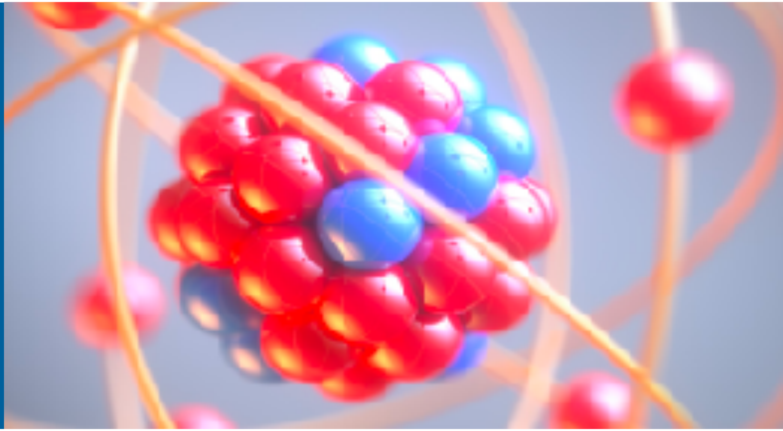
UNCERTAINTY QUANTIFICATION IN NUCLEAR MANY-BODY THEORY



ALESSANDRO LOVATO

Argonne NATIONAL LABORATORY

PRISMA+ Colloquium

University of Mainz

June 26, 2024

CAREER RECAP

2006: *Bachelor in Physics from "Sapienza" University (Rome, Italy)*

2008: *Master in Particle Physics from "Sapienza" University (Rome, Italy)*

2012: *PhD in Astro-Particle Physics from "SISSA" (Trieste, Italy)*

2012 - 2014: *Postdoc in the ALCF Division at Argonne*

2014 - present: *Staff Scientist in the Physics Division at Argonne*

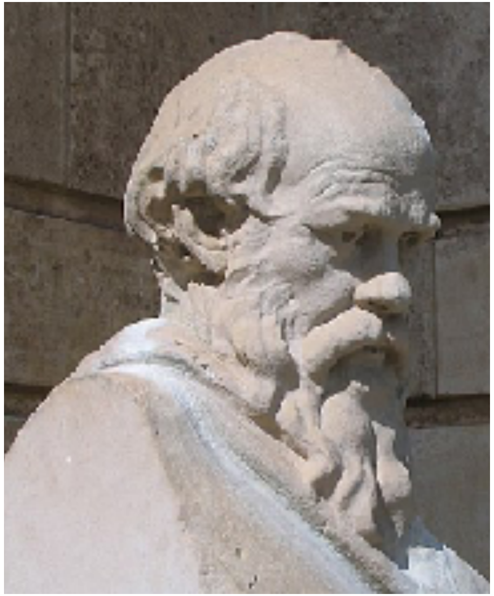
2018 - present: *(on leave) Researcher at INFN-TIFPA in Italy*

HISTORICAL INTRODUCTION

Voltaire *(attributed to): Uncertainty is an uncomfortable position. But certainty is a ridiculous one.*

Information and Statistics in Nuclear Experiment and Theory (ISNET) News Article

HISTORICAL INTRODUCTION



Plato, The Apology of Socrates*: Although I do not suppose that either of us knows anything really beautiful and good, I am better off than he is – for he knows nothing, and thinks he knows. I neither know nor think I know.*

HISTORICAL INTRODUCTION

June 2008

Policy Statement on the Inclusion of Uncertainty Estimates for Theoretical Papers in *Physical Review A*

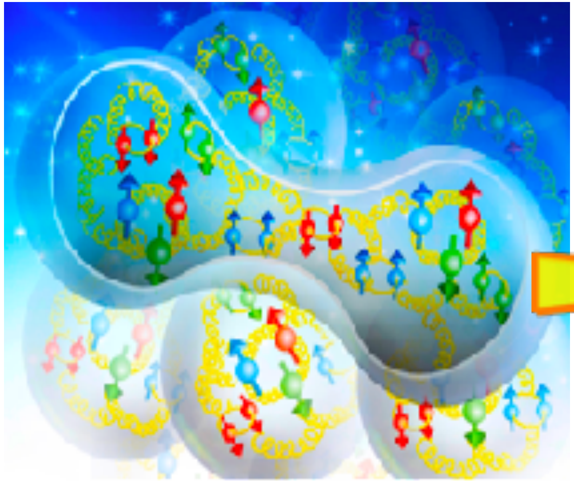
The following policy statement was discussed and approved by the Editorial Board of *Physical Review A* in May 2008.

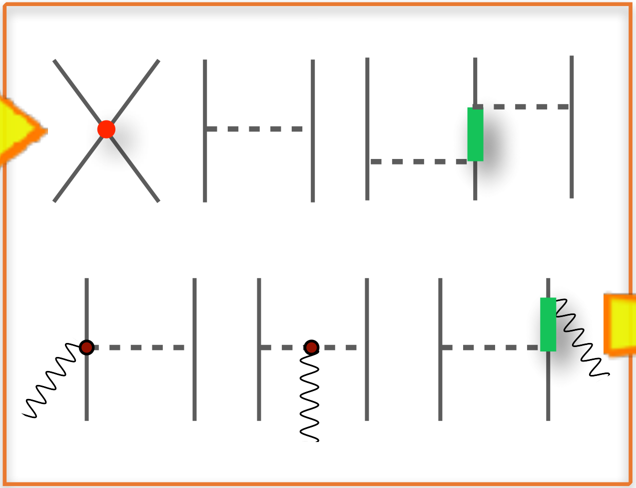
Papers presenting the results of theoretical calculations are expected to include uncertainty estimates for the calculations whenever practicable, and especially under the following circumstances:

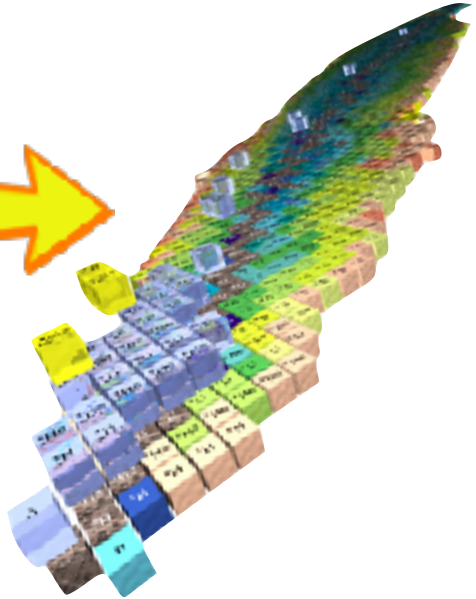
a. If the authors claim high accuracy, or improvements on the accuracy of previous work.
b. If the primary motivation for the paper is to make comparisons with present or future high precision experimental data.
c. If the primary motivation is to provide interpolations or extrapolations of known experimental data.

The Editors

"AB-INITIO" NUCLEAR THEORY







SOURCES OF UNCERTAINTIES

$$H\left|\Psi_n\right\rangle = E_n\left|\Psi_n\right\rangle \quad ; \quad M_{mn} = \left\langle\Psi_m\right| J \left|\Psi_n\right\rangle$$

SOURCES OF UNCERTAINTIES

$$H |\Psi_n\rangle = E_n |\Psi_n\rangle \quad ; \quad M_{mn} = \langle \Psi_m | J | \Psi_n \rangle$$

- Modeling the Hamiltonian and currents is a long-standing problem of Nuclear Physics

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- Solving the quantum many-body problems entails approximations

SOURCES OF UNCERTAINTIES

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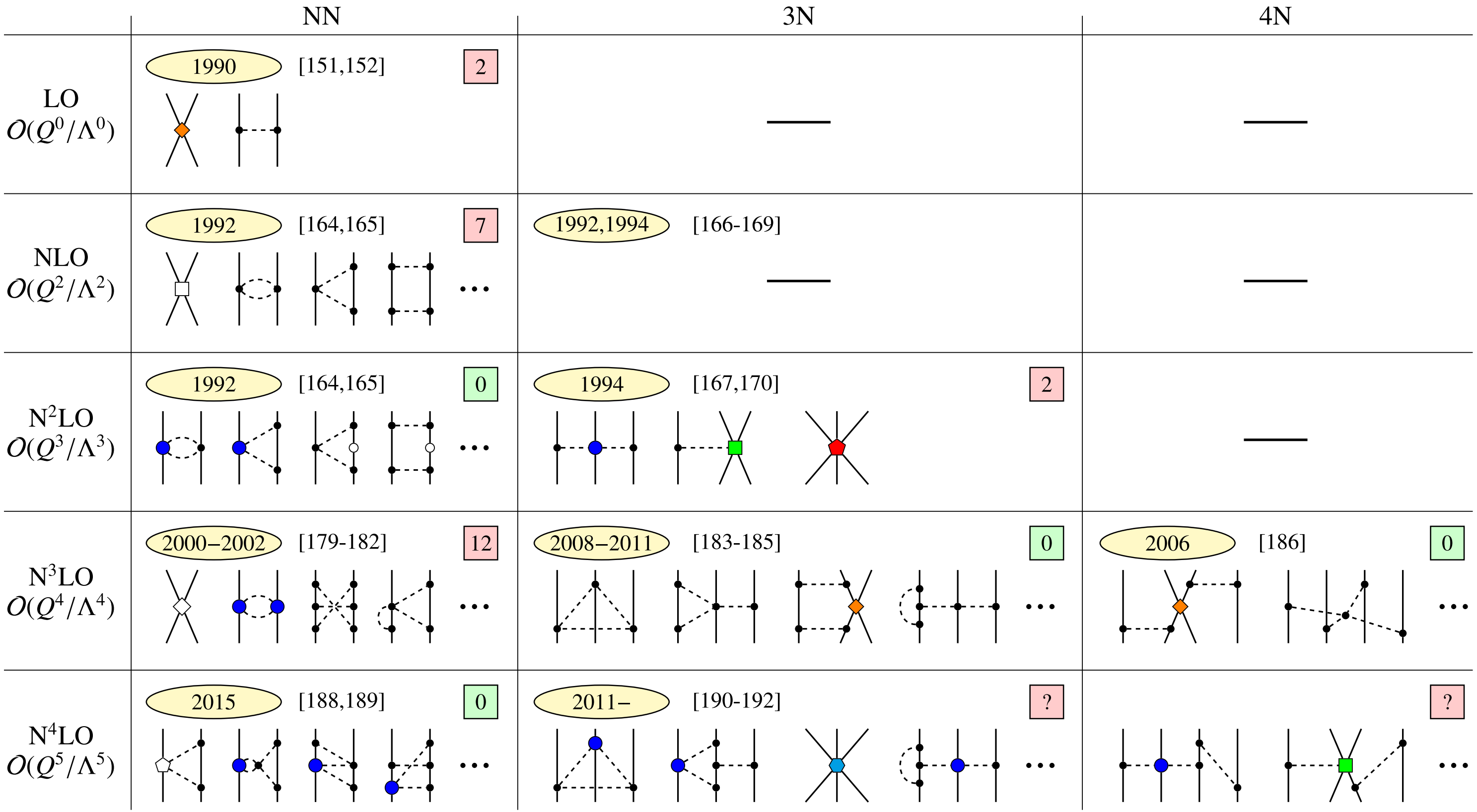
- Modeling the Hamiltonian and currents is a long-standing problem of Nuclear Physics.
- Solving the quantum many-body problems entails approximations.
- These two sources of uncertainties can be correlated.

HAMILTONIAN



K. Hebeler et al., *Phys. Rept.* **890** (2021) 1-116

UQ FOR THE TWO-BODY FORCE

- Bayes's theorem to include prior information in a transparent way

$$\mathrm{pr}(\vec{\alpha}|D,I) = \frac{\mathrm{pr}(D|\vec{\alpha},I)\cdot\mathrm{pr}(\vec{\alpha}|I)}{\mathrm{pr}(D|I)}$$

- Keep track of both experimental and theory uncertainties

$$y_{\mathrm{exp}} = y_{\mathrm{true}} + \delta y_{\mathrm{exp}} \qquad\qquad y_{\mathrm{true}} = y_{\mathrm{th}} + \delta y_{\mathrm{th}}$$

- Theory uncertainties dominated by EFT truncation

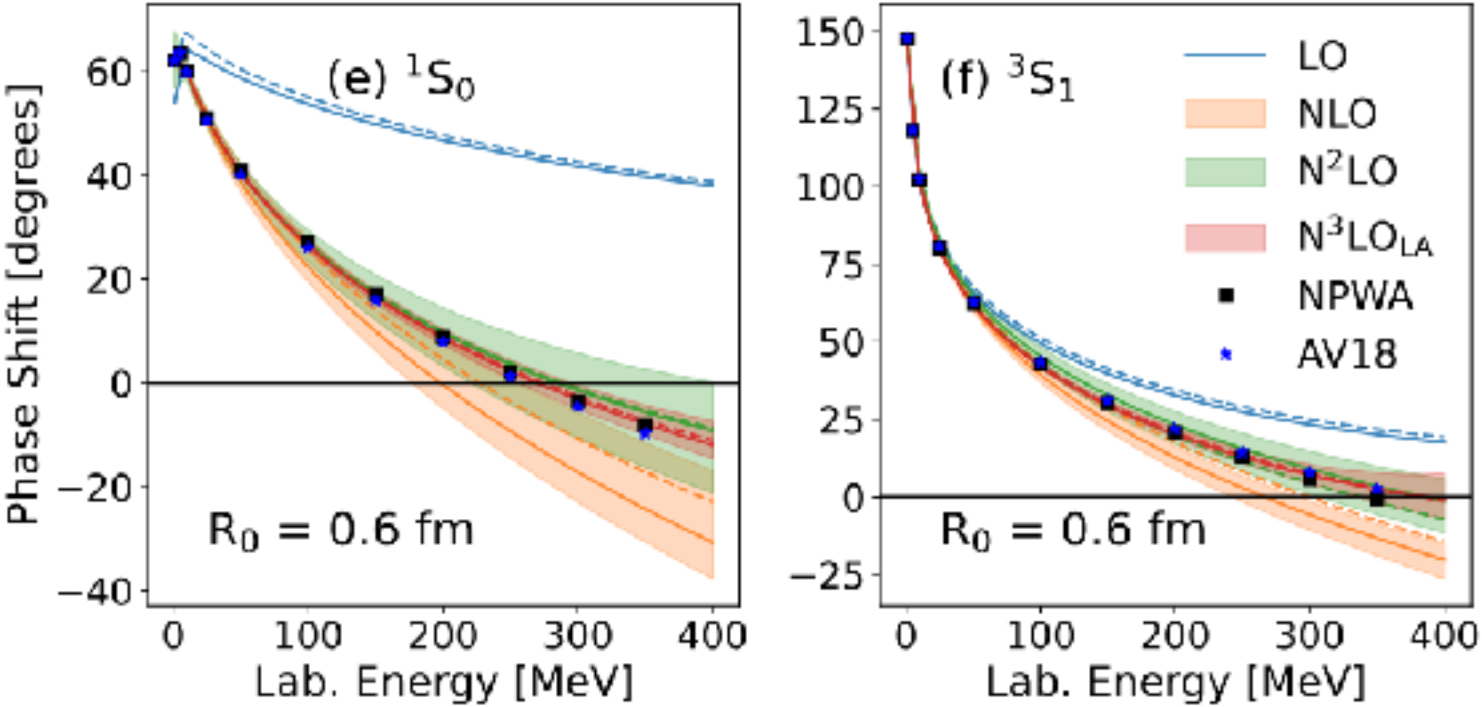
$$y_{\mathrm{th}}^{(k)} = y_{\mathrm{ref}} \sum_{\nu=0}^{k} c_\nu Q^\nu \quad ; \quad Q = \frac{\max(m_\pi, p)}{\Lambda_b} \quad ; \quad \delta y_{\mathrm{th}}^{(k)} = y_{\mathrm{ref}} \sum_{\nu=k+1}^{\infty} c_\nu Q^\nu$$

