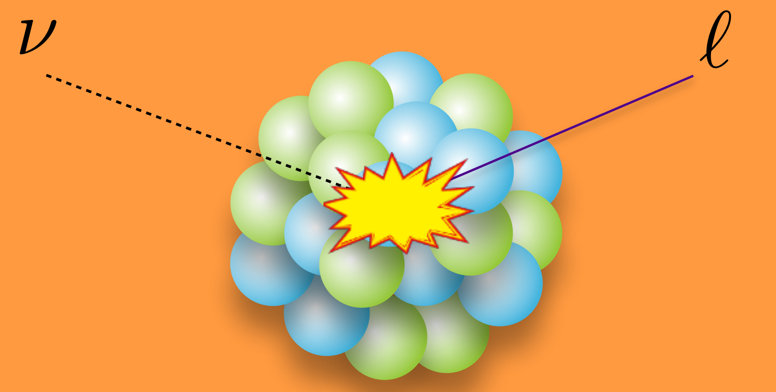
LEPTON-NUCLEUS SCATTERING WITHIN QUANTUM MONTE CARLO APPROACHES



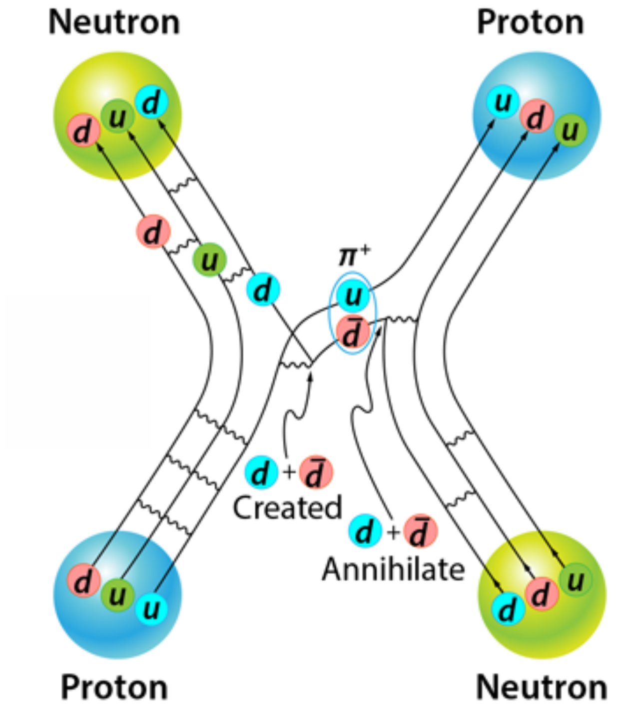
ALESSANDRO LOVATO

Argonne NATIONAL LABORATORY

MITP Scientific Program:
Neutrino-Nucleus Interactions in the Standard Model and Beyond

May 15, 2025

“AB-INITIO” NUCLEAR THEORY



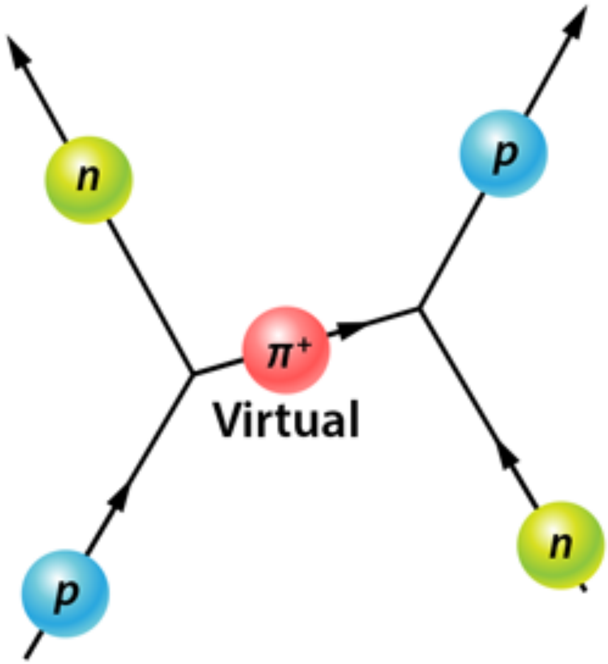
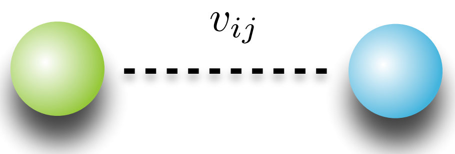


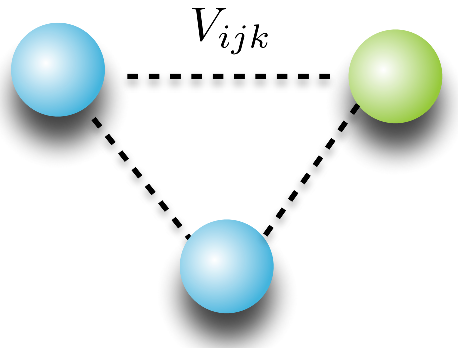
Illustration by APS / Alan Stonebraker

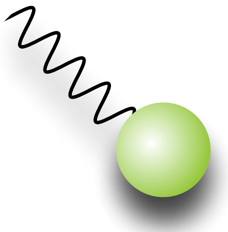
CONSISTENT HAMILTONIAN AND CURRENTS

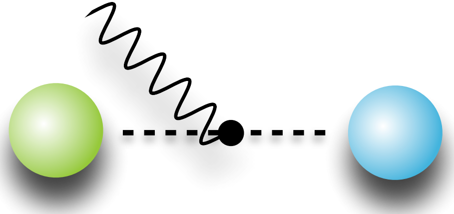
$$H = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

$$J = \sum_i j_i + \sum_{i<j} j_{ij}$$



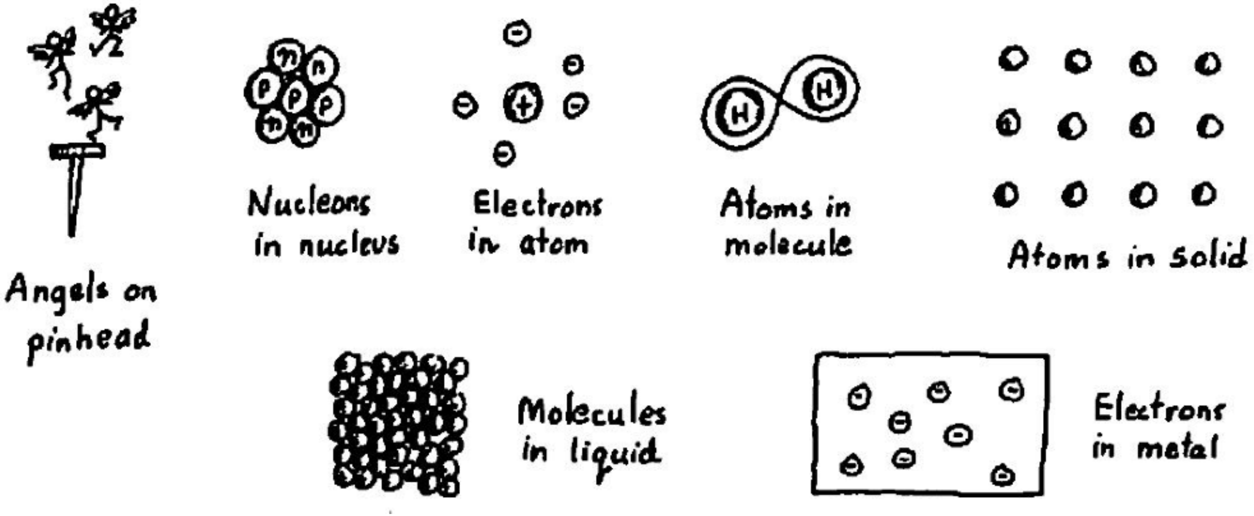






THE QUANTUM MANY-BODY PROBLEM

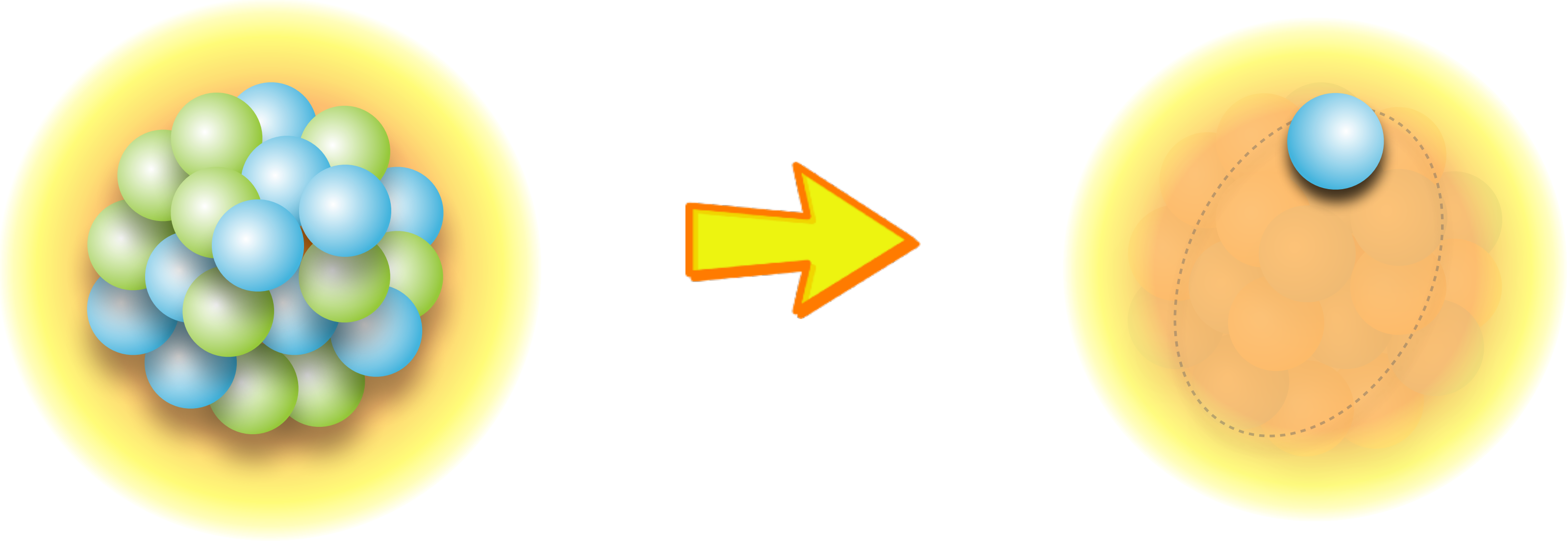
$$H\,|\Psi_n\rangle = E_n\,|\Psi_n\rangle \qquad\qquad M_{mn} = \langle\Psi_m|\,J\,|\Psi_n\rangle$$



A guide to Feynman diagrams in the many-body problem

THE MEAN-FIELD APPROXIMATION

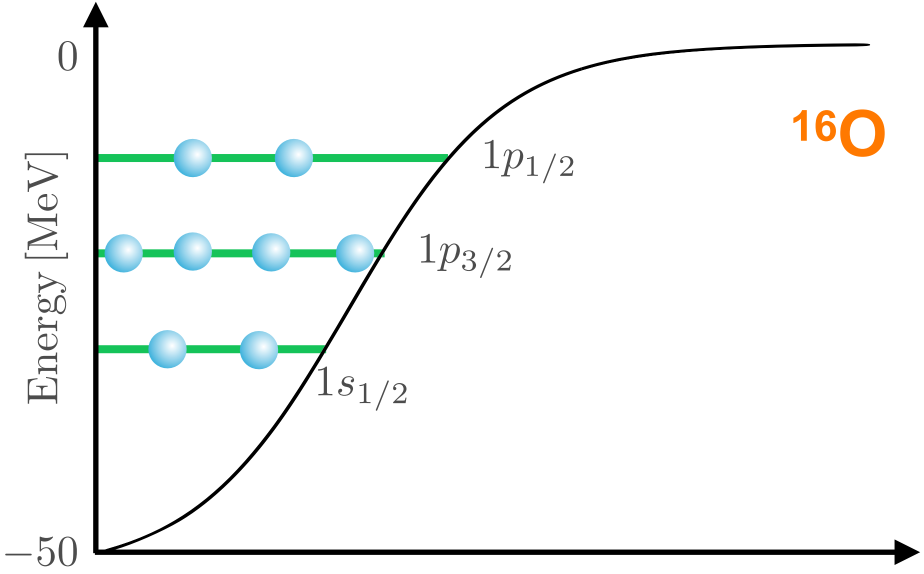
Mean field: nucleons are independent particles subject to an average nuclear potential



$$\sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk} \longrightarrow \sum_{i} U_i$$

THE MEAN-FIELD APPROXIMATION

The mean-field ground-state wave function is a Slater determinant

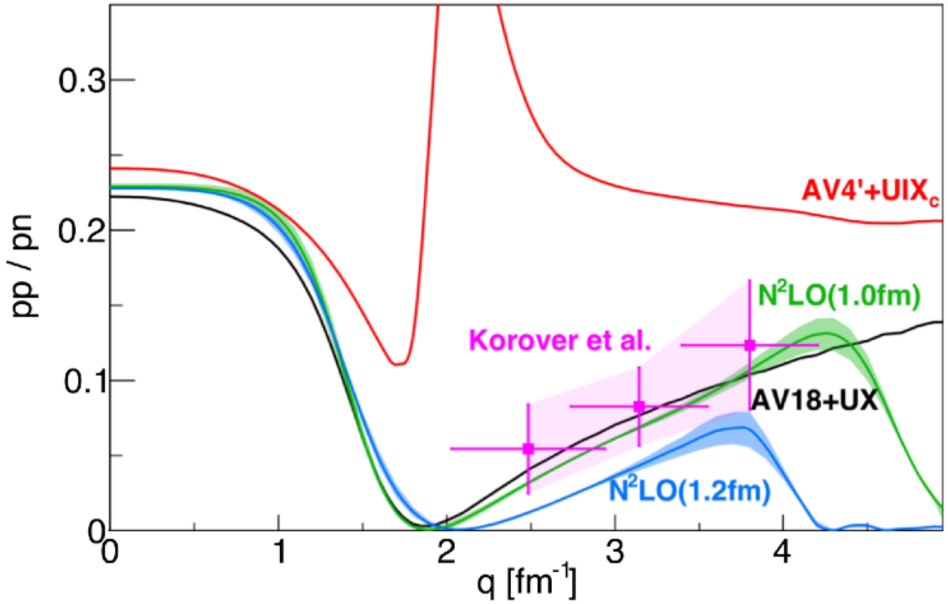


$$\Phi_0(x_1, \ldots, x_A) = \mathcal{A}[\phi_{n_1}(x_1) \ldots \phi_{n_A}(x_A)]$$

QUANTUM MONTE CARLO METHODS

Continuum nuclear QMC uses a coordinate-space representation of many-body wave functions.

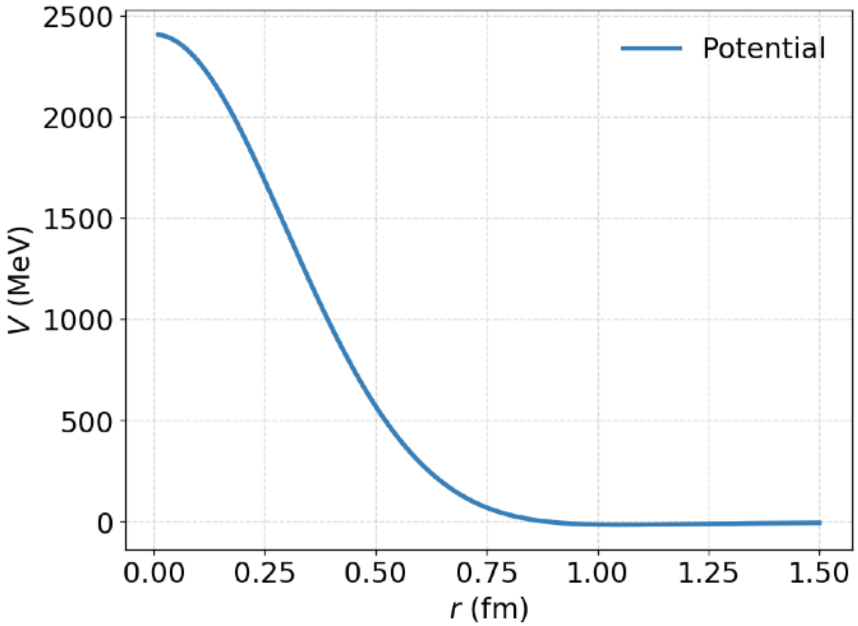
- No difficulties in treating high-resolution nuclear forces
- Access to high-momentum components of the nuclear wave functions;
- Limited to relatively light nuclear systems

