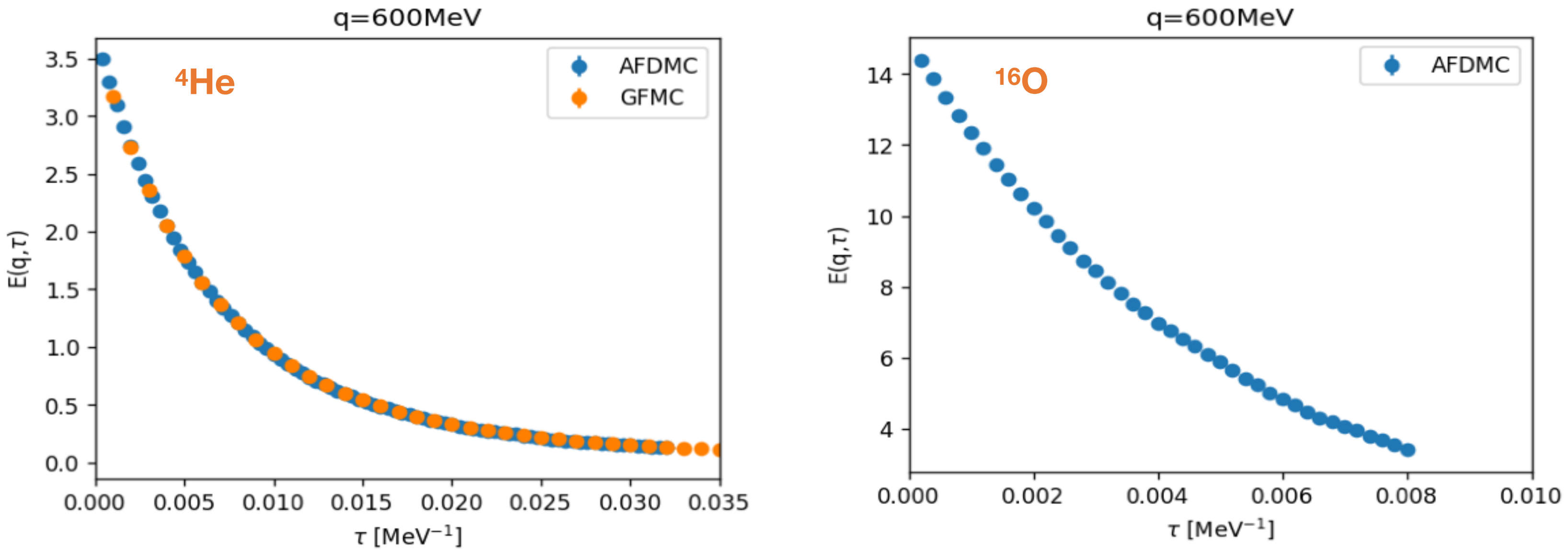
HOW TO TACKLE LARGER NUCLEI?



BEYOND ^{12}C: AFDMC AND MACHINE LEARNING

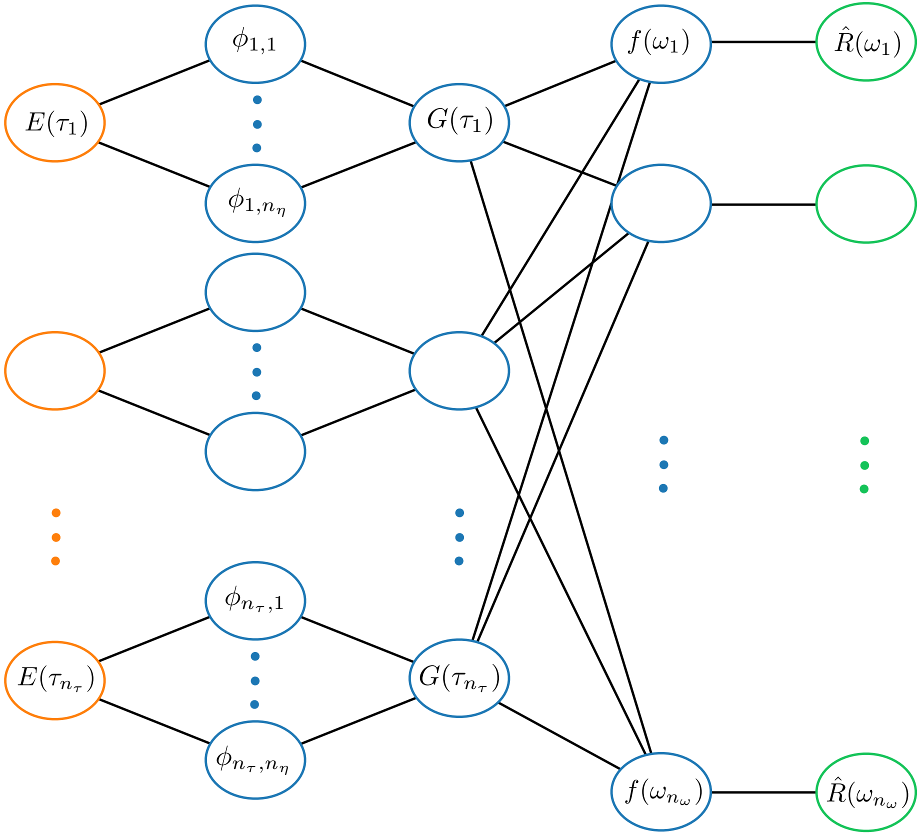
The auxiliary-field diffusion Monte Carlo method can treat ^{16}O sampling the spin-isospin