D. Furnstahl, Phys. Rev. C ***92****, 024005 (2015)*

S. Wesolowski, J. Phys. G ***46****, 045102 (2019)*

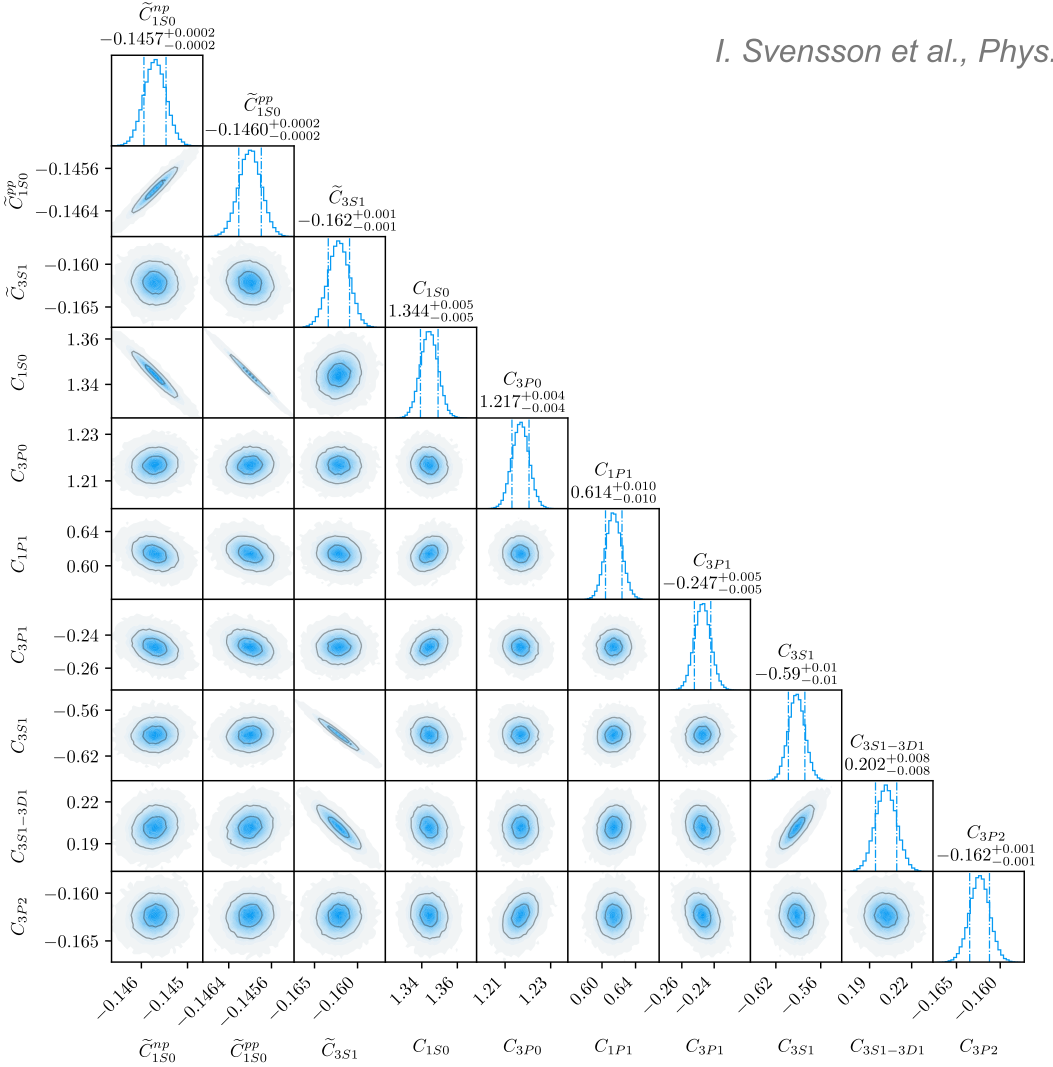
I. Svensson et al., Phys.Rev.C ***105****, 014004 (2022)*

UQ FOR THE TWO-BODY FORCE

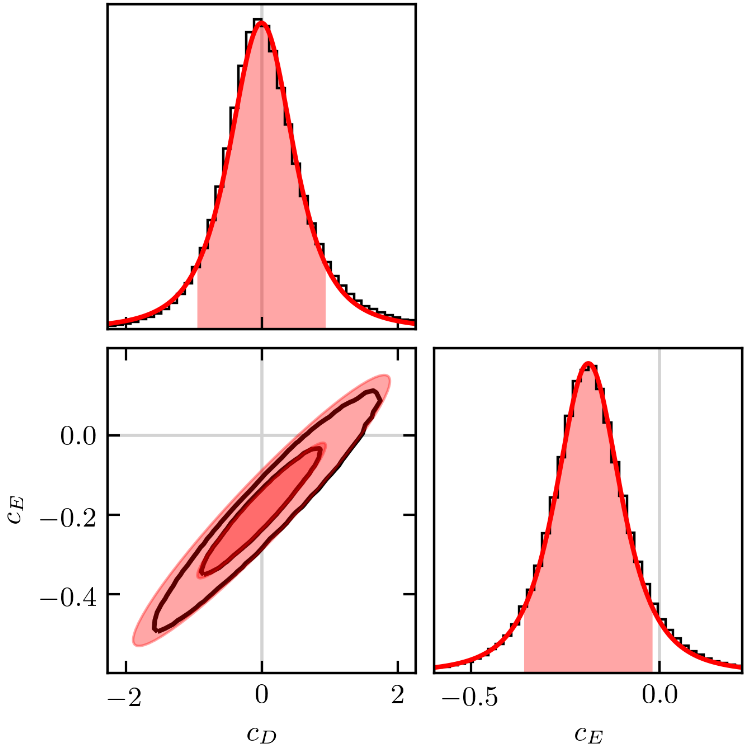


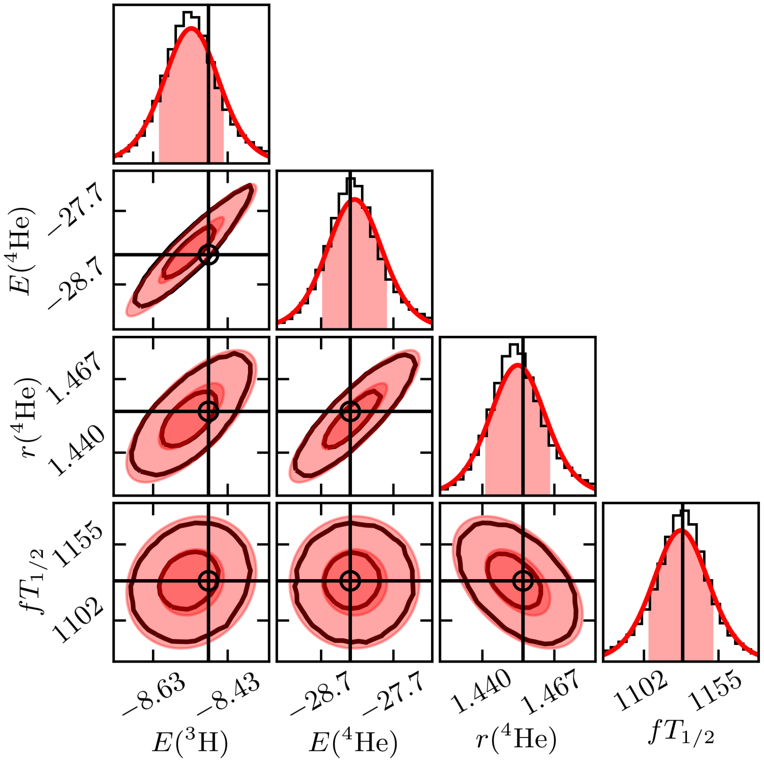
*R. Somasundaram, Phys.Rev.C **109** (2024) 3, 3*

I. Svensson et al., Phys.Rev.C ***105*** *(2022), 014004*



UQ FOR THE THREE-BODY FORCE





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

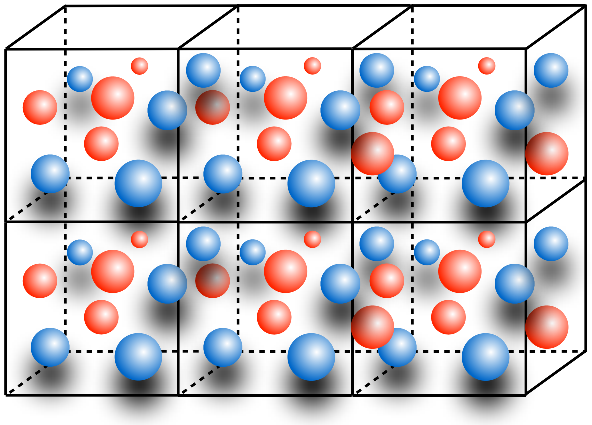
THE MEAN-FIELD APPROXIMATION

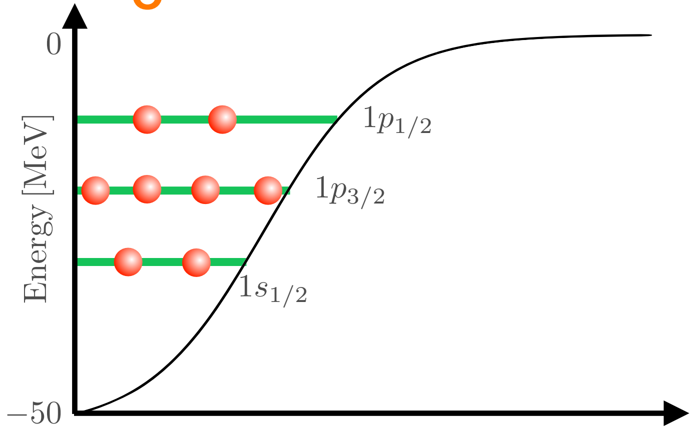
The mean field ground-state wave function is a Slater determinant

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

$$\Phi_0(x_1, x_2) = \phi_1(x_1)\phi_2(x_2) - \phi_2(x_1)\phi_1(x_2)$$

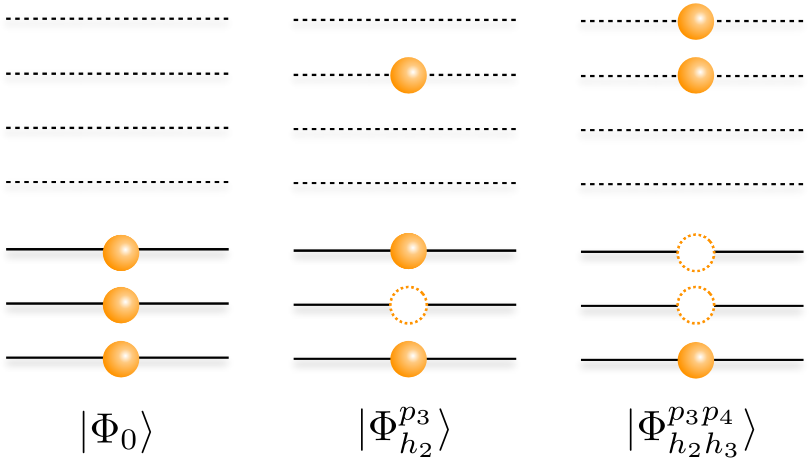
Infinite matter





CONFIGURATION-INTERACTION METHODS

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



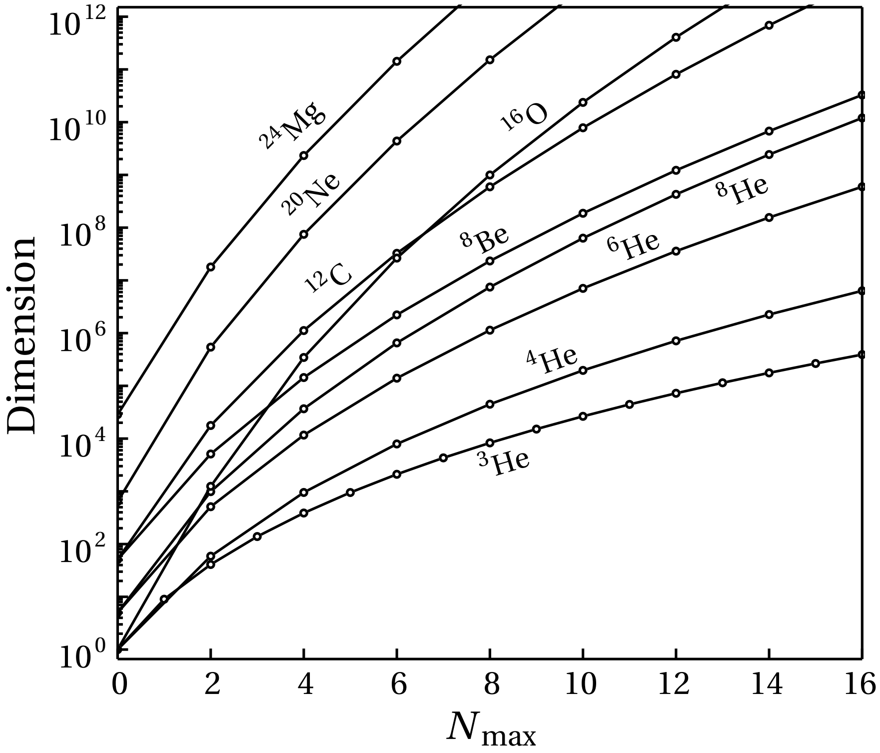
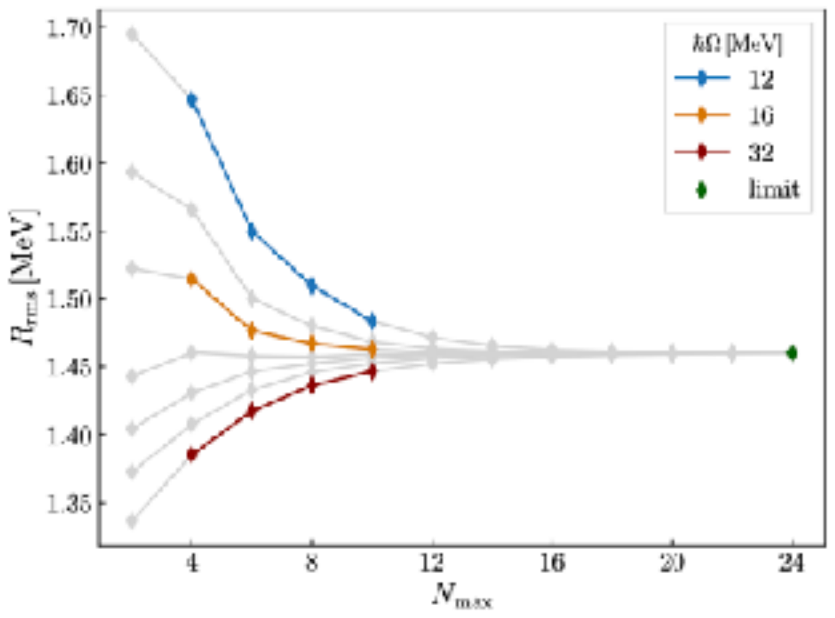
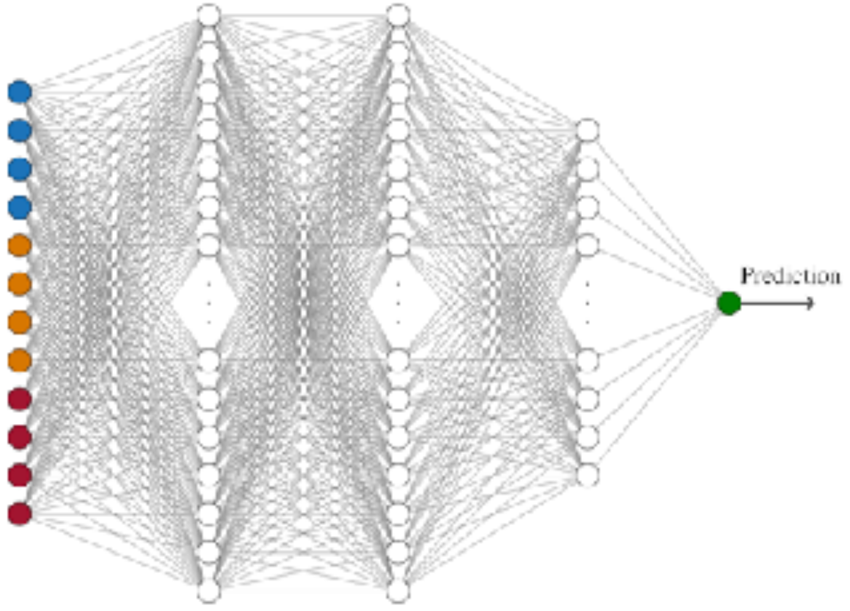


