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THE HEBREW UNIVERSITY OF JERUSALEM

Nuclear Responses with Neural-Network Quantum States

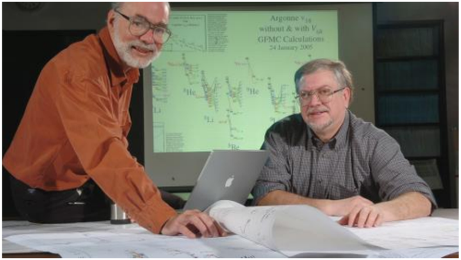
Nir Barnea

ESNT Workshop, June 29 - July 4, 2026

Saclay

OCTOBER 29, 2009

Steven Pieper and Robert Wiringa, senior scientists at the U.S. Department of Energy's (DOE) Argonne National Laboratory, have won the 2010 Tom W. Bonner Prize in nuclear physics. The award will be presented by the American Physical Society in Washington, D.C., in February 2010.



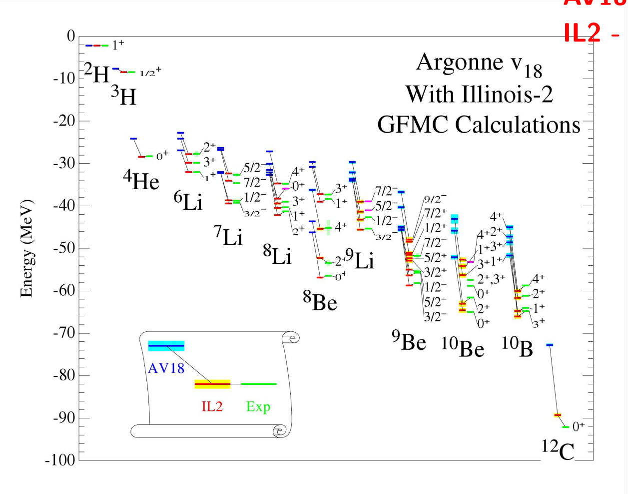
Steven Pieper (left) and Robert Wiringa, senior scientists at Argonne National Lab, have won the 2010 Tom W. Bonner Prize in nuclear physics.

Pieper and Wiringa, who are theoretical physicists, won the prize for developing and applying models of nuclear forces and methods to calculate the properties of light nuclei. The prize typically recognizes outstanding experimental research in nuclear physics, but in special circumstances it may be awarded for outstanding theoretical work.

The spectra of light nuclei

AV18 - NN force

IL2 - NNN force



S. Pieper and R. Wiringa, Ann. Rev. Nucl. Part. Sci. **51**, 53 (2001)

The VMC-GFMC method

- VMC - Variational Monte-Carlo

$$E = \langle \Psi_T | H | \Psi_T \rangle / \langle \Psi_T | \Psi_T \rangle \geq E_0$$

- GFMC -Green's Function Monte-Carlo

$$\exp(-H\tau)|\Psi_T\rangle \rightarrow |\Psi_0\rangle$$

- **Limitations:**

  DMC unstable, needs very good starting WF,

  $A \leq 12$

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- **Limitations:**
  DMC unstable, needs very good starting WF,
  $A \leq 12$

The trial wave-function

The trial wave-function

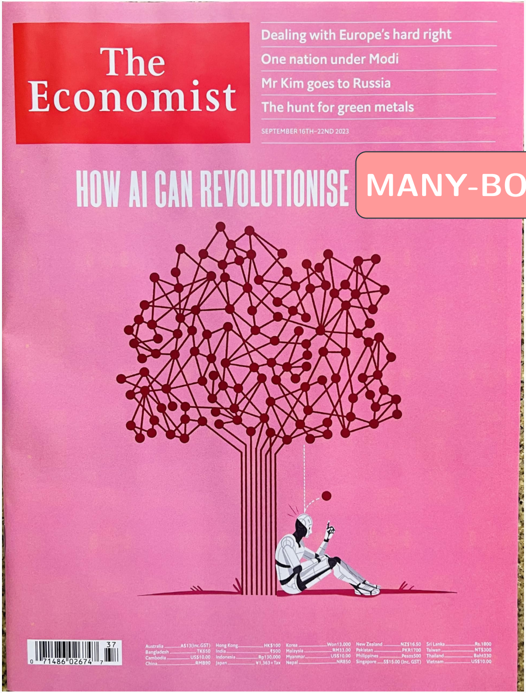
$$\boxed{|\Psi_T\rangle = \mathcal{F}|\Phi\rangle}$$