We developed the AFDMC to allow for the calculation of Euclidean response functions



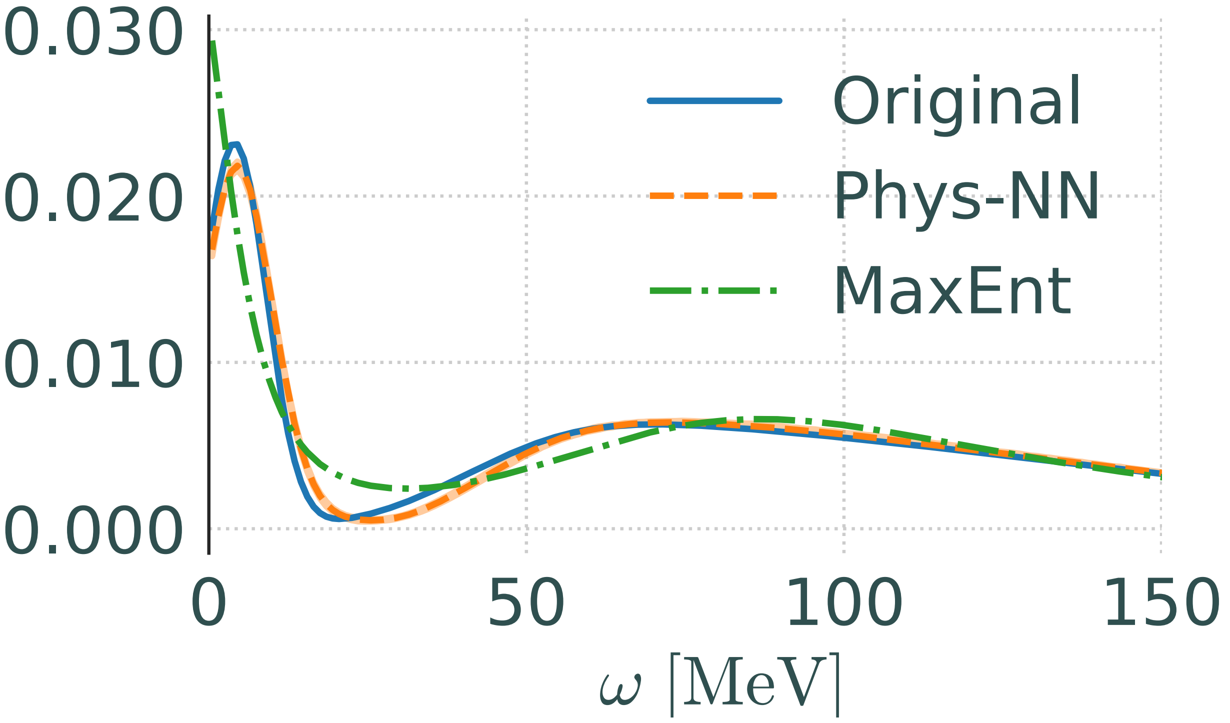
N. Rocco, AL et al., in preparation

BEYOND ^{12}C: AFDMC AND MACHINE LEARNING



*K. Raghavan, AL, al., PRC **103**, 035502 (2021)*

BEYOND ^{12}C: AFDMC AND MACHINE LEARNING

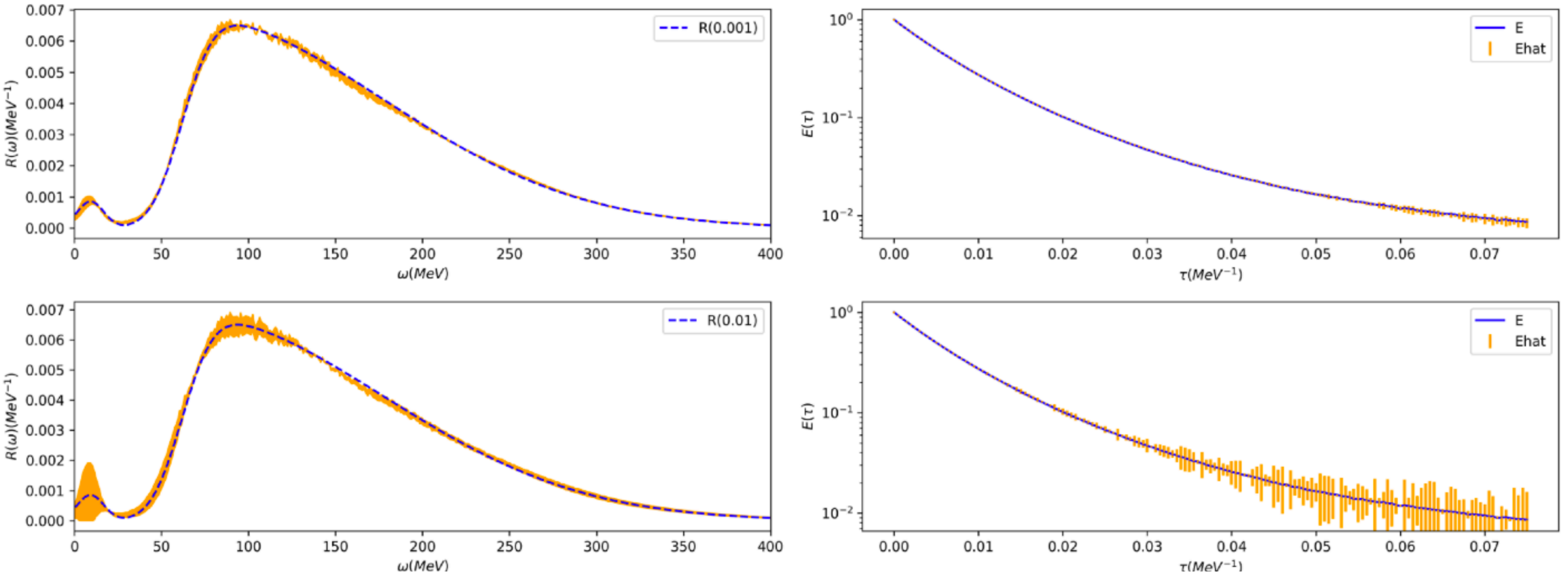


*K. Raghavan, AL, al., PRC **103**, 035502 (2021)*

BEYOND ^{12}C: AFDMC AND MACHINE LEARNING