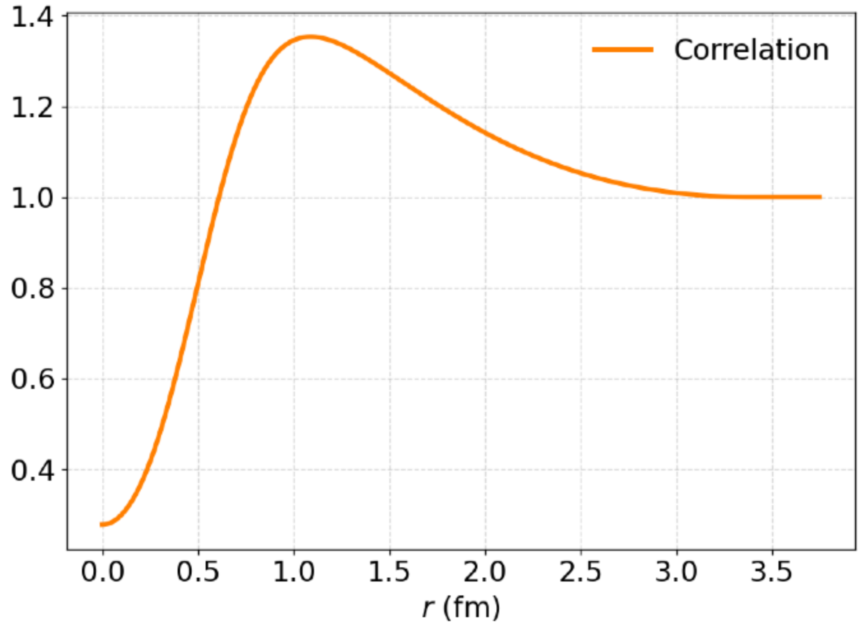


R. Cruz-Torres et al., Nature Phys. ***17*** *(2021) 3, 306*

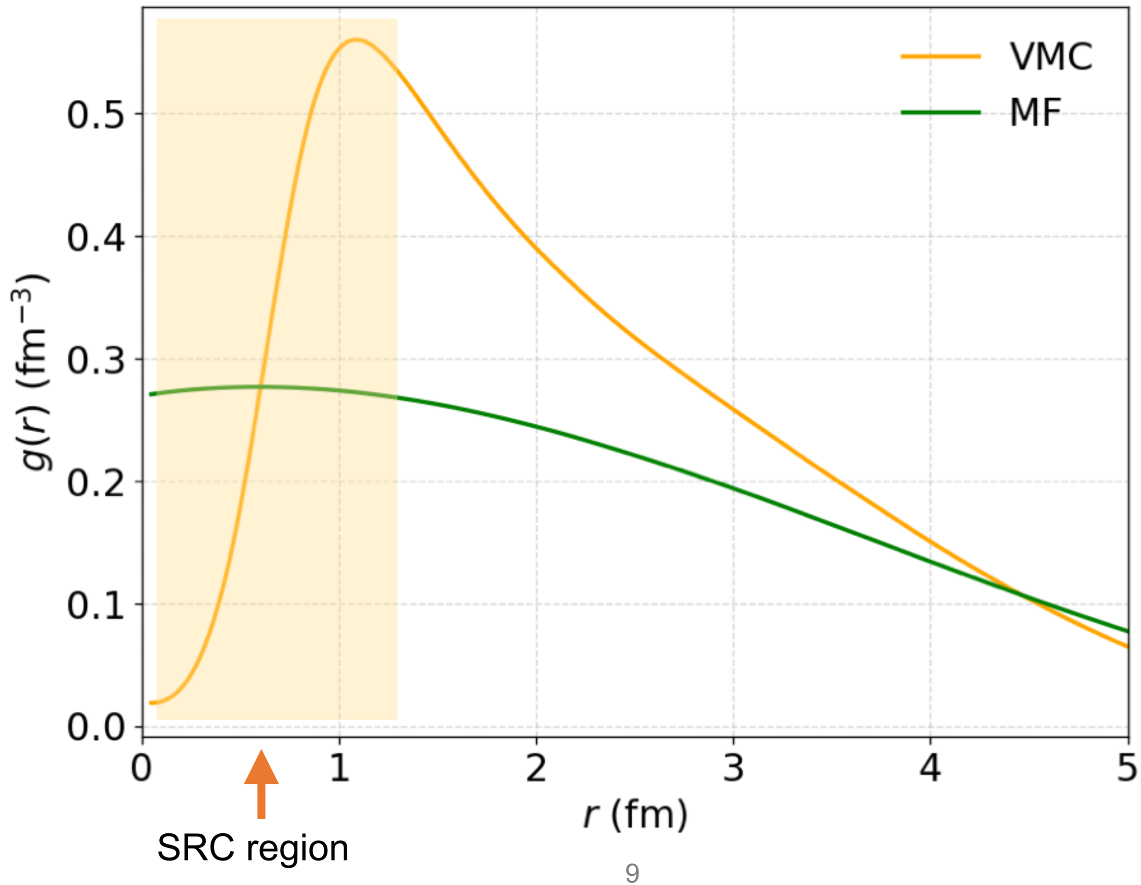
VARIATIONAL MONTE CARLO

$$|\Psi_V\rangle = \Big(1 + \sum_{ijk} F_{ijk}\Big)\Big(\mathcal{S}\prod_{i<j} F_{ij}\Big)|\Phi_{\mathrm{MF}}\rangle \quad \longleftrightarrow \quad E_V \equiv \frac{\langle\Psi_V|H|\Psi_V\rangle}{\langle\Psi_V|\Psi_V\rangle} > E_0$$





VARIATIONAL MONTE CARLO

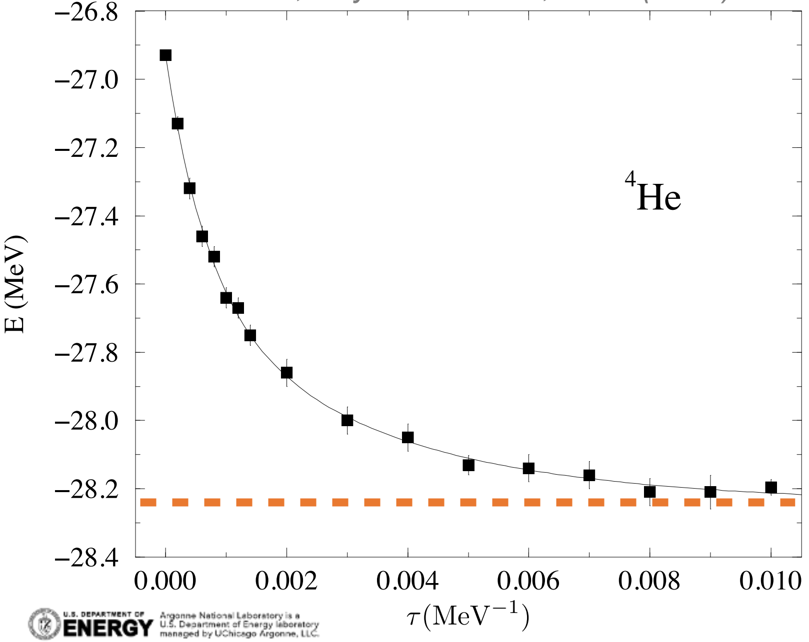


DIFFUSION MONTE CARLO

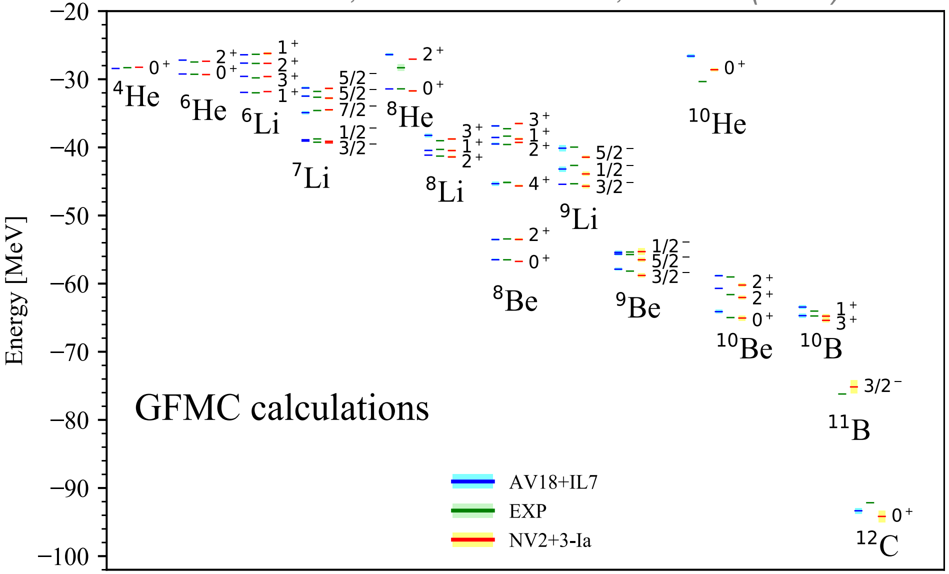
DMC methods project out the ground-state using an imaginary-time propagation

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

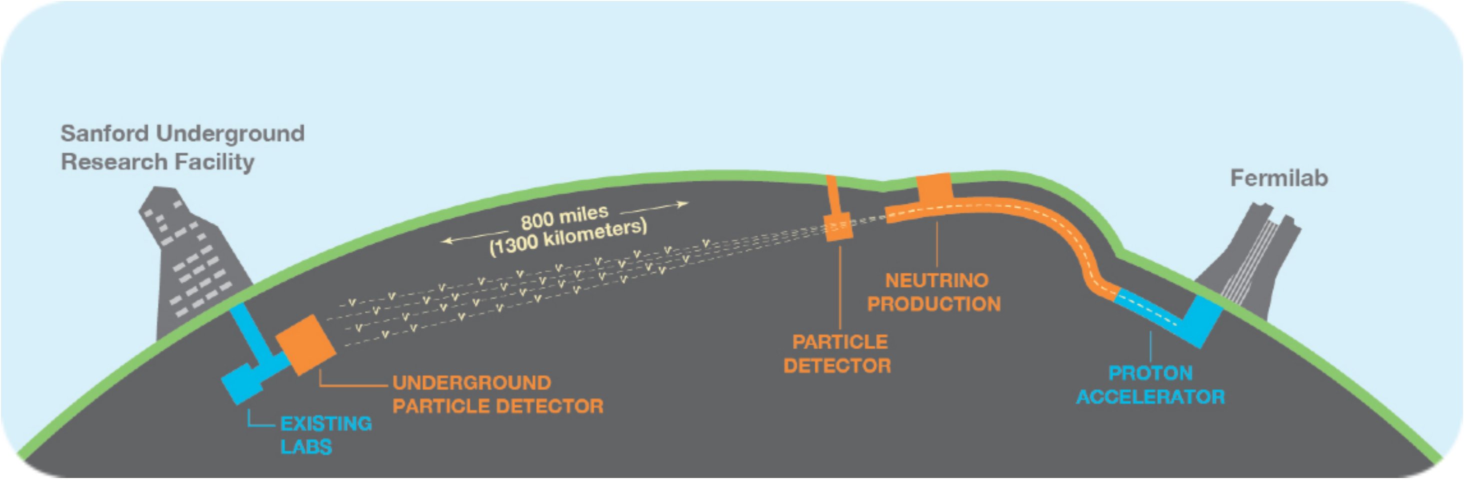
*J. Carlson, Phys. Rev. C **36**, 2026 (1987)*



*M. Piarulli, AL et al. PRL **120**, 052503 (2018)*



NEUTRINO-NUCLEUS SCATTERING



RESPONSE FUNCTIONS

$$R(\omega, \mathbf{q}) = \sum_f \langle \Psi_0 | J^\dagger | \Psi_f \rangle \langle \Psi_f | J | \Psi_0 \rangle \delta(\omega - E_f + E_0)$$

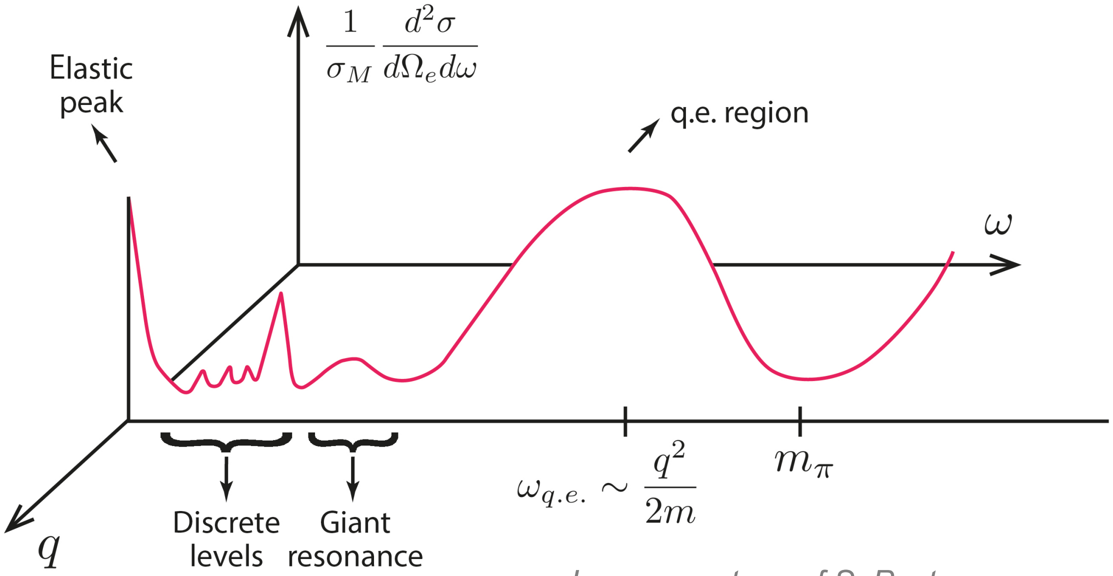
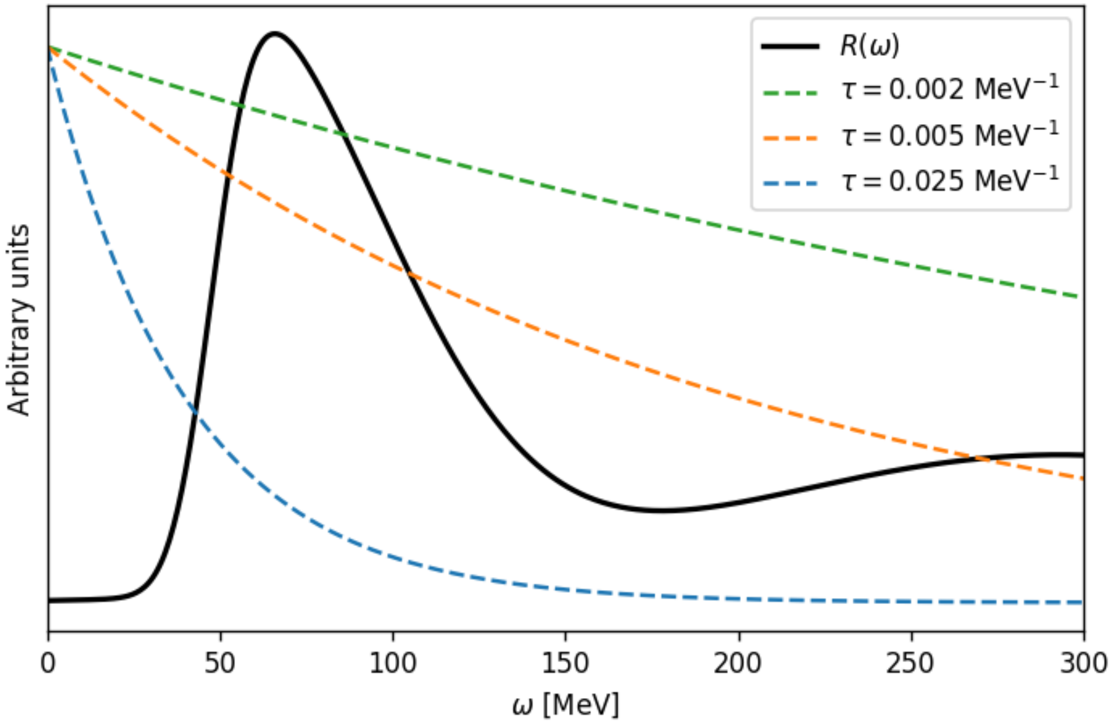


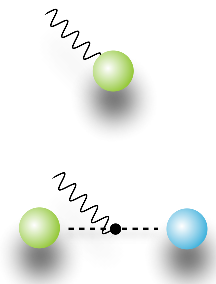
Image courtesy of S. Pastore

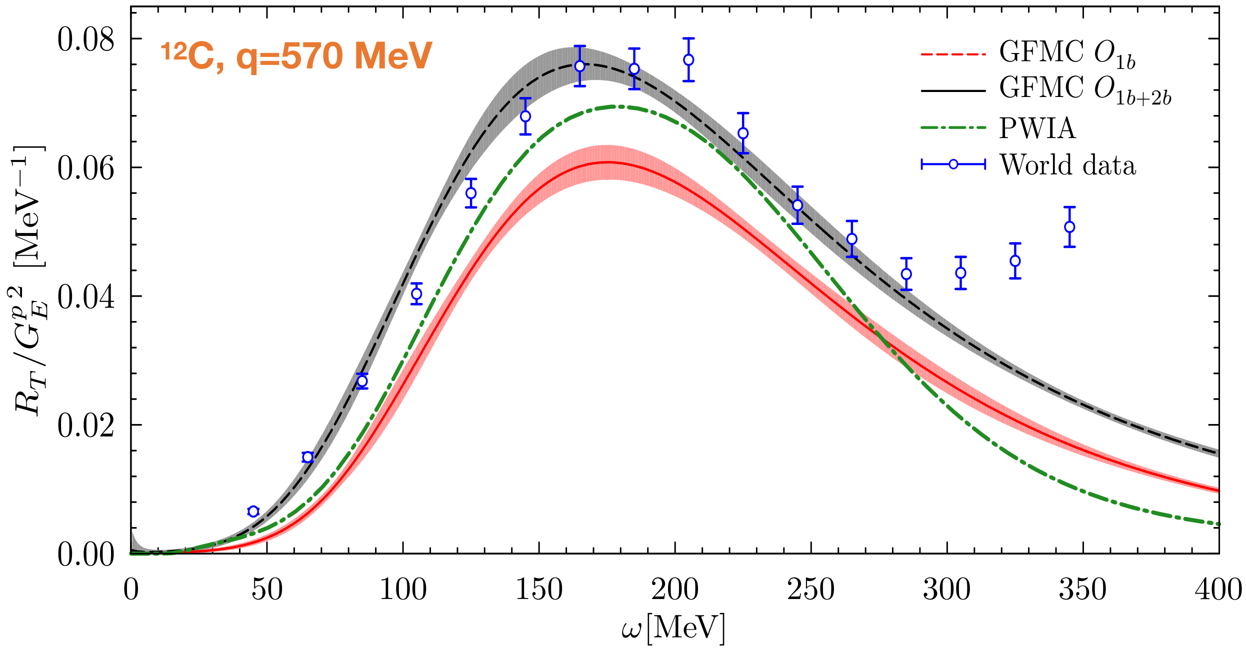
EUCLIDEAN RESPONSES

$$E(\tau, \mathbf{q}) = \int d\omega e^{-\omega\tau} R(\omega, \mathbf{q}) = \langle \Psi_0 | J^\dagger e^{-(H-E_0)\tau} J | \Psi_0 \rangle$$



