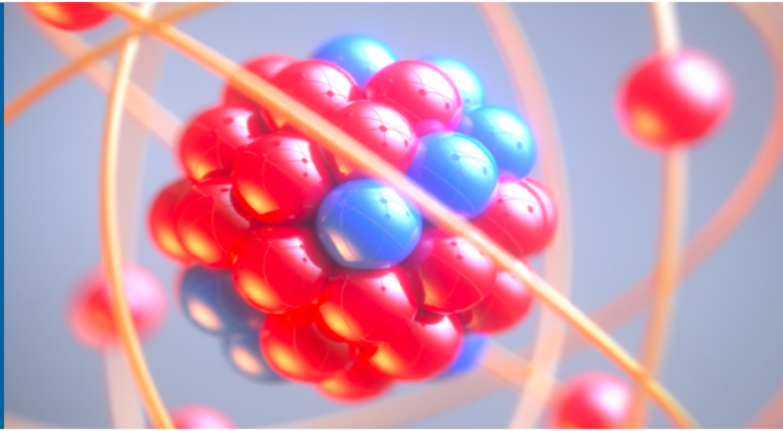
UNCERTAINTY QUANTIFICATION IN QMC CALCULATIONS OF LEPTON-NUCLEUS SCATTERING



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Argonne NATIONAL LABORATORY

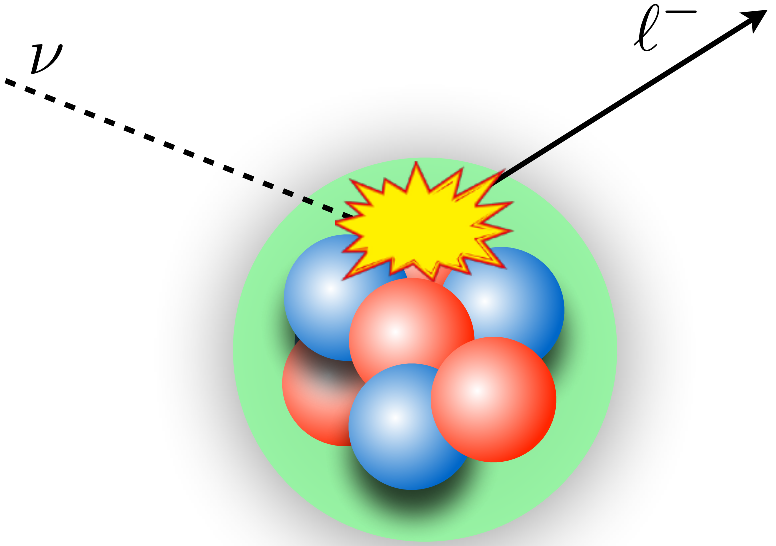
Theoretical Physics Uncertainties to Empower Neutrino Experiments

Seattle, October 31, 2023

INTRODUCTION

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

$$N_{\rm near} \approx \int dE\, \Phi_{\rm near}(E) \times \underline{\sigma(E)} \qquad N_{\rm far} \approx \int dE\, P(E) \times \Phi_{\rm far}(E) \times \underline{\sigma(E)}$$



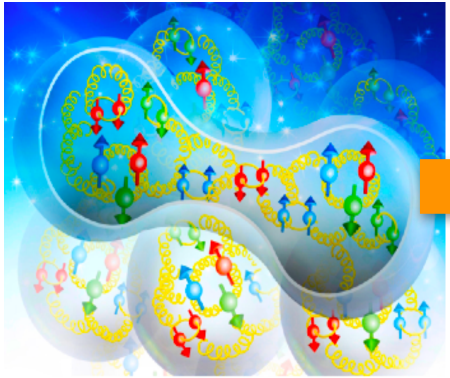
PART 1

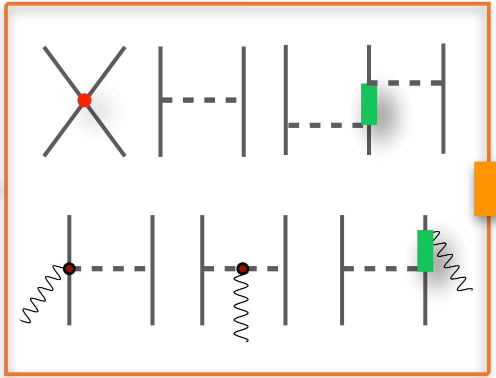
THE NUCLEAR MANY-BODY PROBLEM

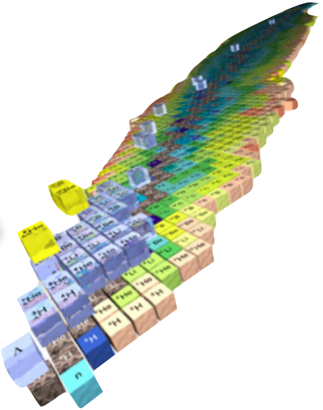
THE NUCLEAR MANY-BODY PROBLEM

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 connect QCD with nuclear observables.



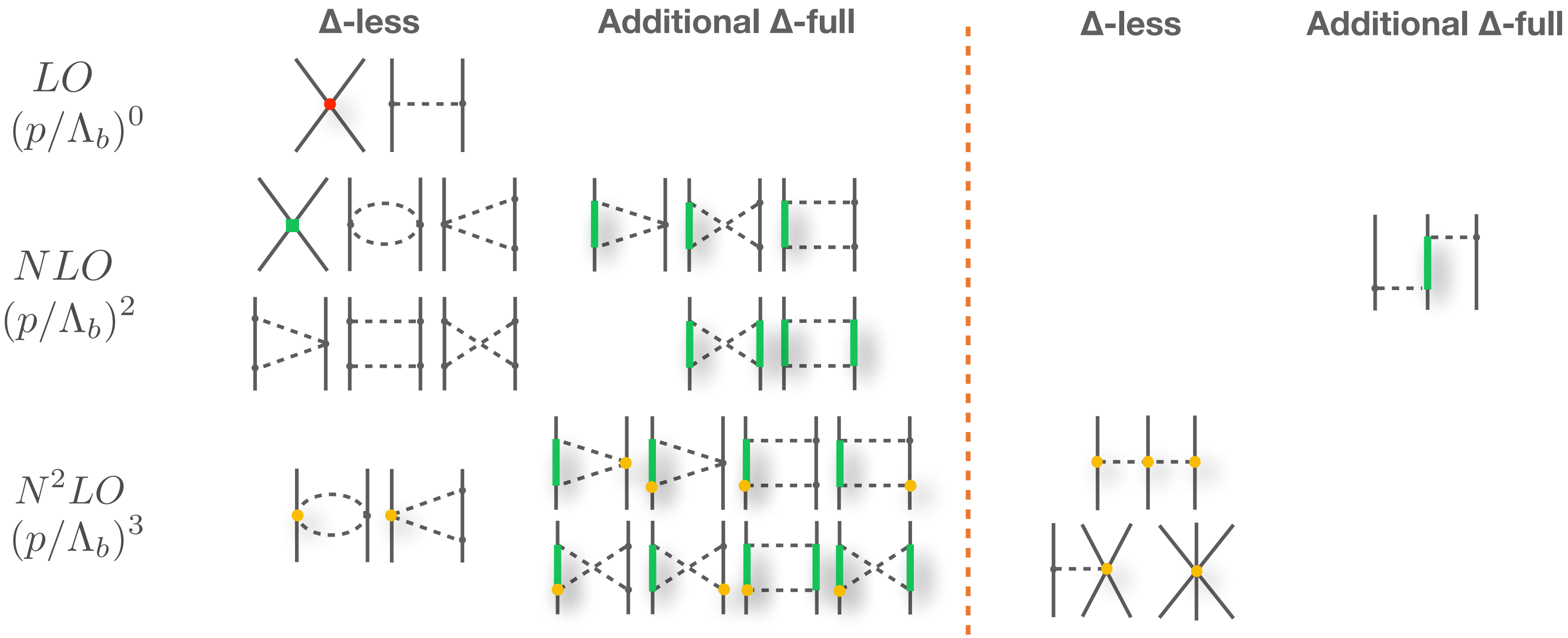




$$H = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk} \qquad J = \sum_i j_i + \sum_{i<j} j_{ij}$$

NUCLEAR HAMILTONIANS

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



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

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

UQ FOR NUCLEAR HAMILTONIANS

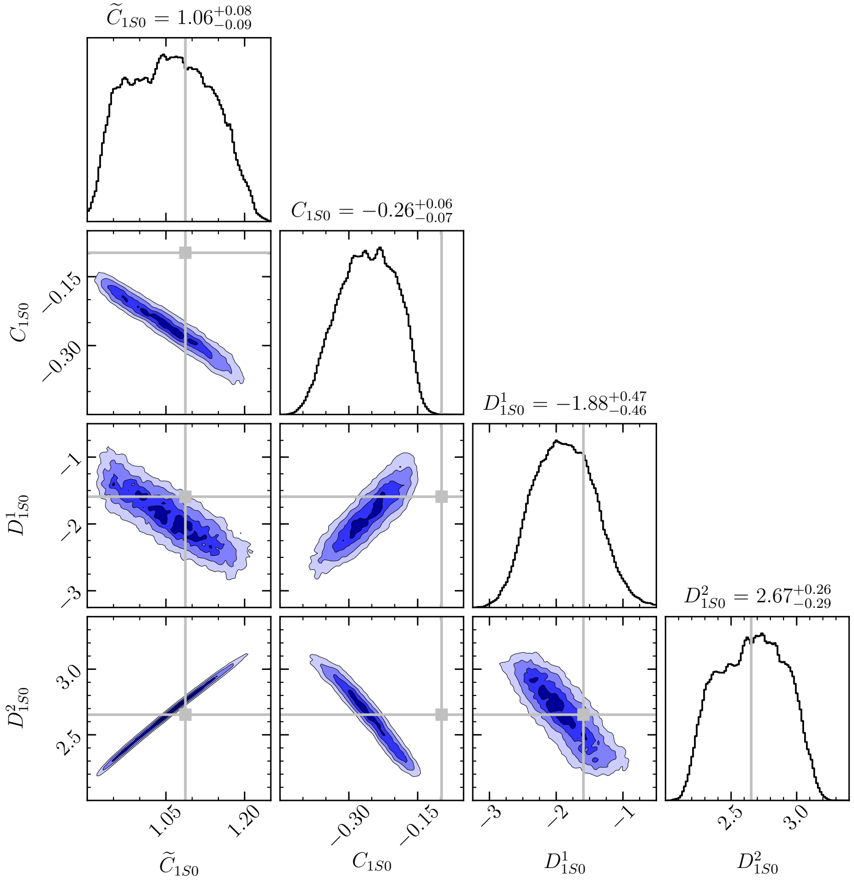
- EFTs enables to rigorously estimate the uncertainties originating in the nuclear Hamiltonian
- Bayesian frameworks recently developed for parameter estimation in nuclear EFTs
- Correlations among different low-energy constants

S. Wesolowski et al., Phys.Rev.C 104 (2021) 6, 064001

S. Wesolowski et al., J. Phys. G 46 (2019) 4, 045102

R. J. Furnstahl et al., Phys. Rev. C 92 (2015) 2, 024005

R. J. Furnstahl et al., J.Phys. G 42 (2015) 3, 034028



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SOLVING THE NUCLEAR MANY-BODY PROBLEM

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

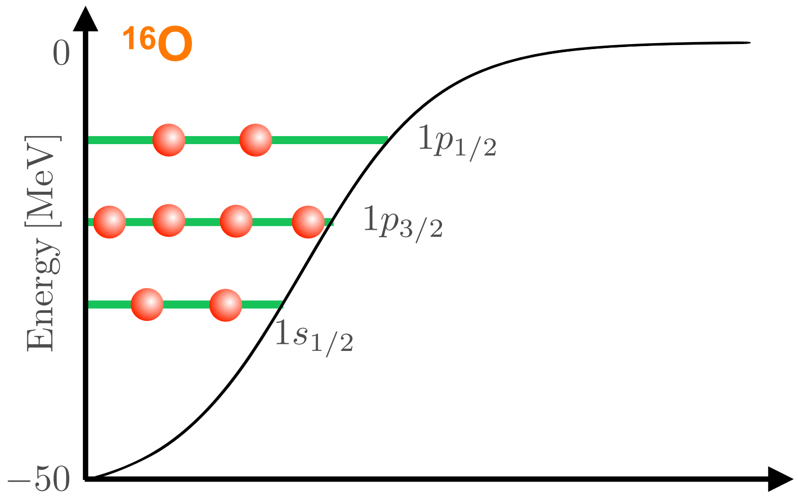
$$H\Psi_0(x_1,\dots,x_A) = E_0\Psi_0(x_1,\dots,\dots,x_A) \quad \longleftrightarrow \quad x_i \equiv \{\mathbf{r}_i, s_i^z, t_i^z\}$$

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

- Mean field: the ground-state wave function is a single Slater determinant

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

- Only statistical, no dynamical correlations



CONFIGURATION-INTERACTION METHODS

The exact ground-state wave function can be expressed as a sum of Slater determinants

$$\Psi_0(x_1,\dots,x_A)=\sum_n c_n\Phi_n(x_1,\dots,x_A)$$

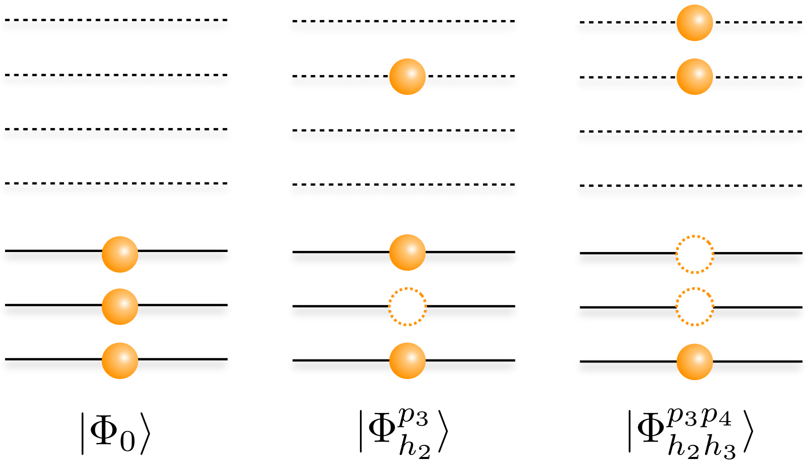
The occupation-number representation automatically encompass the fermion antisymmetry

$$|\Psi_0\rangle = \sum_{h_1\dots,p_1\dots} c_{h_1\dots}^{p_1\dots}|\Phi_{h_1\dots}^{p_1\dots}\rangle$$

$$|\Phi_{h_1\dots}^{p_1\dots}\rangle = a_{p_1}^\dagger \dots a_{h_1}\dots|\Phi_0\rangle$$