We developed an artificial-neural network approach suitable to invert the Laplace transform that:

- Provides robust estimates of the uncertainty of the inversion;



K. Raghavan, AL, in preparation)

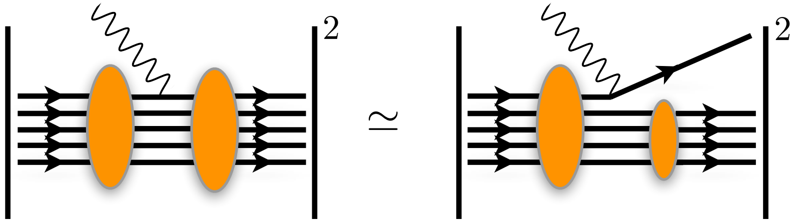
FACTORIZATION SCHEME

At large momentum transfer, the scattering reduces to the sum of individual terms

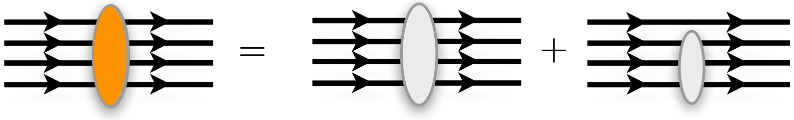
$$J^\mu \to \sum_i j_i^\mu \qquad |\psi_f^A\rangle \to |p\rangle \otimes |\psi_f^{A-1}\rangle \qquad E_f = E_f^{A-1} + e(\mathbf{p})$$