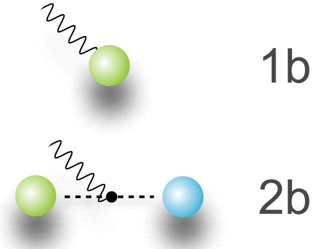
VALIDATION WITH ELECTRON SCATTERING

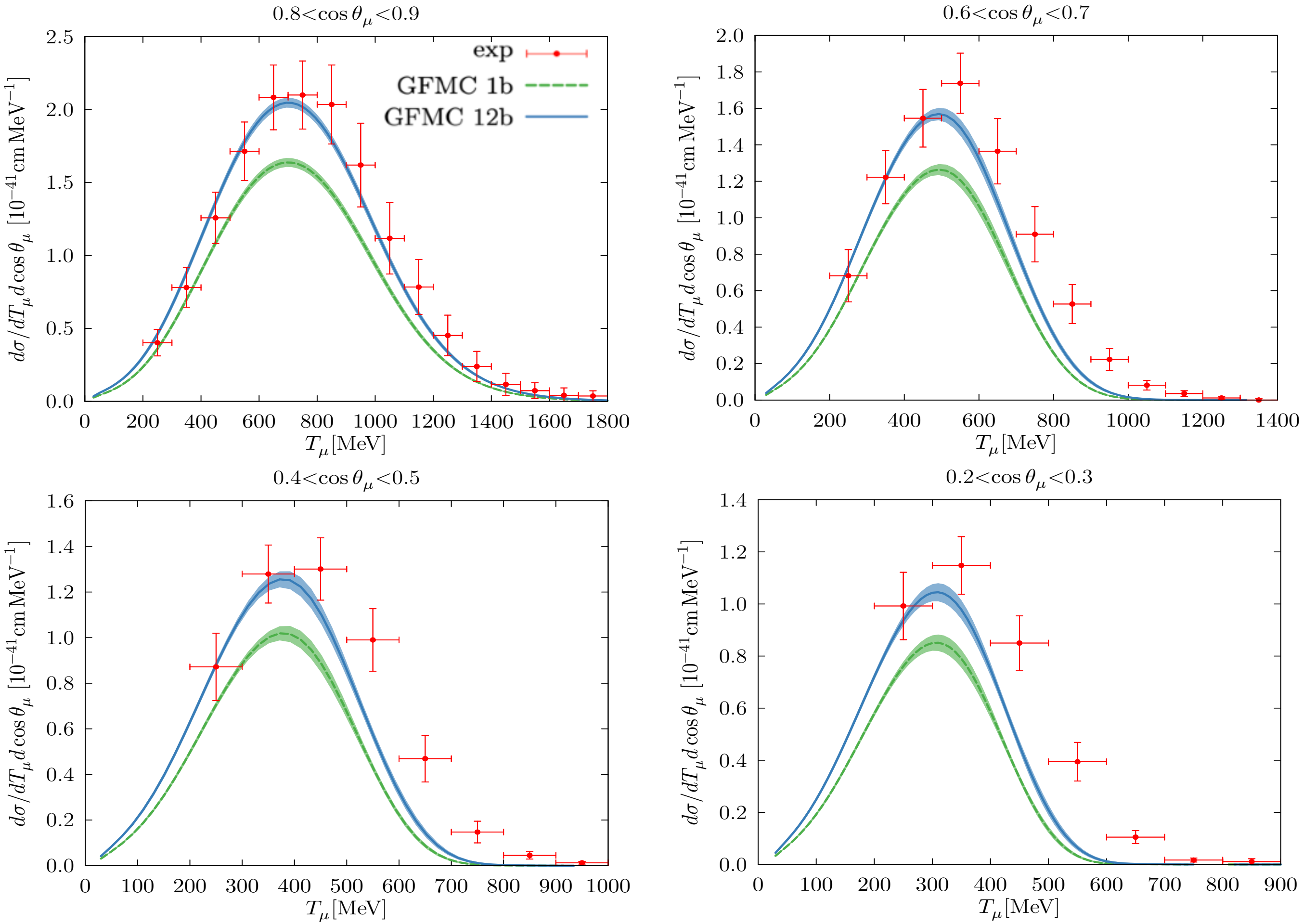




AL et al. Physical Review Letters **117** 082501 (2016)

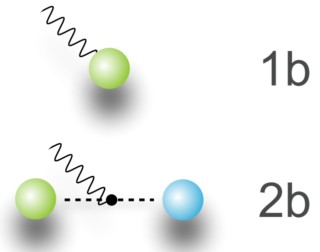
MINIBOONE

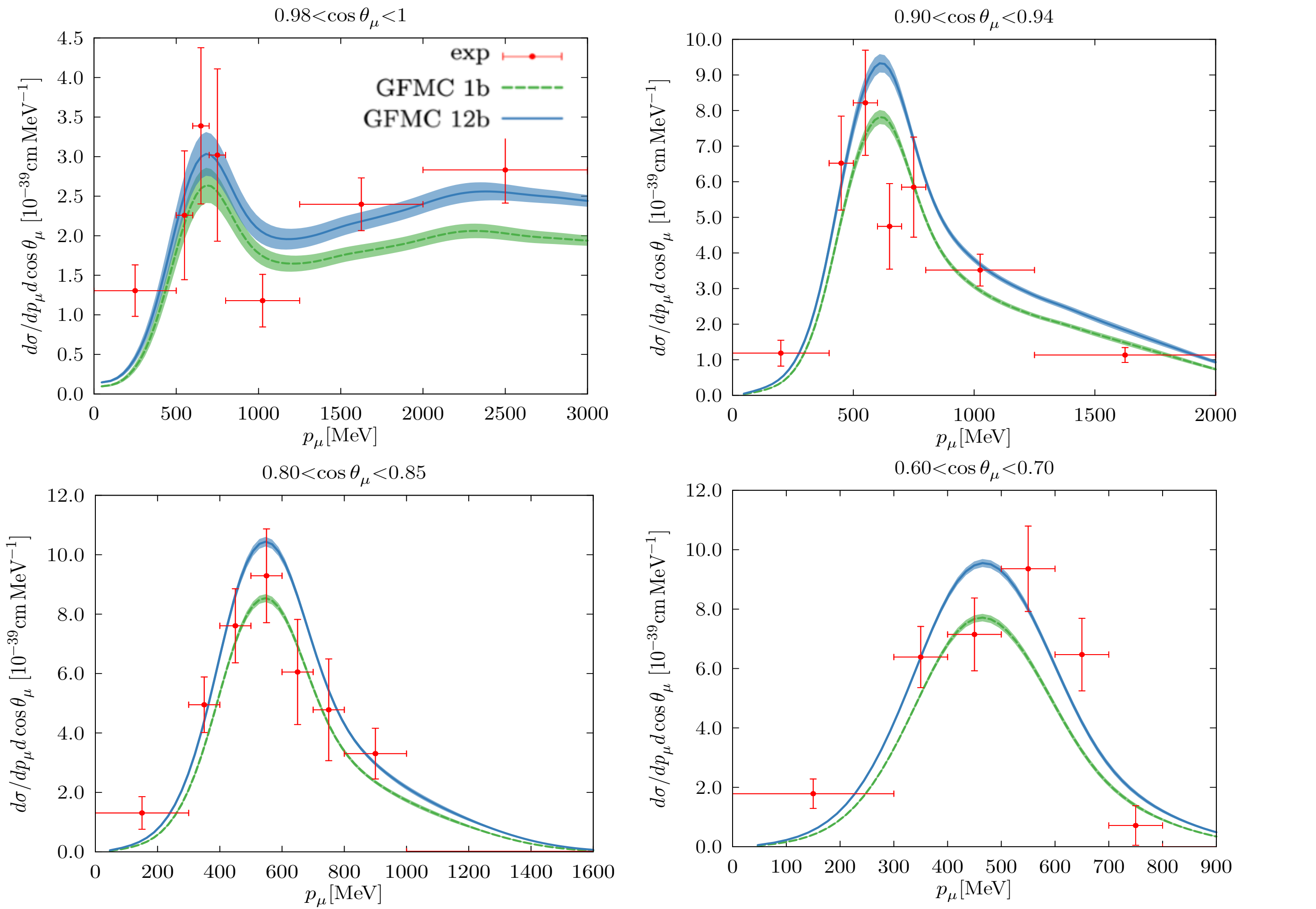




*AL et al., Physical Review X **10**, 031068 (2020)*

T2K





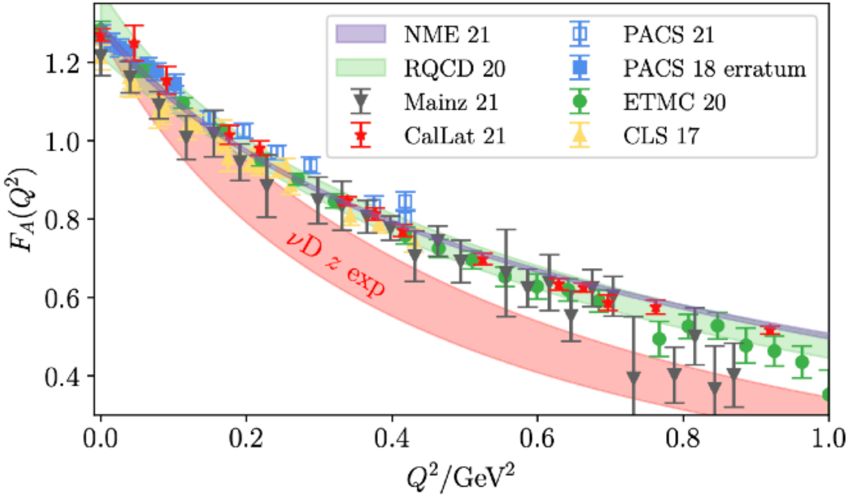
*AL et al., Physical Review X **10**, 031068 (2020)*

ELEMENTARY AMPLITUDES

The nucleon's axial form factor is crucial for modeling neutrino-nucleus interactions;

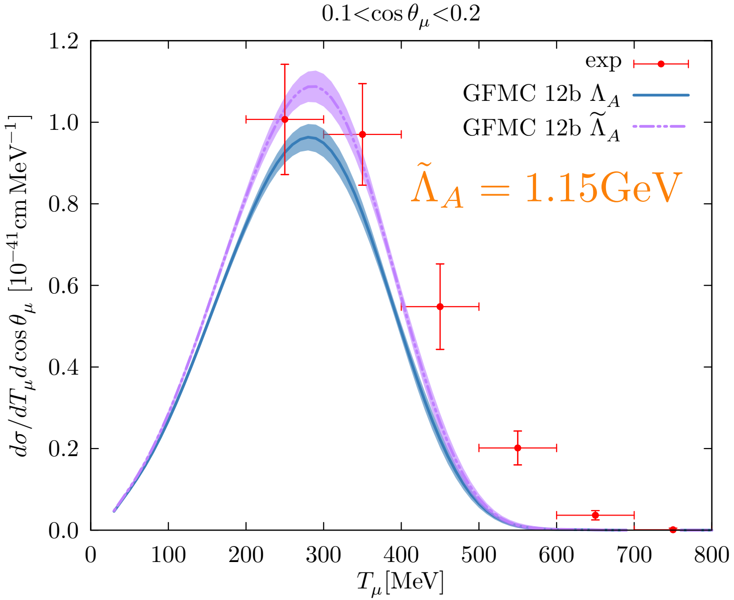
Scarce (old) experimental data available

Lattice-QCD calculations are essential



A. Meyer et al., Ann. Rev. Nucl. Part. Sci. **72** (2022) 205

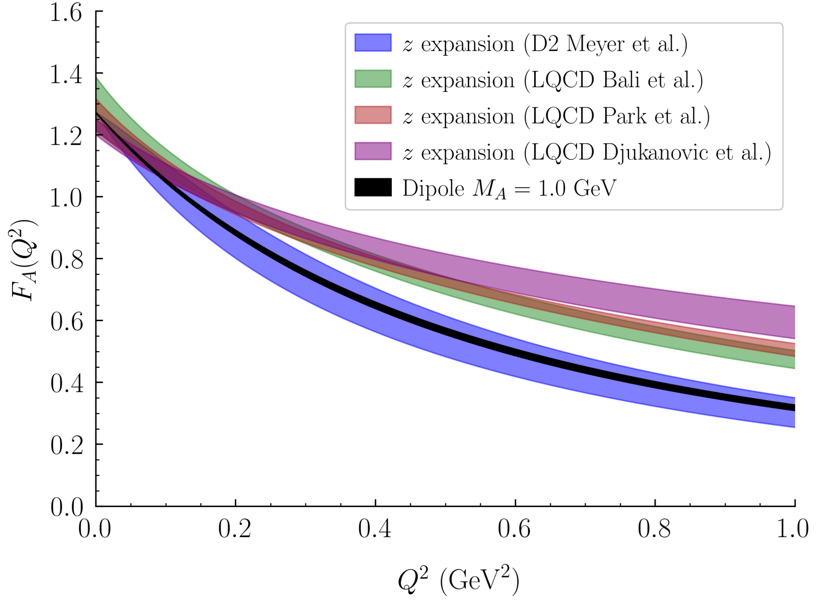
We have considered a value of the axial mass more in line with recent LQCD determinations



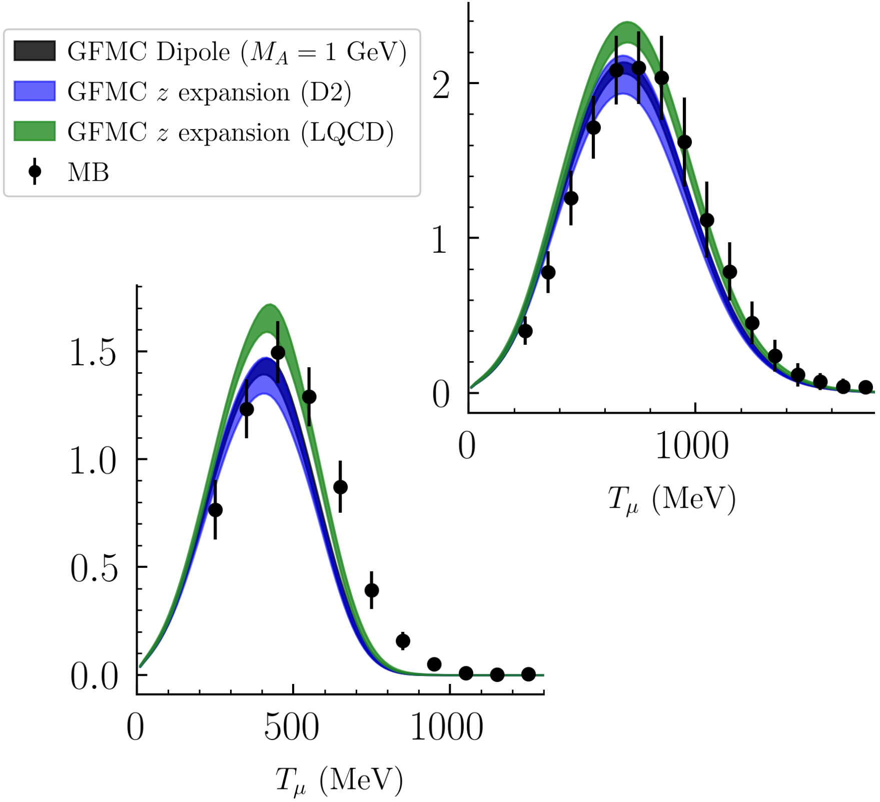
AL et al., Physical Review X **10**, 031068 (2020)

ELEMENTARY AMPLITUDES

Z-expansion parameterizations of axial form factors, consistent with experimental or LQCD data

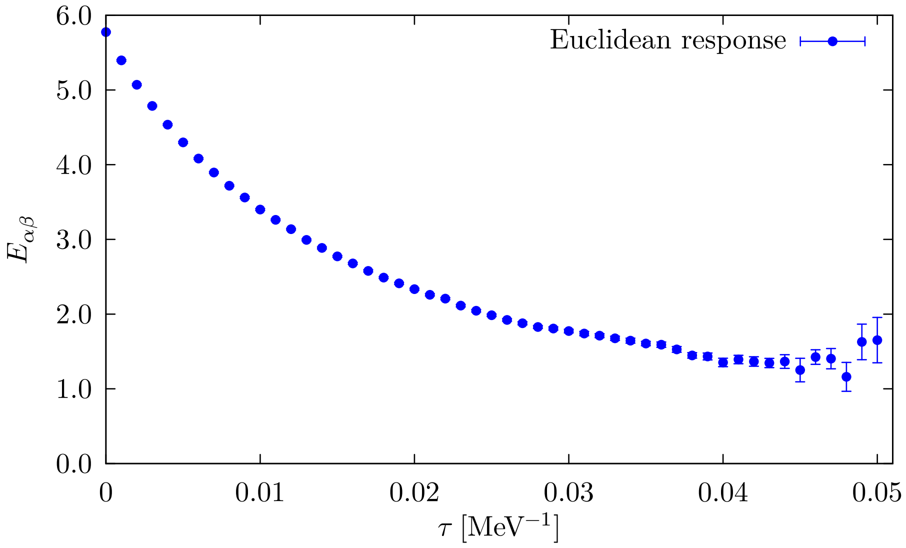


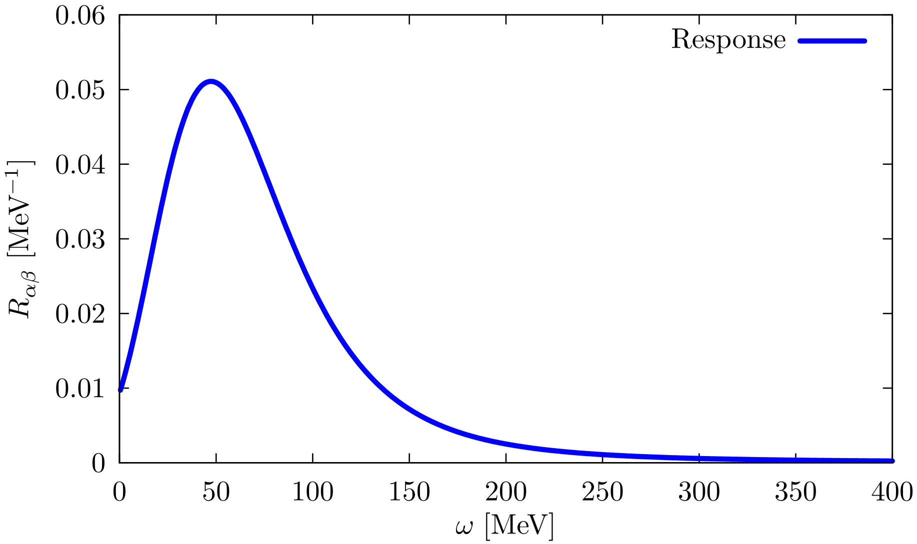
D. Simons, et al, JPG in press (2025)