The dimensionality explodes quickly

$$\binom{N}{A}=\frac{N!}{(N-A)!A!}$$

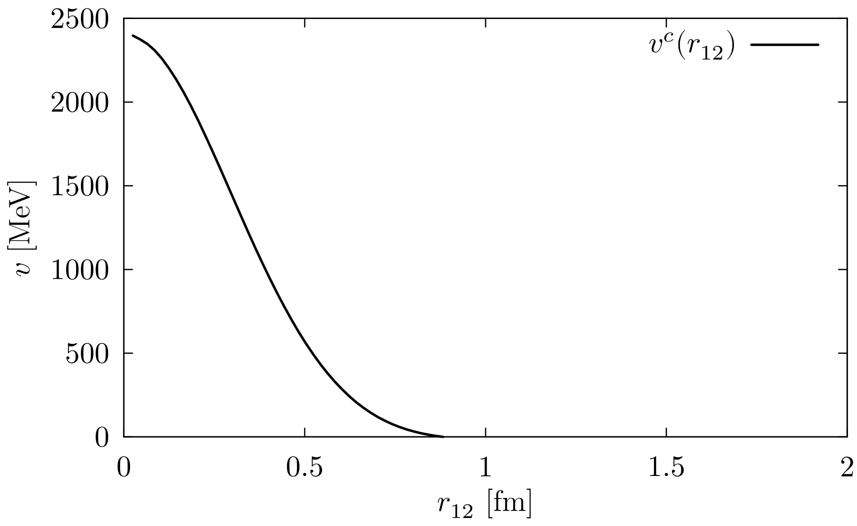


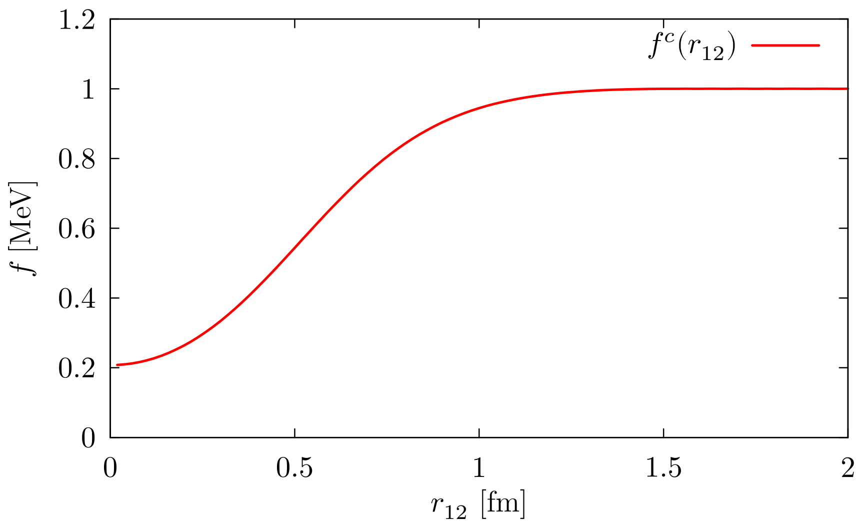
VARIATIONAL MONTE CARLO

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

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

The correlations are consistent with the underlying nuclear interaction





GREEN'S FUNCTION MONTE CARLO

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

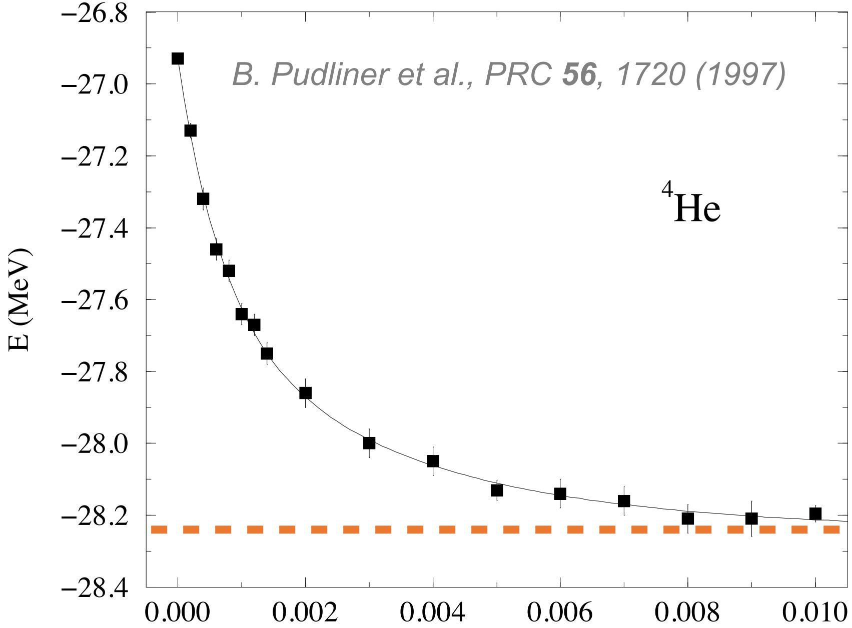
$$|\Psi_T\rangle = \sum_n c_n |\Psi_n\rangle \qquad H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

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.

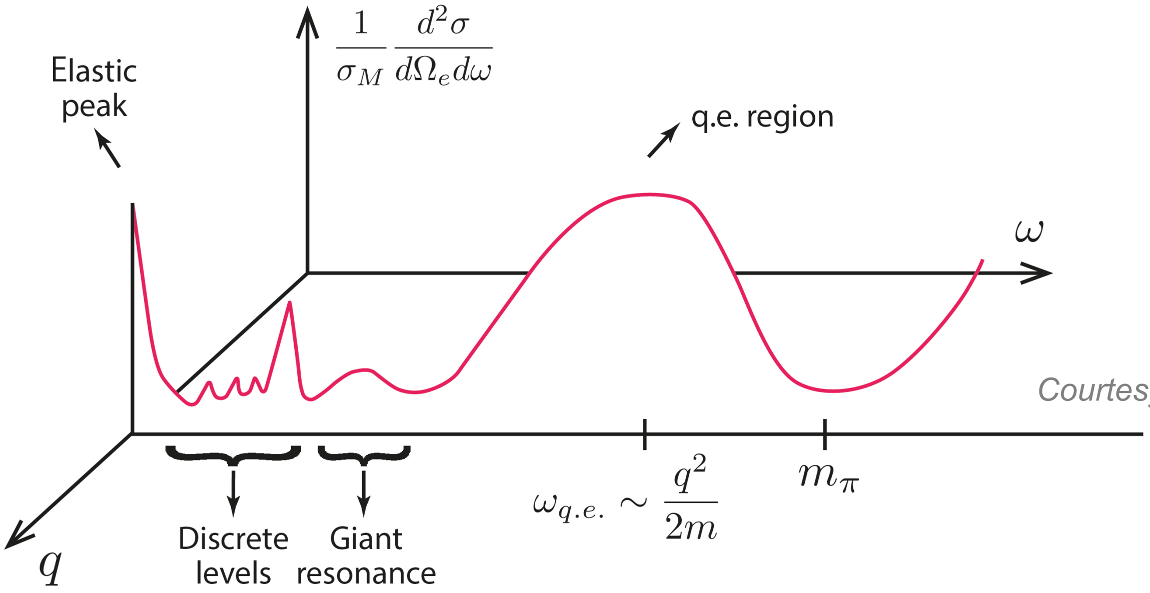


PART 2.A.

INCLUSIVE LEPTON-NUCLEUS SCATTERING

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

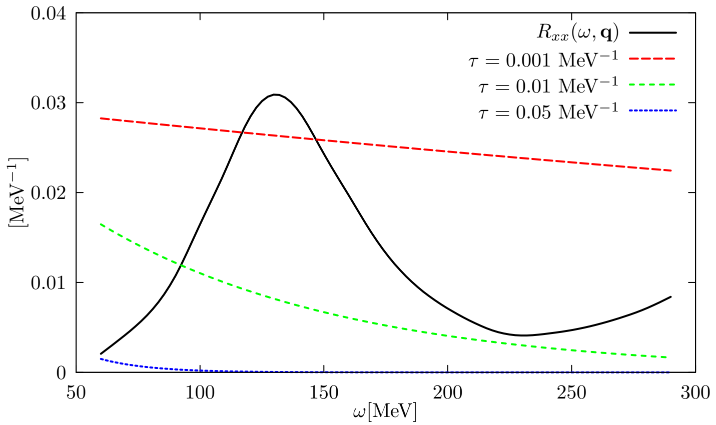
$$R_{\alpha\beta}(\omega, \mathbf{q}) = \sum_f \langle\Psi_0|J_\alpha^\dagger(\mathbf{q})|\Psi_f\rangle\langle\Psi_f|J_\beta(\mathbf{q})|\Psi_0\rangle\delta(\omega - E_f + E_0)$$

EUCLIDEAN RESPONSES

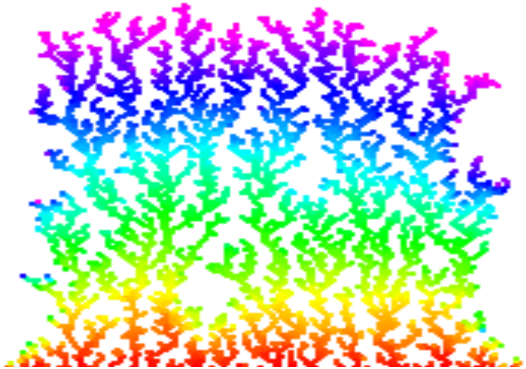
Our GFMC calculations rely on the Laplace kernel

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

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



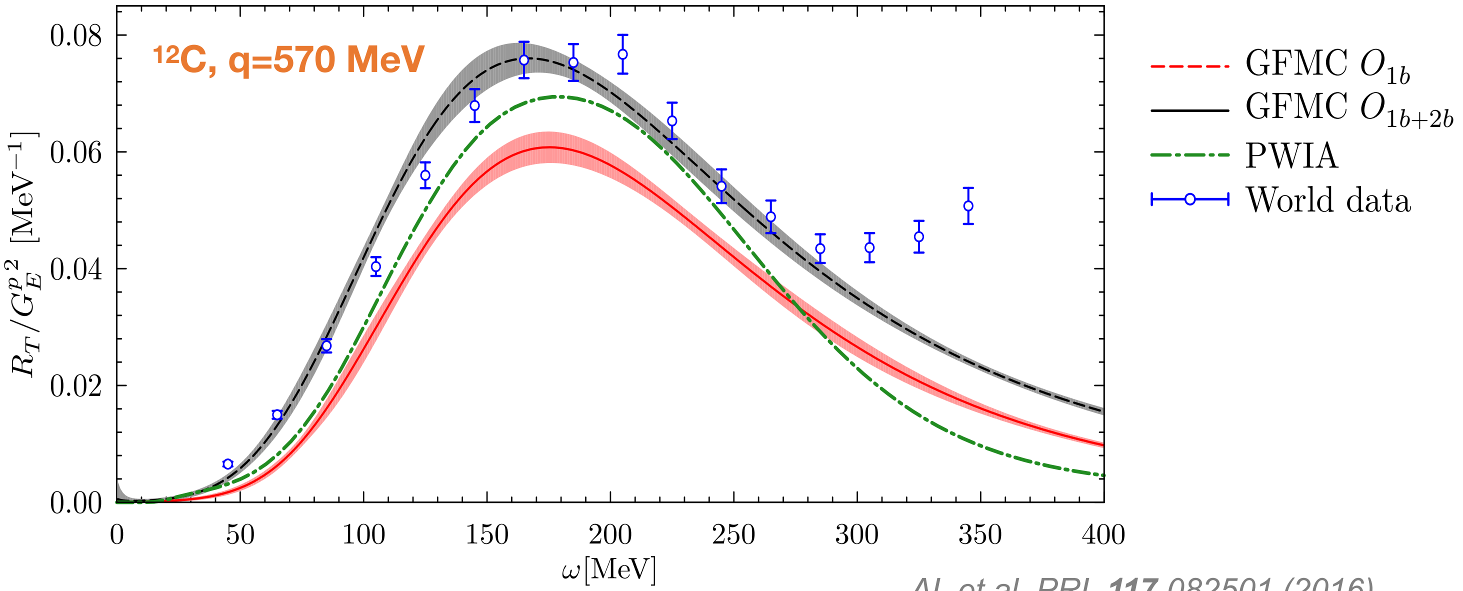
The system is first heated up by the transition operator. Its cooling determines the Euclidean response of the system