The incoherent contribution of the one-body response reads

$$R_{\alpha\beta} \simeq \int \frac{d^3k}{(2\pi)^3} dE P_h(\mathbf{k}, E) \sum_i \langle k | {j_\alpha^i}^\dagger | k+q \rangle \langle k+q | j_\beta^i | k \rangle \delta(\omega + E - e(\mathbf{k}+\mathbf{q}))$$



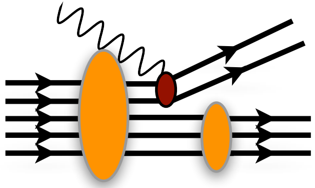
We include excitations of the A-1 final state with two nucleons in the continuum



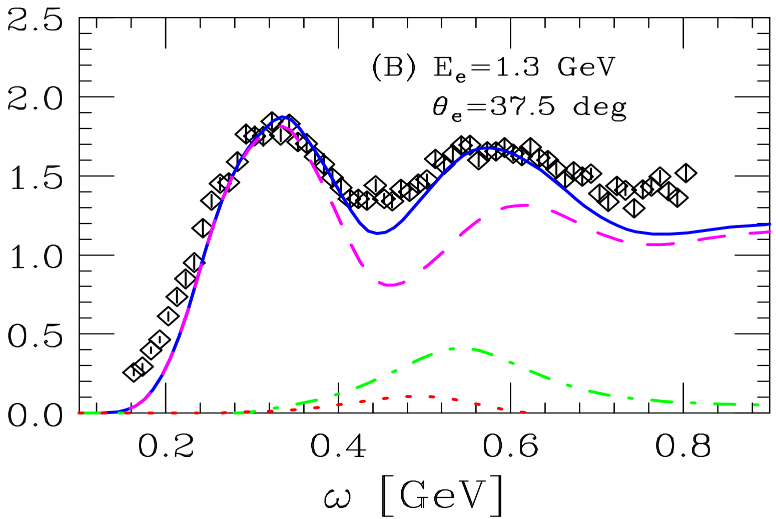
EXTENDED FACTORIZATION SCHEME

Using relativistic MEC requires extending the factorization scheme to two-nucleon emissions

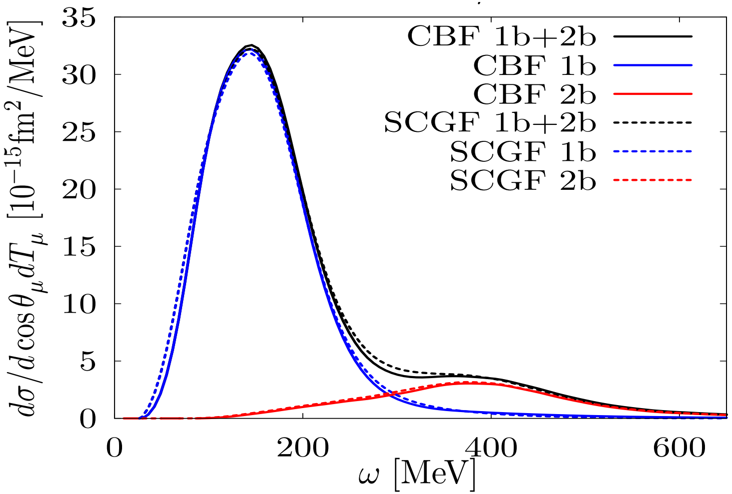
$$|\Psi_f^A\rangle \to |p_1 p_2\rangle \otimes |\Psi_f^{A-2}\rangle$$



We compute electron and neutrino inclusive cross sections using CBF and SCGF spectral functions