Image courtesy of Patrick Fasano

UQ IN CONFIGURATION-INTERACTION METHODS



(a) NCSM results

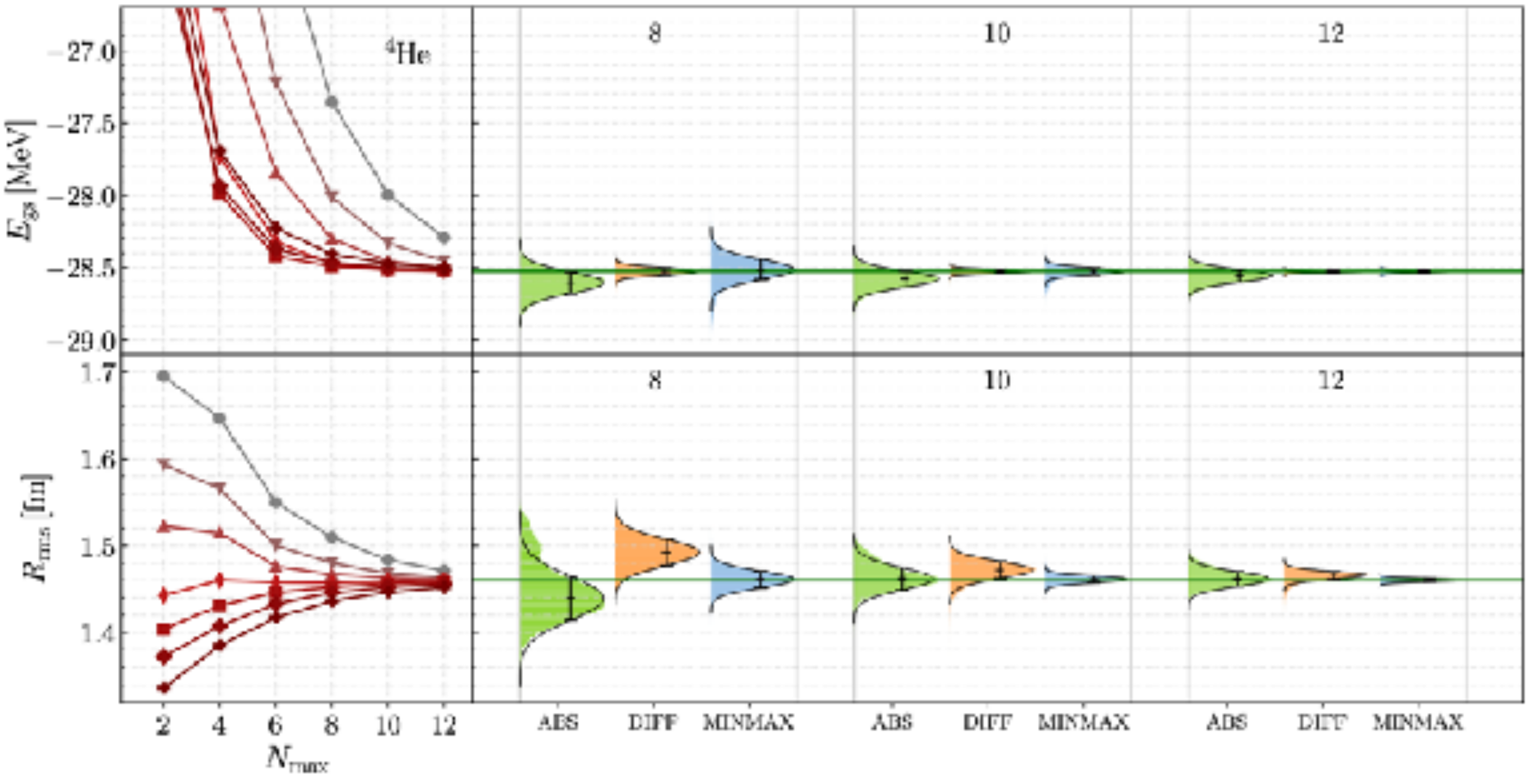


(b) network topology

M. Knöll et al., Phys. Lett.B ***839*** *(2023) 137781*

T. Wolfgruber et al., arXiv:2310.05256

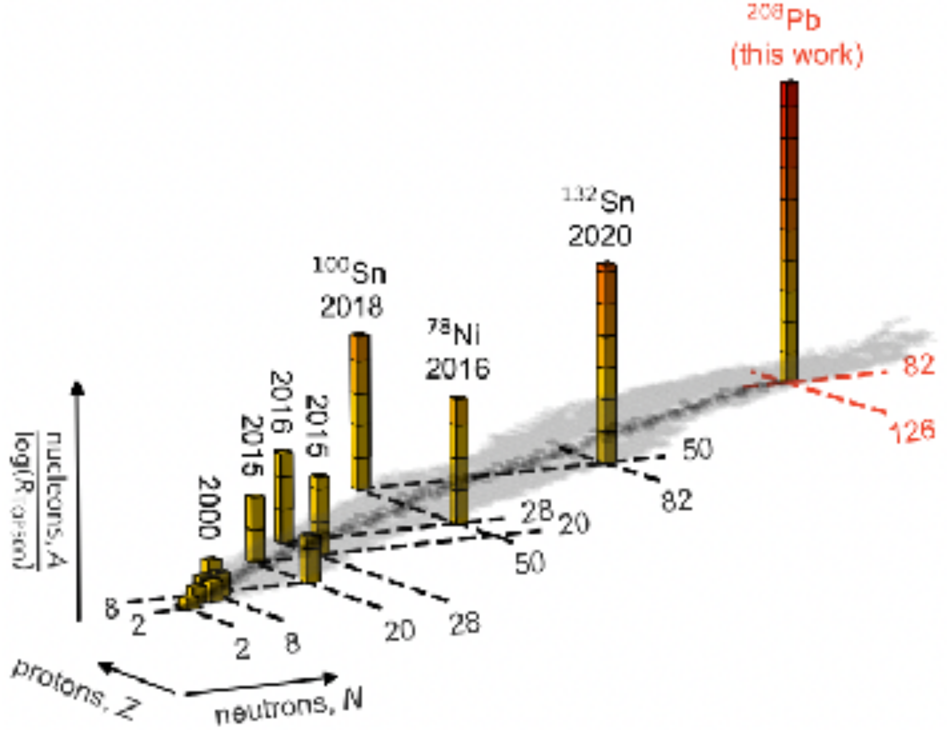
UQ IN CONFIGURATION-INTERACTION METHODS



T. Wolfgruber et al., arXiv:2310.05256

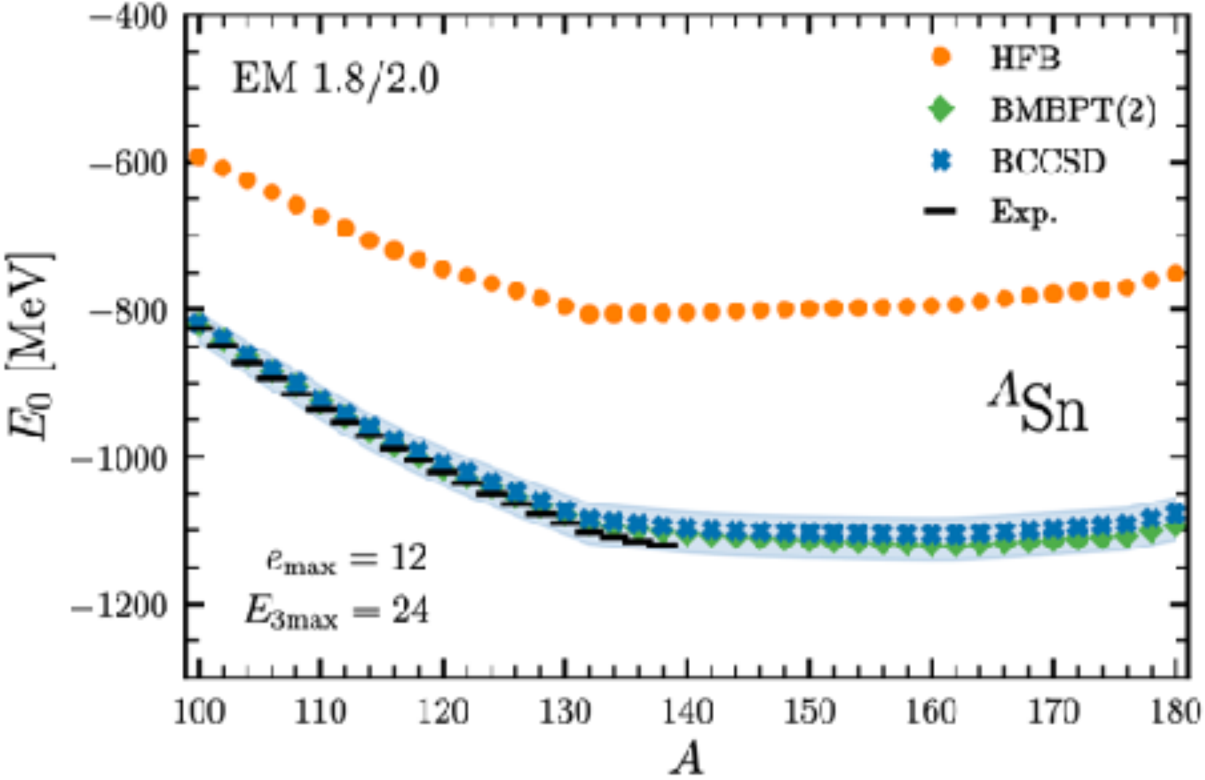
TACKLE LARGER SYSTEMS

Polynomially-scaling methods reach (much) larger systems with controlled approximations



B. S. Hu et al., Nature Phys. ***18*** *(2022) 10, 1196*

TACKLE LARGER SYSTEMS



A. Tichai et al., Phys. Lett. B **851** (2024) 138571

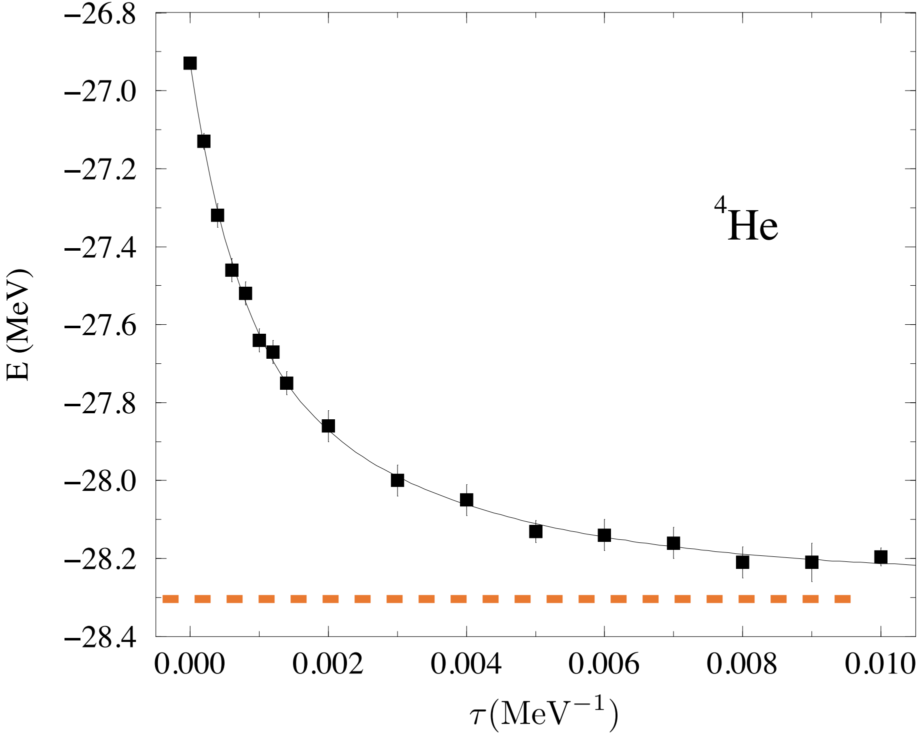
CONTINUUM QUANTUM MONTE CARLO

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

$$|\Psi_V\rangle = \sum_n c_n |\Psi_n\rangle$$

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

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



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

B. Pudliner et al., PRC ***56****, 1720 (1997)*

UQ IN CONTINUUM QUANTUM MONTE CARLO

The fermion ground state is (typically) an excited state of the Hamiltonian

$$E_0^S \leq E_0^A \quad \longleftrightarrow \quad \lim_{\tau \to \infty} e^{-(H - E_0^A)\tau} |\Psi_V\rangle = \sum_n c_n^S e^{-(E_n^S - E_0^A)\tau} |\Psi_n\rangle + c_0^A |\Psi_0^A\rangle + \dots$$

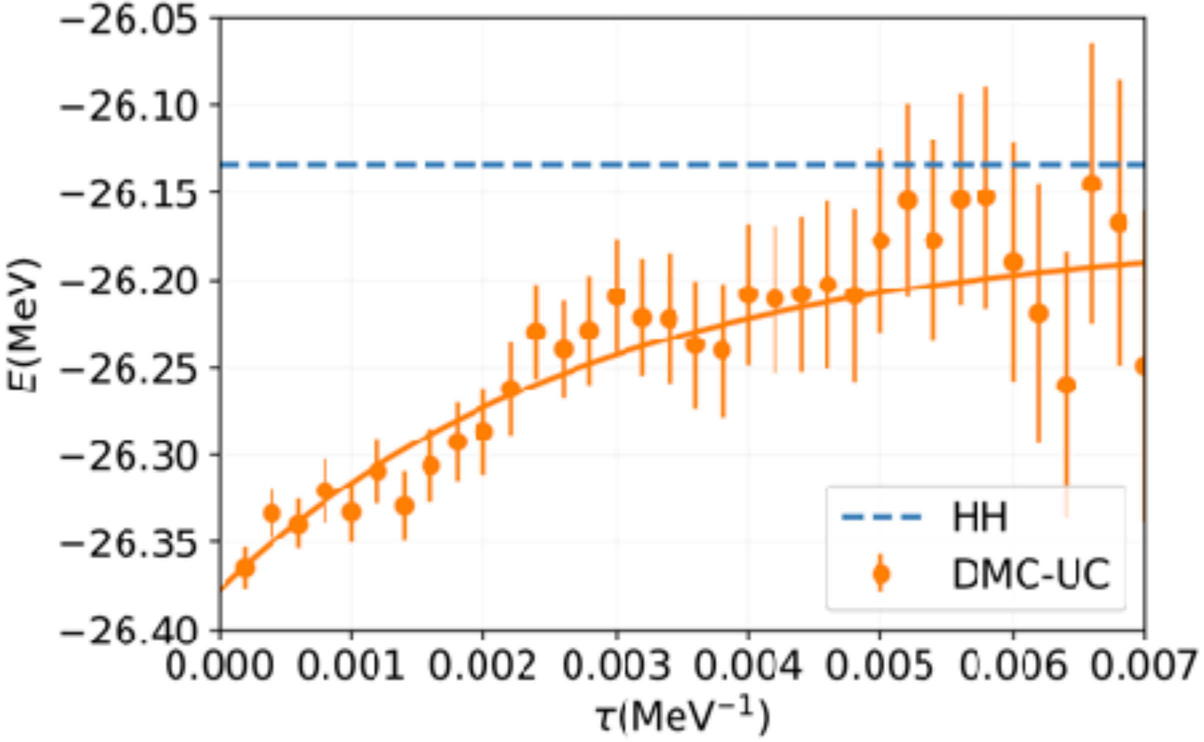
The boson ground-state component does not affect the Hamiltonian expectation value

$$\langle H \rangle = \int dR_N \langle \Psi_V | H | R_N \rangle \langle R_N | e^{-(E_n^S - E_0^A)\tau} | \Psi_n \rangle = 0$$

Problem: The variance diverges exponentially

$$\langle H^2 \rangle = \int dR_N \langle \Psi_V | H | R_N \rangle^2 \langle R_N | e^{-(E_n^S - E_0^A)\tau} | \Psi_n \rangle$$