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

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

VALIDATION WITH ELECTRON SCATTERING



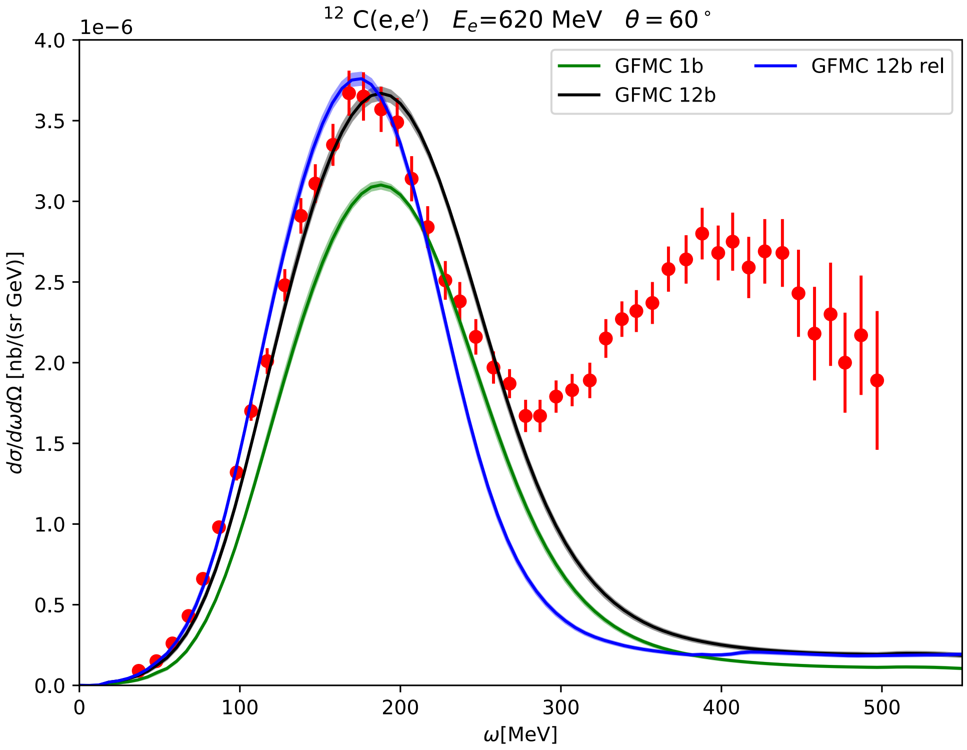
*AL et al. PRL **117** 082501 (2016)*

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

VALIDATION WITH ELECTRON SCATTERING

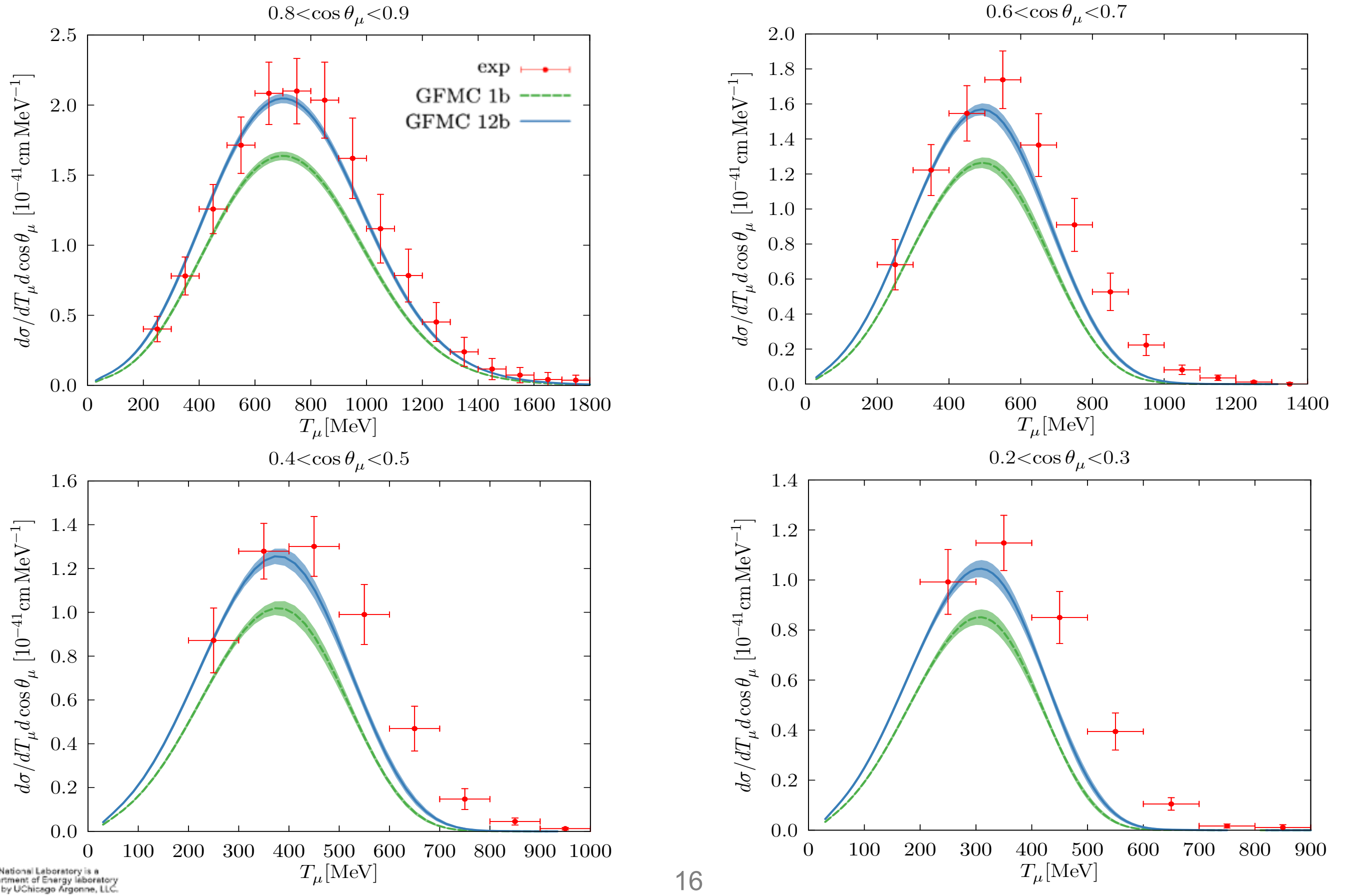
Included relativistic effects in inclusive cross section



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

MINIBOONE CROSS SECTIONS

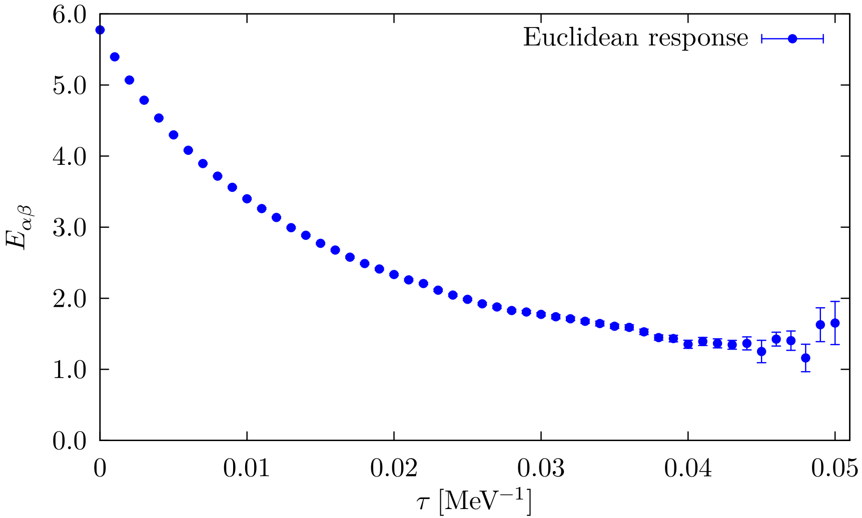
*AL et al., PRX **10**, 031068 (2020)*

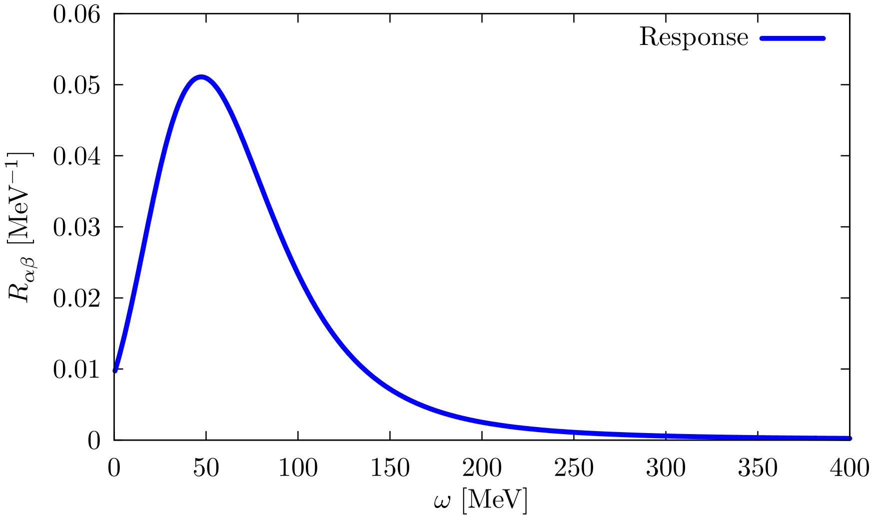


UQ IN INVERTING THE LAPLACE TRANSFORM

Inverting the Euclidean response is an ill posed problem: any set of observations is limited and noisy and the situation is even worse since the kernel is a smoothing operator.

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





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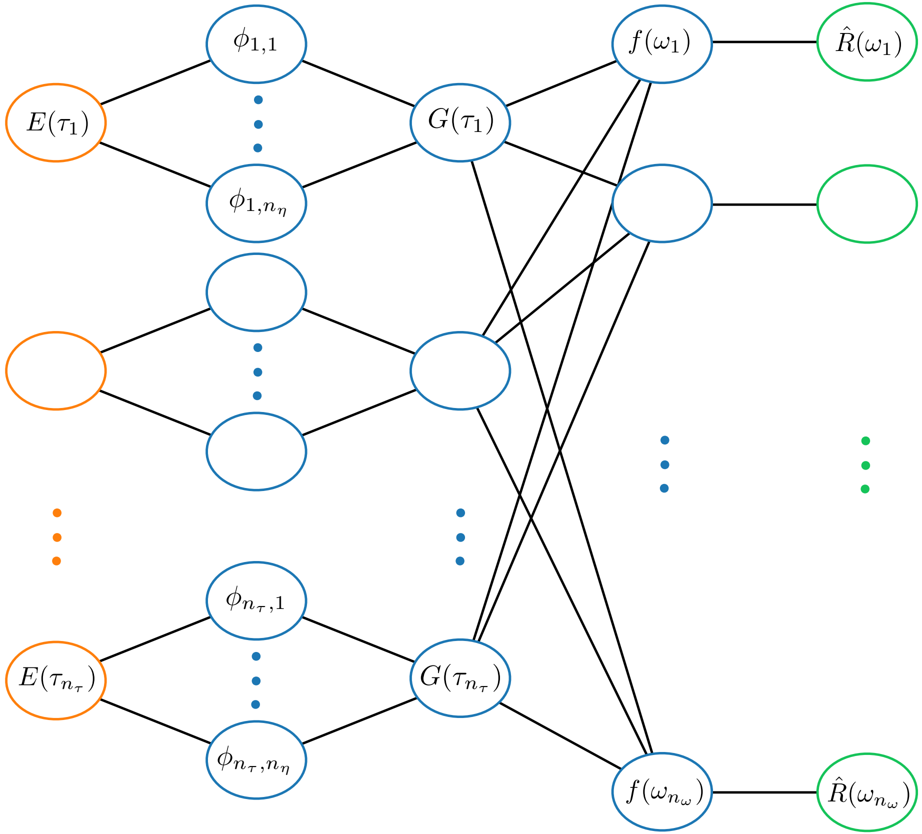
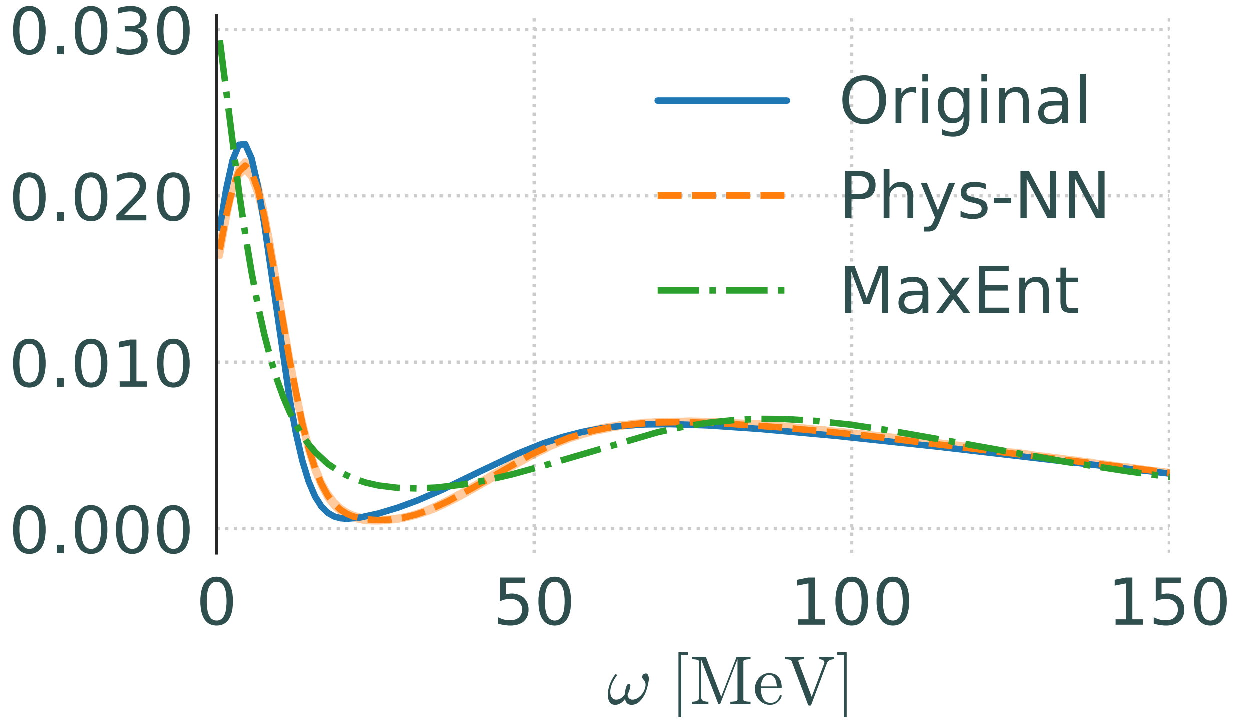