N. Rocco, et al. PRL. **116** 192501 (2016)

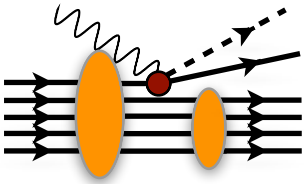


N. Rocco, et al. PRC **99** 025502 (2019)

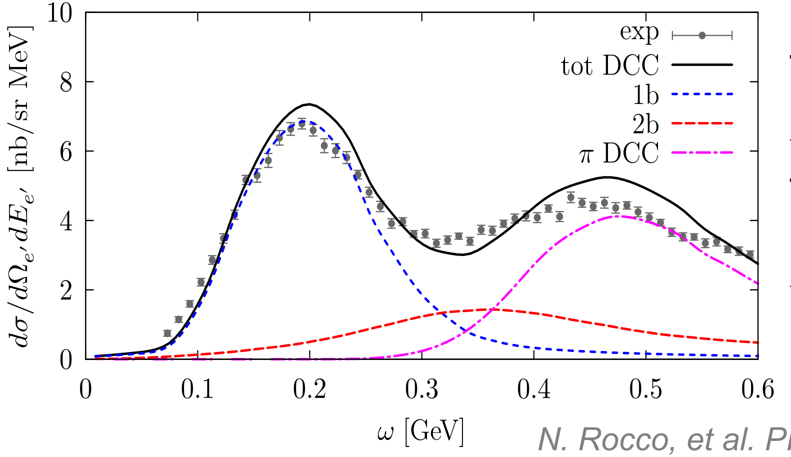
EXTENDED FACTORIZATION SCHEME

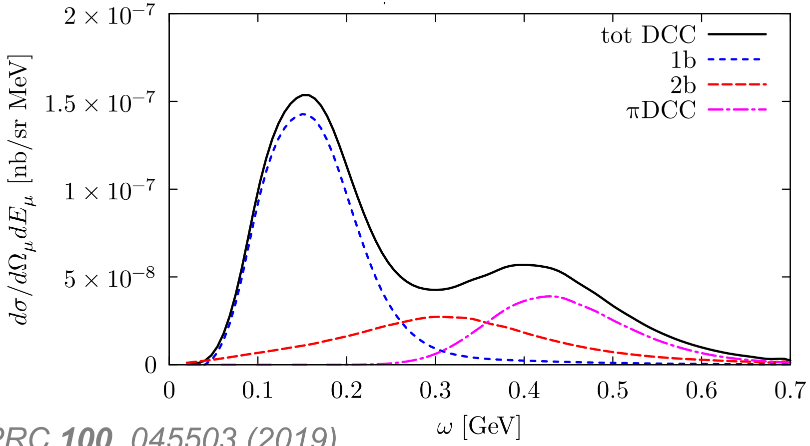
The factorization scheme can be further extended to include real pions in the final state

$$|\Psi_f^A\rangle \rightarrow |p_1, p_\pi\rangle \otimes |\Psi_f^{A-1}\rangle$$



The DCC model, suitable to accurately describe single-nucleon pion-production, is folded with a realistic spectral function





*N. Rocco, et al. PRC **100**, 045503 (2019)*

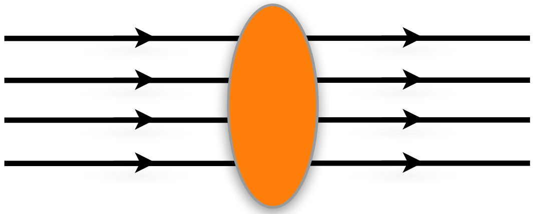
QMC-BASED SPECTRAL FUNCTION

The hole spectral function is a sum of two contributions

$$P_h(\mathbf{k},E)=\sum_n |\langle\Psi_0^A|[|k\rangle\times|\Psi_n^{A-1}\rangle]|^2\delta(E+E_0^A-E_n^{A-1})=P_h^{MF}(\mathbf{k},E)+P_h^{corr}(\mathbf{k},E)$$

Mean-field component

$$|\bar{\Psi}_n^{A-1}\rangle =$$



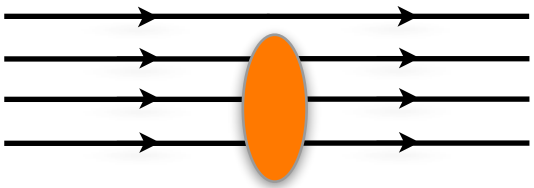
$$P_h^{MF}(\mathbf{k},E)=\sum_n |\langle\Psi_0^A|[|k\rangle\times|\bar{\Psi}_n^{A-1}\rangle]|^2$$