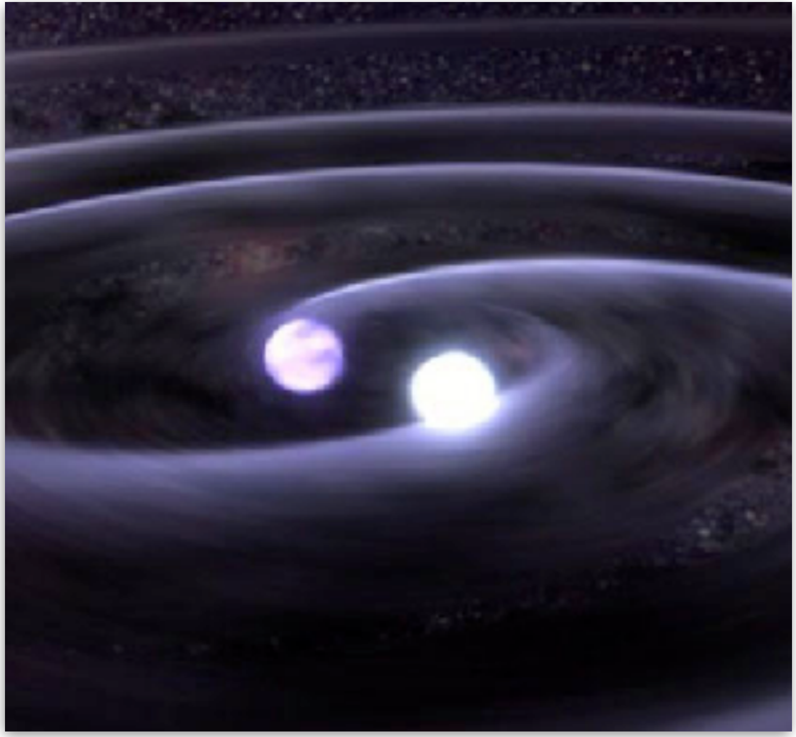
UQ IN CONTINUUM QUANTUM MONTE CARLO

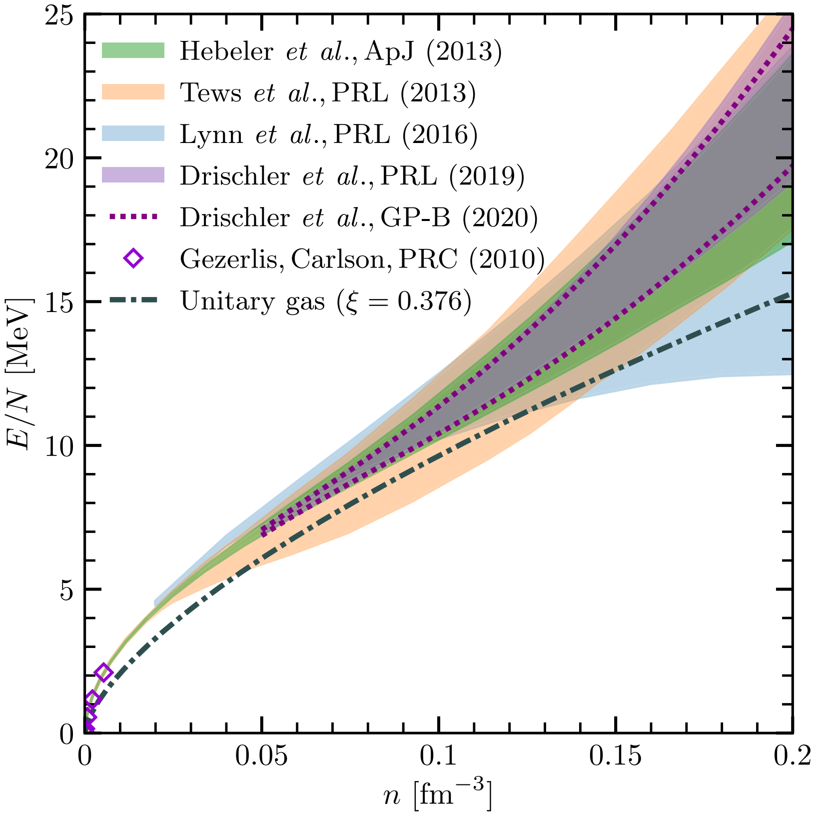


A. Gnech et al., arXiv:2405.14916

SELECTED APPLICATIONS

UQ FOR THE NUCLEAR EQUATION OF STATE

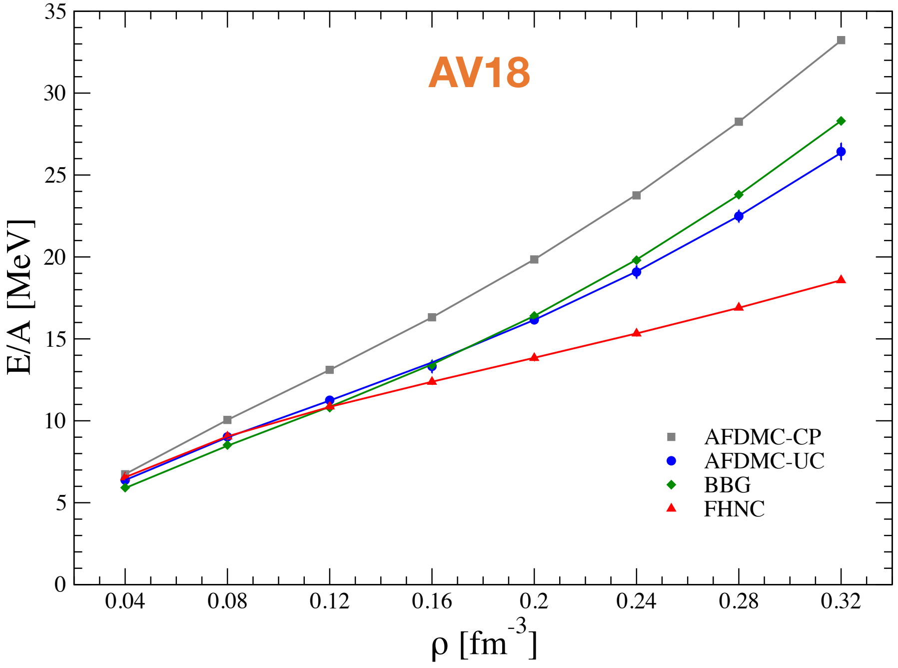


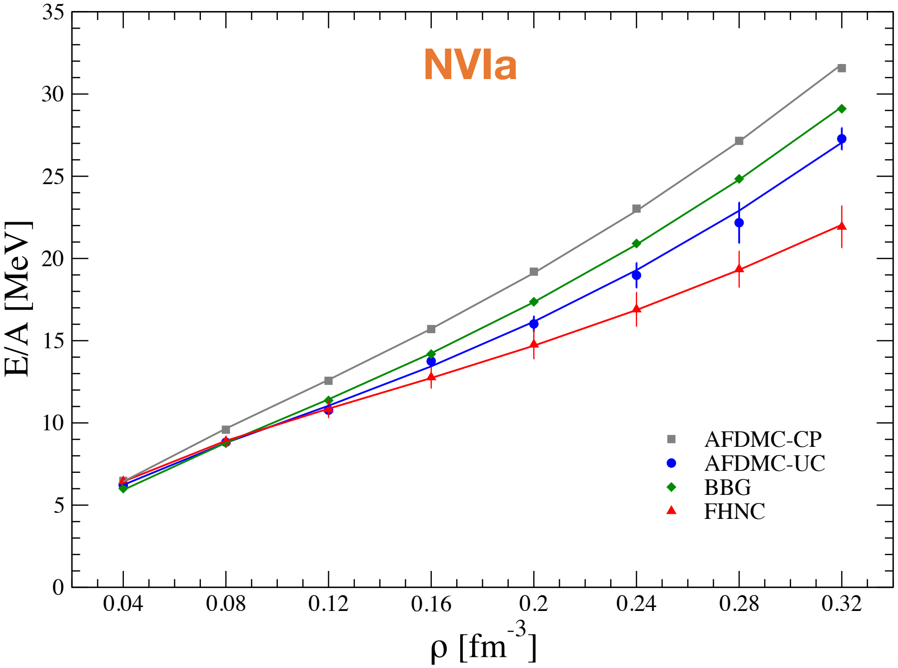


S. Huth, et al., Phys. Rev. C, **103**, 025803 (2021)

NEUTRON-MATTER EQUATION OF STATE

We benchmarked three many-body methods using the AV18 and chiral-EFT interactions

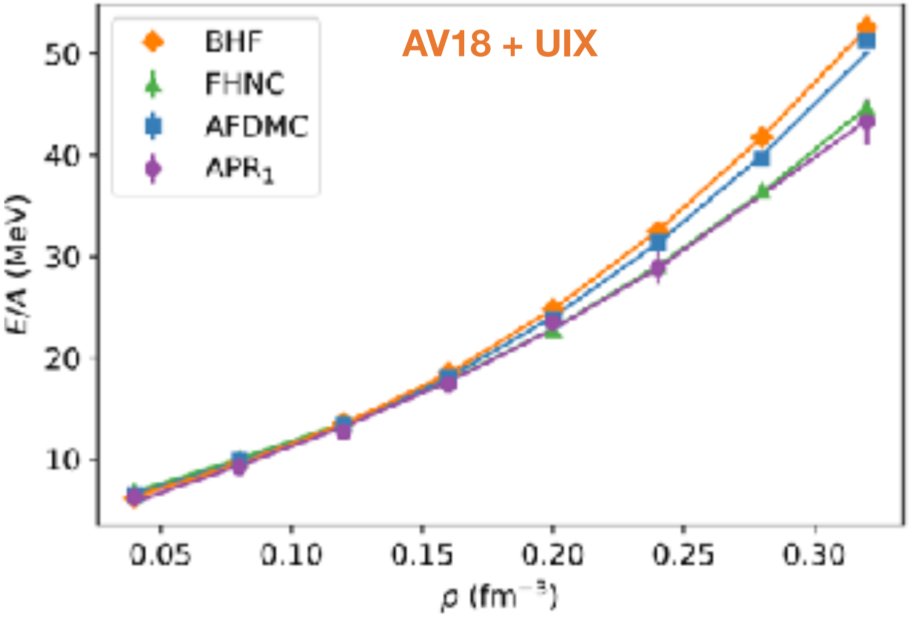


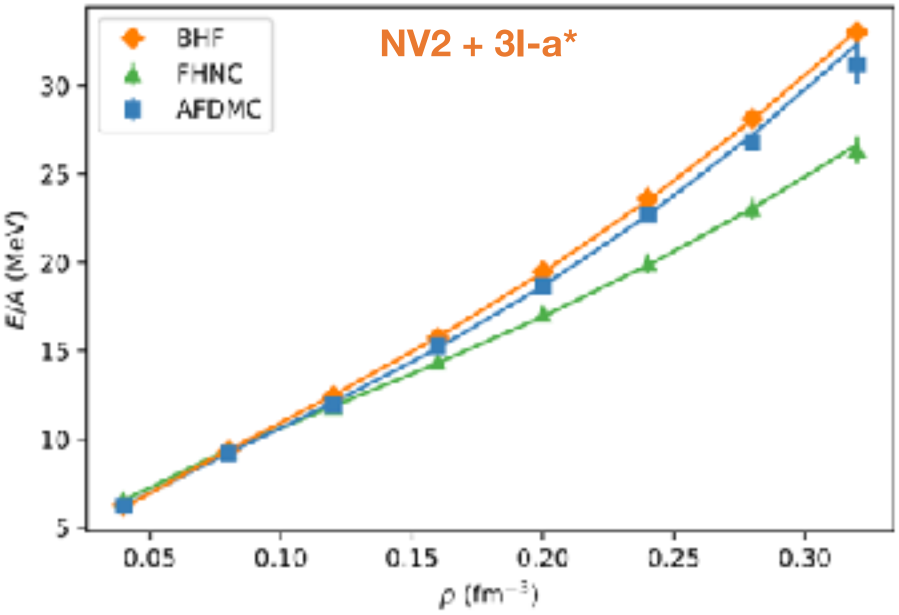


*M. Piarulli, et al., Phys.Rev.C **101**, 045801(2020)*

NEUTRON-MATTER EQUATION OF STATE

Extended the benchmark calculations to phenomenological and chiral-EFT three-body forces





AL et al., Phys.Rev.C ***105*** *(2022) 5, 055808*

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UQ FOR NEUTRINO-OSCILLATION PHYSICS

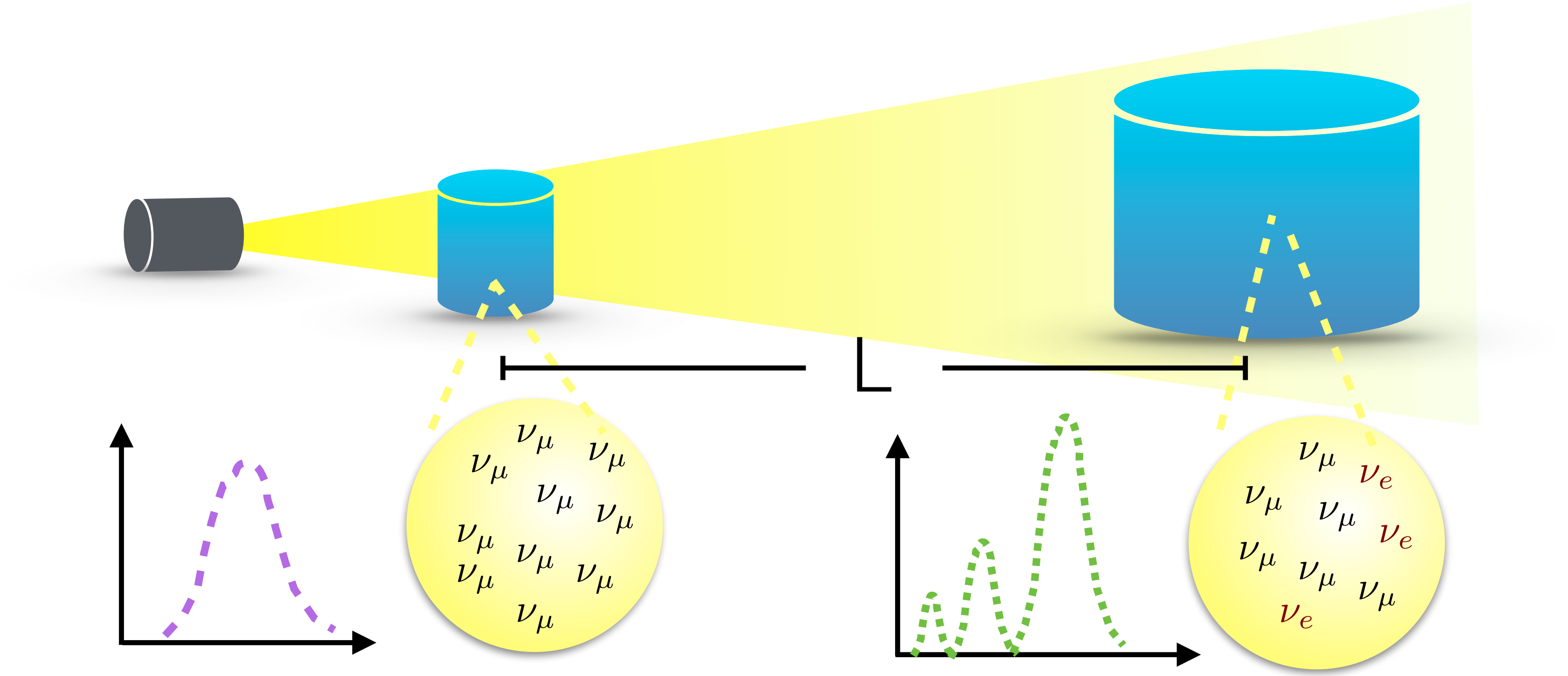
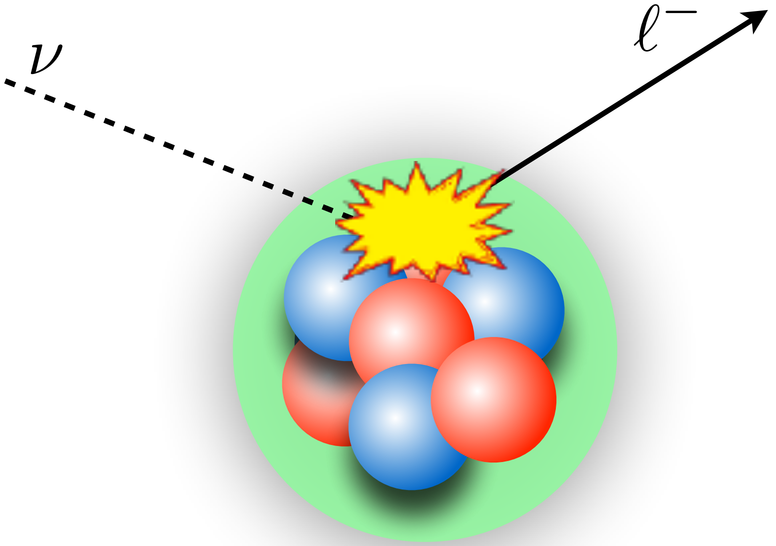