*K. Raghavan, AL, al., PRC **103**, 035502 (2021)*

UQ IN INVERTING THE LAPLACE TRANSFORM



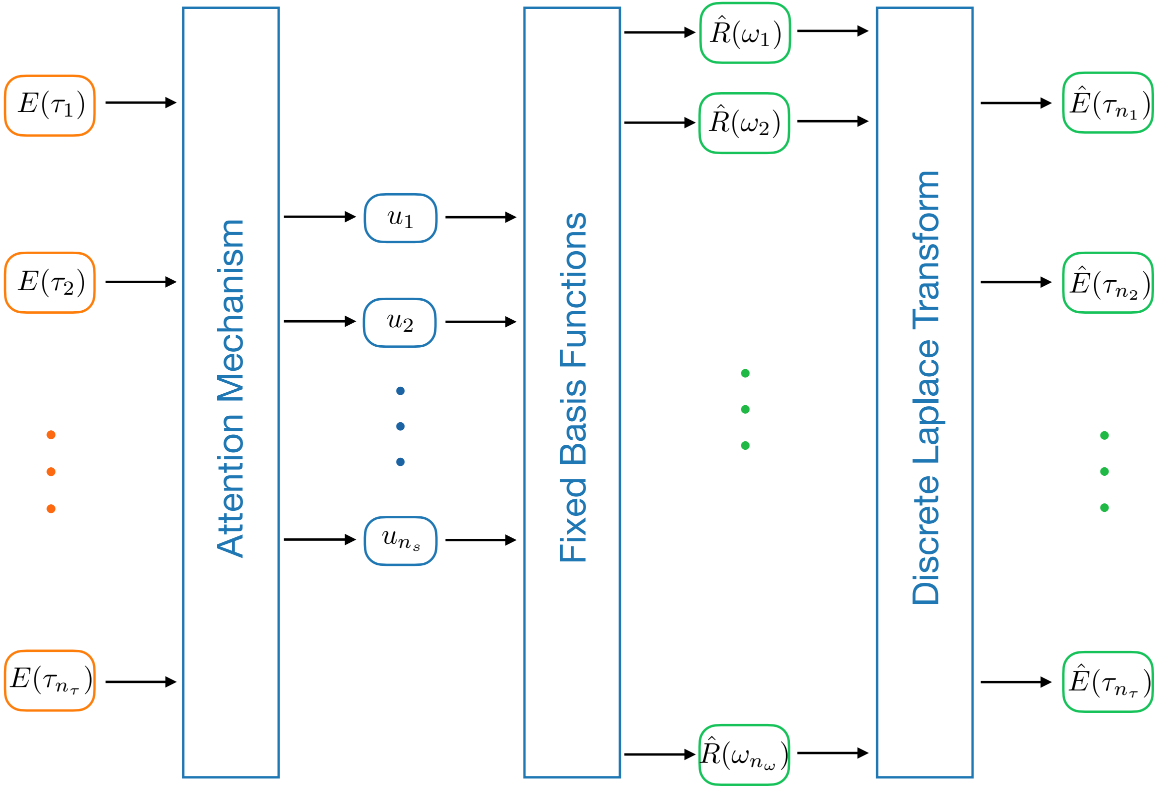
UQ IN INVERTING THE LAPLACE TRANSFORM

Expand in a basis function inspired by MaxEnt

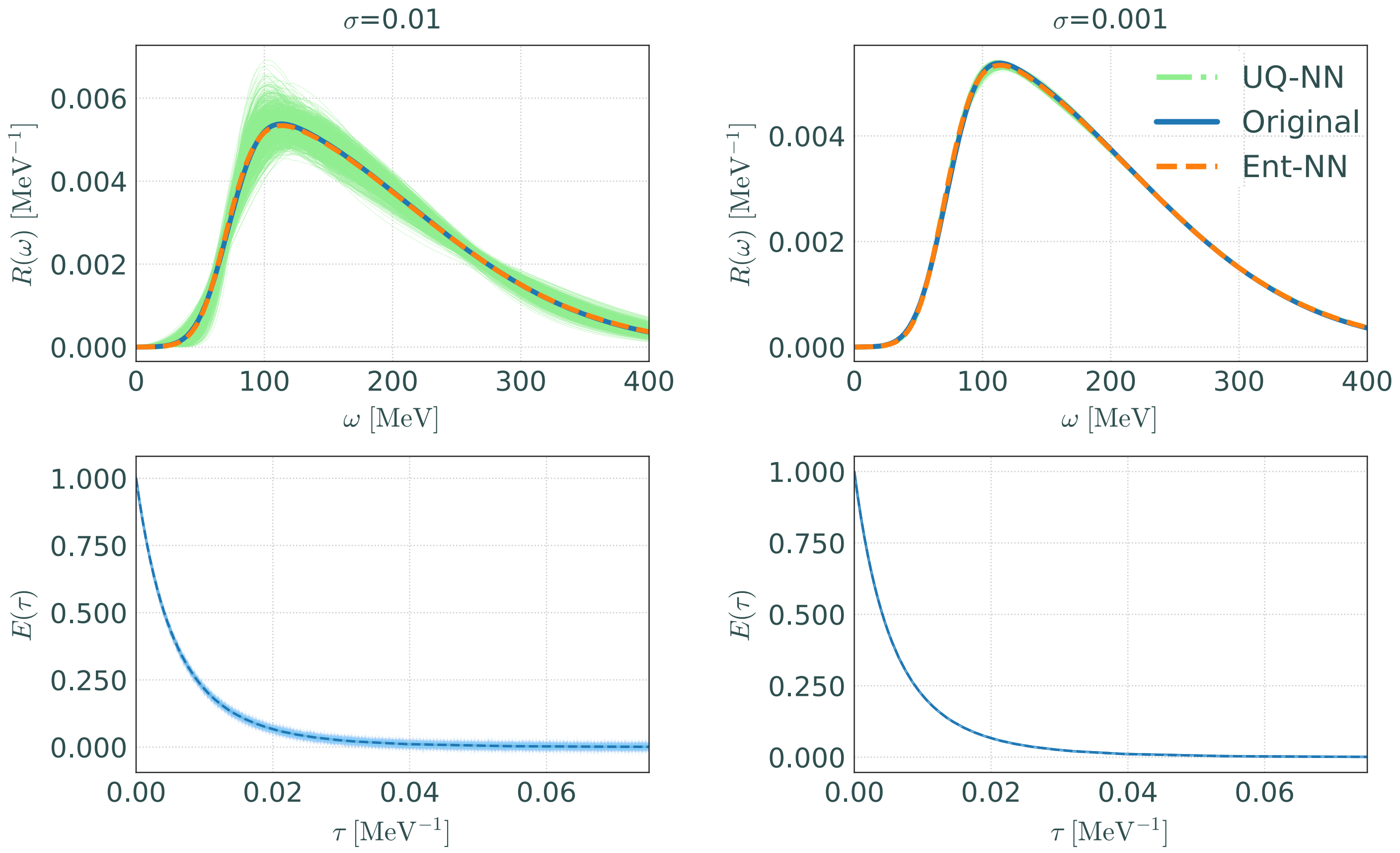
$$\begin{cases} R_i = M_i \exp\left(\sum_{j=1}^{n_s} U_{ij} u_j\right) \\ K = V \Sigma U^T \\ K_{ij} = e^{-\omega_j \tau_i} \Delta\omega_j \end{cases}$$

Augment the training dataset with noisy Euclidean responses

$$E_i^\sigma = \bar{E}_i + \epsilon_i \,,$$

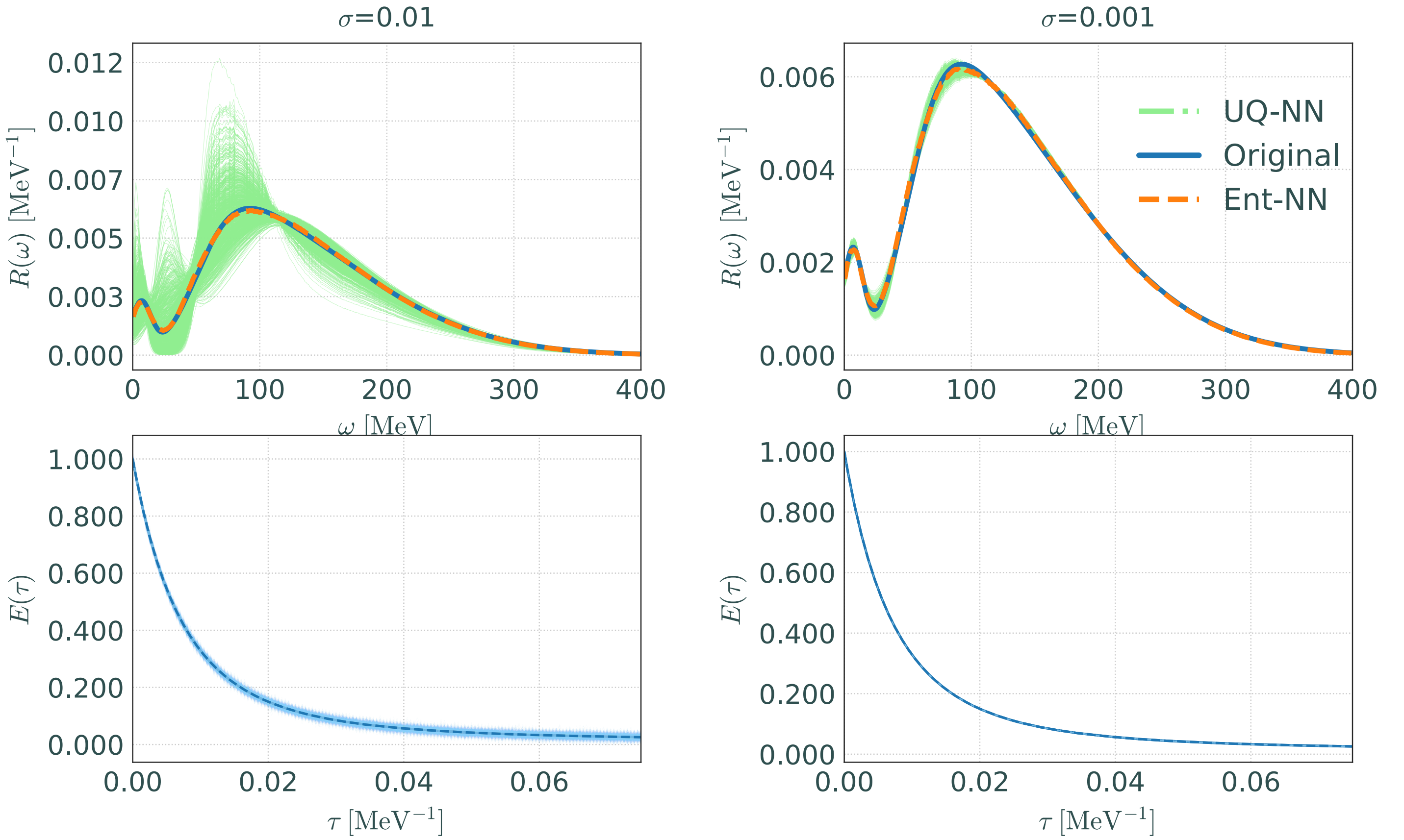


UQ IN INVERTING THE LAPLACE TRANSFORM



K. Raghavan, AL, al., arXiv:

UQ IN INVERTING THE LAPLACE TRANSFORM



K. Raghavan, AL, al., arXiv:

PART 2.B.
ELEMENTARY AMPLITUDES INPUT

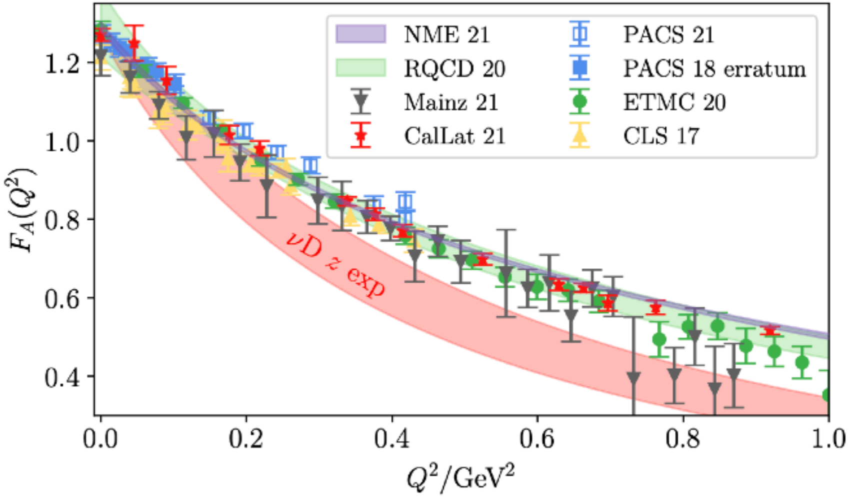
AXIAL FORM FACTOR

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

Scarce (old) experimental data available

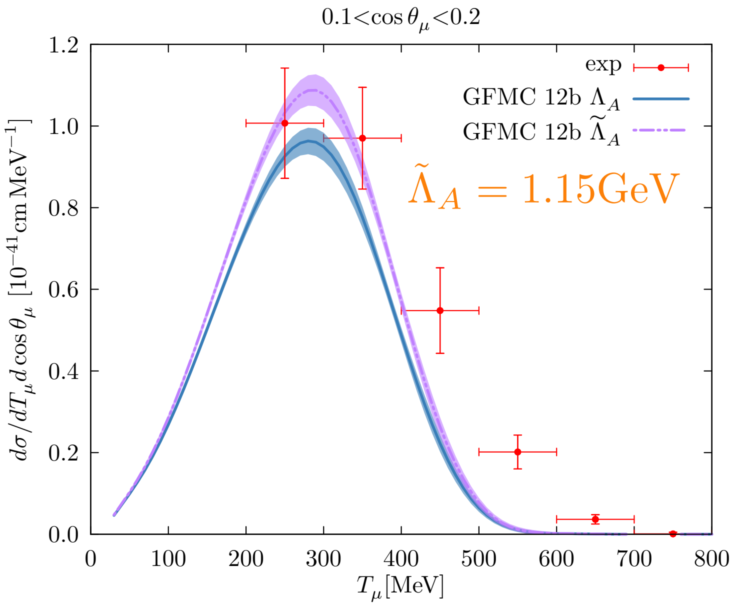
↕

Lattice-QCD calculations are essential



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

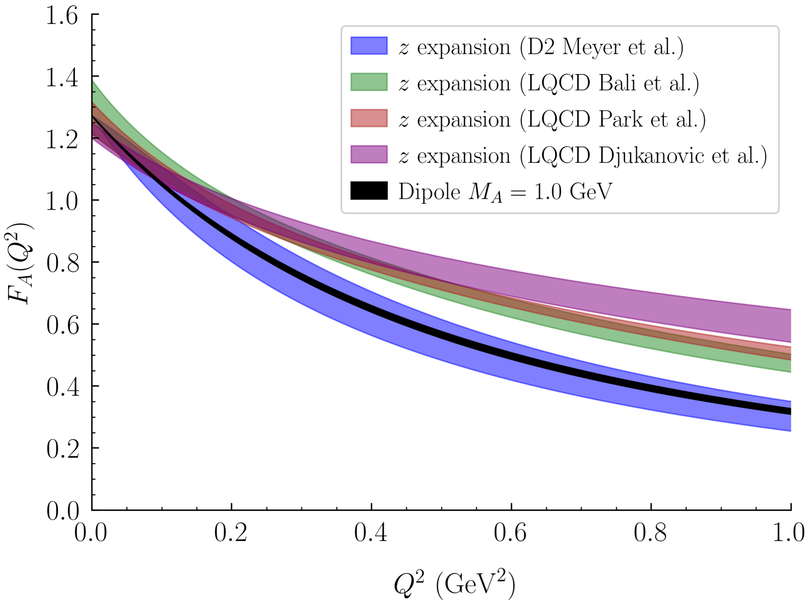
We have considered a value of the axial mass more in line with recent LQCD determinations