$|\Phi\rangle$ - anti symmetric wave-function
$\mathcal{F}$ - correlation operator

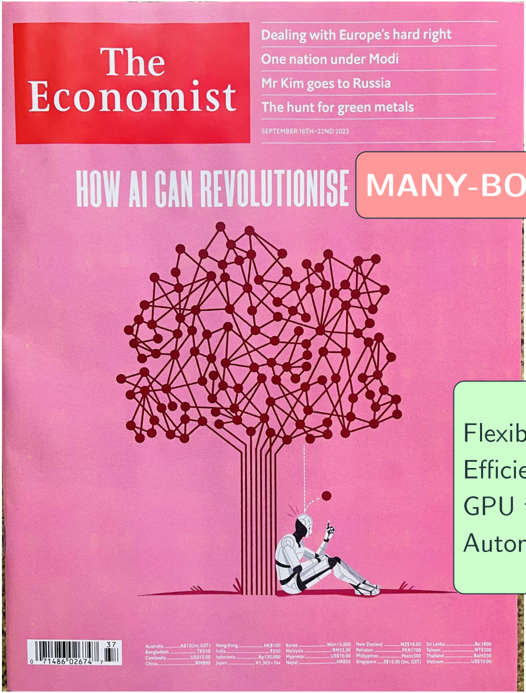
$$\boxed{\mathcal{F} = \left(\mathcal{S}\prod_{i<j<k}(1+F_{ijk})\right)\left(\mathcal{S}\prod_{i<j}F_{ij}\right)|\Psi_T\rangle}$$

VMC-GFMC handles interactions with large cutoff.
The large spin-isospin vector $\approx 4^A$ creates a limitations


The Economist
Dealing with Europe's hard right
One nation under Modi
Mr Kim goes to Russia
The hunt for green metals
SEPTEMBER 16TH–22ND 2023
HOW AI CAN REVOLUTIONISE SCIENCE