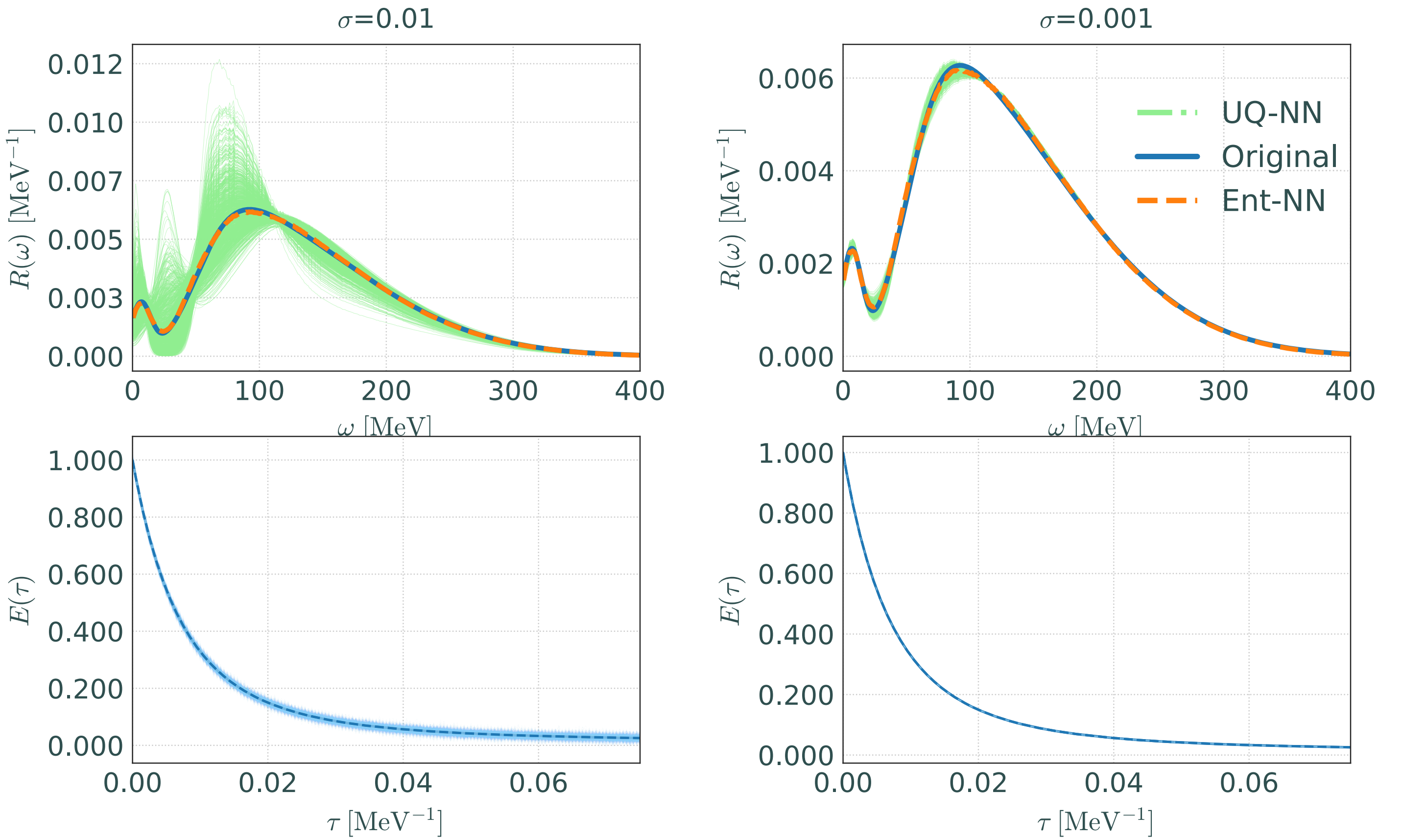
INVERTING THE LAPLACE TRANSFORM

$$E_{\alpha\beta}(\tau, \mathbf{q}) \quad \Rightarrow \quad R_{\alpha\beta}(\omega, \mathbf{q})$$



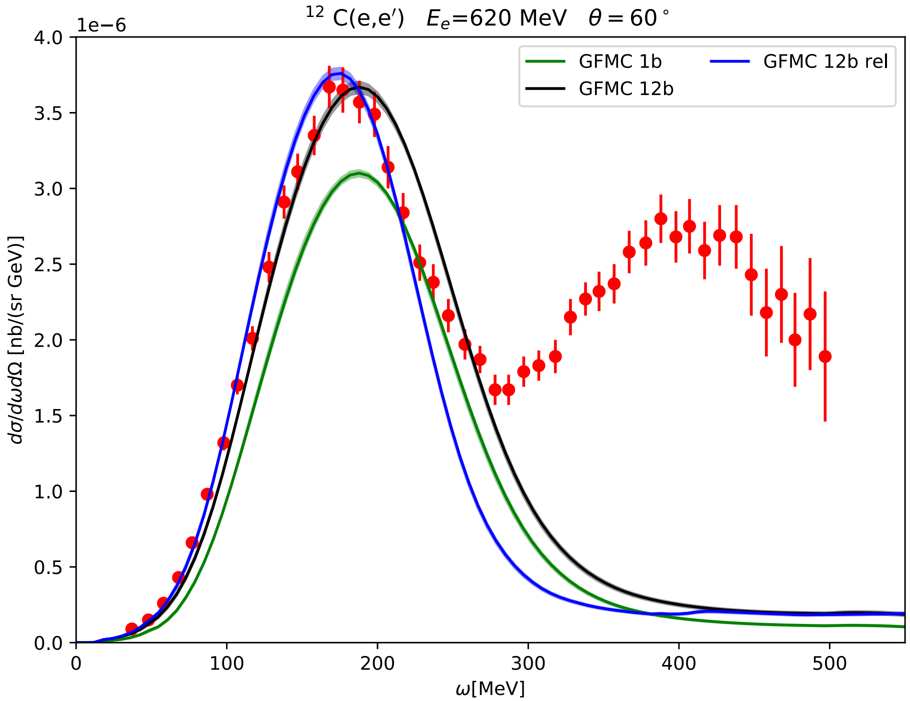


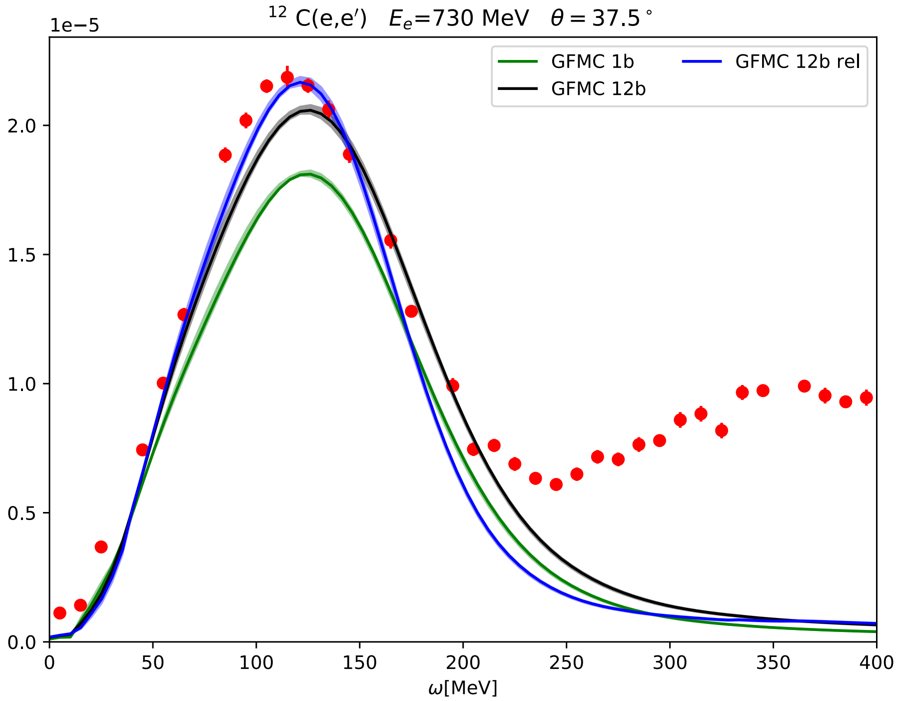
QUANTIFYING THE INVERSION UNCERTAINTY



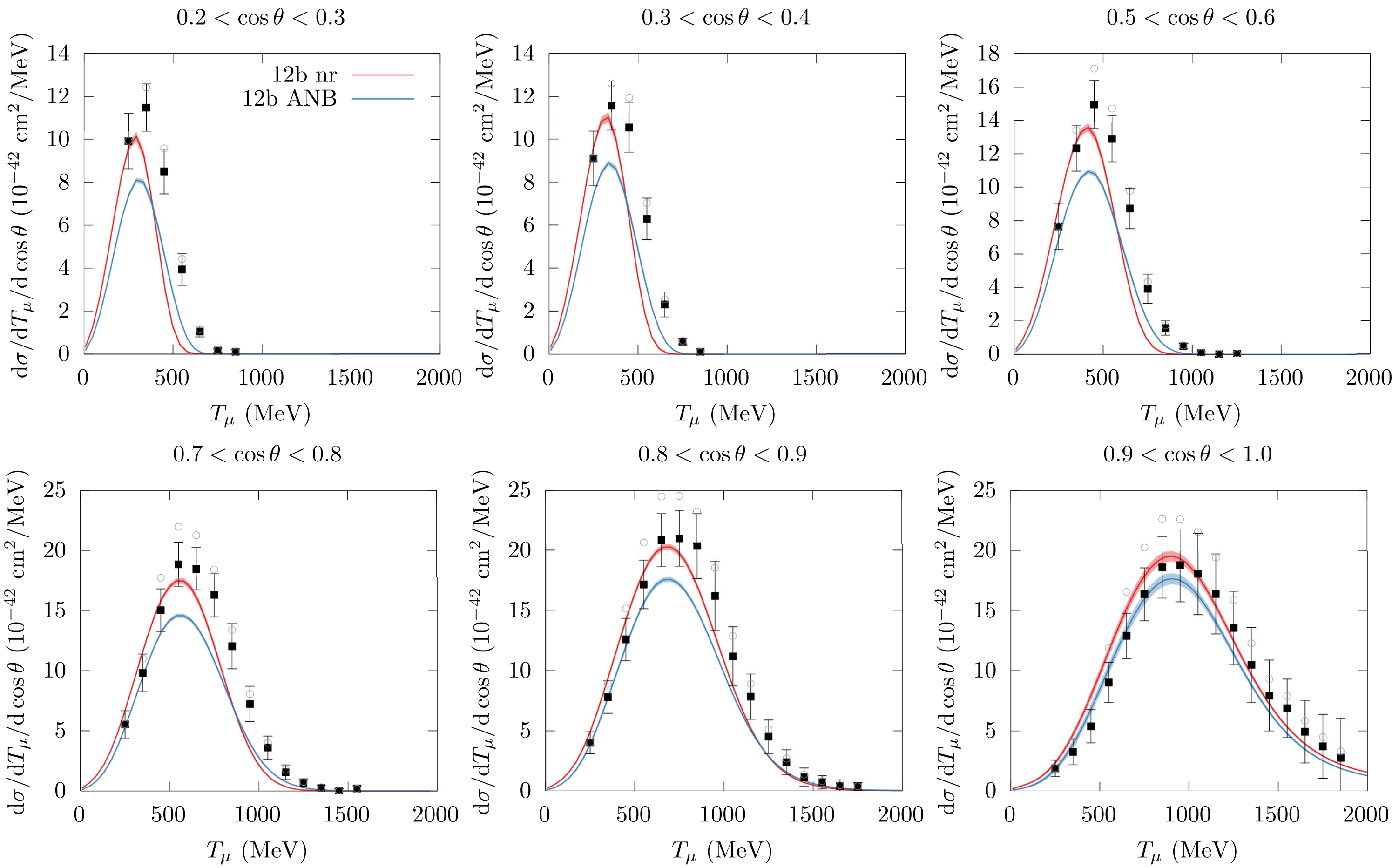
K. Raghavan, AL, Phys.Rev.C **110** (2024) 2, 025504

RELATIVISTIC EFFECTS





N. Rocco et al., Universe ***9*** *(2023) 8, 367*

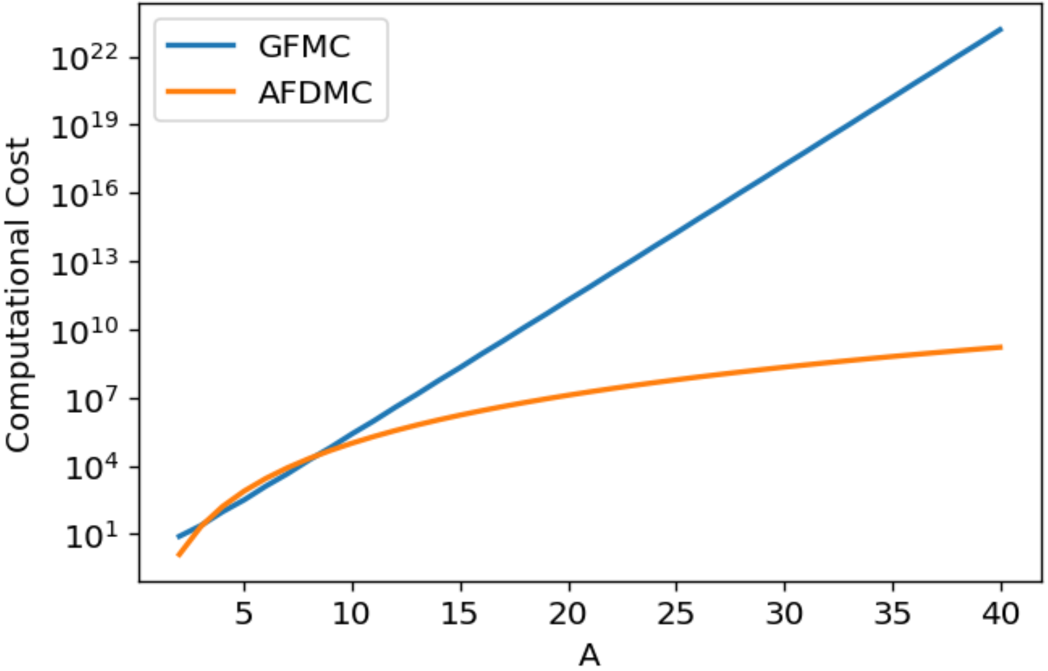


A. Nikolakopoulos, at al., *Phys. Rev. C* ***109*** *(2024) 1, 014623*

BEYOND ^{12}C WITH THE AFDMC

GFMC: many-body basis → $|S\rangle \equiv C_{\uparrow\uparrow\uparrow}|\uparrow\uparrow\uparrow\rangle + C_{\uparrow\uparrow\downarrow}|\uparrow\uparrow\downarrow\rangle + \cdots + C_{\downarrow\downarrow\downarrow}|\downarrow\downarrow\downarrow\rangle$

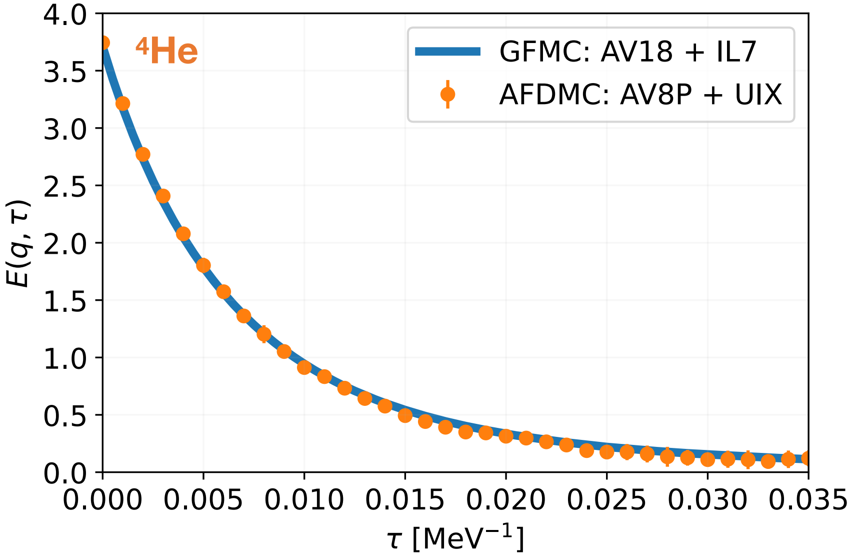
AFDMC: single-spinor basis → $|S\rangle \equiv (u_1|\uparrow\rangle_1 + d_1|\downarrow\rangle_1) \otimes \ldots (u_A|\uparrow\rangle_A + d_A|\downarrow\rangle_A)$

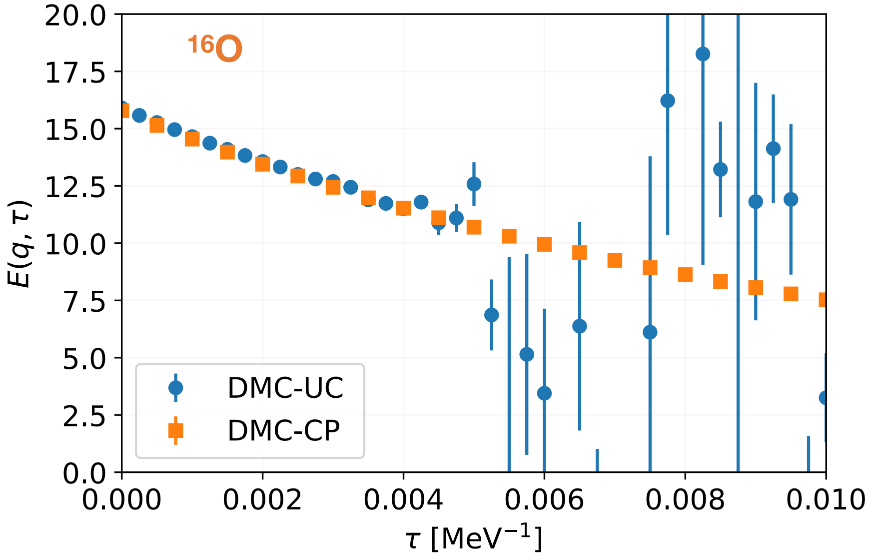


BEYOND ^{12}C WITH THE AFDMC

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

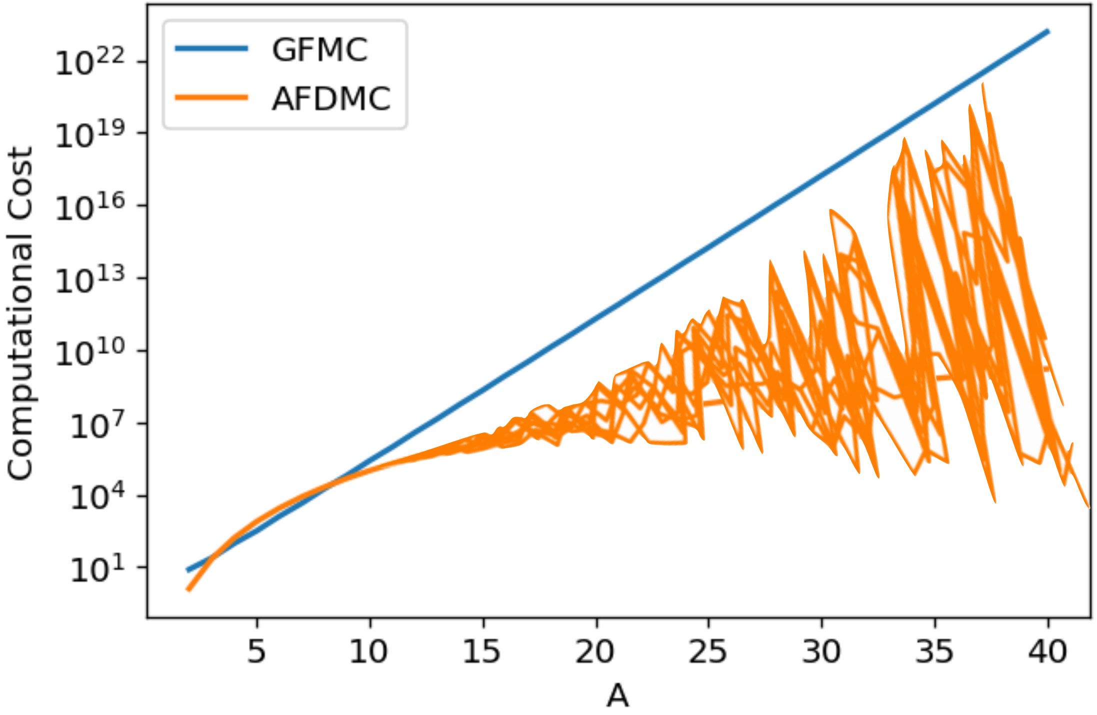
We developed the AFDMC to allow for the calculation of Euclidean response functions





*A. Gnech, et al., Phys.Rev. C **111** (2025) 2, 024314*

HOW TO TACKLE (EVEN) LARGER NUCLEI?