Image courtesy of Noemi Rocco

UQ FOR NEUTRINO-OSCILLATION PHYSICS

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

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



UQ FOR NEUTRINO-OSCILLATION PHYSICS

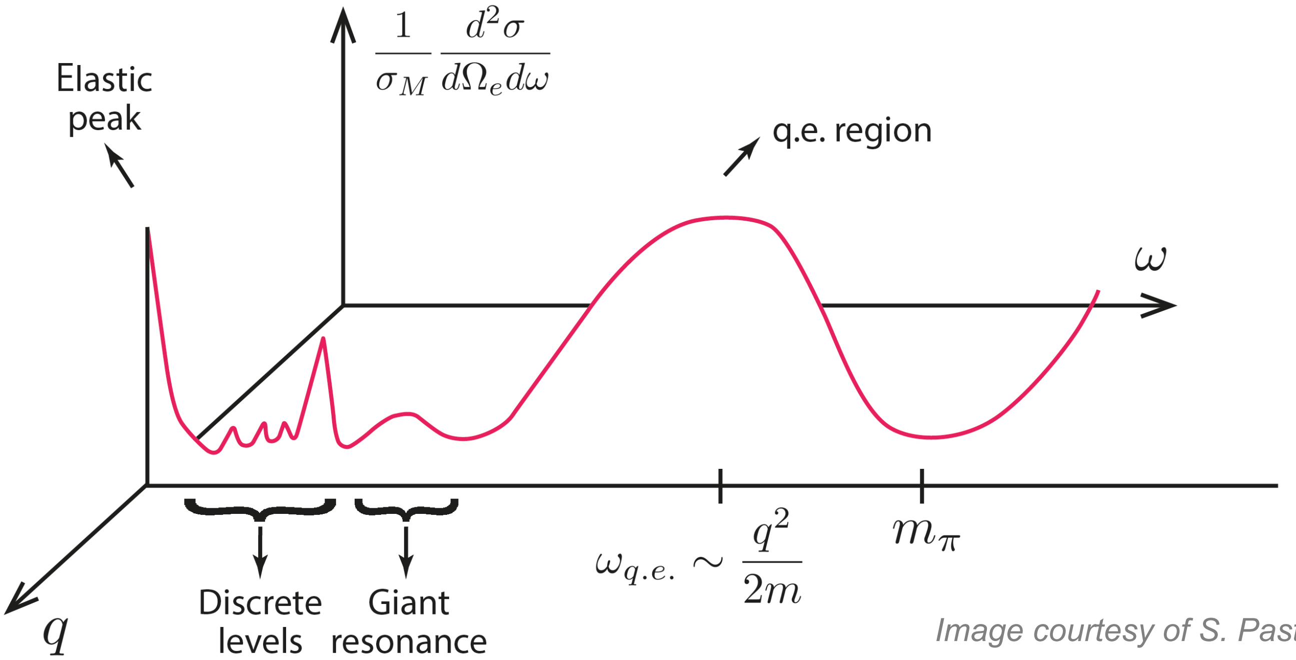


Image courtesy of S. Pastore

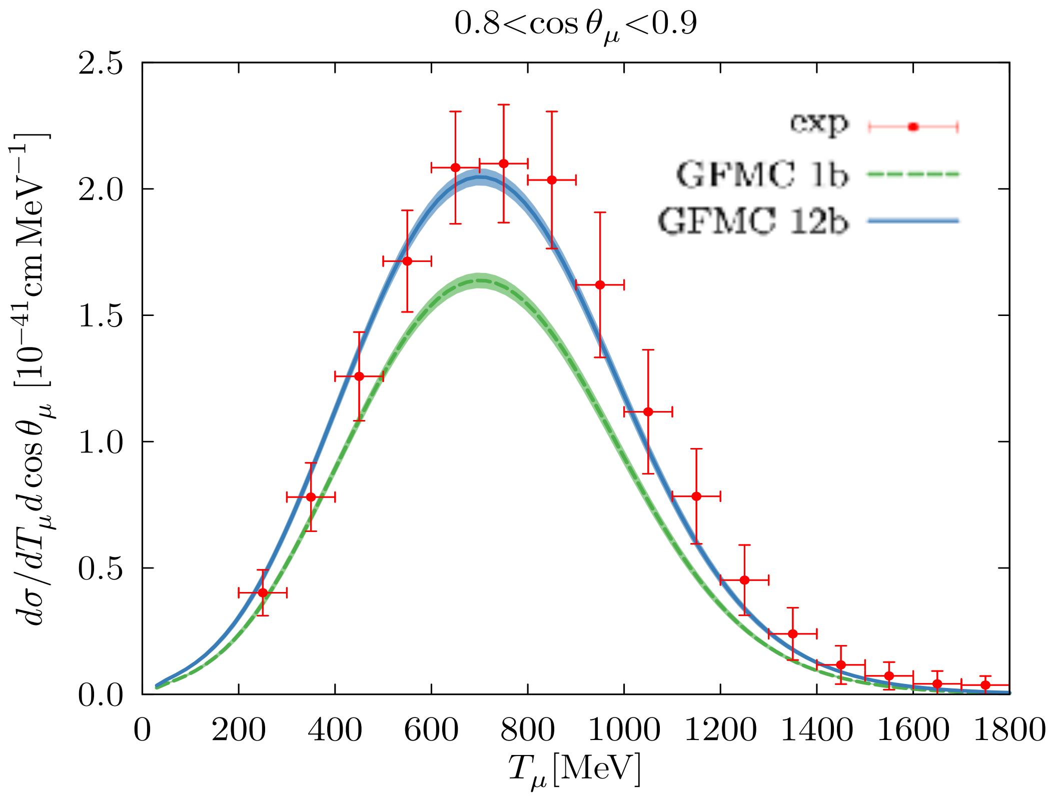
UQ FOR NEUTRINO-OSCILLATION PHYSICS

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

$$\Downarrow$$

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

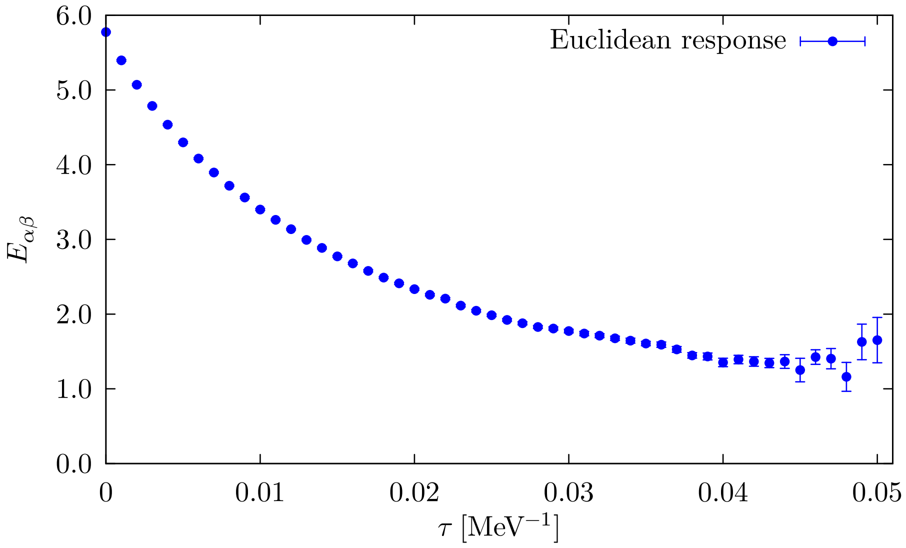
UQ FOR NEUTRINO-OSCILLATION PHYSICS

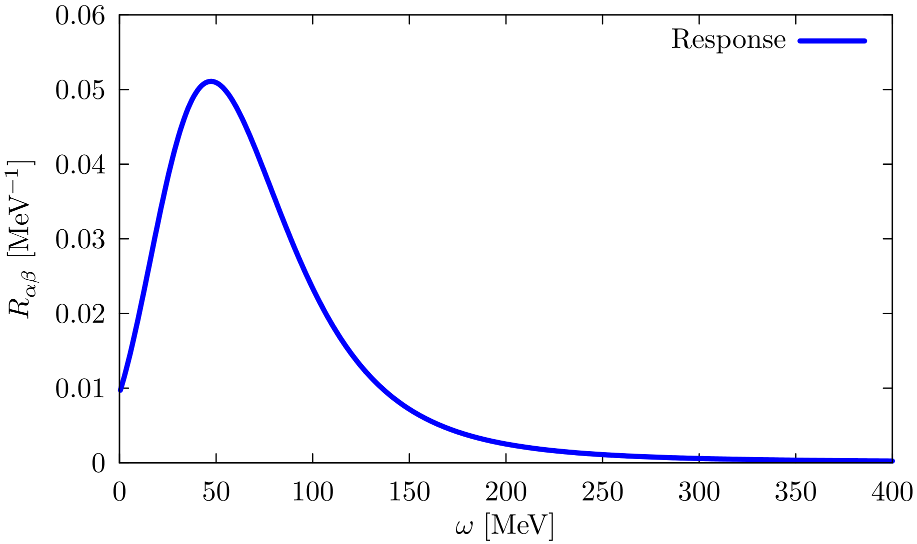


AL et al., PRX **10**, 031068 (2020)

UQ IN THE MANY-BODY METHOD

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





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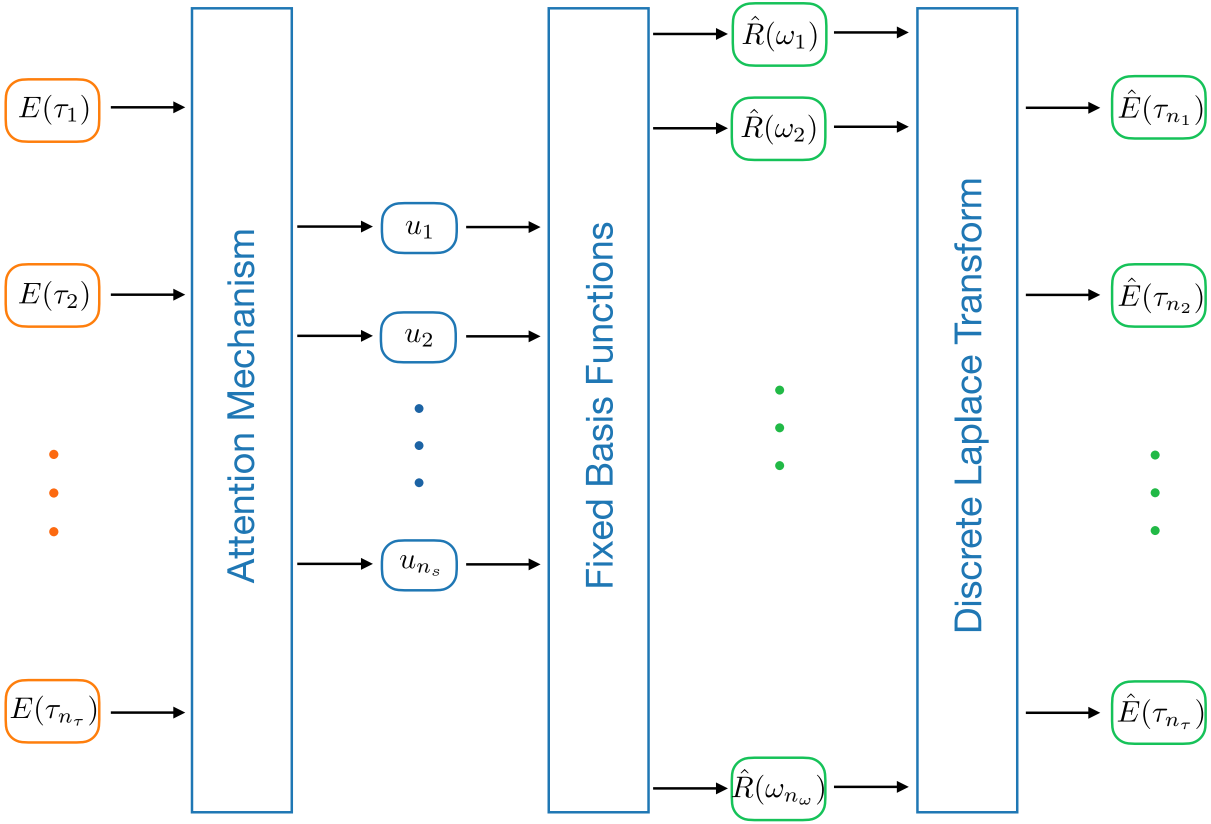
UQ IN THE MANY-BODY METHOD

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

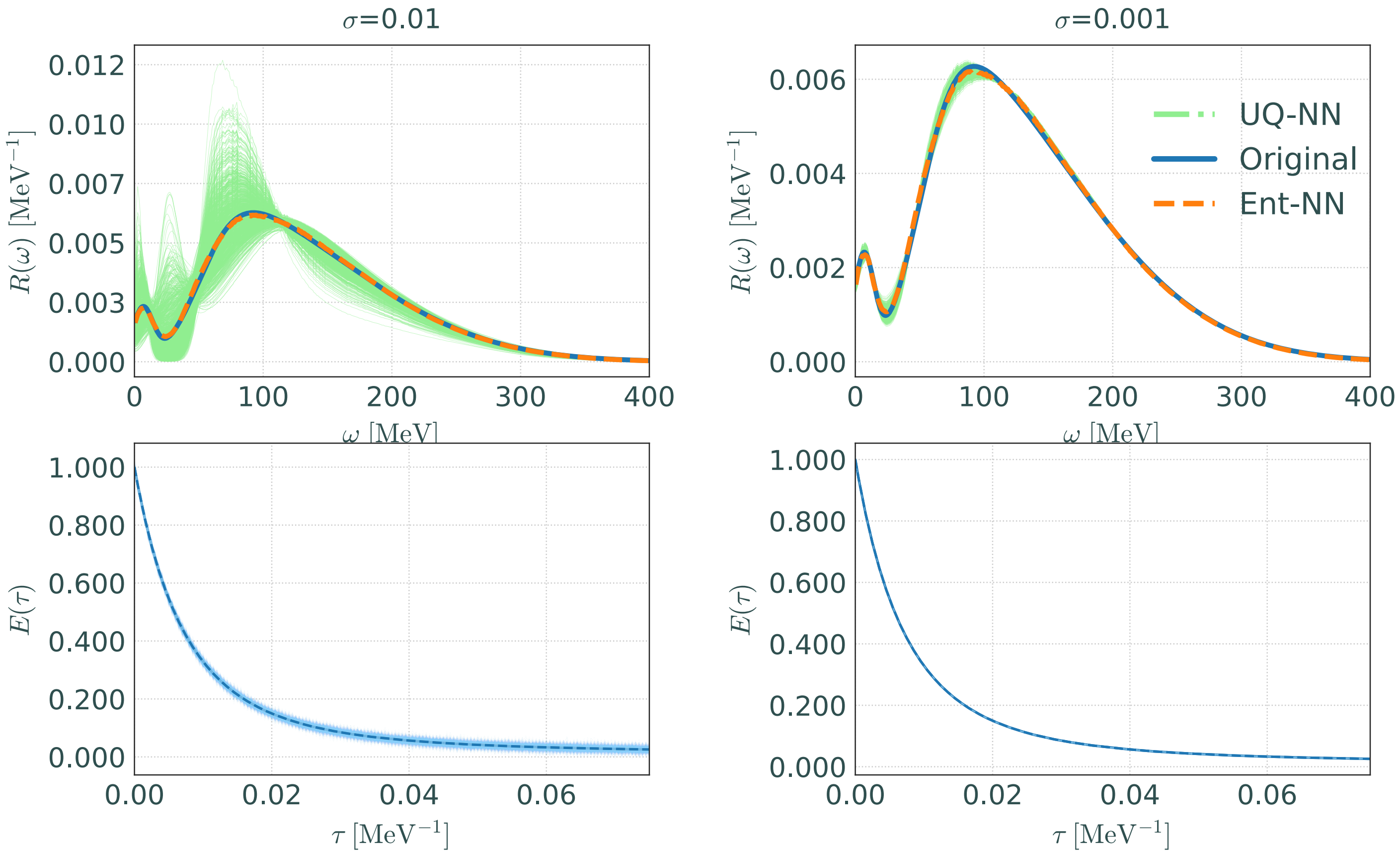
Augment the training dataset with noisy Euclidean responses