$$\times\,\delta\left(E-B_0^A+B_n^{A-1}-\frac{k^2}{2M^{A-1}}\right)$$

Computed using VMC spectroscopic overlaps

Correlation component

$$|k'\rangle\times|\Psi_0^{A-2}\rangle =$$



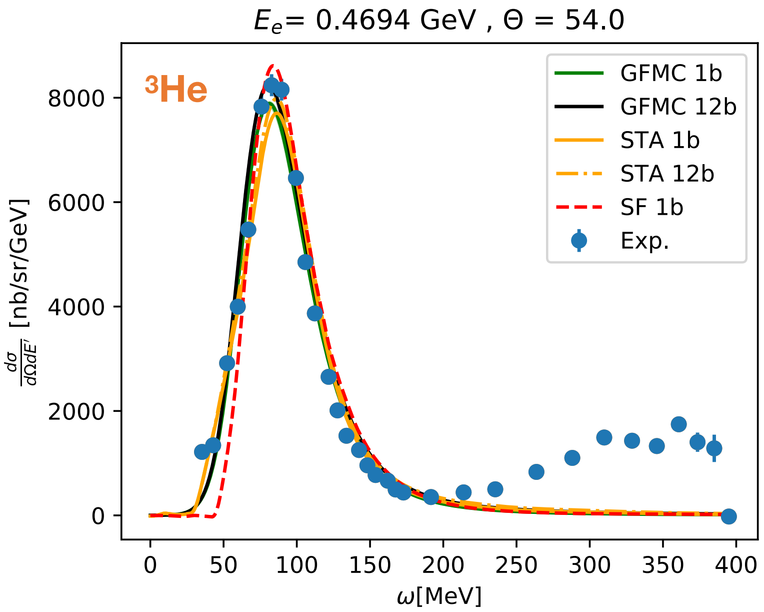
$$P_h^{corr}(\mathbf{k},E)\simeq\sum_{k'} |\langle\Psi_0^A|[|kk'\rangle\times|\bar{\Psi}_0^{A-2}\rangle]|^2$$

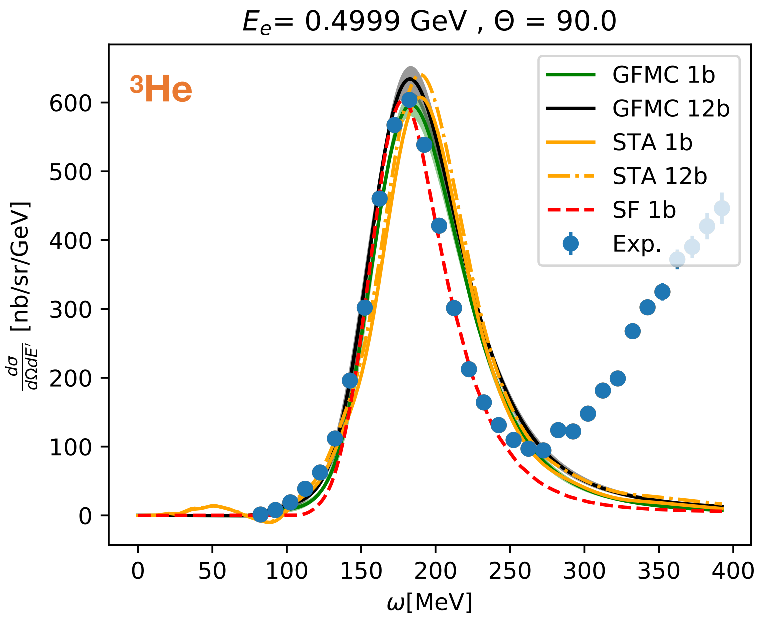
$$\times\,\delta\left(E-B_0^A-e(k')+B_0^{A-2}-\frac{(\mathbf{k}+\mathbf{k}')^2}{2M^{A-2}}\right)$$

Computed from the short-range contributions of VMC two-body momentum distributions

QMC-BASED SPECTRAL FUNCTION

We compare the inclusive electron-^{3}He cross section obtained with the QMC spectral functions and those computed within the GFMC and STA approaches