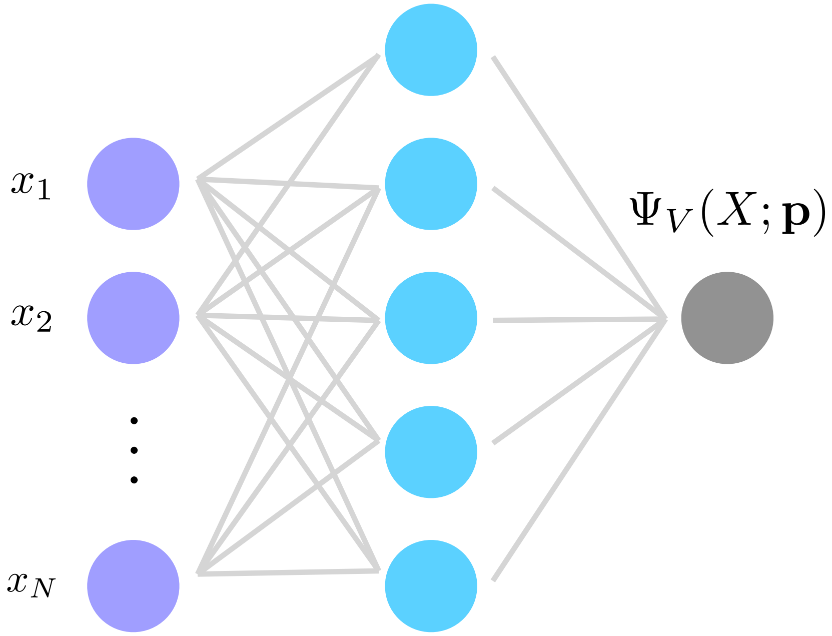
GFMC

$$|\Psi_T\rangle \sim \prod_{i<j} F_{ij}|\Phi\rangle$$

AFDMC

$$|\Psi_T\rangle \sim (1 + \sum_{i<j} F_{ij})|\Phi\rangle$$

NEURAL-NETWORK QUANTUM STATES



$$E_V \equiv \frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} > E_0$$

$$E_V \simeq \frac{1}{N} \sum_{X \in |\Psi_V(X)|^2} \frac{\langle X | H | \Psi_V \rangle}{\langle X | \Psi_V \rangle}$$

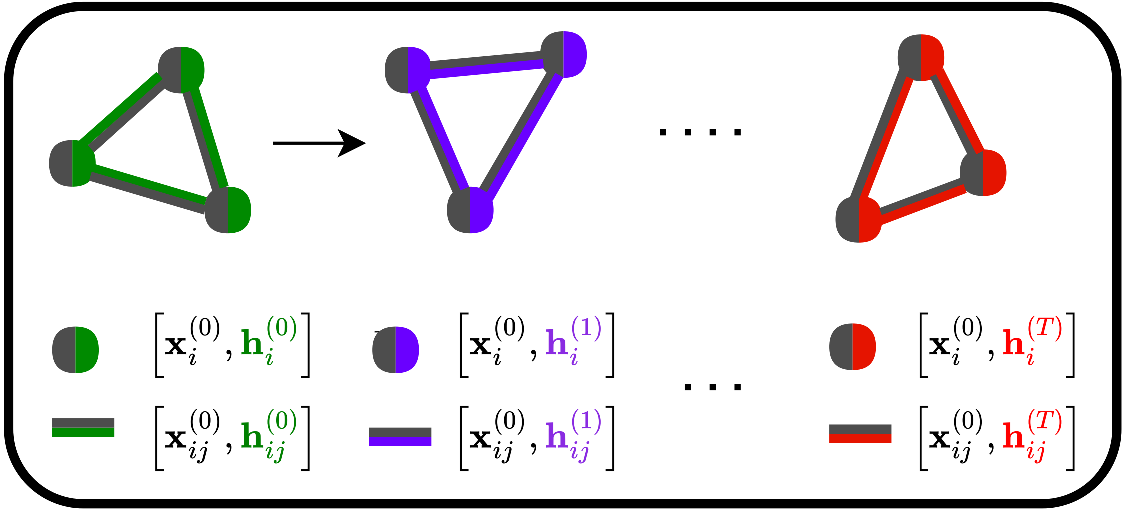
NFS IN COORDINATE SPACE

Antisymmetry is built in the ansatz

$$\Psi_V(X;\mathbf{p}) = e^{\mathcal{U}(X;\mathbf{p})} \times \Phi(X;\mathbf{p})$$

The expressivity is augmented through message-passing back flow transformations

$$\mathbf{x}_i \longrightarrow \mathbf{y}_i(\mathbf{x}_i;\mathbf{x}_{j\neq i})$$

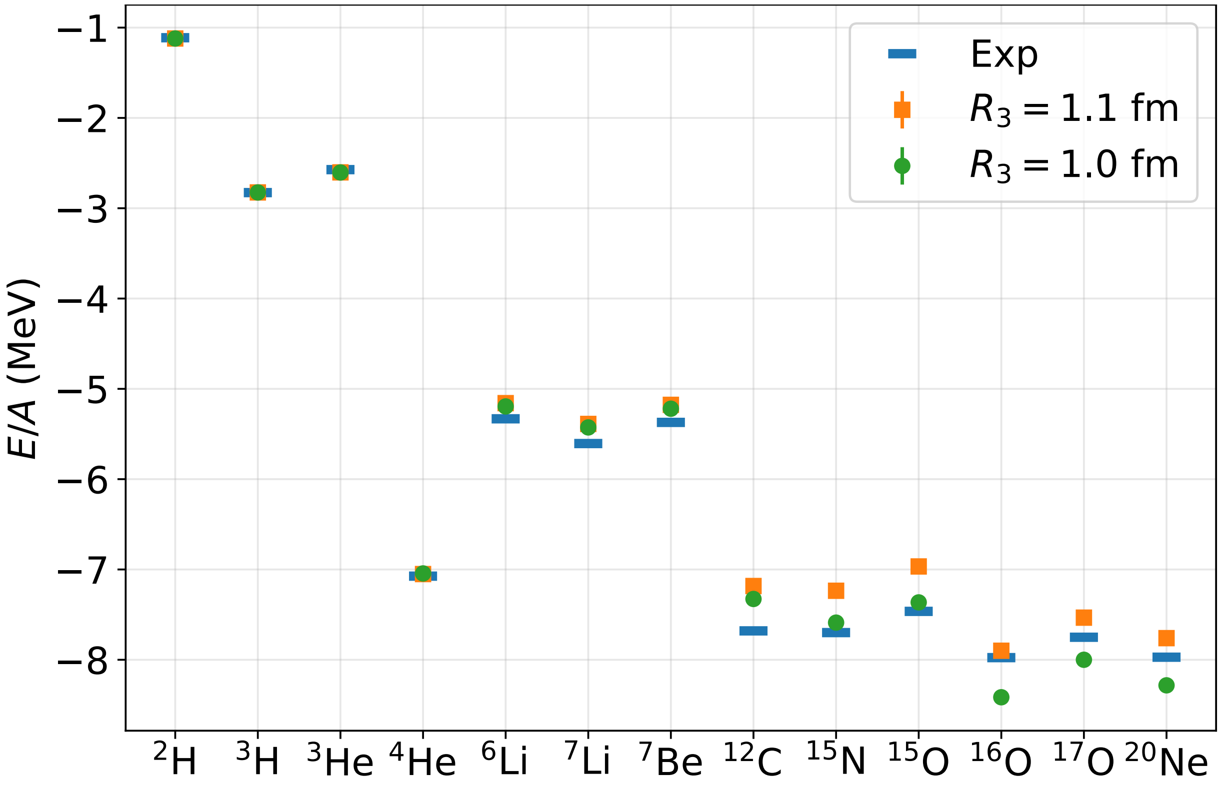


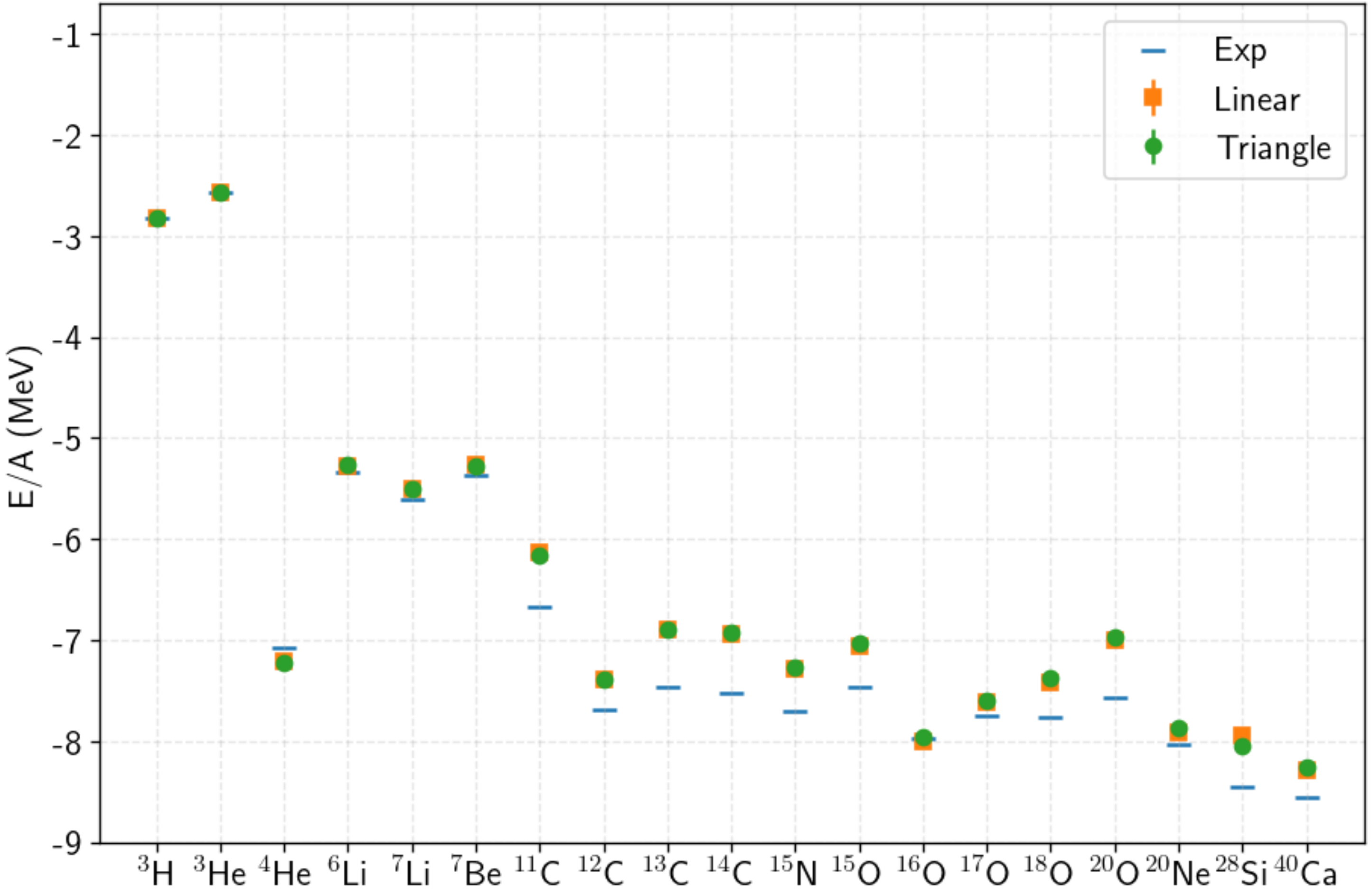
*G. Pescia, et al., Phys. Rev. B **110** (2024), 035108*

*J. Kim, et al., Commun.Phys. **7** (2024), 148*

*B. Fore, at al., Commun.Phys. **8** (2025), 108*

NQS TO EXTEND QMC TO A=20



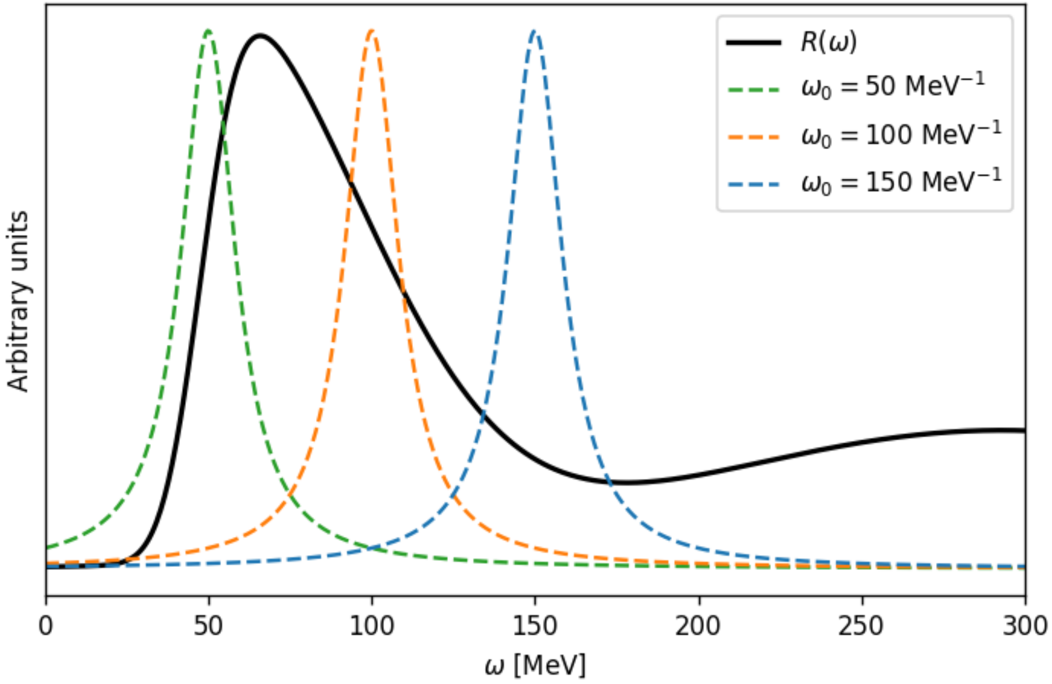


Bryce Fore, in preparation

NUCLEAR RESPONSES WITH NQS

We consider the Lorentz Kernel
(see Sonia's talk on Monday)

$$L(\omega_0, \Gamma, \mathbf{q}) = \int_{\omega_{th}}^{\infty} d\omega \frac{R(\omega, \mathbf{q})}{(\omega - \omega_0)^2 + \Gamma^2}$$



NUCLEAR RESPONSES WITH NQS

The first step in computing the LIT involves solving the inhomogeneous Schrödinger equation

$$(H - E_0 - \omega_0 - i\Gamma)|\Psi_L\rangle = J|\Psi_0\rangle$$

The LIT can be computed from the norm

$$\langle\Psi_L|\Psi_L\rangle = \Psi_0|J^\dagger \frac{1}{H - E_0 - \omega_0 + i\Gamma} \frac{1}{H - E_0 - \omega_0 - i\Gamma} J|\Psi_0\rangle$$

Leveraging the Hermiticity of the Hamiltonian, we recast the norm as an overlap

$$\langle\Psi_L|\Psi_L\rangle = \frac{1}{\Gamma}\,\mathrm{Im}\langle\Psi_L|J|\Psi_0\rangle$$

E. Parnes, et al., arXiv:2504.20195 [nucl-th]

NUCLEAR RESPONSES WITH NQS

Resolvent equation:

$$(H - E_0 - \omega_0 - i\Gamma)|\Psi_L\rangle = J|\Psi_0\rangle$$

1) Maximize the fidelity

$$\mathcal{F}(\Psi, \Phi) = \frac{\langle\Psi|\Phi\rangle\langle\Phi|\Psi\rangle}{\langle\Psi|\Psi\rangle\langle\Phi|\Phi\rangle}$$

$$\begin{cases} |\Psi\rangle = (\hat{H} - E_0 - \omega_0 + i\Gamma)|\Psi_L\rangle \\ |\Phi\rangle \equiv J|\Psi_0\rangle \end{cases}$$