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



K. Raghavan, AL, al., arXiv:2310.18756

UQ IN THE MANY-BODY METHOD



K. Raghavan, AL, al., arXiv:2310.18756

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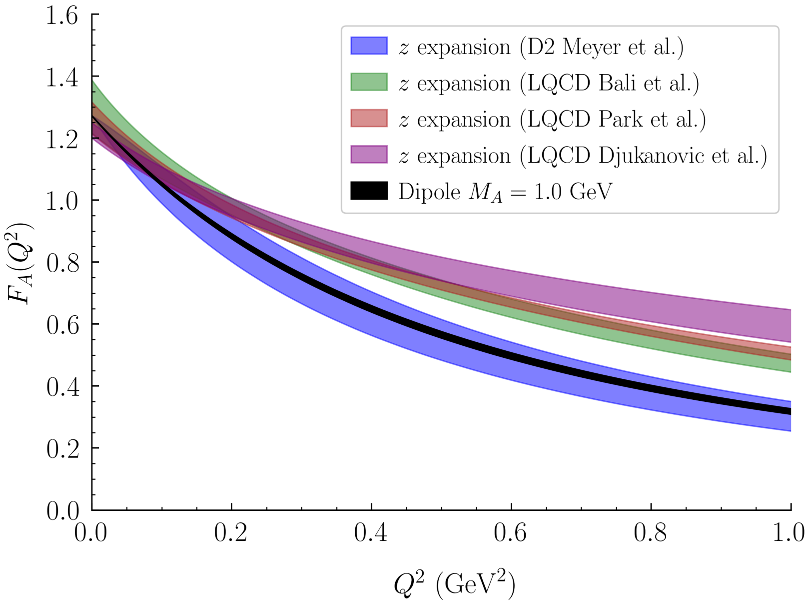
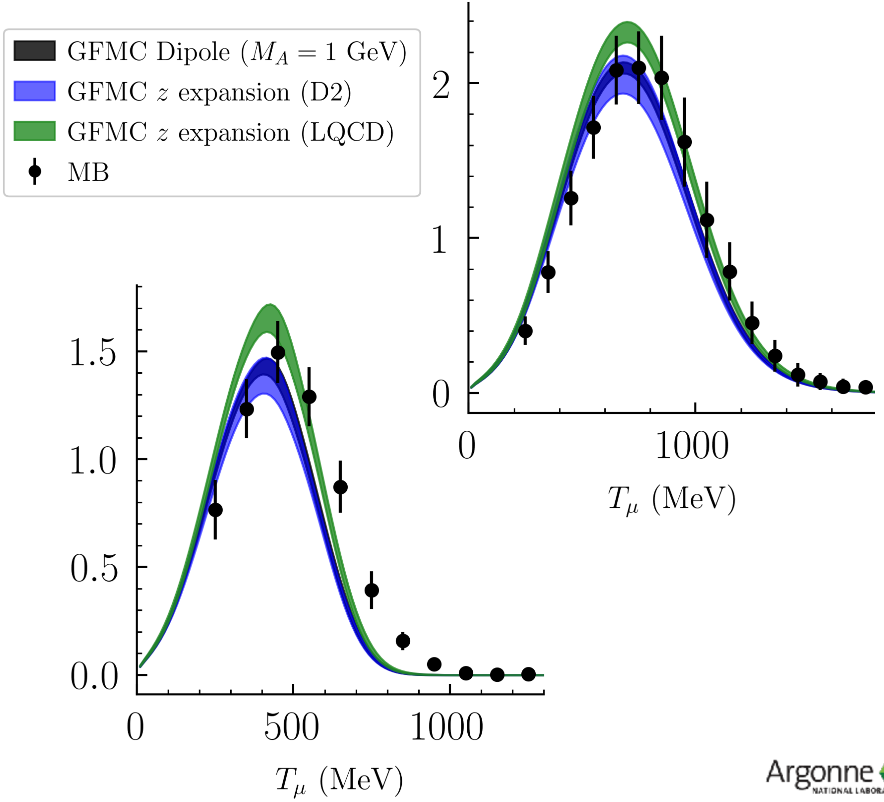
UQ IN THE INPUT CURRENT

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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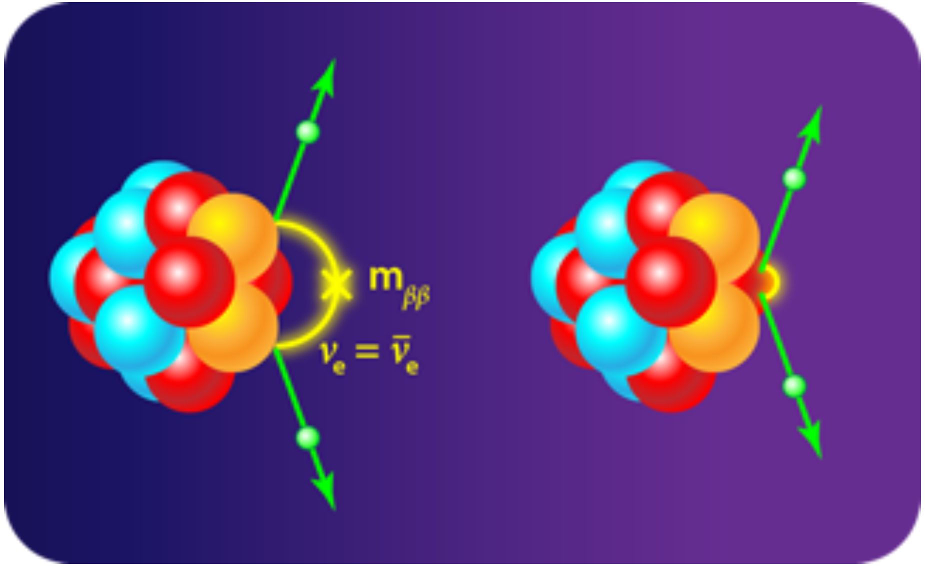
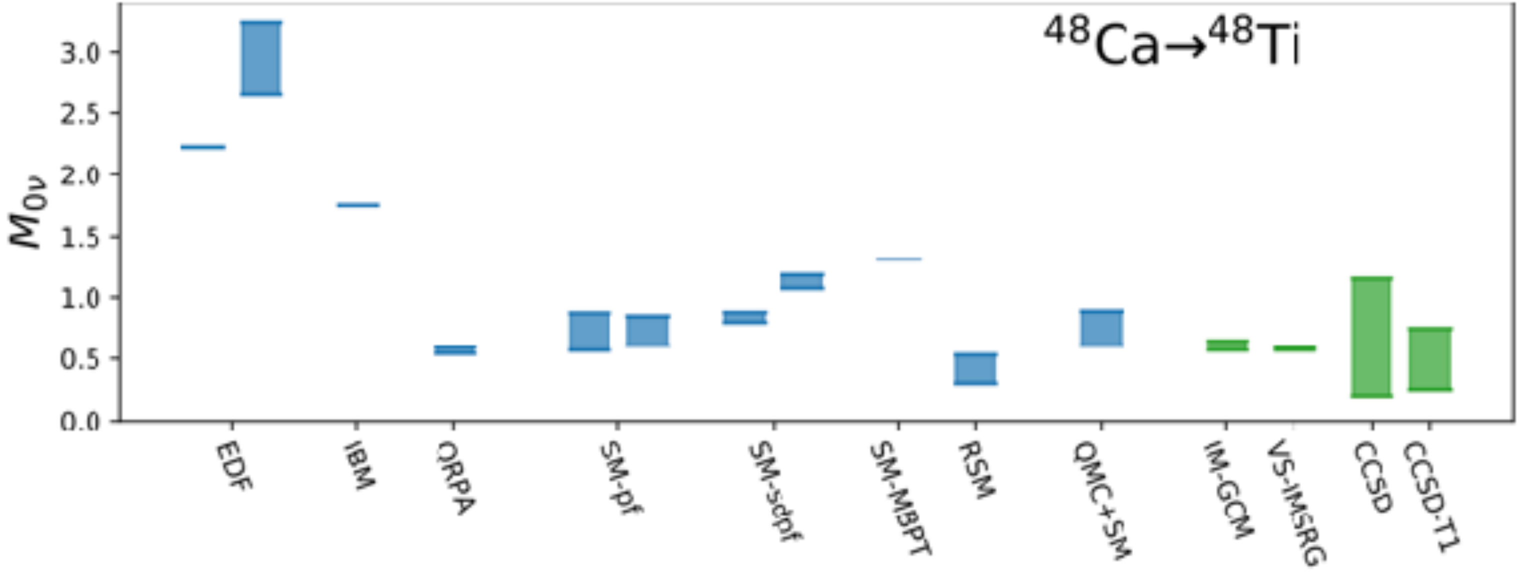
NEUTRINOLESS DOUBLE-BETA DECAY

- Lepton number not conserved.
- Neutrino mass has a Majorana component.
- Provide crucial information about neutrino mass generation.
- Suggest that the matter-antimatter asymmetry in the universe originated in leptogenesis.



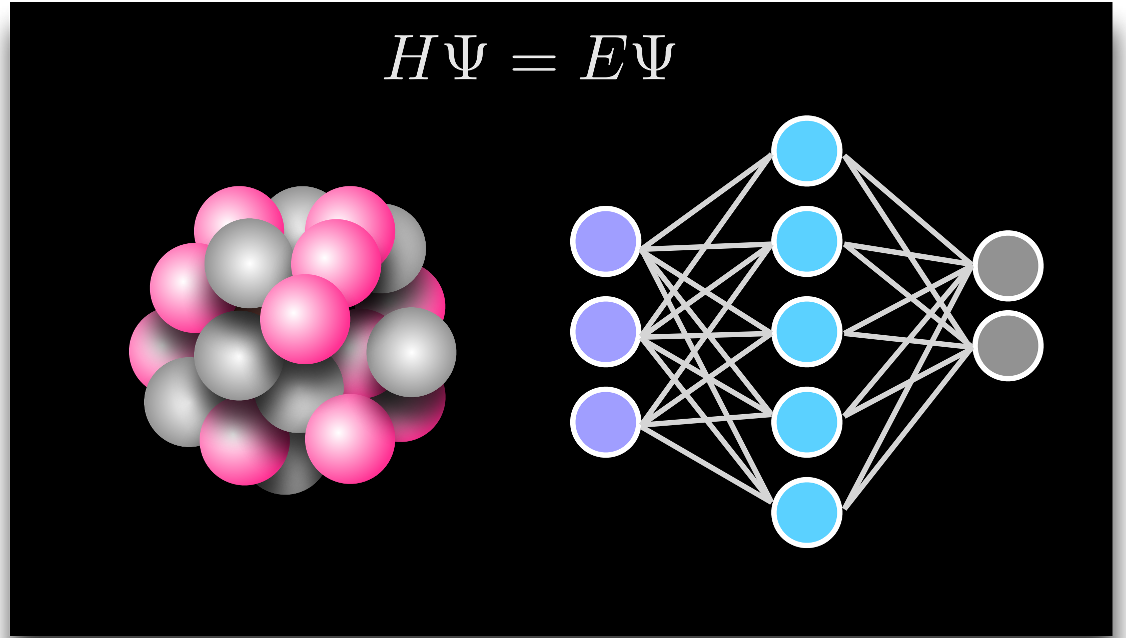
NEUTRINOLESS DOUBLE-BETA DECAY

$$[T_{1/2}]^{-1} = G^{0\nu}|M^{0\nu}|^2\langle m_{\beta\beta}\rangle^2 \quad ; \quad m_{\beta\beta} = \left|\sum_k m_k U_{ek}\right|^2 \quad ; \quad M^{0\nu} = \langle\Psi_f|O^{0\nu}|\Psi_i\rangle$$



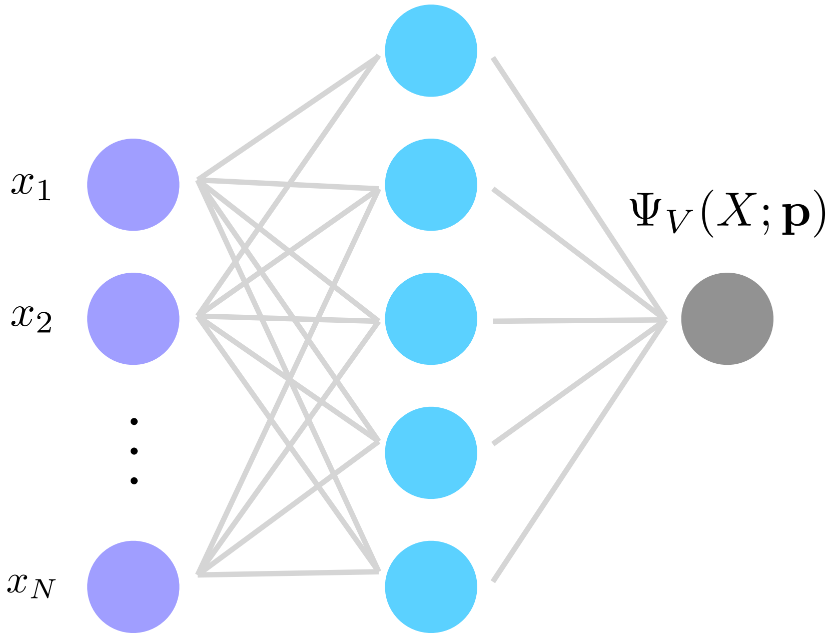
V. Cirigliano et al., J.Phys. G **49** (2022) 12, 120502

NEURAL NETWORK QUANTUM STATES



NEURAL-NETWORK QUANTUM STATES

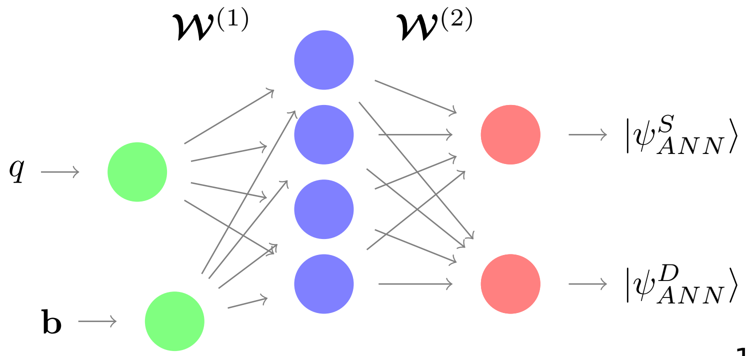
NQS are now widely and successfully applied to study condensed-matter systems



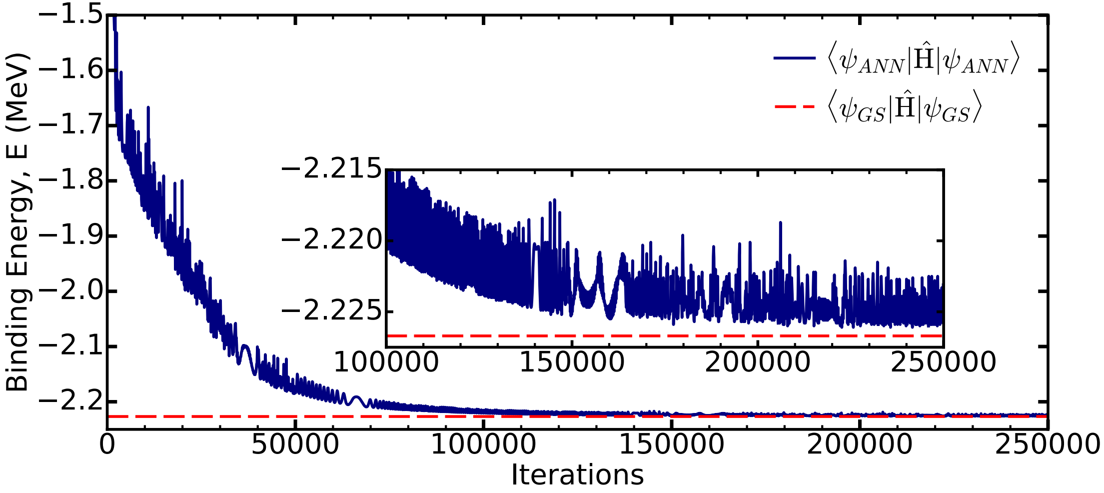
$$E_V \equiv \frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} > E_0$$

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

NEURAL-NETWORK QUANTUM STATES



$$E^{\mathcal{W}} = \frac{\left\langle \Psi^{\mathcal{W}}_{\text{ANN}} \right| \hat{H} \left| \Psi^{\mathcal{W}}_{\text{ANN}} \right\rangle}{\left\langle \Psi^{\mathcal{W}}_{\text{ANN}} \middle| \Psi^{\mathcal{W}}_{\text{ANN}} \right\rangle}$$



*Keeble, Rios, PLB **809**, 135743 (2020)*

*Sarmiento, et al., EPJ **139** (2024) 2, 189*

NEURAL-NETWORK QUANTUM STATES

Nucleons are fermions

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

Slater-Jastrow ansatz

$$\Psi_V(X) = e^{J(X)}\Phi(X) \quad ; \quad \Phi(X) = \det \begin{bmatrix} \phi_1(\mathbf{x}_1) & \phi_1(\mathbf{x}_2) & \cdots & \phi_1(\mathbf{x}_N) \\ \phi_2(\mathbf{x}_1) & \phi_2(\mathbf{x}_2) & \cdots & \phi_2(\mathbf{x}_N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_N(\mathbf{x}_1) & \phi_N(\mathbf{x}_2) & \cdots & \phi_N(\mathbf{x}_N) \end{bmatrix}$$