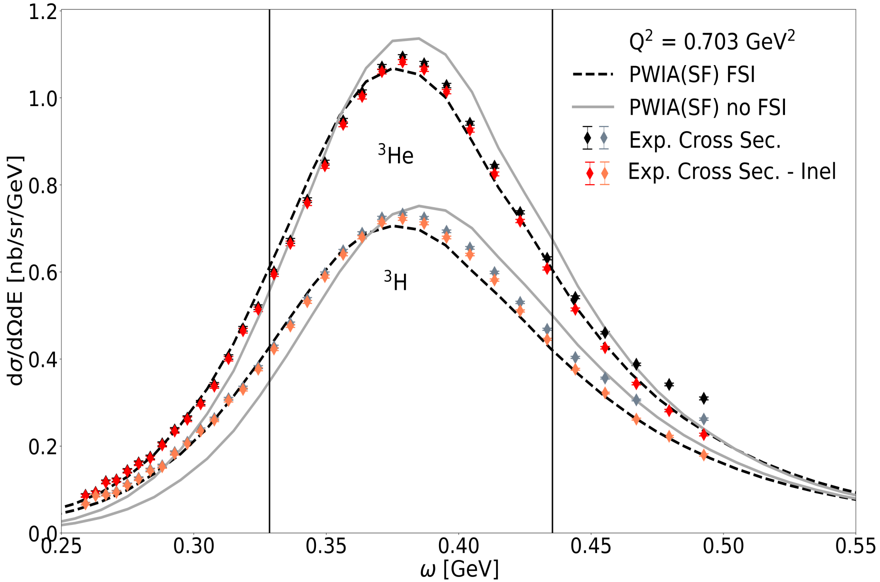


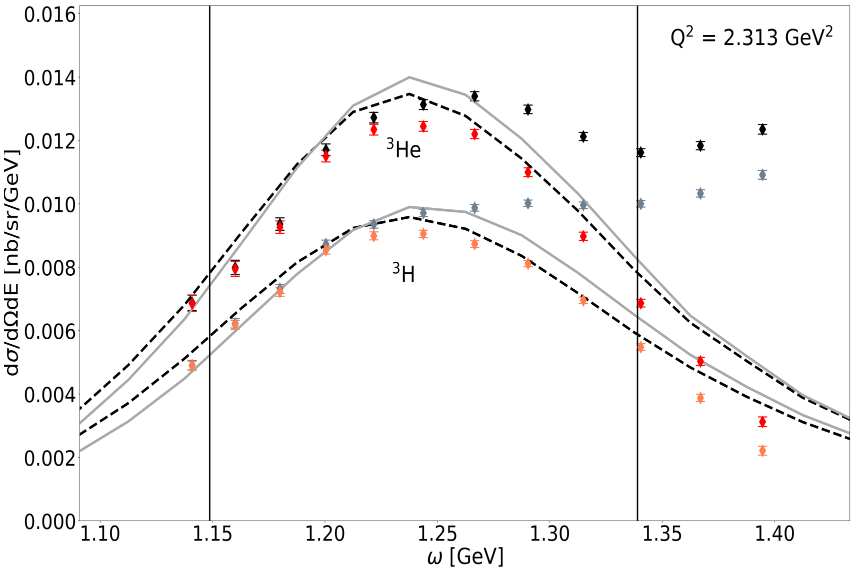


*L. Andreoli, AL, et al. PRC **105**, 014002 (2022)*

QMC-BASED SPECTRAL FUNCTION

The QMC-BASED spectral function has aided a novel measurement of the neutron magnetic form factor from A=3 mirror nuclei





S.N. Santiesteban et al. 2304.13770 [nucl-ex]

QMC-BASED SPECTRAL FUNCTION

Using a similar strategy, we obtained the mean-field spectral function of ^{12}C

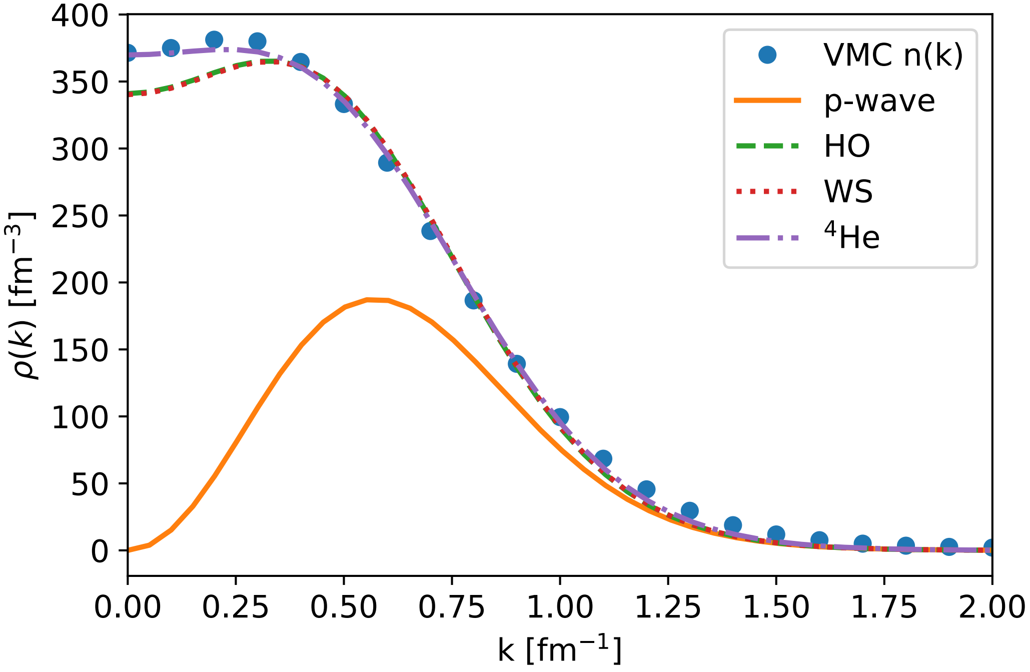
- p-shell overlaps: computed by Fourier transforming VMC radial overlaps