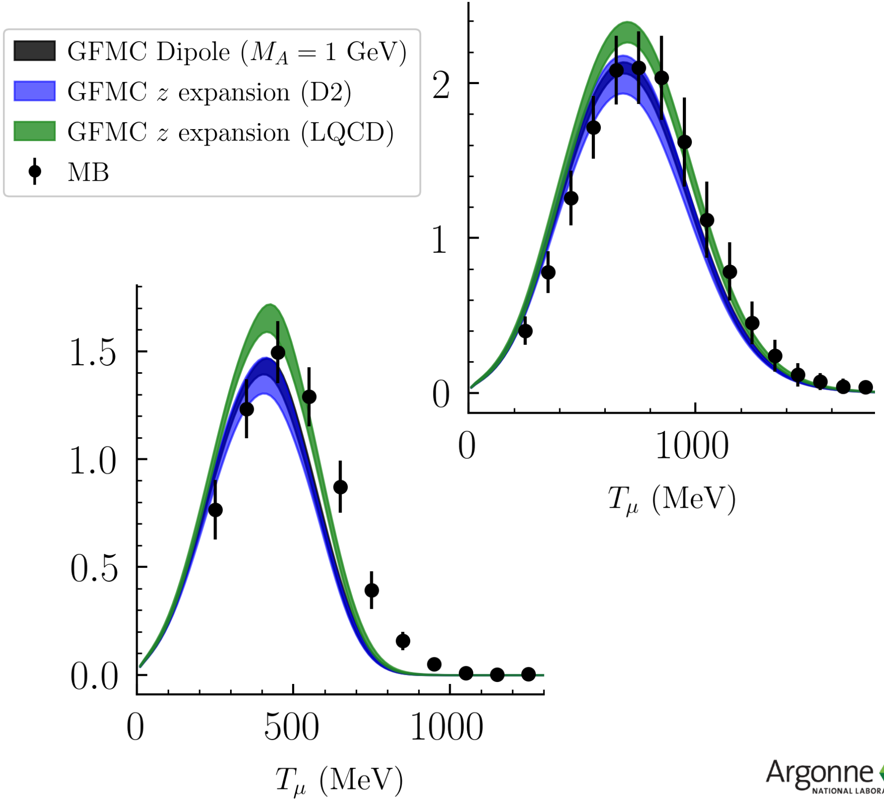
*AL et al., PRX **10**, 031068 (2020)*

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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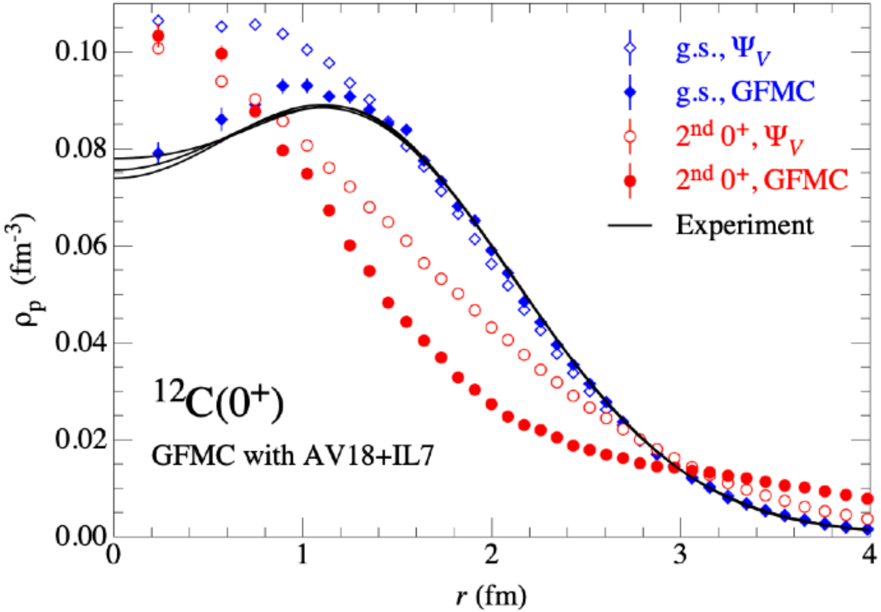
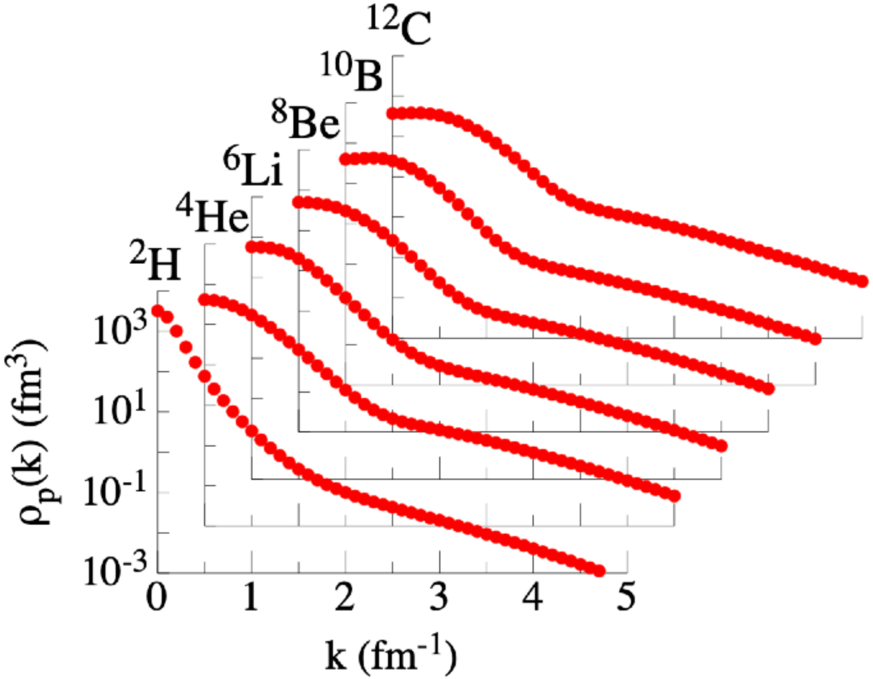
PART 3
DISTRIBUTIONS RELEVANT TO EVENT GENERATORS

SPATIAL AND MOMENTUM DISTRIBUTIONS

QMC methods provide information on the spatial and momentum distributions





J. Carlson et al., Rev. Mod. Phys. 87 (2015) 1067

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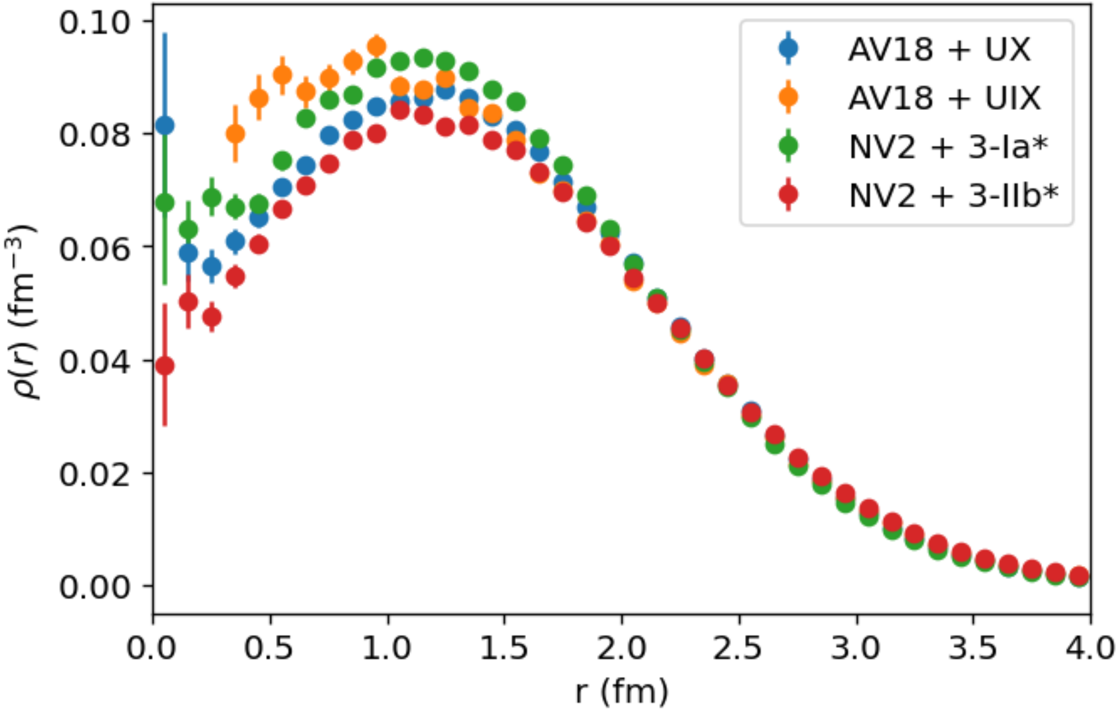
UQ ON SINGLE-NUCLEON DISTRIBUTIONS

UQ using different realistic input Hamiltonians



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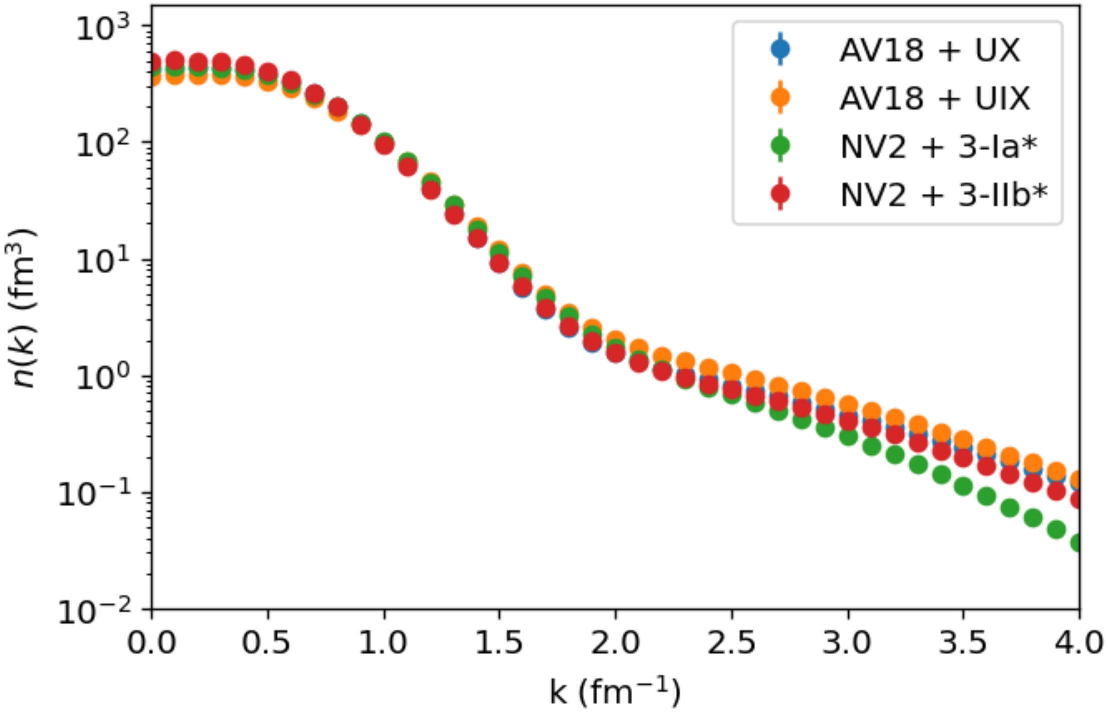
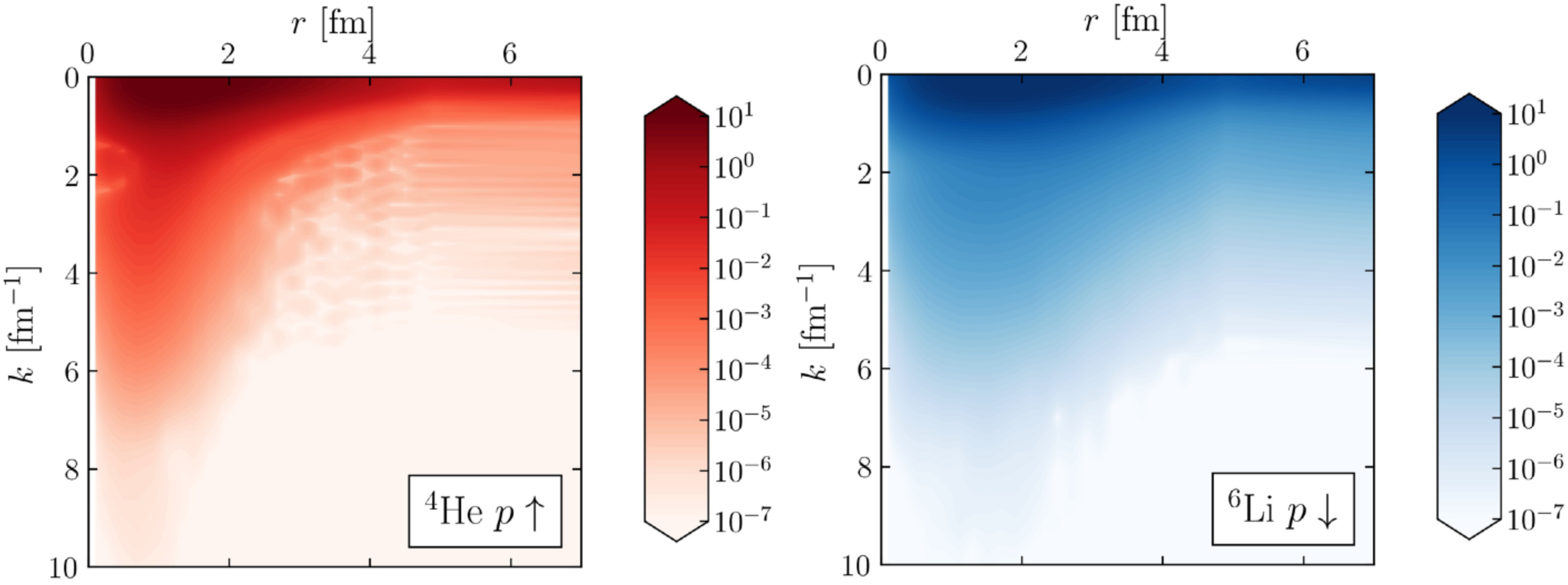