2) Compute the global phase and norm

$$|\bar{\Psi}\rangle \approx \mathcal{N}|\Psi\rangle \longrightarrow \mathcal{N} = \frac{\langle\Phi|\bar{\Psi}\rangle}{\langle\Phi|\Phi\rangle}$$

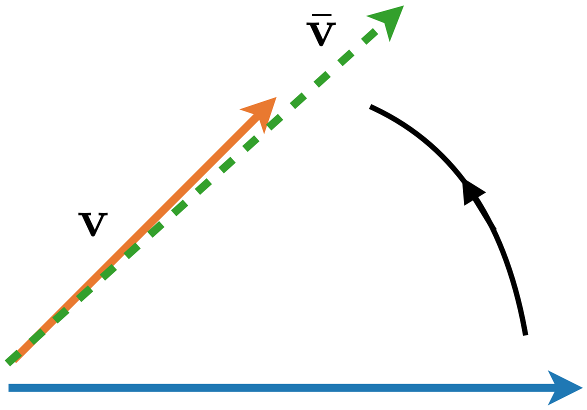
E. Parnes, et al., arXiv:2504.20195 [nucl-th]

NUCLEAR RESPONSES WITH NQS

In matrix form

$$\hat{H}\mathbf{v} = \mathbf{u}$$

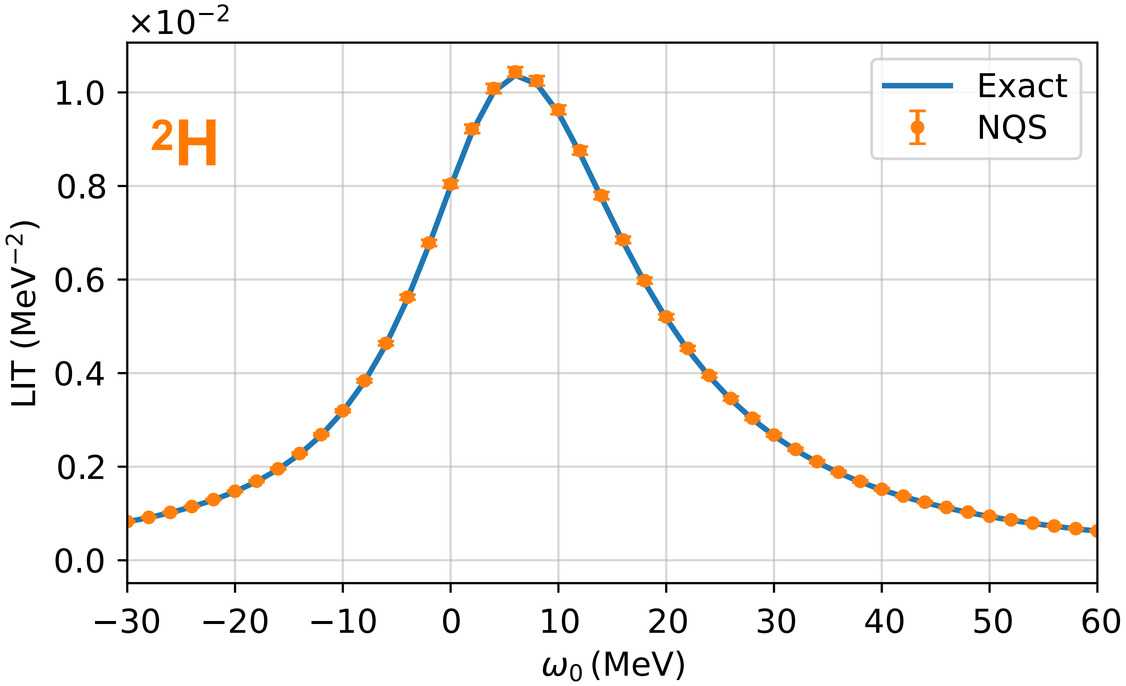
Maximizing the fidelity and then finding the norm



E. Parnes, et al., arXiv:2504.20195 [nucl-th]

NUCLEAR RESPONSES WITH NQS

We considered a dipole transition $$J = \sum_{i}^{A} q_i \left(z_i - Z_{cm} \right)$$



E. Parnes, et al., arXiv:2504.20195 [nucl-th]

NUCLEAR RESPONSES WITH NQS

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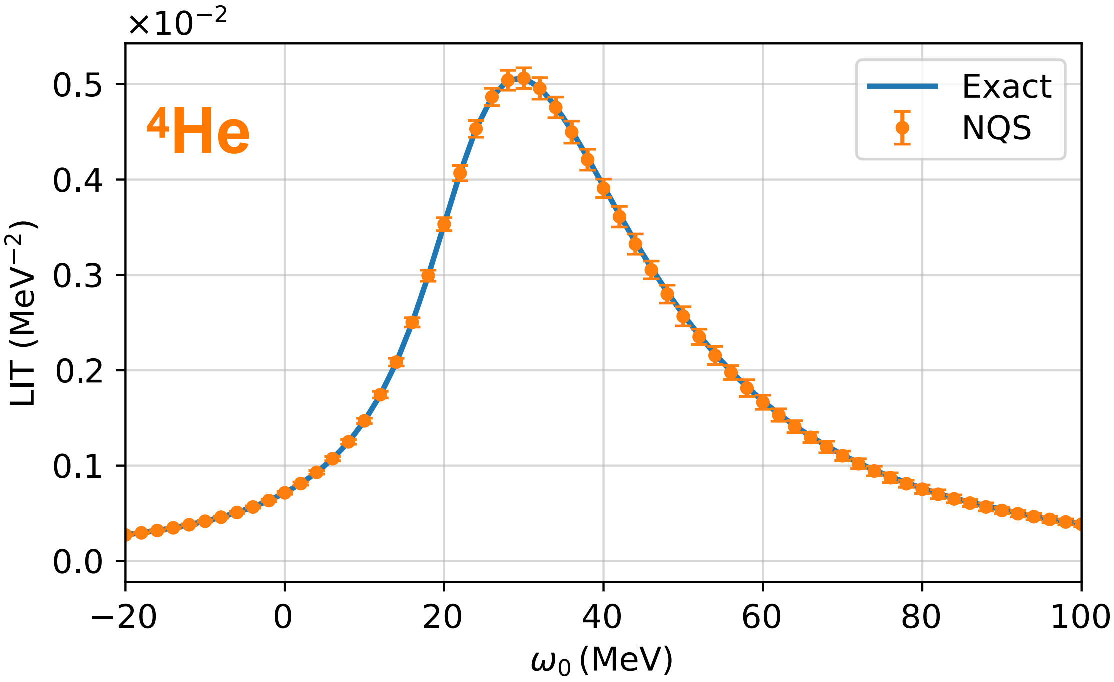


E. Parnes, et al., arXiv:2504.20195 [nucl-th]

NUCLEAR RESPONSES WITH NQS

We invert the LIT with an improved maximum-entropy approach

$$P(R|L) = P(L|R)\frac{P(R)}{P(L)}$$

Likelihood function with Monte Carlo and systematic error

$$P(L|R) = \frac{e^{-\chi^2/2}}{Z_L} \qquad \chi^2 = \sum_{i=1}^{N_{\omega_0}} \frac{(\tilde{L}_i - L_i)^2}{\sigma_i^2}$$

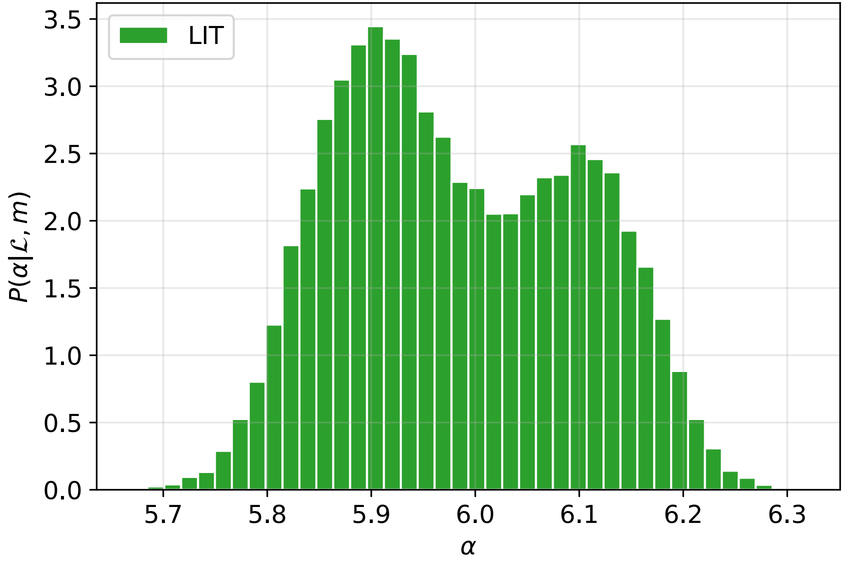
Entropic prior

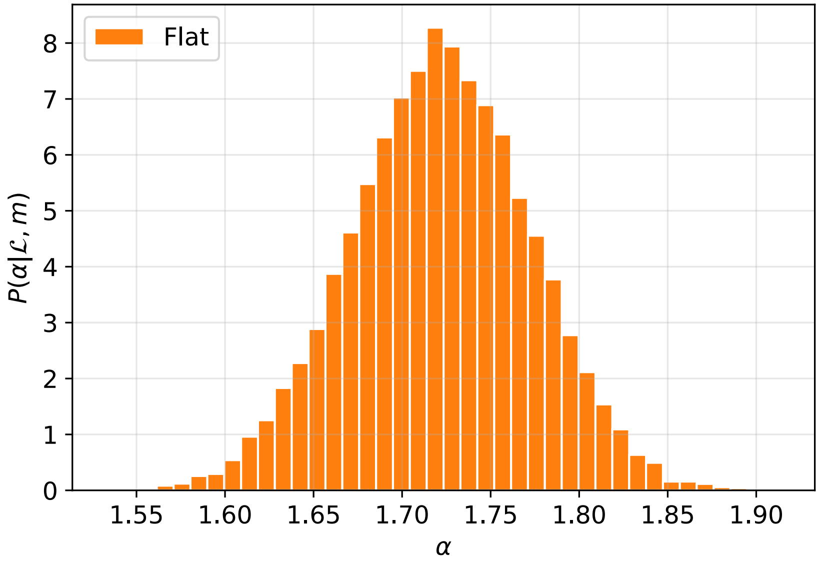
$$P(R) = e^{\alpha S} \longrightarrow S = \int d\omega \left[R(\omega) - m(\omega) - R(\omega)\log\left(\frac{R(\omega)}{m(\omega)}\right)\right]$$

E. Parnes, et al., arXiv:2504.20195 [nucl-th]

NUCLEAR RESPONSES WITH NQS

MCMC “with swap” used to sample the posterior: no need to fix α

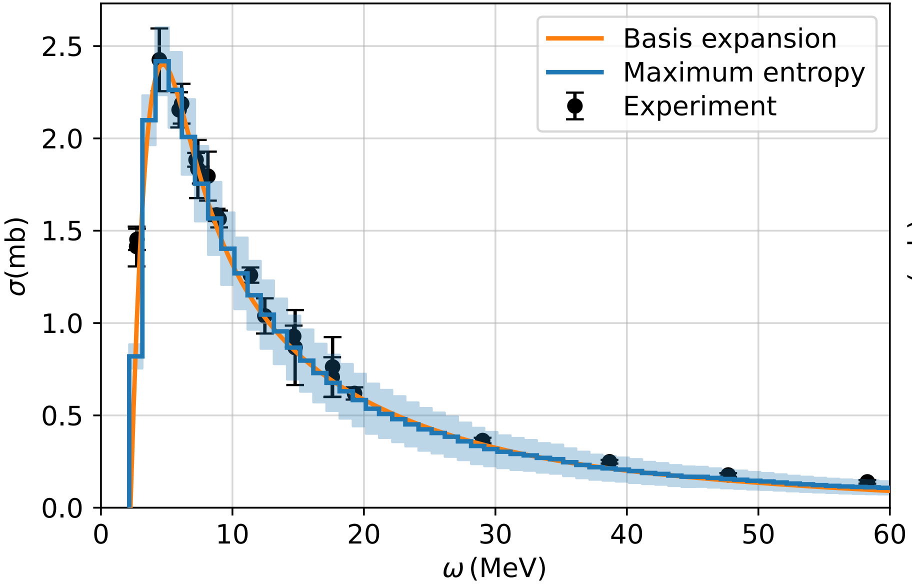


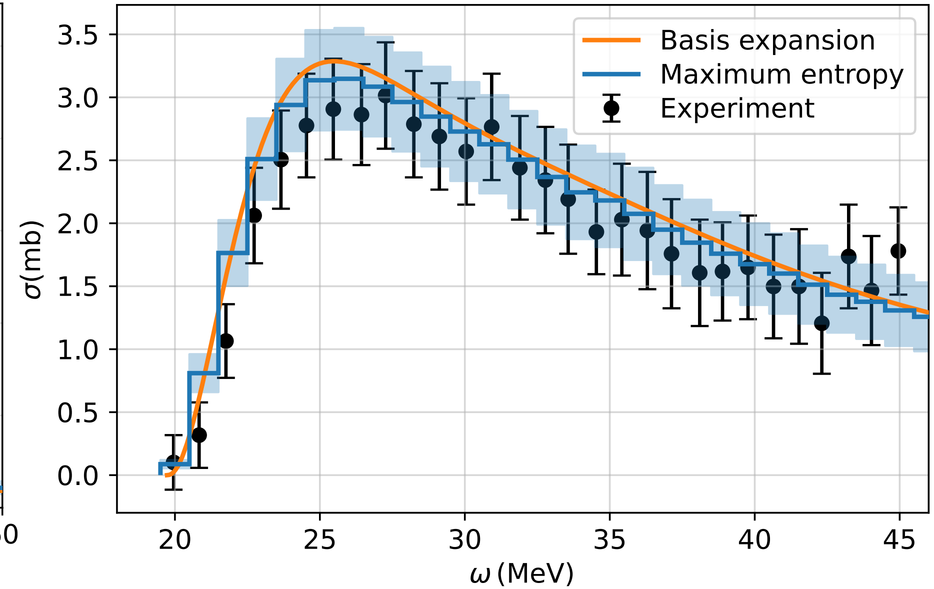


E. Parnes, et al., arXiv:2504.20195 [nucl-th]

NUCLEAR RESPONSES WITH NQS

Computed the photo-absorption cross section with quantified uncertainties

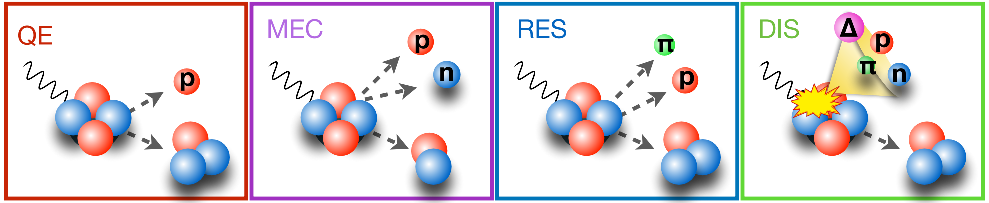


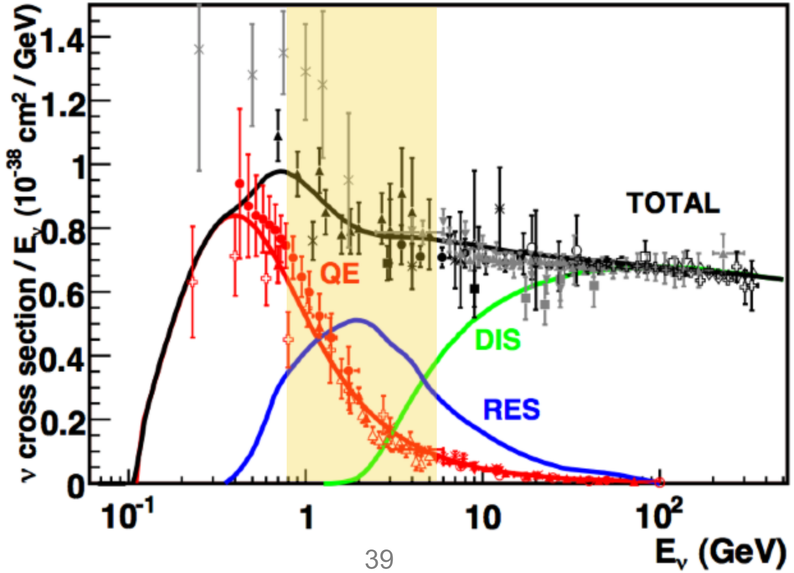


E. Parnes, et al., arXiv:2504.20195 [nucl-th]

HIGHER ENERGY REGION

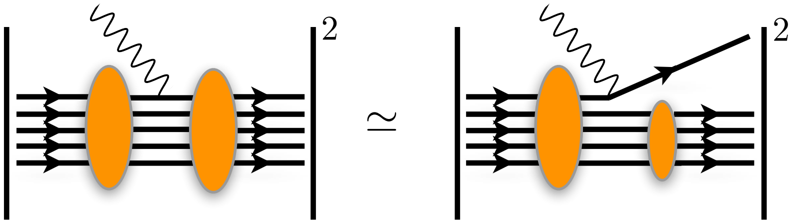
Describing all the reaction mechanisms at play in accelerator-neutrino experiments is a formidable challenge



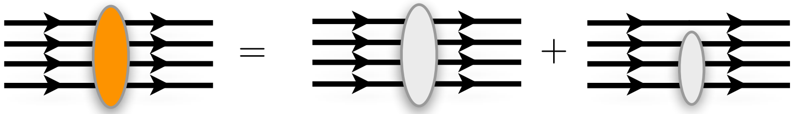


EXTENDED FACTORIZATION SCHEME

One-body current

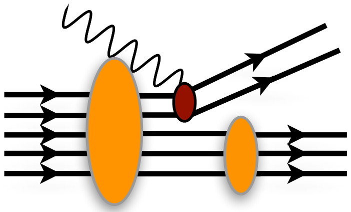


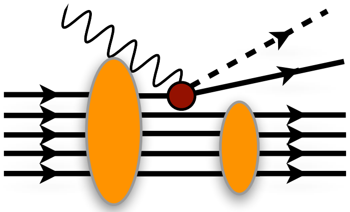
The spectral function includes excitations of the A-1 final state with two nucleons in the continuum