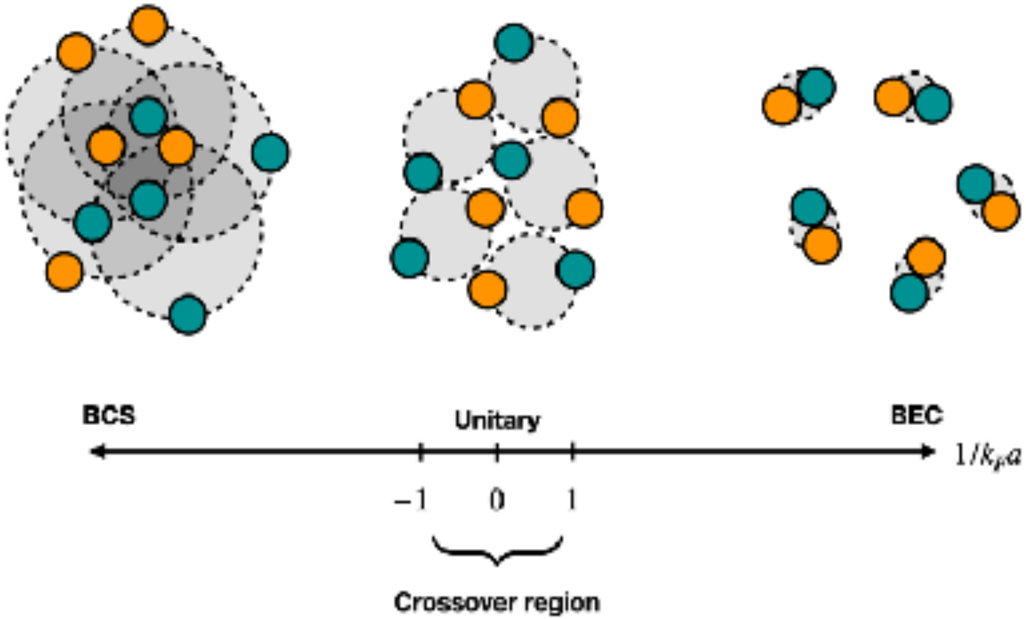
*J. Stokes et al., PLB, **102**, 205122 (2020)*

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

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

COLD FERMI GASES

Periodic-NQS to solve the two-components Fermi gas in the BCS- BEC crossover region



$$H = \sum_i \frac{p_i^2}{2m} + \sum_{i<j} v_{ij}$$

$$v_{ij} = (\delta_{s_i,s_j} - 1) v_0 \frac{2\hbar^2}{m} \frac{\mu^2}{\cosh^2(\mu r_{ij})}$$

NEURAL PFAFFIAN

Pfaffian-Jastrow ansatz

$$\Phi_{PJ}(X) = \mathrm{pf}\begin{bmatrix} 0 & \phi(x_1,x_2) & \cdots & \phi(x_1,x_N) \\ \phi(x_2,x_1) & 0 & \cdots & \phi(x_2,x_N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi(x_N,x_1) & \phi(x_N,x_2) & \cdots & 0 \end{bmatrix}$$

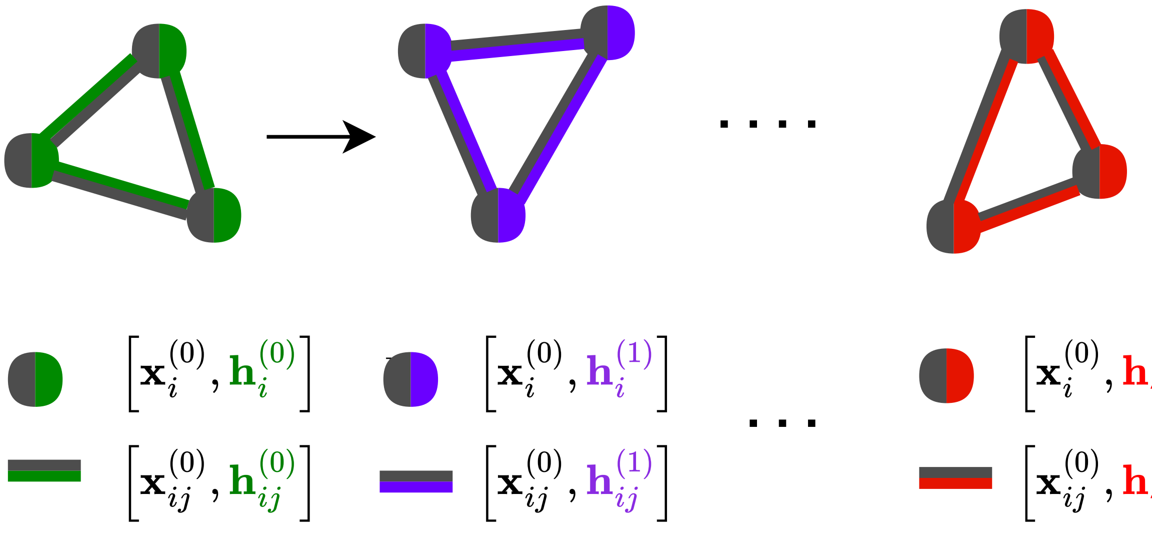
In order for the above matrix to be skew-symmetric, the neural pairing orbitals are taken to be

$$\phi(x_i,x_j) = \eta(x_i,x_j) - \eta(x_j,x_i)$$

Example: $$\mathrm{pf}\begin{bmatrix} 0 & \phi_{12} & \phi_{13} & \phi_{14} \\ -\phi_{12} & 0 & \phi_{23} & \phi_{24} \\ -\phi_{13} & -\phi_{23} & 0 & \phi_{34} \\ -\phi_{14} & -\phi_{24} & -\phi_{34} & 0 \end{bmatrix} = \phi_{12}\phi_{34} - \phi_{13}\phi_{24} + \phi_{14}\phi_{23}$$

NEURAL BACKFLOW CORRELATIONS

The nodal structure is improved with neural back-flow transformations $\mathbf{x}_i \rightarrow \mathbf{y}_i(\mathbf{x}_i; \mathbf{x}_{j\neq i})$

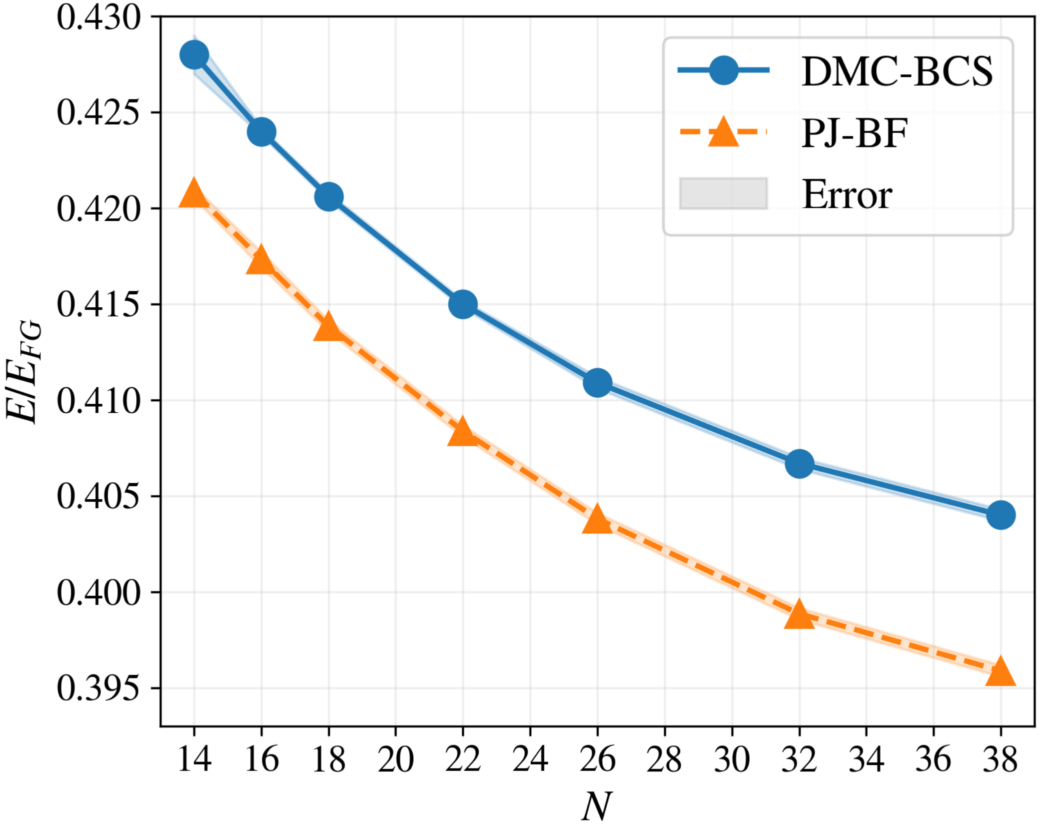


$\left[\mathbf{x}_i^{(0)}, \mathbf{h}_i^{(0)}\right]$ $\left[\mathbf{x}_i^{(0)}, \mathbf{h}_i^{(1)}\right]$ $\left[\mathbf{x}_i^{(0)}, \mathbf{h}_i^{(T)}\right]$

$\left[\mathbf{x}_{ij}^{(0)}, \mathbf{h}_{ij}^{(0)}\right]$ $\left[\mathbf{x}_{ij}^{(0)}, \mathbf{h}_{ij}^{(1)}\right]$ $\left[\mathbf{x}_{ij}^{(0)}, \mathbf{h}_{ij}^{(T)}\right]$

G. Pescia, et al., 2305.08831 [cond-mat.quant-gas]

COLD FERMI GASES



$$\left(\frac{E}{E_{FG}}\right)_{\text{exp}} = \xi = 0.376(5)$$

J. Kim, B. Fore, AL, et al. Commun.Phys. **7** (2024) 1, 148

BACK TO NUCLEAR PHYSICS

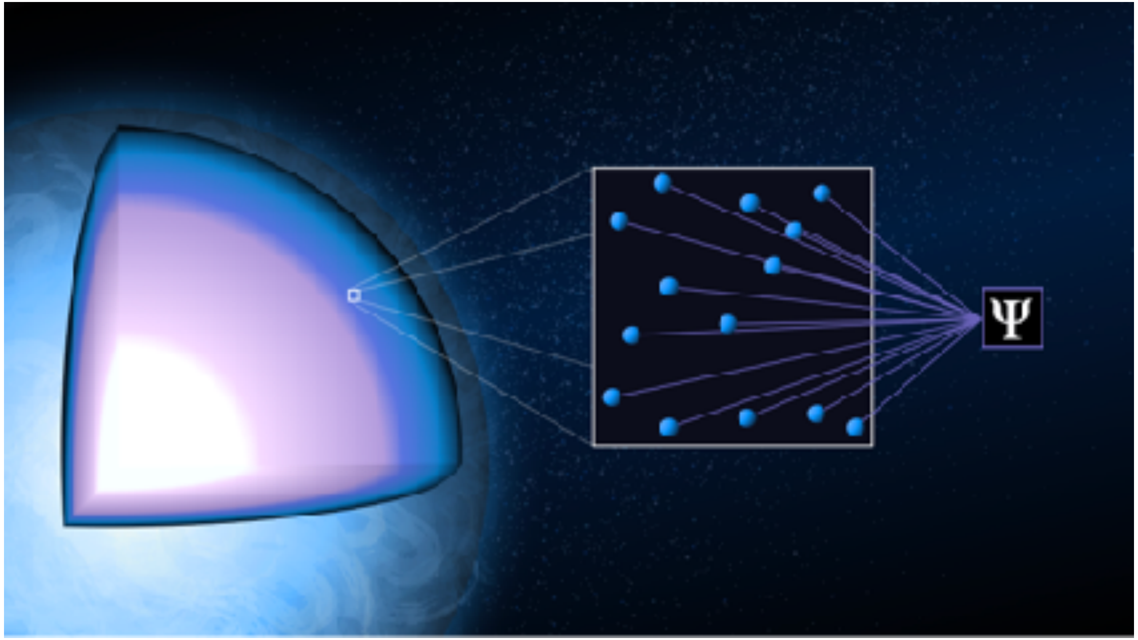


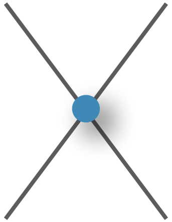
Image Credit: Jane Kim

“ESSENTIAL" HAMILTONIAN

Input: Hamiltonian inspired by a LO pionless-EFT expansion

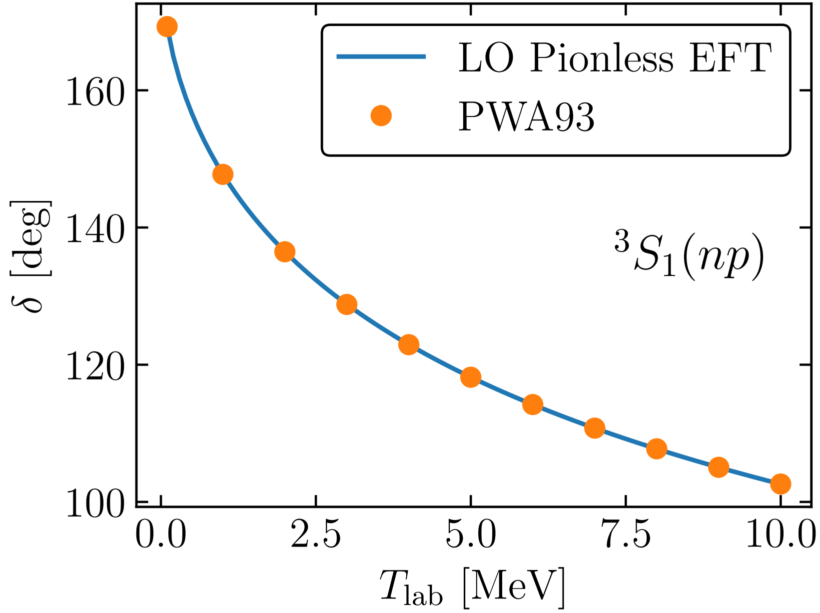
$$H_{LO} = -\sum_i \frac{\vec{\nabla}_i^2}{2m_N} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

- NN potential fit to s-wave np scattering lengths and effective ranges



$$v_{ij}^{\mathrm{CI}} = \sum_{p=1}^{4} v^p(r_{ij}) O_{ij}^p \,,$$

$$O_{ij}^{p=1,4} = (1, \tau_{ij}, \sigma_{ij}, \sigma_{ij}\tau_{ij})$$



R. Schiavilla, AL, PRC **103**, 054003 (2021)

“ESSENTIAL" HAMILTONIAN

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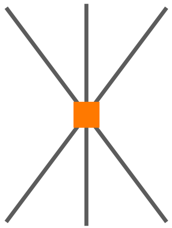
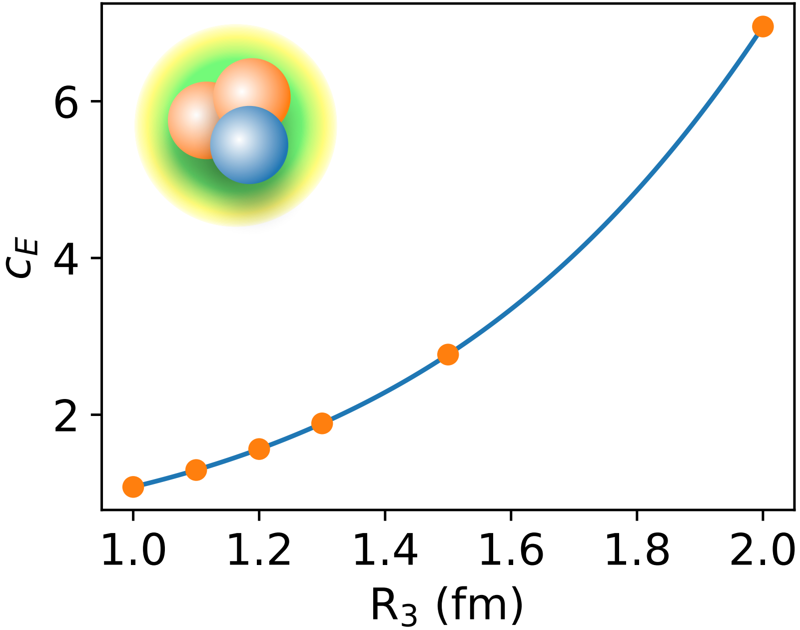
- 3NF adjusted to reproduce the energy of ^{3}H.