WIGNER FUNCTIONS

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



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

SIMILARITY RENORMALIZATION GROUP

We can use renormalization-group to reduce the resolution of the starting "bare" Hamiltonian

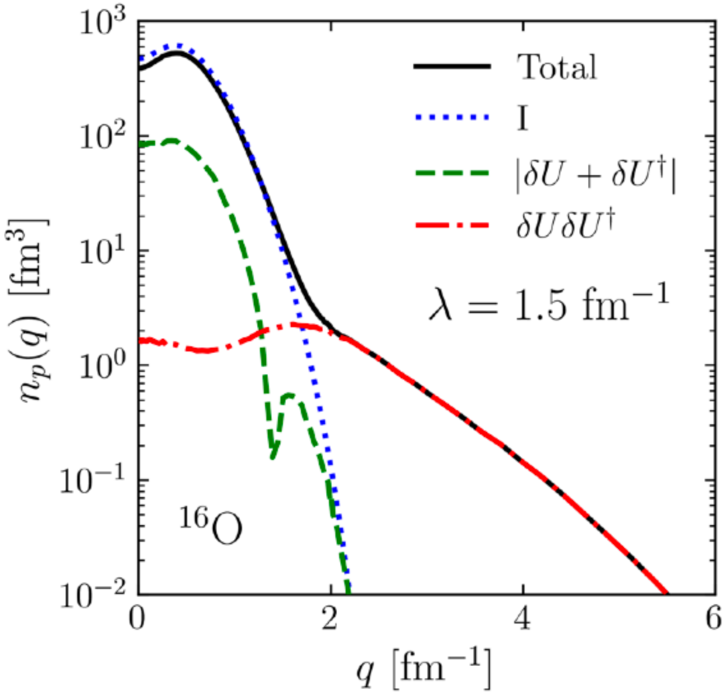
$$H(\lambda) = U(\lambda) H_0 U^\dagger(\lambda)$$

Use low-resolution, mean-field, wave functions and evolved operators

$$n(\mathbf{q}) = \langle \Psi_0 | a^\dagger_{\mathbf{q}} a_{\mathbf{q}} | \Psi_0 \rangle = \langle \Psi_\lambda | a^\dagger_{\mathbf{q}}(\lambda) a_{\mathbf{q}}(\lambda) | \Psi_\lambda \rangle$$

Expand the SRG operator and keep two-body terms only

$$U(\lambda) = 1 + \delta U(\lambda)$$



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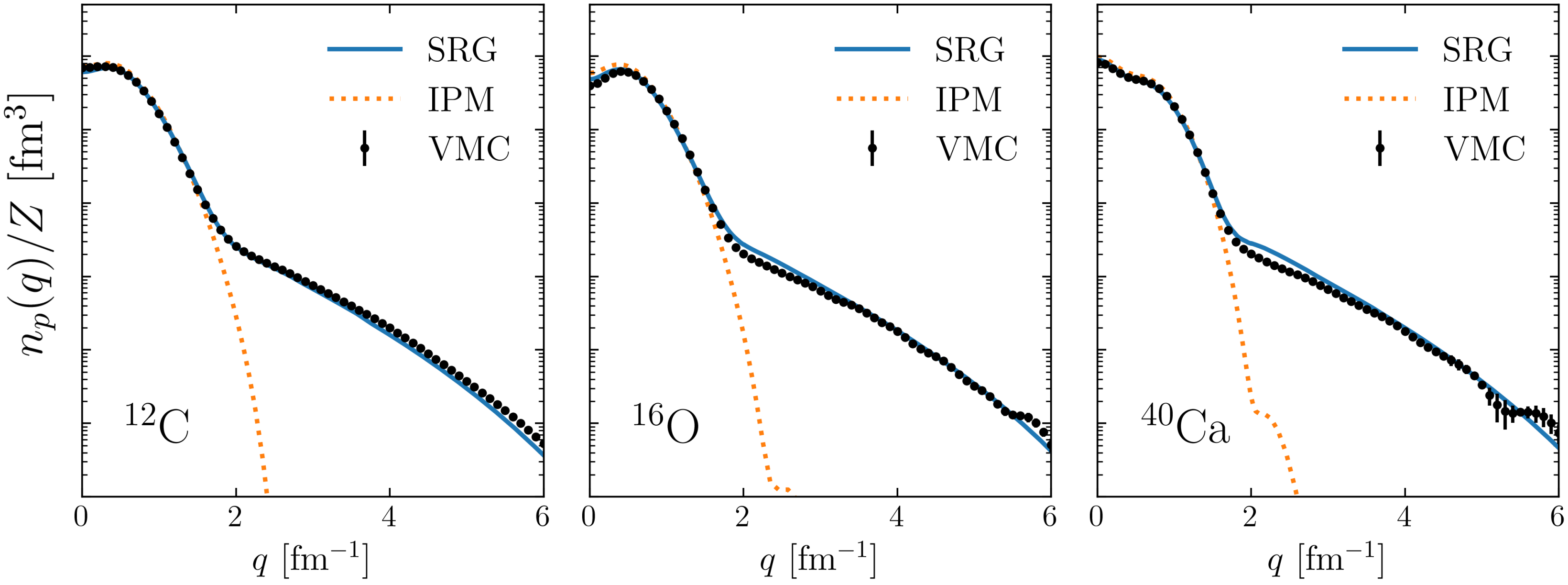


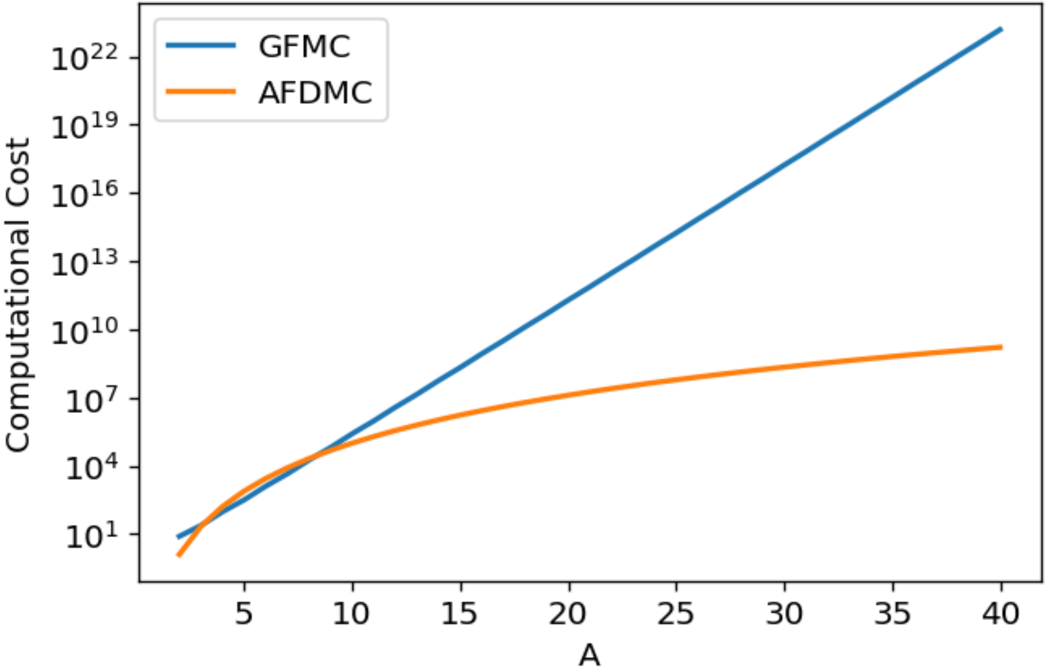
A. Tropiano et al., in preparation

TREAT LARGER NUCLEI

GFMC VS AFDMC

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

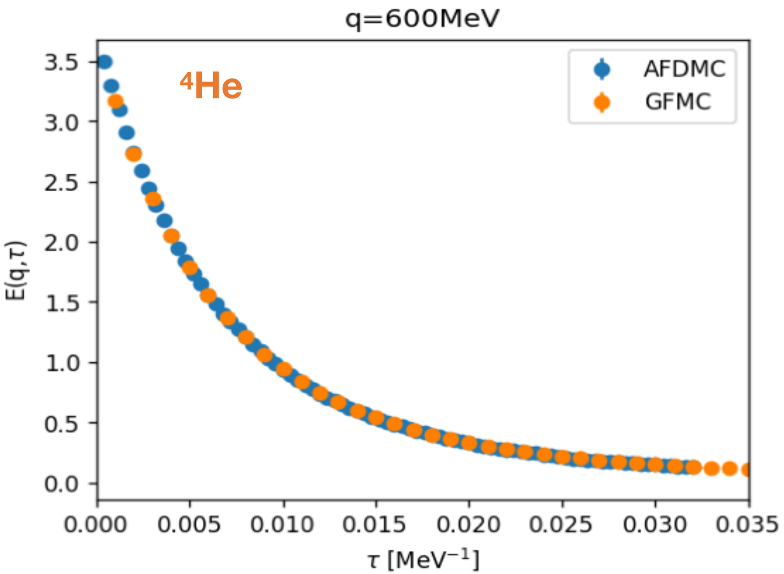
AFDMC: single-spinor basis → $|S\rangle \equiv (u_1|\uparrow\rangle_1 + d_1|\downarrow\rangle_1) \otimes \ldots (u_A|\uparrow\rangle_A + d_A|\downarrow\rangle_A)$

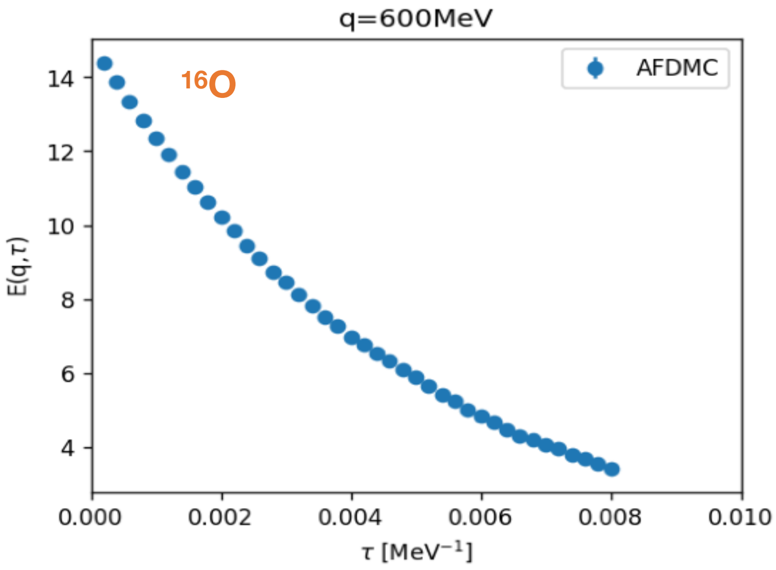


BEYOND ^{12}C WITH THE AFDMC

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

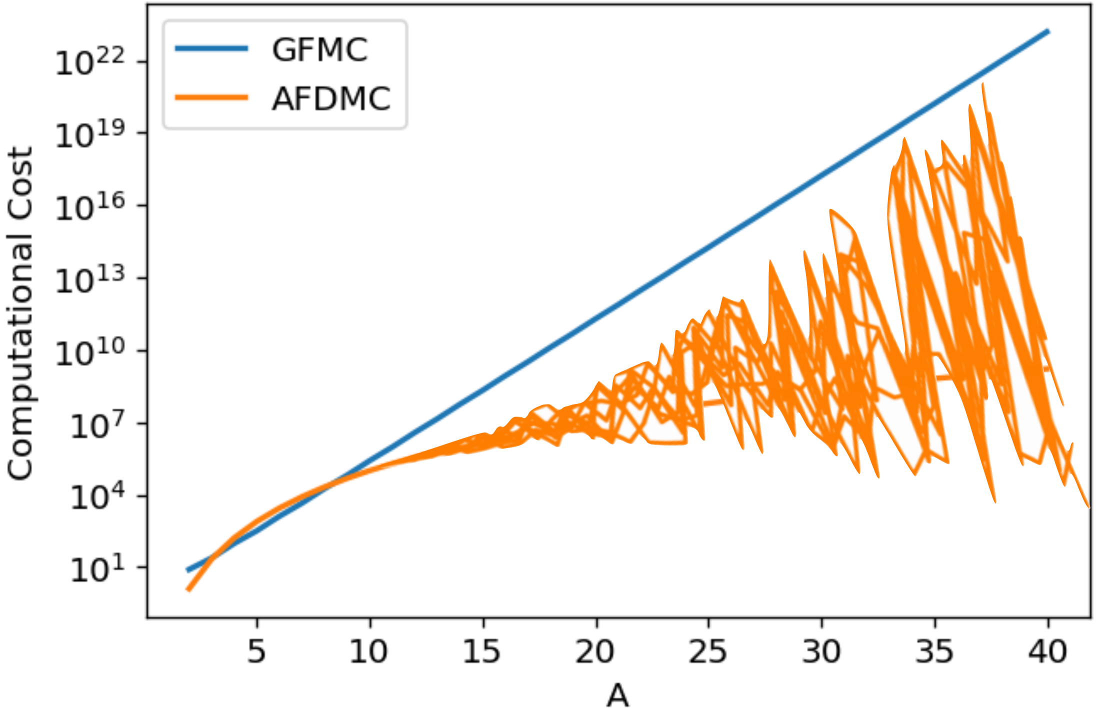
We developed the AFDMC to allow for the calculation of Euclidean response functions





N. Rocco, AL et al., in preparation

HOW TO TACKLE (EVEN) LARGER NUCLEI?