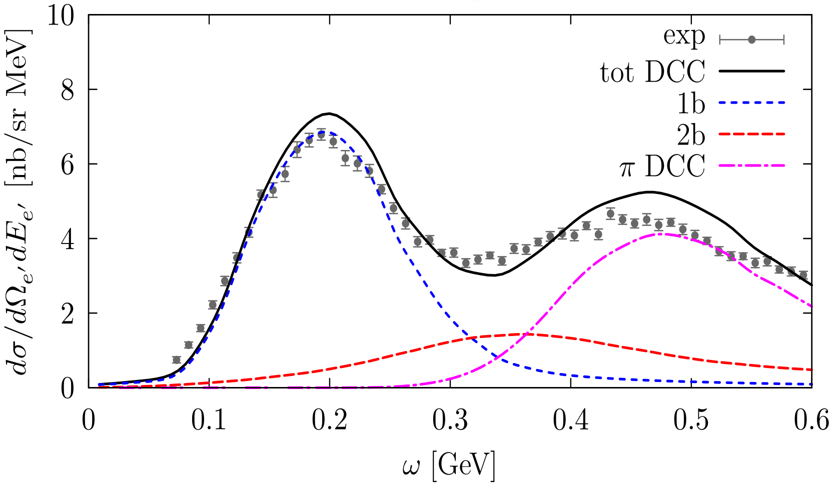


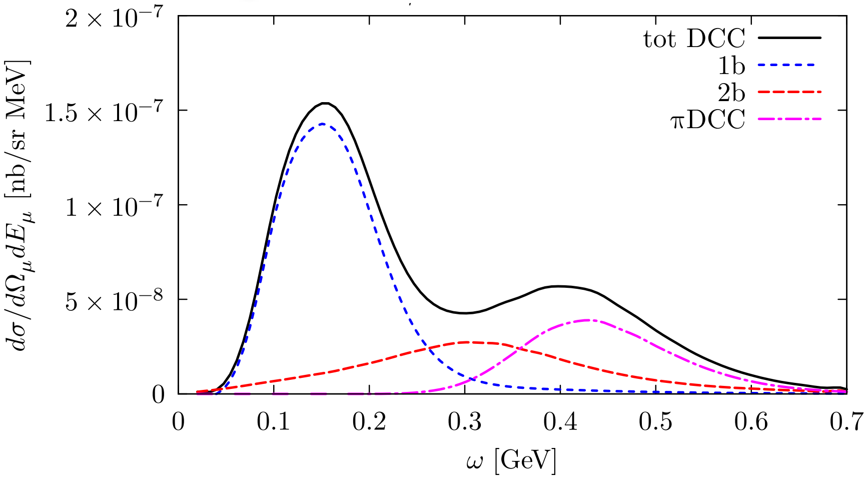
EXTENDED FACTORIZATION SCHEME

Two-body currents and pion-production



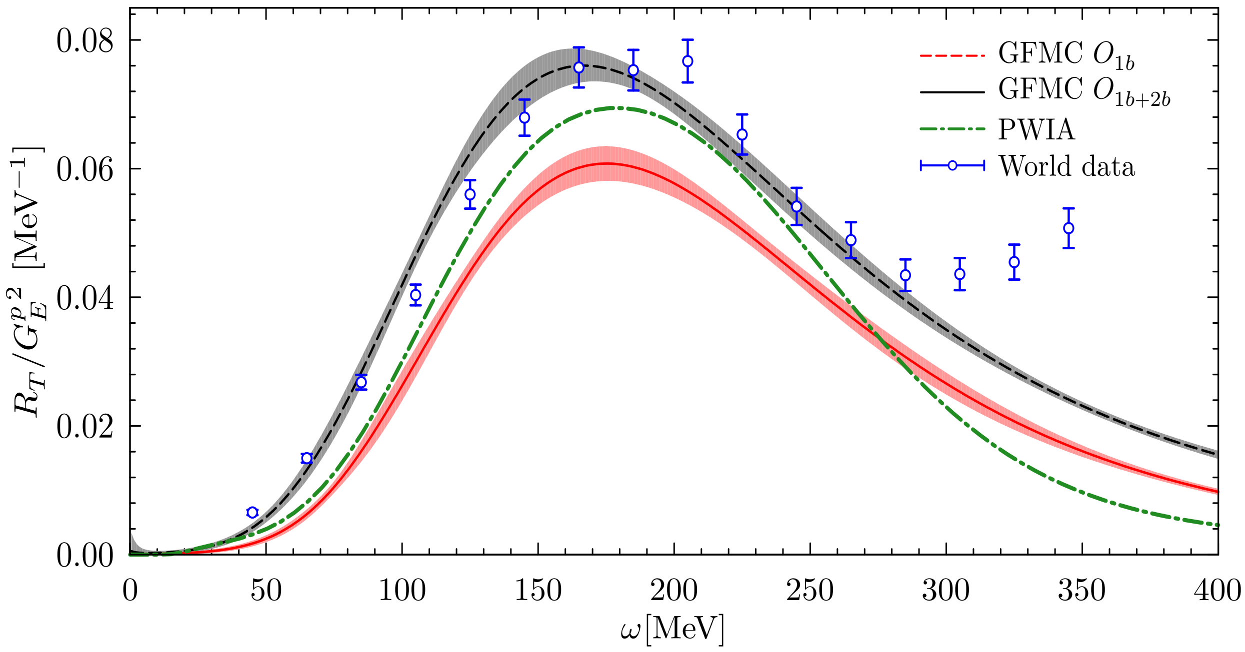






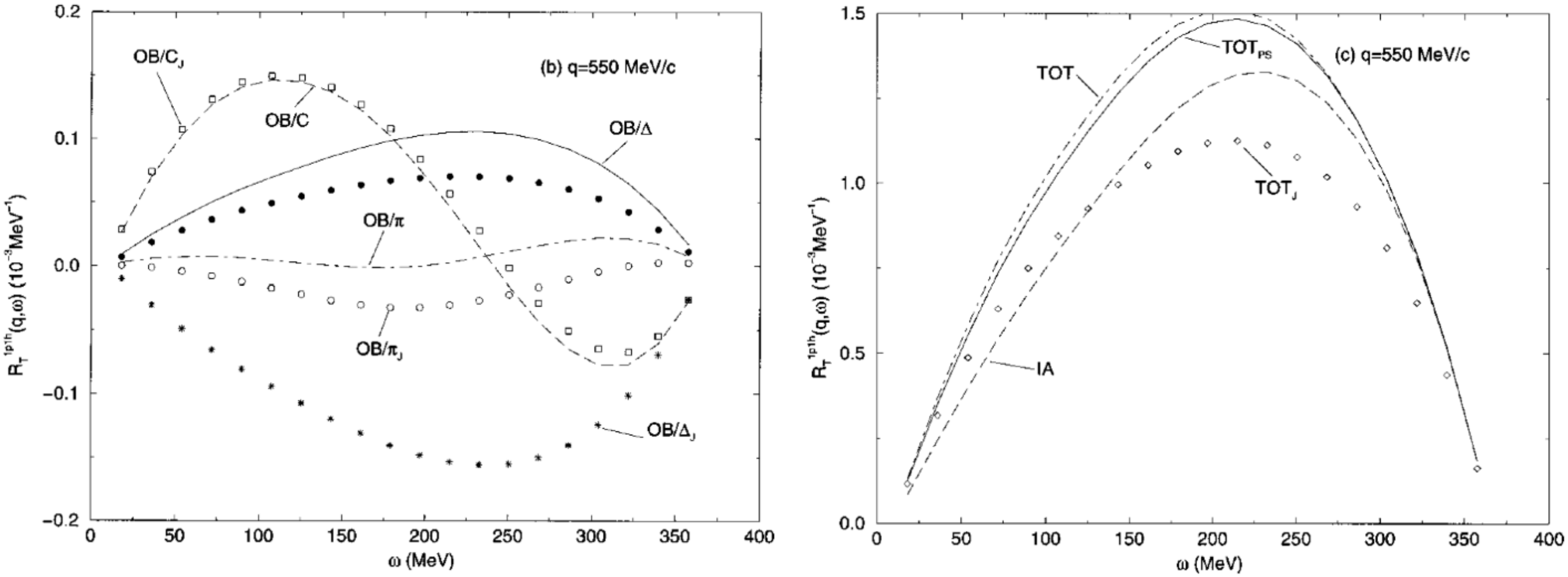
N. Rocco, et al. Physical Review C ***100****, 045503 (2019)*

INTERFERENCE PUZZLE



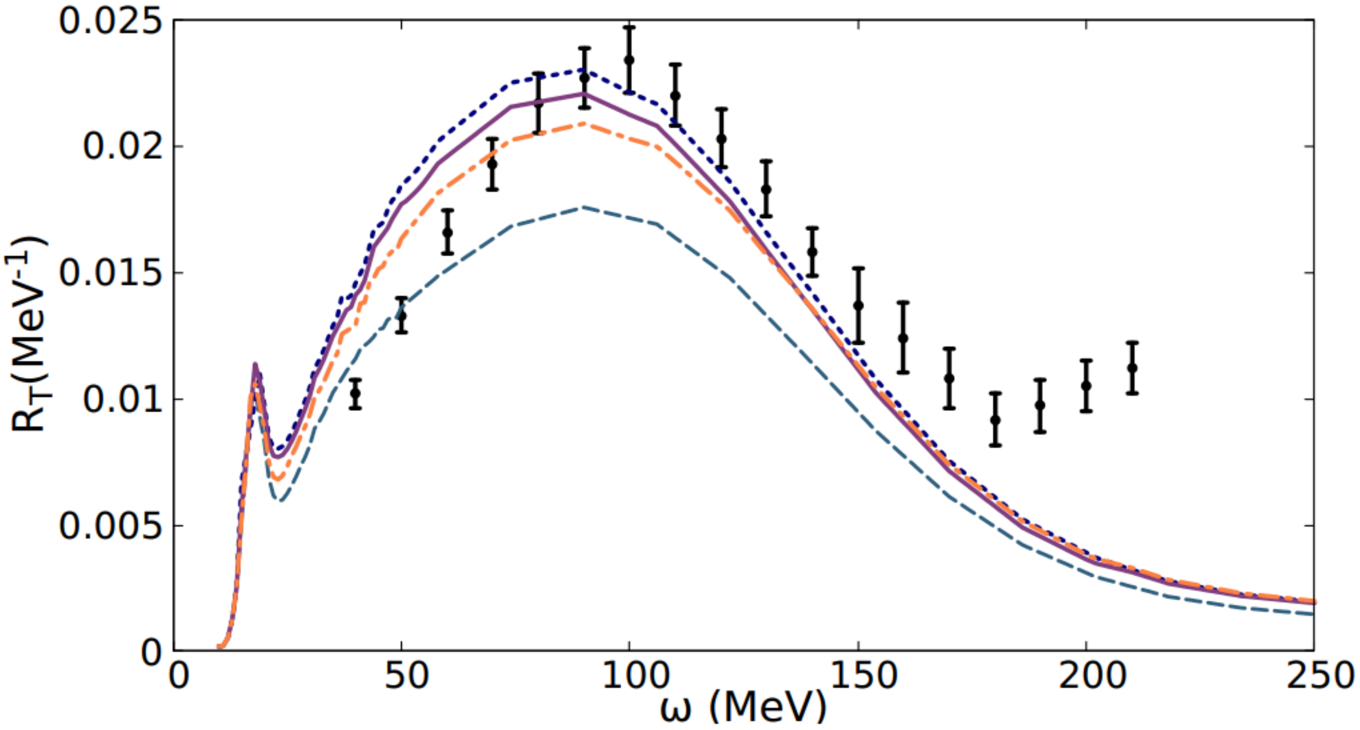
AL et al. Physical Review Letters ***117*** *082501 (2016)*

INTERFERENCE PUZZLE



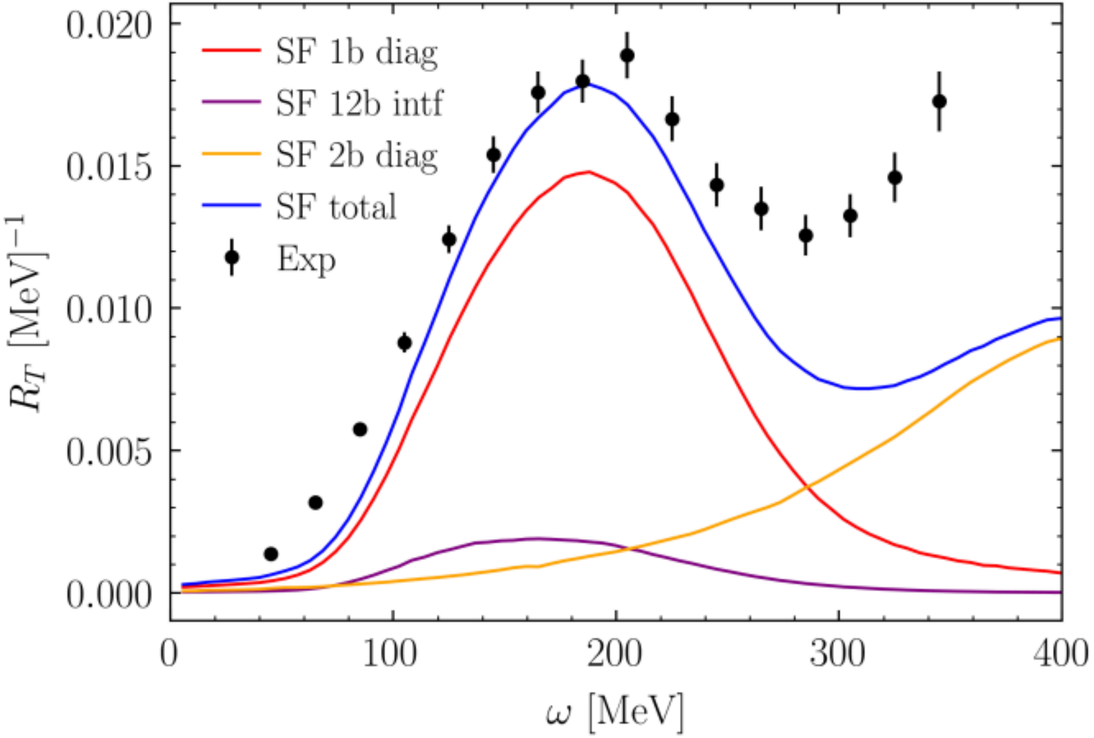
A. Fabrocini, Physical Review C **55**, 338 (1997)

INTERFERENCE "PUZZLE"



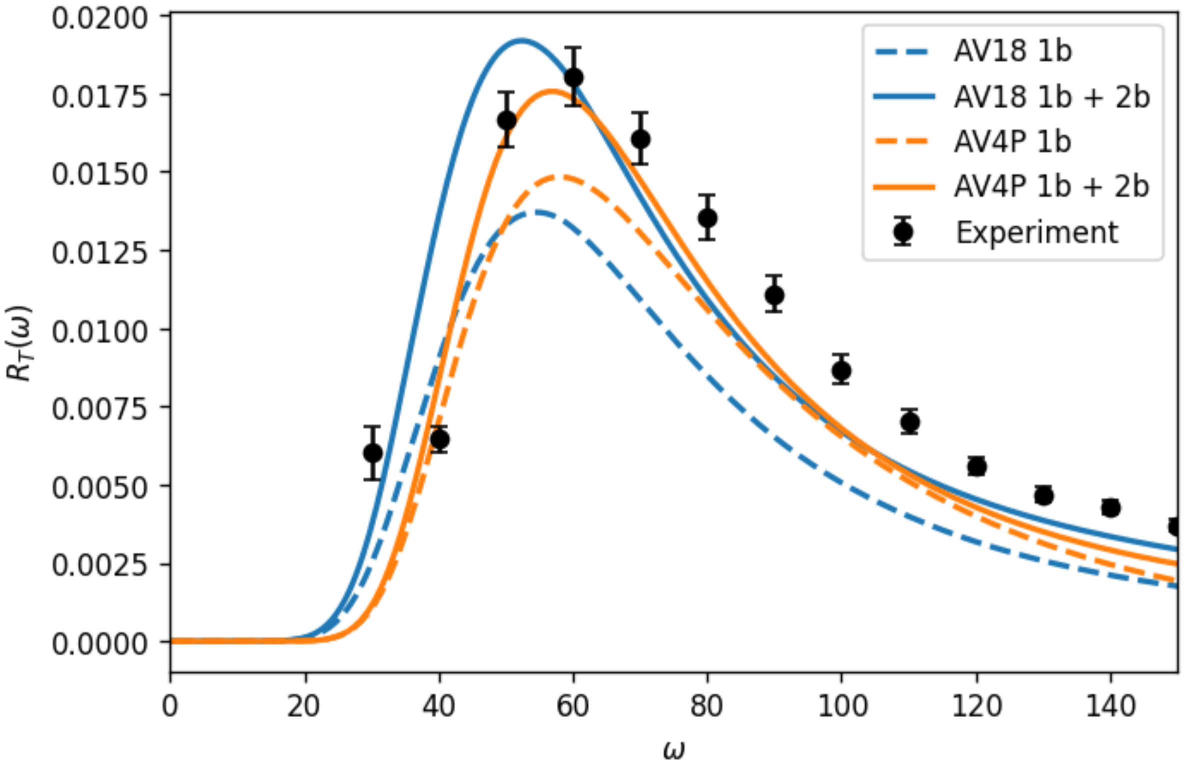
T. Franco-Munoz et al., Phys. Rev. C **108** (2023) 6, 064608

INTERFERENCE “PUZZLE”



AL et al., 2312.12545 [nucl-th]

INTERFERENCE "PUZZLE"



QMC-BASED INTRANUCLEAR CASCADE

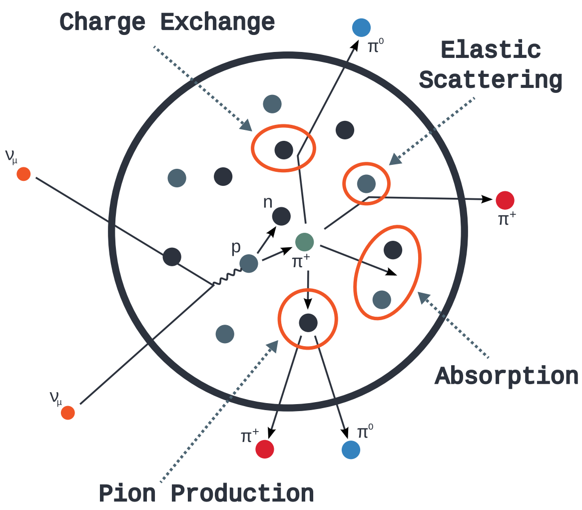


Figure from T. Golan

Ingredients:

- Propagation of particles
- Elastic scattering
- Pion Production
- Pion Absorption

Developed a semi-classical intra-nuclear cascade that assume classical propagation between consecutive scatterings and use QMC configurations as inputs;

QMC-BASED INTRANUCLEAR CASCADE

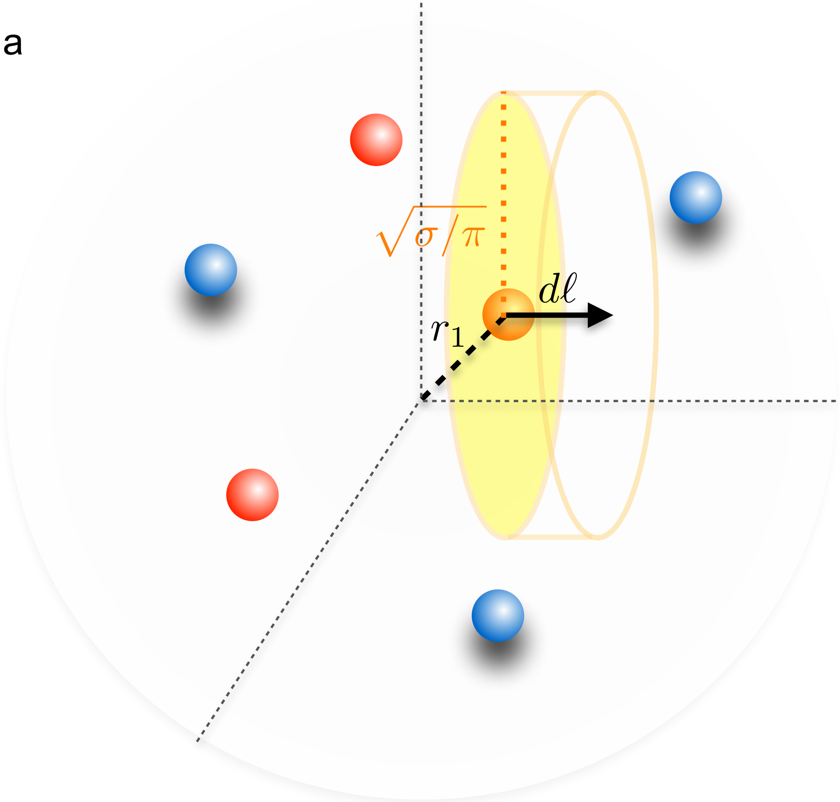
Accept/reject algorithm based on a “cylinder” and a “gaussian” distributions

$$P_{\text{cyl}}(b) = \theta(\sigma/\pi - b^2)$$

$$P_{\text{Gau}}(b) = \exp\left(-\frac{\pi b^2}{\sigma}\right)$$

A standard mean free path approach is also implemented

$$P_{\text{int}} = (\rho_p \sigma_p + \rho_n \sigma_n) d\ell$$



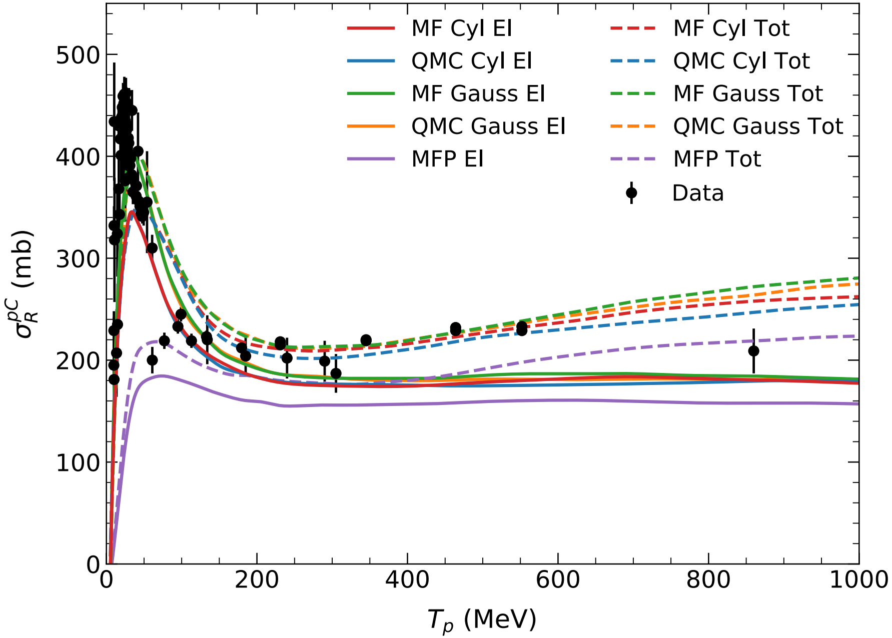
PROTON-CARBON CROSS SECTION

- Define a proton bean with kinetic energy T_p, uniformly distributed over A

- Propagate each proton in time and check for scattering at each step;

- Monte Carlo cross section defined as:

$$\sigma_{\mathrm{MC}} = A\frac{N_{\mathrm{scat}}}{N_{\mathrm{tot}}}$$

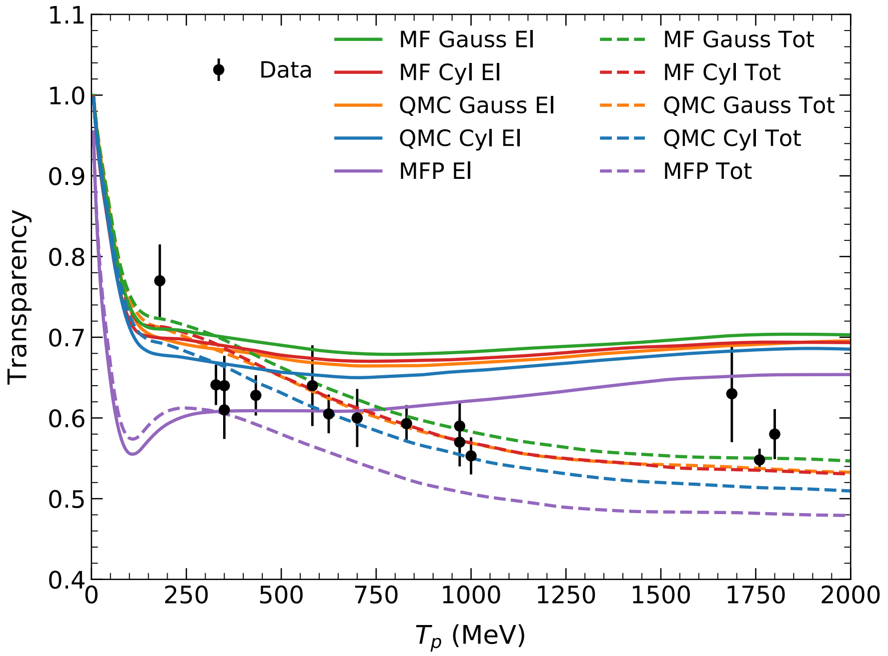


*J. Isaacson, et al., Physical Review C **103**, 015502 (2021)*

NUCLEAR TRANSPARENCY

- Randomly sample a nucleon inside the nucleus from our configurations
- Give the nucleon a kinetic energy T_p and propagate it in the nuclear medium

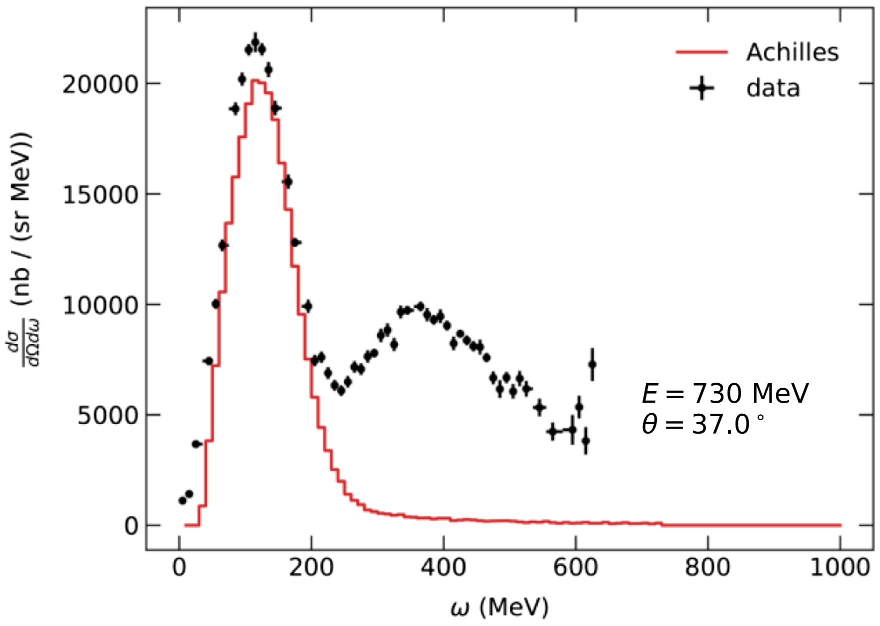
$$T_{\mathrm{MC}} = 1 - \frac{N_{\mathrm{hits}}}{N_{\mathrm{tot}}}$$

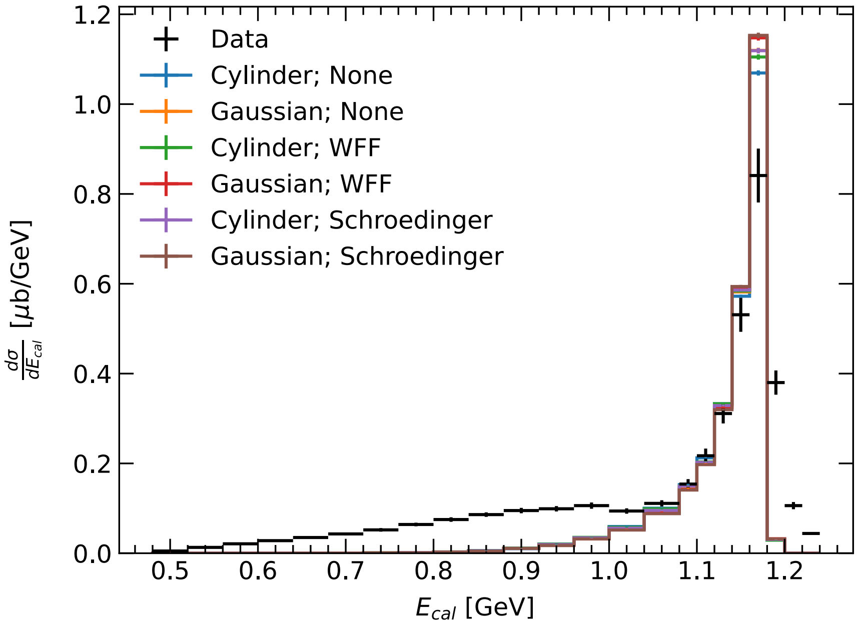


*J. Isaacson, et al., Physical Review C **103**, 015502 (2021)*

ACHILLES

"A CHIcago Land Lepton Event Simulator", ACHILLES.

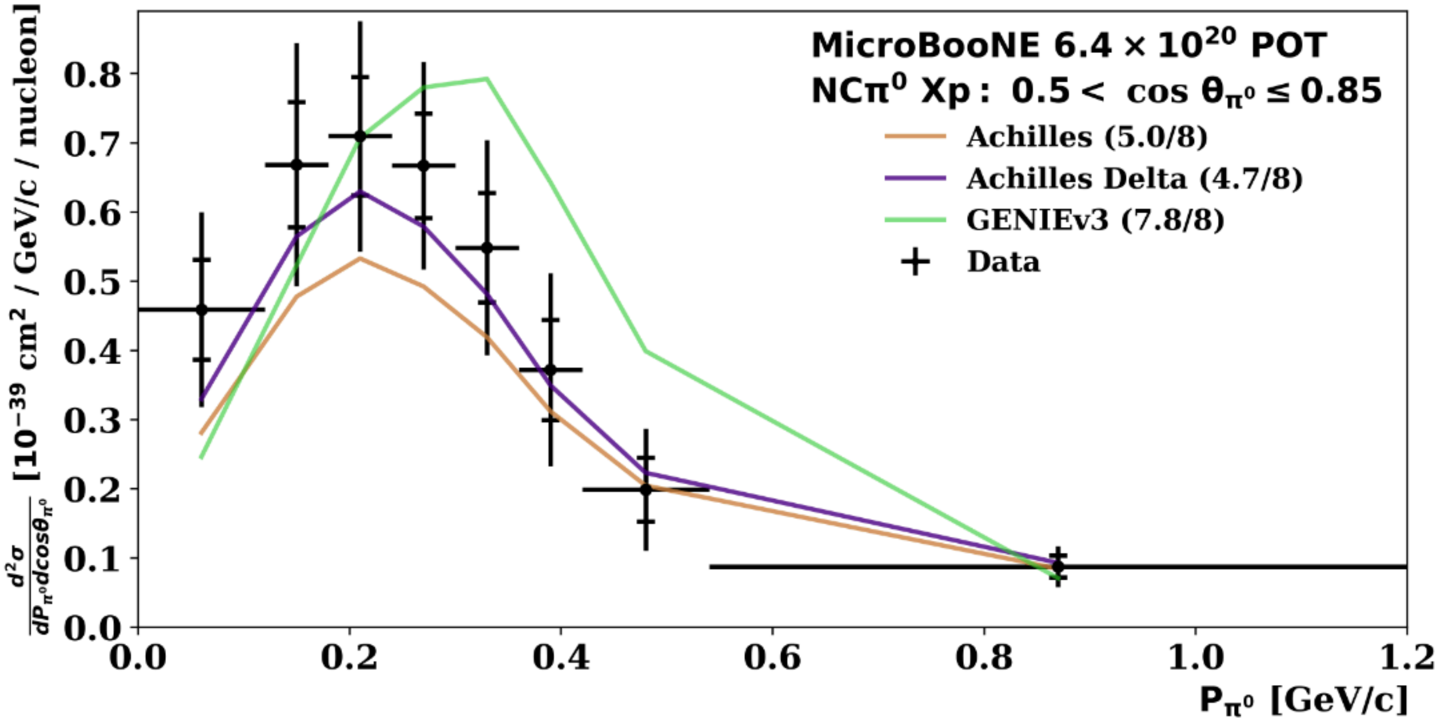




*J. Isaacson, et al., Physical Review D **107**, 033007 (2023)*

ACHILLES

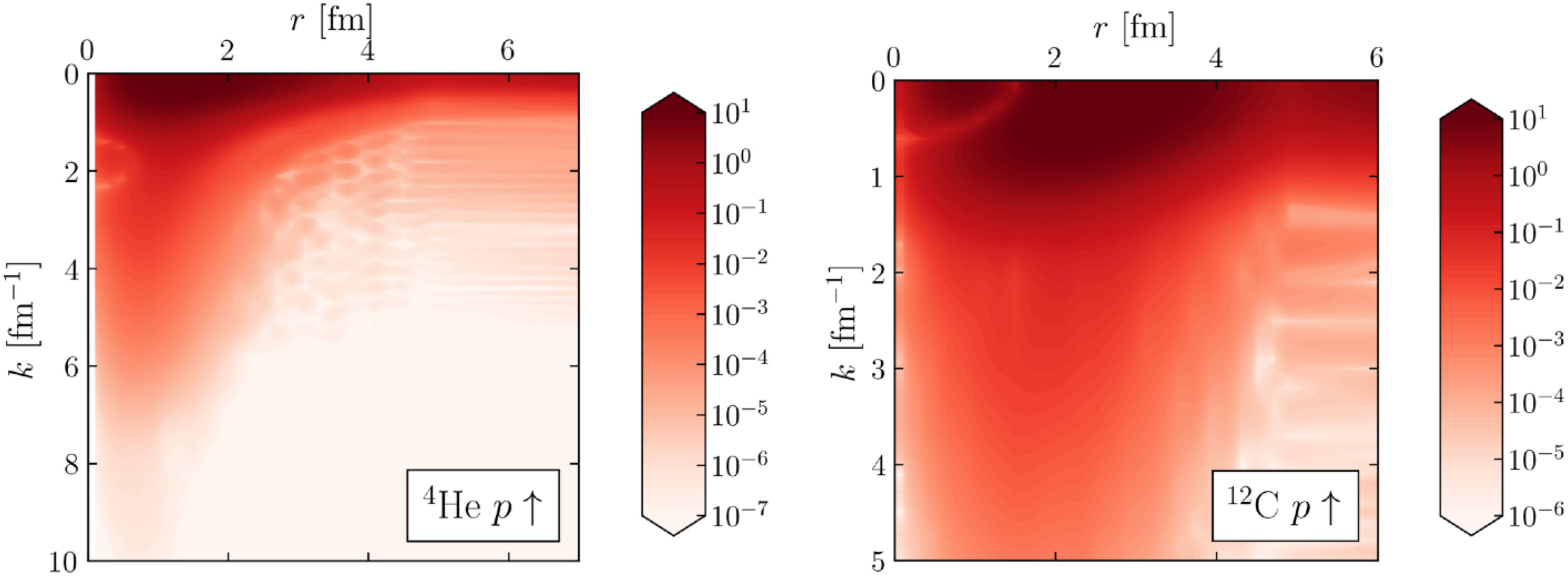
Included pion-production based on the DCC model and consistent pion propagation



J. Isaacson, N. Steinberg et al., in preparation

WIGNER FUNCTIONS

Wigner quasi-probability distributions retain the correlations between positions and momenta



A. Tropiano, N. Rocco, R. B. Wiringa, in preparation

CONCLUSIONS AND OUTLOOK

- QMC methods allow for a multi-scale description of atomic nuclei, including:
  - ➡ Response functions.
  - ➡ Coordinate and momentum-space distributions.
  - ➡ Wigner quasi-probability distributions.
  - ➡ Spectral functions (not shown in this talk)
- NQS are promising to extend the QMC to larger systems and to low-energy responses
  - ➡ Inclusion of high-resolution interactions underway (positive test in cold atoms).
  - ➡ Real-time dynamics in progress.
- The extended factorization scheme allows to reach larger energy and model pion production
  - ➡ Ongoing implementation in ACHILLES