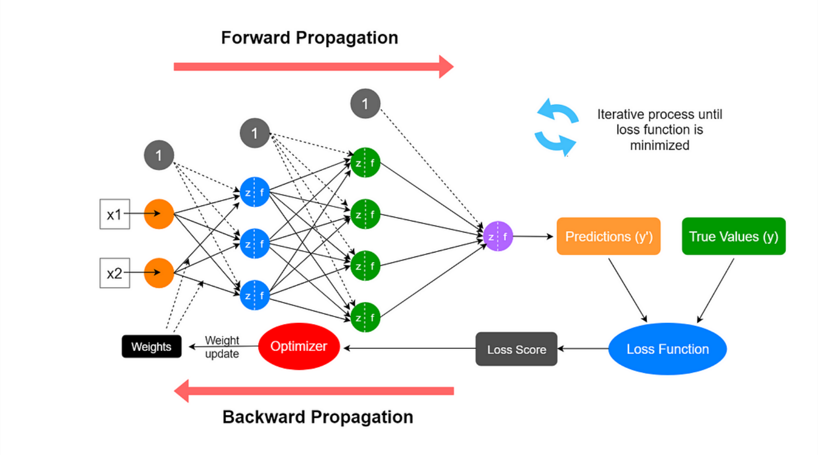


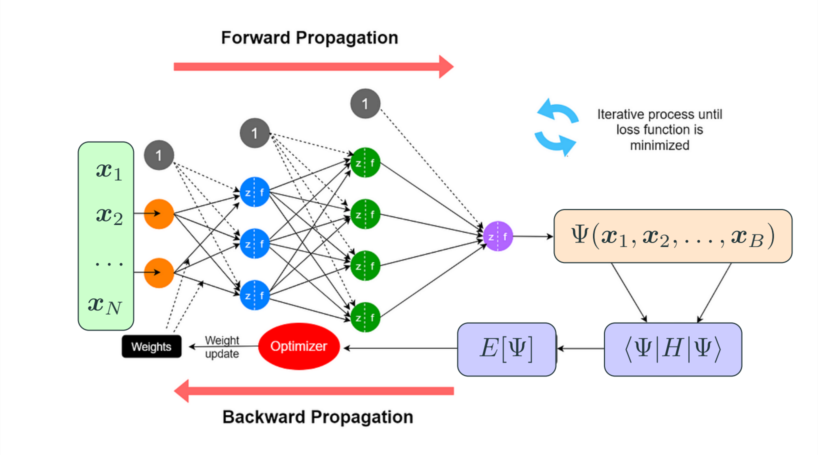
MANY-BODY THEORY



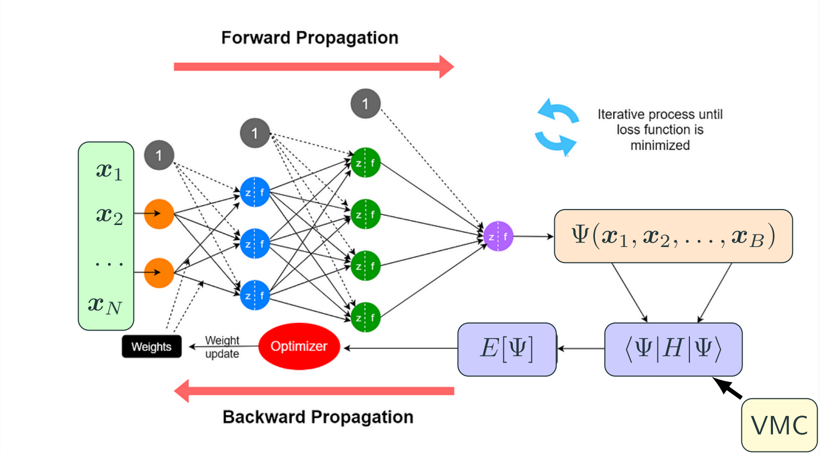
MANY-BODY THEORY

- Flexible-model
- Efficient minimization
- GPU tech
- Automatic differentiation


Forward Propagation
Iterative process until loss function is minimized
1
1
1
x1
x2
z f
Predictions (y')
True Values (y)
Weights
Weight update
Optimizer
Loss Score
Loss Function
Backward Propagation



Forward Propagation
Iterative process until loss function is minimized
x_1
x_2
$\dots$
x_N
1
z f
$\Psi(x_1, x_2, \dots, x_B)$
$\langle\Psi|H|\Psi\rangle$
$E[\Psi]$
Optimizer
Weight update
Weights
Backward Propagation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Weights
Weight update
Optimizer
$E[\Psi]$
$\langle\Psi|H|\Psi\rangle$
VMC
Backward Propagation

Variational principle:

$$\langle E \rangle = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \geq E_0$$

Evaluation of the integral

$$\begin{aligned}
\langle E \rangle &= \frac{\int dX \Psi^*(X) H \Psi(X)}{\int dX \Psi^*(X) \Psi(X)} \\
&= \frac{1}{\int dX |\Psi(X)|^2} \int dX |\Psi(X)|^2 \frac{1}{\Psi(X)} H \Psi(X) \\
&\approx \frac{1}{N} \sum_n^N \frac{1}{\Psi(X_n)} H \Psi(X_n)
\end{aligned}$$