GFMC

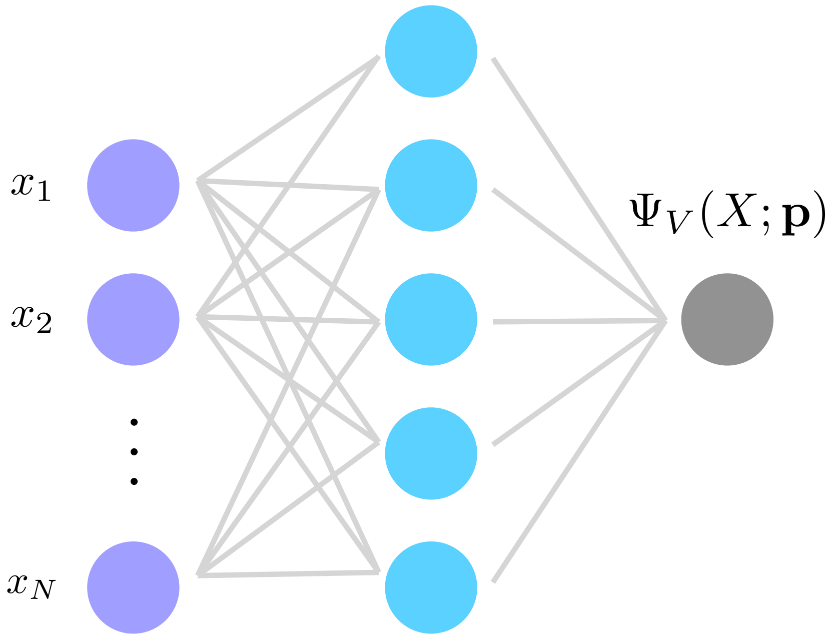
$$|\Psi_T\rangle \sim \prod_{i<j} F_{ij} |\Phi\rangle$$

AFDMC

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

NEURAL-NETWORK QUANTUM STATES

Originally introduced by Carleo and Troyer for spin systems, NQS are now widely and successfully applied to study condensed-matter systems



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

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

$$\mathbf{p}_{\tau+\delta\tau} = \mathbf{p}_\tau - \eta (S_\tau + \epsilon I)^{-1} \mathbf{g}_\tau$$

NQS IN REAL SPACE (1ST QUANTIZATION)

NQS in 1st quantization must explicitly encode the antisymmetry of the wave function

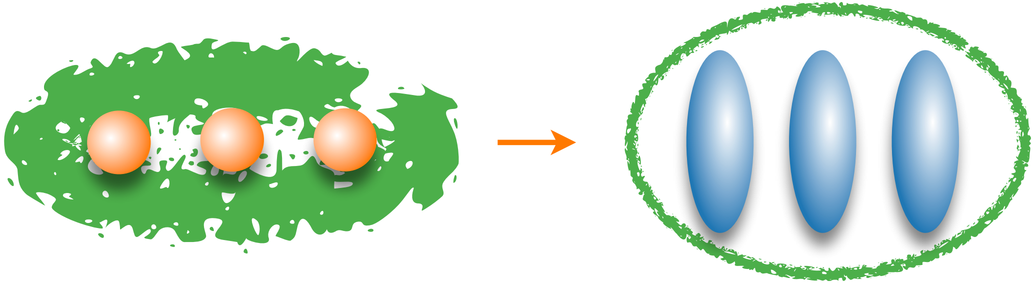
$$\Psi_V(x_1,\dots,x_i,\dots,x_j,\dots x_A;\mathbf{p}) = -\Psi_V(x_1,\dots,x_j,\dots,x_i,\dots x_A;\mathbf{p})$$

Usually expressed as product of permutation-invariant and anti-symmetric functions

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

Universality through back-flow transformations, “hidden” degrees of freedom, or both

$$x_i \longrightarrow y_i(x_i;x_1,\dots,x_A;\mathbf{p})$$



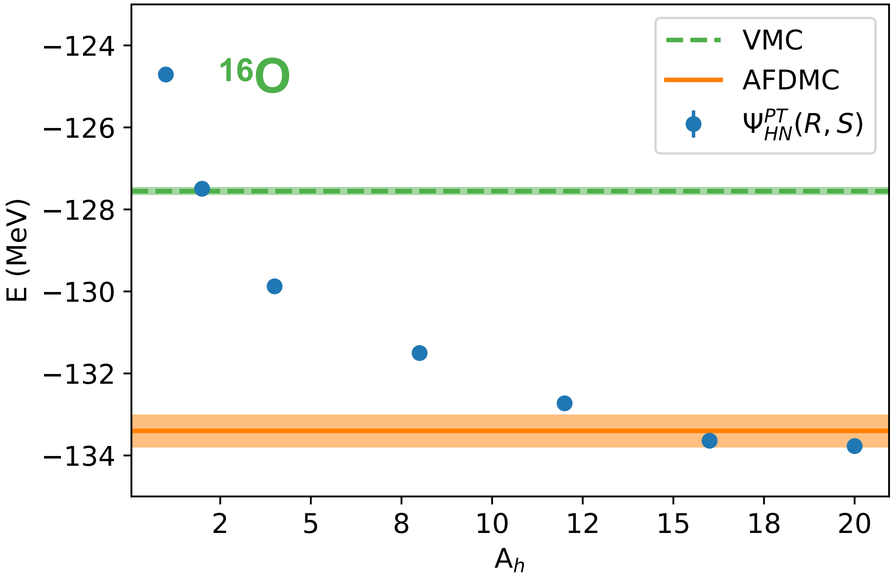
Pfau et al., PRR **2**, 033429 (2020)

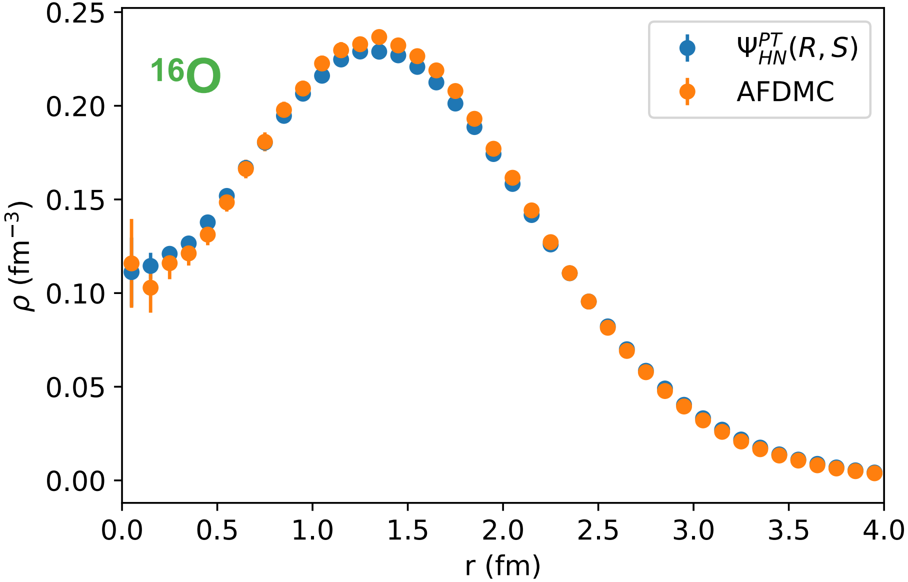
Hermann et al., Nature Chemistry, **12**, 891 (2020)

J. R. Moreno, et al., PRL **125**, 076402 (2022)

NQS: HIDDEN NUCLEONS

In addition to its ground-state energy, we evaluate the point-nucleon density of ^{16}O with A_h=16

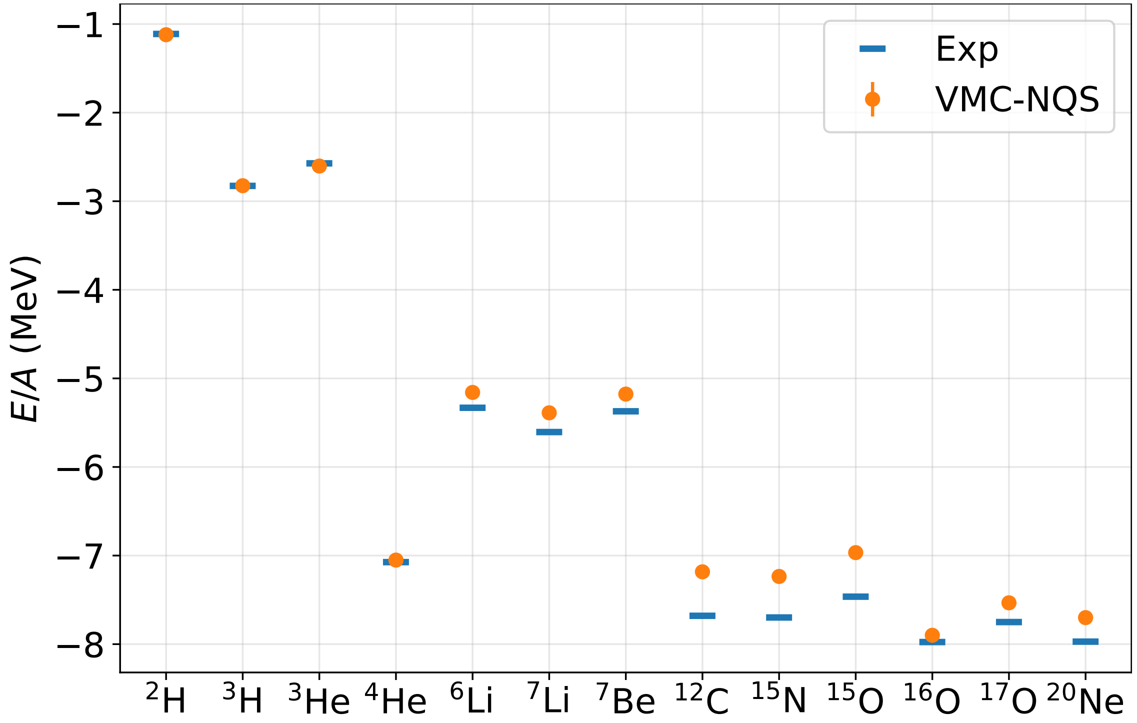




AL, et al., Phys.Rev.Res. ***4*** *(2022) 4, 043178*

ESSENTIAL ELEMENTS OF NUCLEAR BINDING

A simple pionless-EFT Hamiltonian reproduces well the spectrum of different nuclei



A. Gnech, et al., 2308.16266

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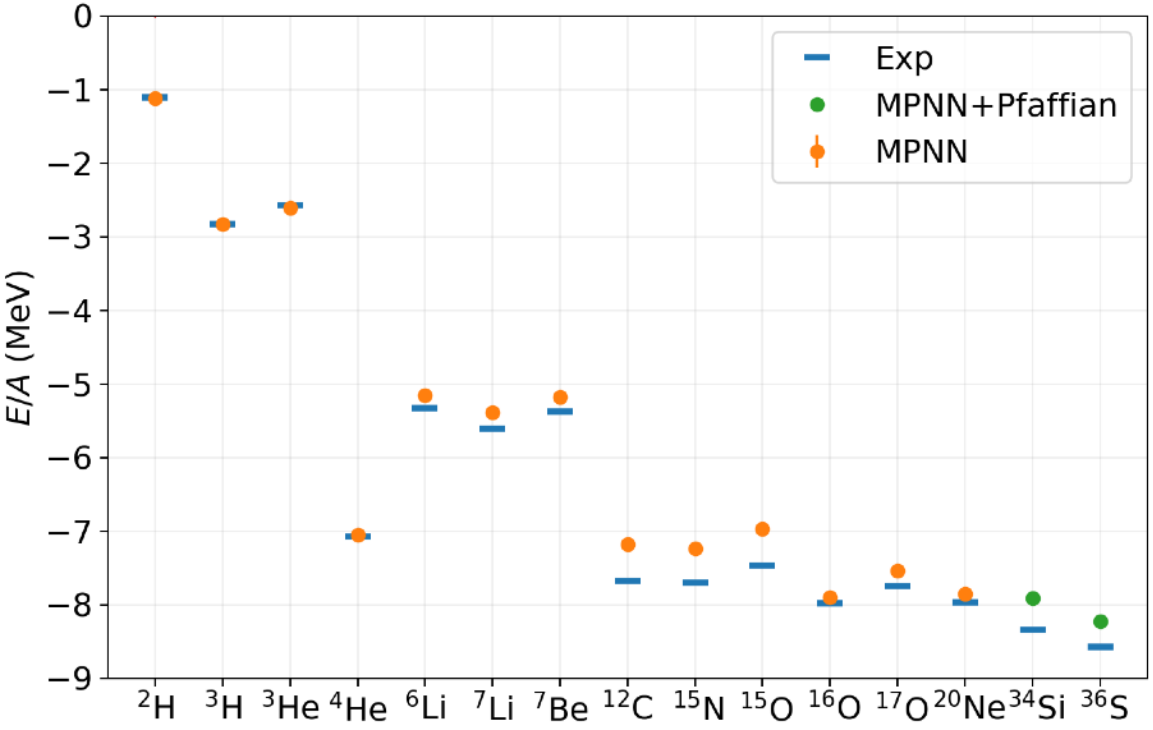
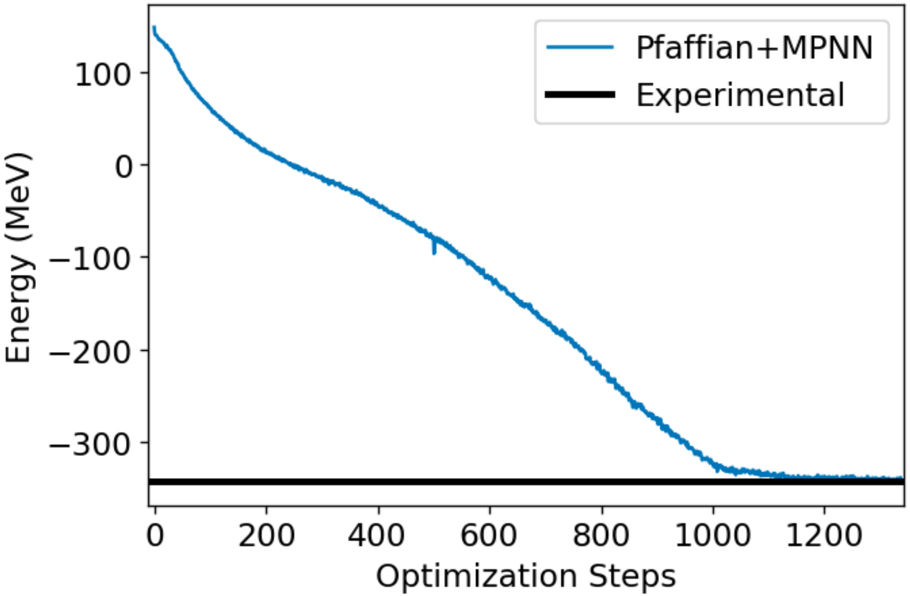
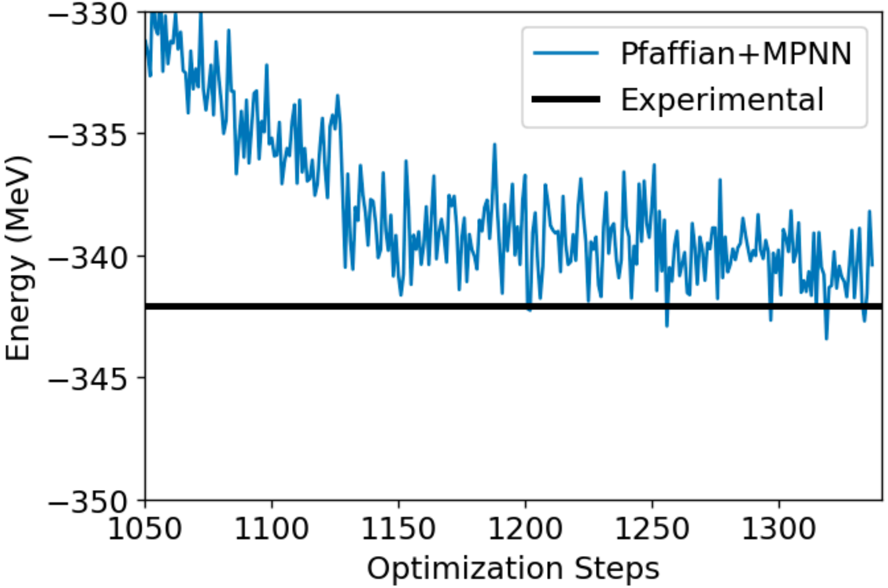