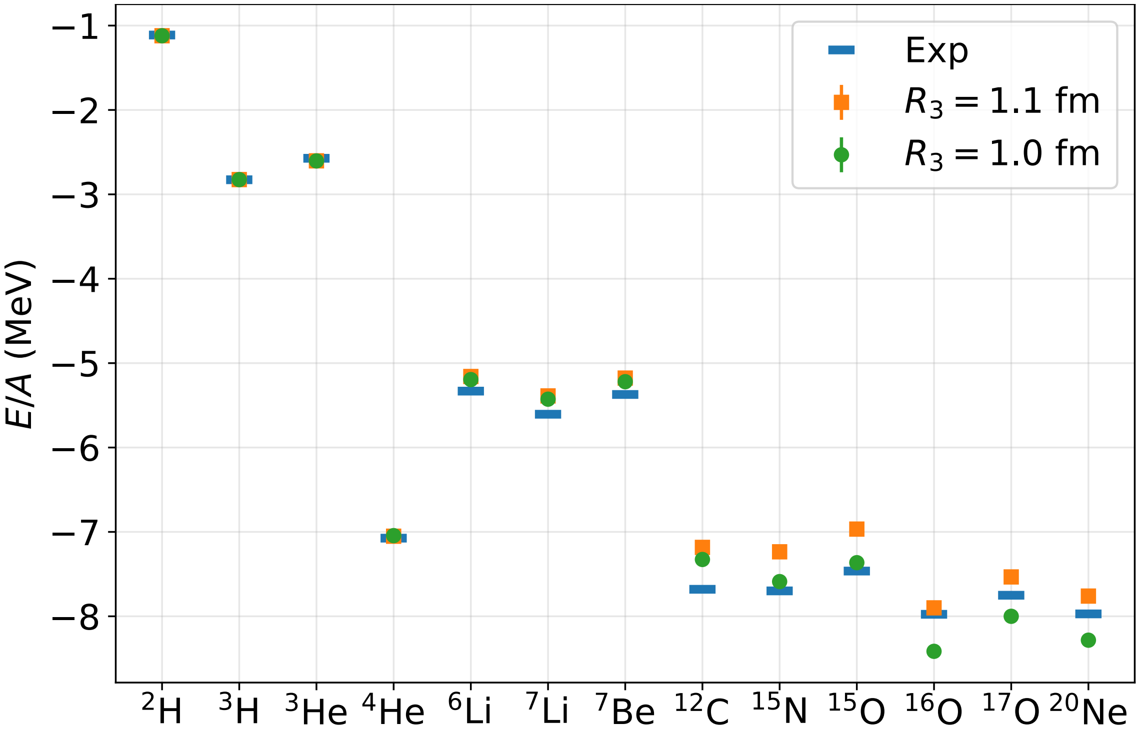
$$V_{ijk} \propto c_E \sum_{\rm cyc} e^{-(r_{ij}^2 + r_{jk}^2)/R_3^2}$$



*R. Schiavilla, AL, PRC **103**, 054003 (2021)*

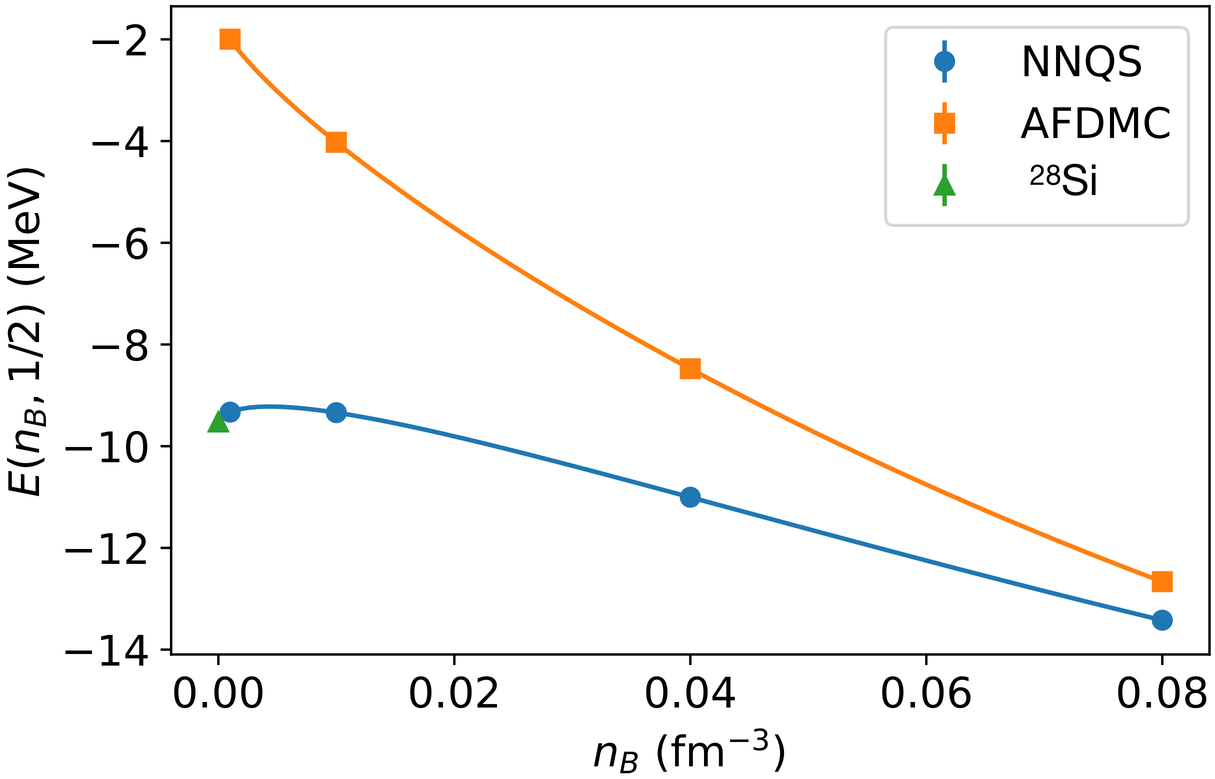
“ESSENTIAL" HAMILTONIAN

Our “essential” Hamiltonian reproduces well the spectrum of different nuclei



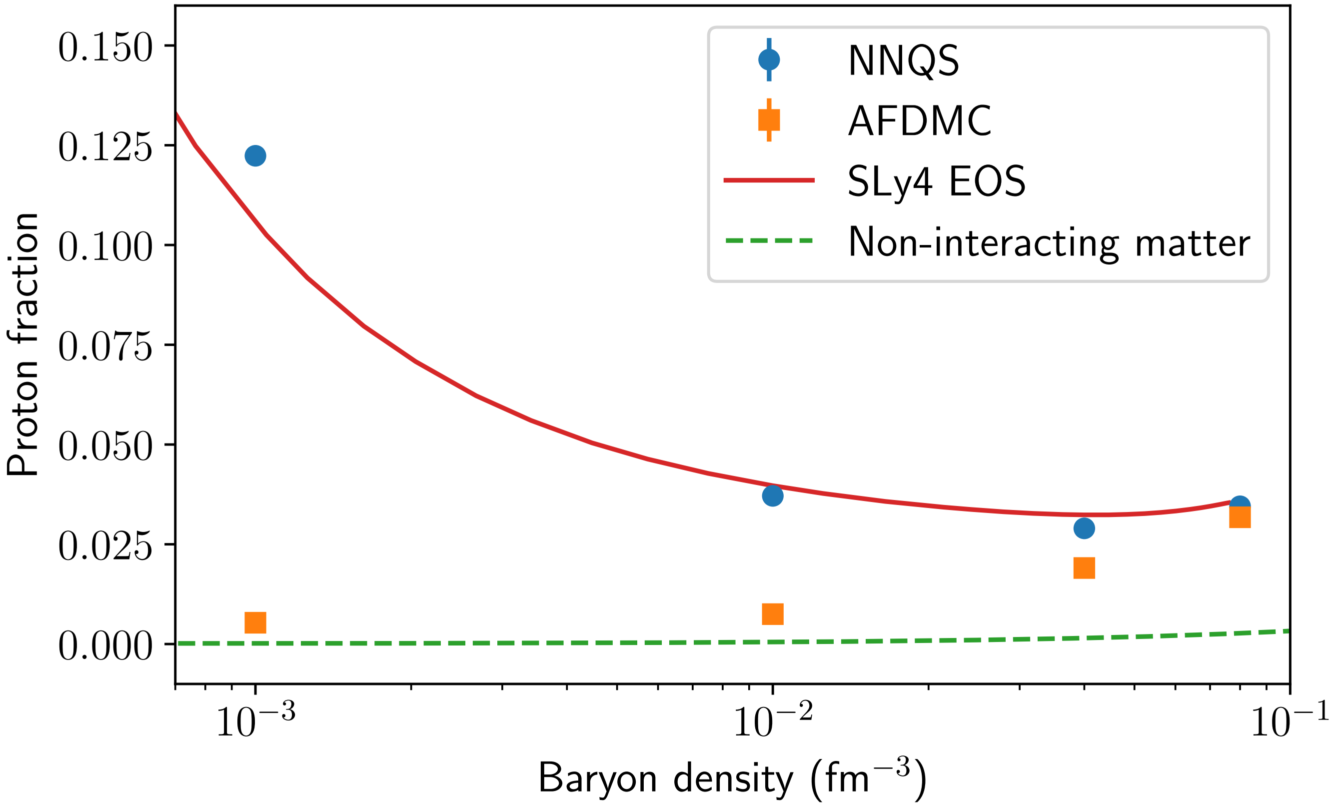
A. Gnech, AL, et al., 2308.16266

DILUTE NUCLEONIC MATTER



B. Fore, AL, et al. in preparation

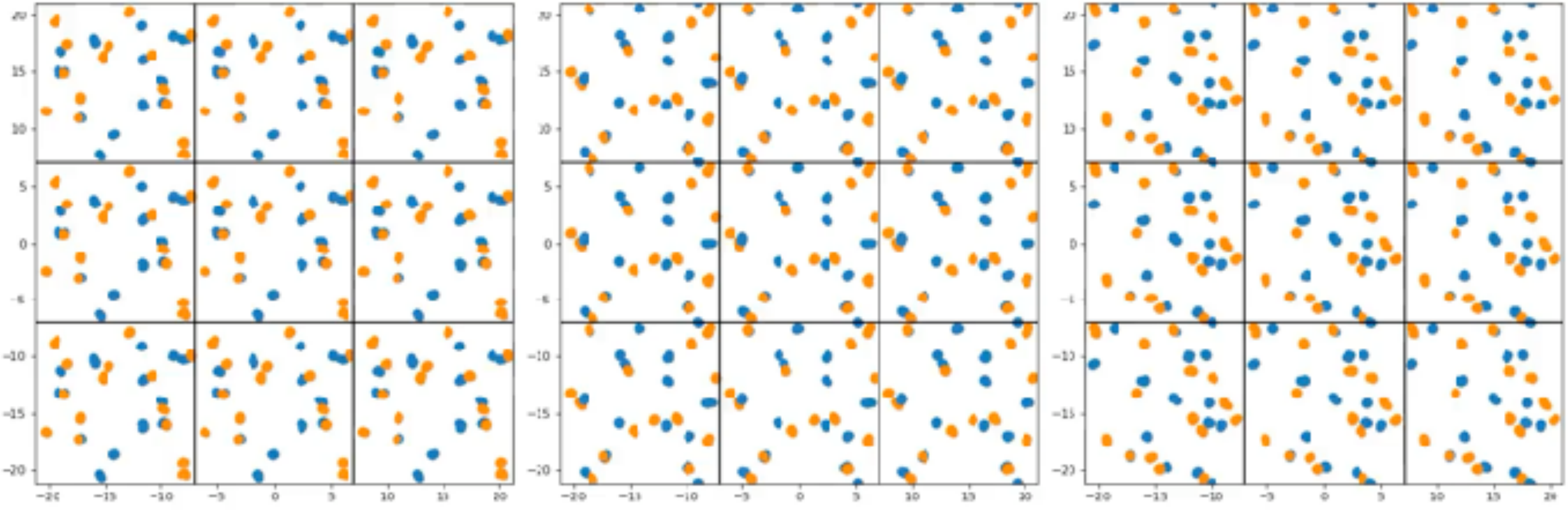
DILUTE NUCLEONIC MATTER



B. Fore, AL, et al. in preparation

DILUTE NUCLEONIC MATTER

14 Neutrons, 14 Protons @ ρ=0.01 fm^{-3}



B. Fore, AL, et al. in preparation

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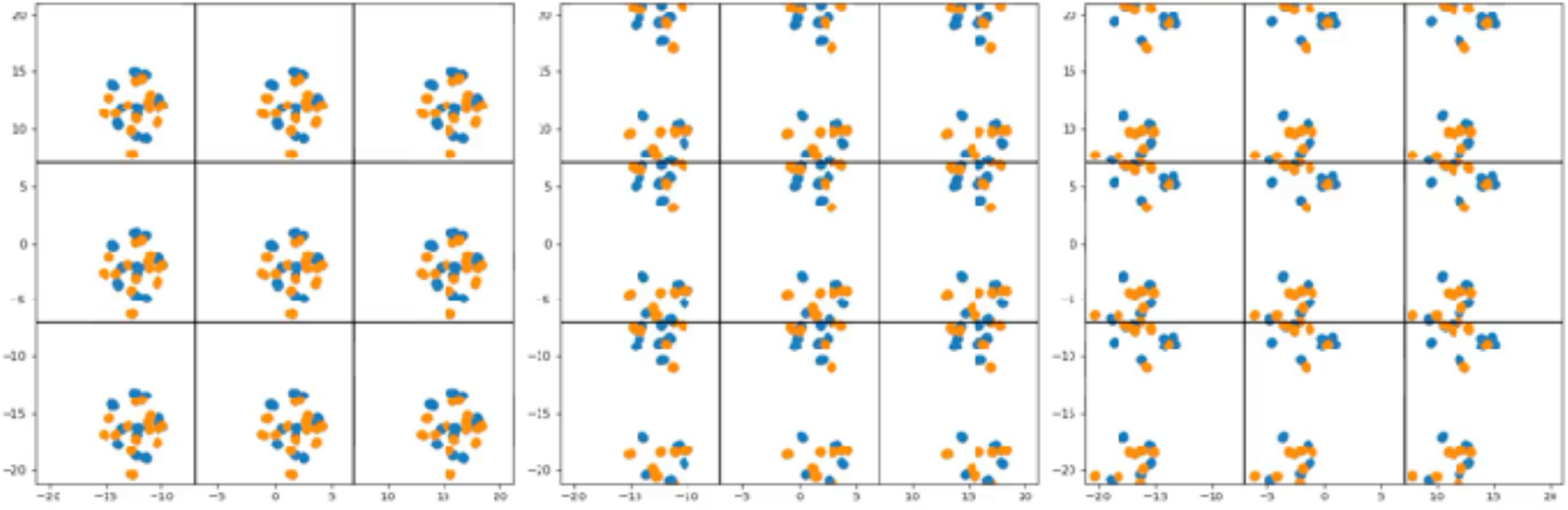

B. Fore, AL, et al. in preparation

CONCLUSIONS

Tremendous progress in estimating uncertainties in theoretical calculations

- Relevant for meaningful “nuclear structure” experiments;
- Essential for Nuclear Astrophysics and Fundamental Physics

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Tremendous progress in estimating uncertainties in theoretical calculations

- Relevant for meaningful “nuclear structure” experiments;
- Essential for Nuclear Astrophysics and Fundamental Physics

***Rumsfeld**: as we know, there are known knowns[…] We also know there are known unknowns […] But there are also unknown unknowns—the ones we don't know we don't know. […] it is the latter category that tends to be the difficult ones.*

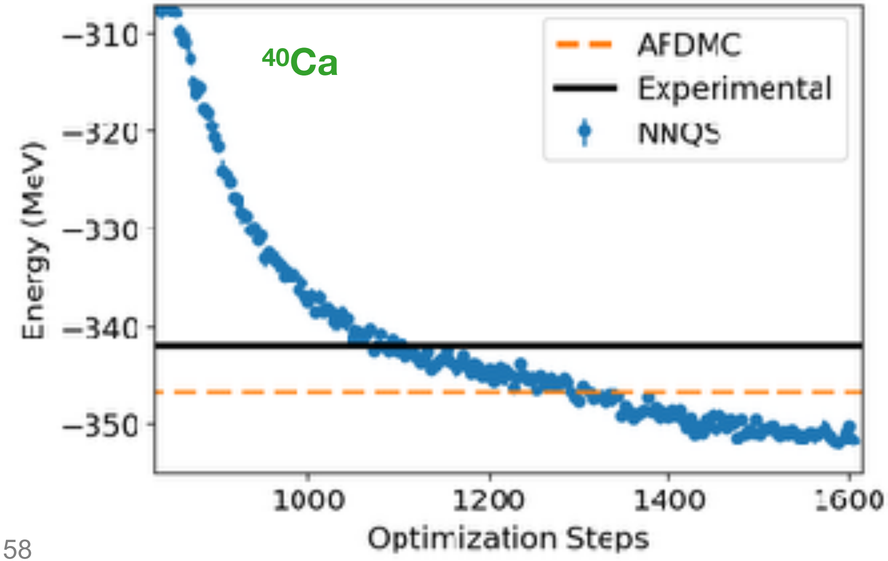
CONCLUSIONS

NQS successfully applied to study:

- ➡ Ultra-cold Fermi gases, outperforming state-of-the-art continuum DMC;
- ➡ Dilute nucleonic matter, including the self-emergence of nuclei;
- ➡ Essential Elements of nuclear binding (including magnetic moments)

Ongoing efforts:

- ➡ Medium-mass nuclei
- ➡ Excited states
- ➡ Chiral-EFT potentials
- ➡ Real-time dynamics
- ➡ UQ in NQS



THANK YOU