$$^{12}\mathrm{C}(0^+) \to ^{11}\mathrm{B}(3/2^-) + p$$
$$^{12}\mathrm{C}(0^+) \to ^{11}\mathrm{B}(1/2^-) + p$$
$$^{12}\mathrm{C}(0^+) \to ^{11}\mathrm{B}(3/2^-)^* + p\,.$$

- s-shell overlaps: rescaling the strength of the transition

$$^{4}\mathrm{He}(0^+) \to ^{3}\mathrm{H}(1/2^+) + p$$

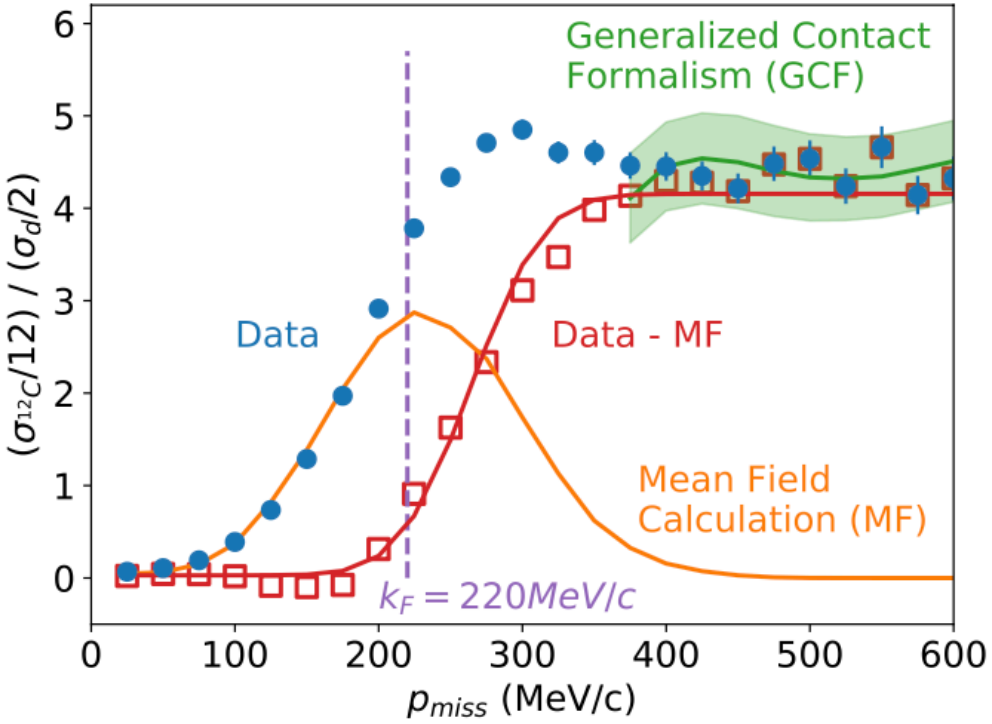
to reproduce the VMC momentum distribution at low momenta



I. Korover, et al Phys.Rev.C ***107*** *(2023) 6, L061301*

QMC-BASED SPECTRAL FUNCTION

This mean-field spectral function automatically includes the quenching of the spectroscopic factors



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CONCLUSIONS

Lepton-nucleus scattering from quantum Monte Carlo

- Validated our approach on electron-^{12}C scattering, including relativistic corrections
- Two-body currents enhance electromagnetic and charged-current responses
- Good agreement with MiniBooNE and T2K inclusive data → First ab-initio results!
- Use the AFDMC and ML methods to reach ^{16}O (and beyond)

Extended factorization scheme

- Two-body currents and pion-production are essential to reproduce electron-scattering data
- Pion production improves agreement with data, need to include DIS
- Used VMC to construct an “ab initio” spectral function

THANK YOU