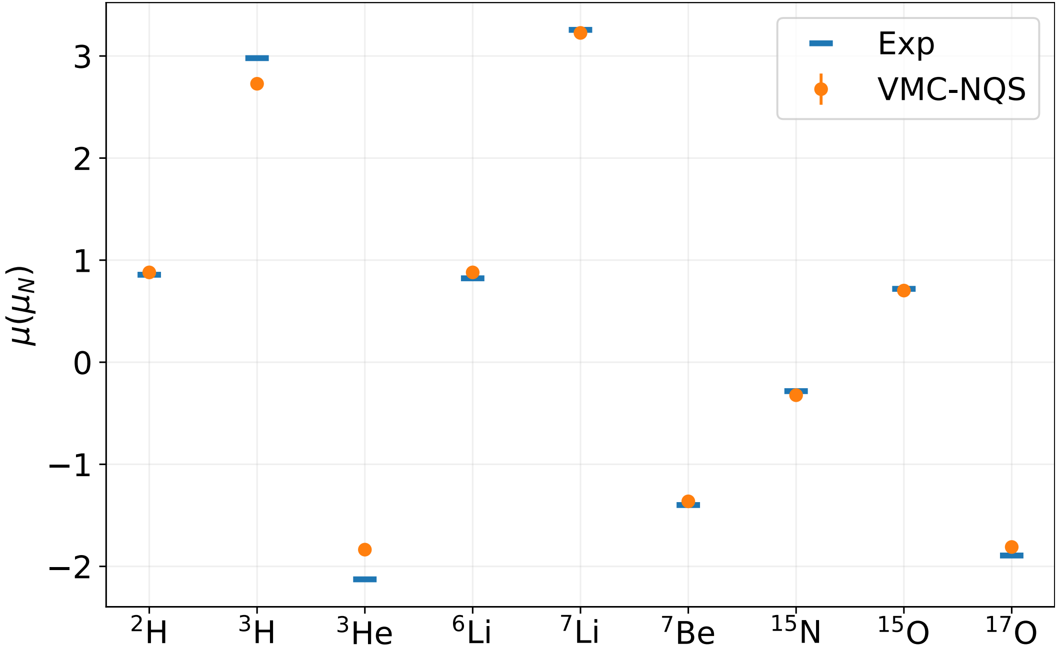
NQS ALLOWS US TO REACH A=40



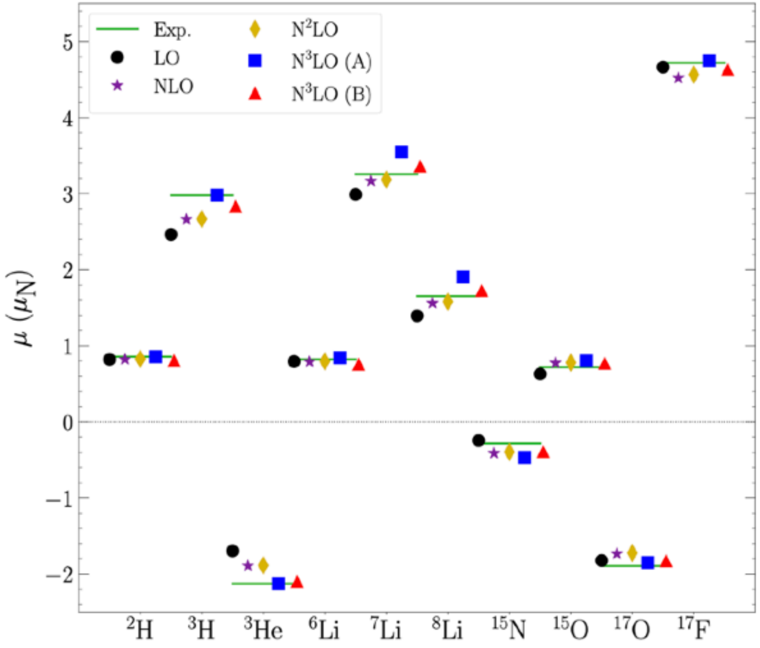


MAGNETIC MOMENTS WITH MPNN

In addition to energies and single-particle densities, we compute electroweak properties



A. Gnech, et al., 2308.16266



J. D. Martin, et al., 2301.08349 [nucl-th]

CONCLUSIONS

- Three main sources of theoretical errors:

  1) Hamiltonian and (hopefully) consistent currents.

  2) Elementary amplitudes: axial form factor…

  3) Nuclear many-body methods of choice.

- QMC allows us to reduce 3) and to explore wide classes of Hamiltonian and currents.

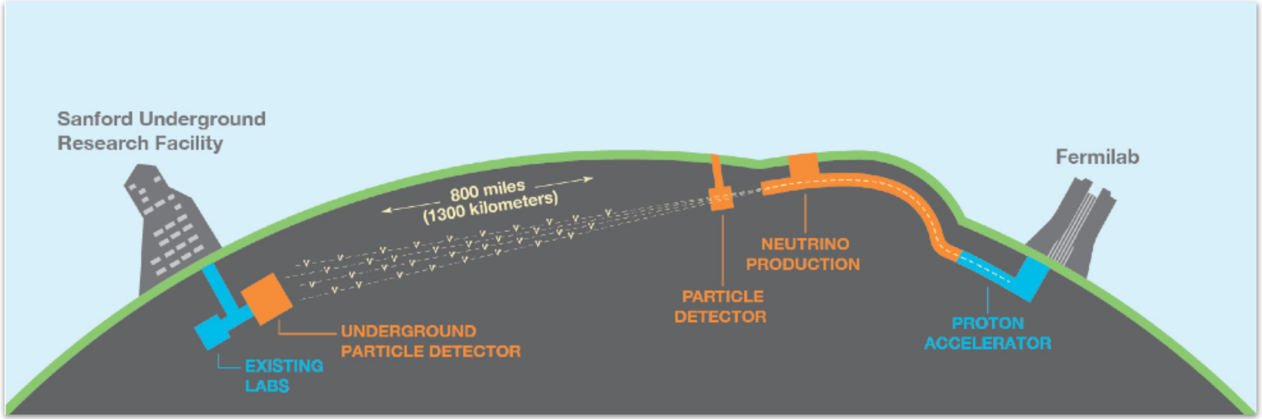
- Neural-network quantum states extend the reach of QMC methods to nuclei used in oscillation experiments.

PERSPECTIVES

- Access “real-time” dynamics: the prototypal exponentially-hard problem in many-body theory

$$\mathcal{D}\left(|\Psi(\mathbf{p}_{t+\delta t})\rangle, e^{-iHt}|\Psi(\mathbf{p}_t)\right)^2 = \arccos\left(\sqrt{\frac{\langle\Psi(\mathbf{p}_{t+\delta t})|e^{-iHt}|\Psi(\mathbf{p}_t)\rangle\langle\Psi(\mathbf{p}_t)|e^{iHt}|\Psi(\mathbf{p}_{t+\delta t})\rangle}{\langle\Psi(\mathbf{p}_{t+\delta t})|\Psi(\mathbf{p}_{t+\delta t})\rangle\langle\Psi(\mathbf{p}_t)|\Psi(\mathbf{p}_{\tau+\delta t})\rangle}}\right)^2$$

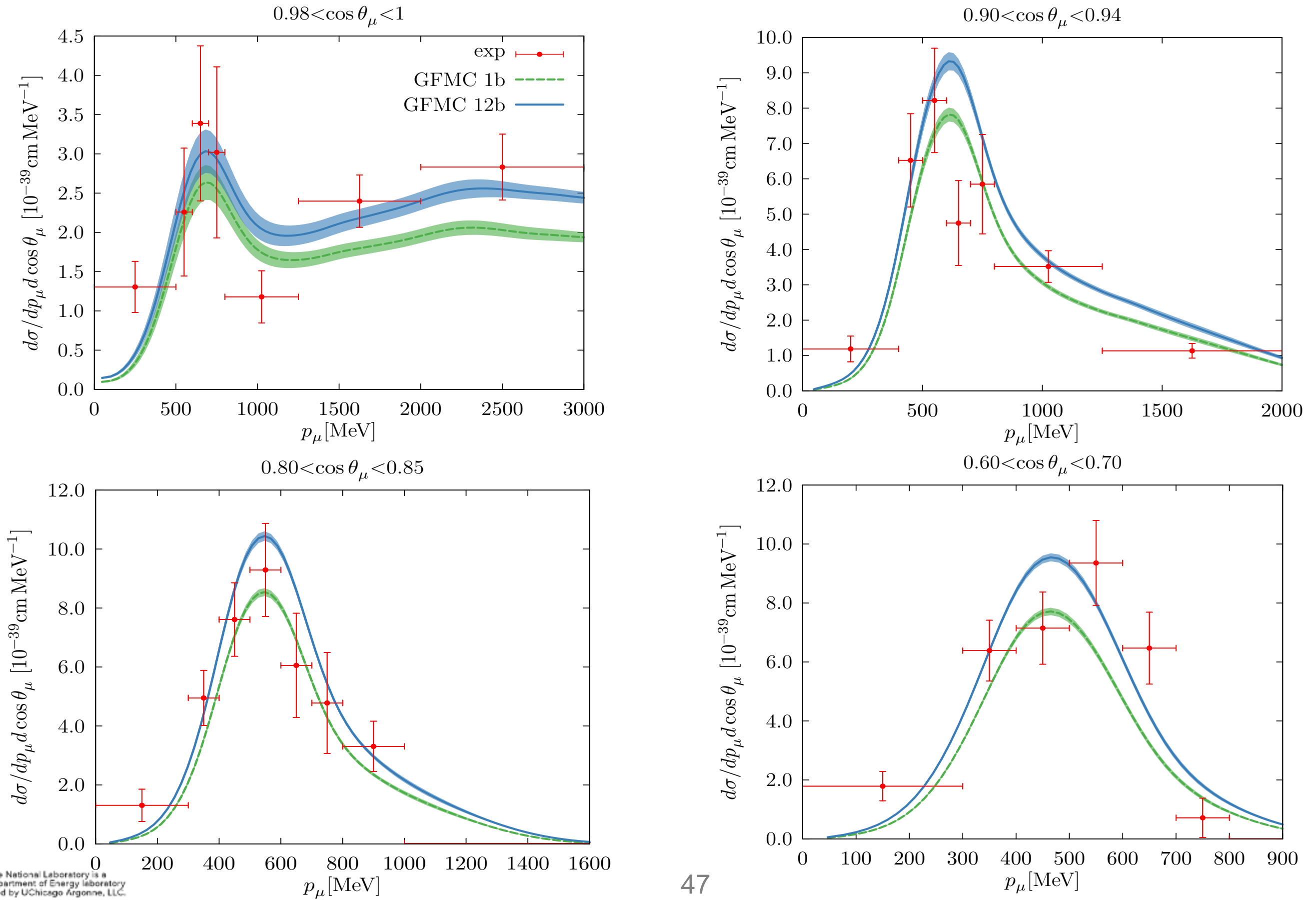
- Relevant for: lepton-nucleus scattering, fusion, and collective neutrino oscillation;



THANK YOU

T2K CROSS SECTIONS

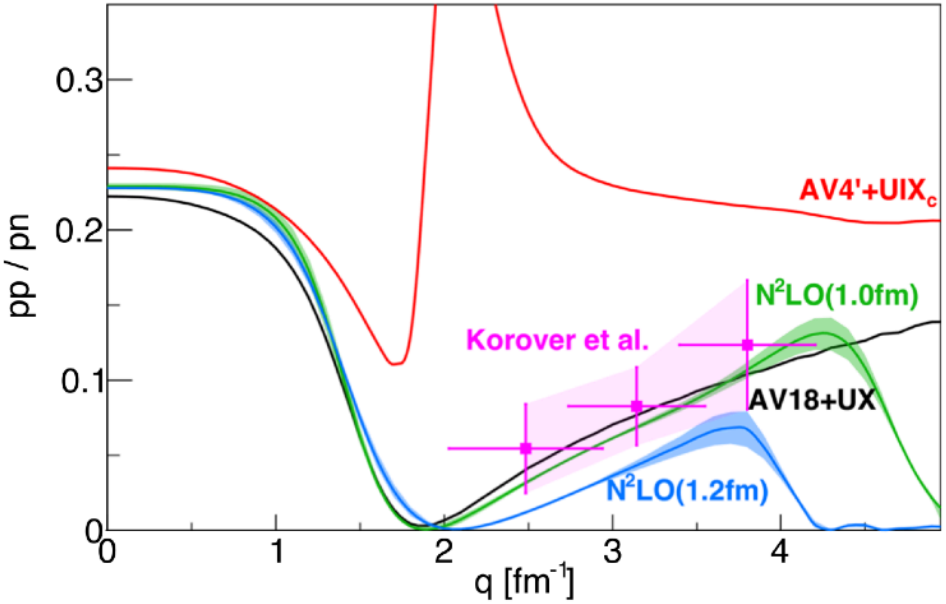
*AL et al., PRX **10**, 031068 (2020)*



QUANTUM MONTE CARLO METHODS

Continuum nuclear quantum Monte Carlo make use of coordinate-space representation of many-body wave functions.

- They have no difficulties in treating "stiff" nuclear forces: test the convergence of nuclear EFTs;
- 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*