X stands for the coordinates and internal dof of all the nucleons

X_n is sampled from the PDF $|\Psi(X)|^2$

Neural Quantum State

AB INITIO CALCULATIONS OF MEDIUM-MASS NUCLEI WITH NEURAL QUANTUM STATES

JANE KIM
Argonne National Laboratory

Challenges in effective field theory descriptions of nuclei
Hirschegg, Austria
21 January 2026

U.S. DEPARTMENT of ENERGY

Argonne NATIONAL LABORATORY

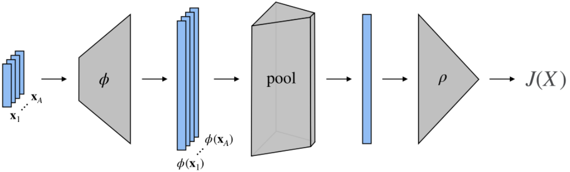
NEURAL QUANTUM STATES

$$\Psi(X) = F(X)\Phi(X)$$

symmetric

antisymmetric

Symmetric part: $F(X) = e^{J(X)}$ (positive definite)



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Zaheer et al., arXiv:1703.06114 (2017)

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NEURAL QUANTUM STATES

$$\Psi(X) = F(X)\Phi(X)$$

symmetric → $F(X)$

antisymmetric → $\Phi(X)$

Antisymmetric part: we use one based on a **Pfaffian**

$$\Phi(X) = \det \begin{bmatrix} \phi_1(\mathbf{x}_1) & \phi_1(\mathbf{x}_2) & \cdots & \phi_1(\mathbf{x}_A) \\ \phi_2(\mathbf{x}_1) & \phi_2(\mathbf{x}_2) & \cdots & \phi_2(\mathbf{x}_A) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_A(\mathbf{x}_1) & \phi_A(\mathbf{x}_2) & \cdots & \phi_A(\mathbf{x}_A) \end{bmatrix}$$

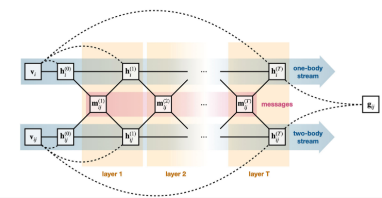
A independent neural networks
or one with A different outputs

$$\Phi(X) = \mathrm{pf} \begin{bmatrix} 0 & \phi(\mathbf{x}_1, \mathbf{x}_2) & \cdots & \phi(\mathbf{x}_1, \mathbf{x}_A) \\ -\phi(\mathbf{x}_1, \mathbf{x}_2) & 0 & \cdots & \phi(\mathbf{x}_2, \mathbf{x}_A) \\ \vdots & \vdots & \ddots & \vdots \\ -\phi(\mathbf{x}_1, \mathbf{x}_A) & -\phi(\mathbf{x}_2, \mathbf{x}_A) & \cdots & 0 \end{bmatrix}$$

One neural network parameterizing the pairing orbital

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

The MPNN Architecture - Message Passing Neural Network architecture - creates antisymmetrized descriptors of particle location that are already well processed by NNs.



$$\Psi(X) = e^{J(X)}\Phi_{PJ}(X)$$

$$\Phi_{PJ}(X) = \mathrm{pf}(P) \quad ; \quad \mathrm{pf}^2(P) = \mathrm{Det}(P)$$

$$P \equiv \begin{pmatrix} 0 & \phi(x_1,x_2) & \cdots & \phi(x_1,x_N) \\ -\phi(x_2,x_1) & 0 & \cdots & \phi(x_2,x_N) \\ \vdots & \vdots & \ddots & \vdots \\ -\phi(x_N,x_1) & -\phi(x_N,x_2) & \cdots & 0 \end{pmatrix}$$

J. Kim, G. Pescia, B. Fore, N. Nys, G. Carleo, S. Gandolfi, M. Hjorth-Jensen, and A. Lovato, Communications Physics 7, 148 (2024)

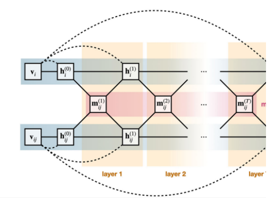
The MPNN Arc[...] [...]k

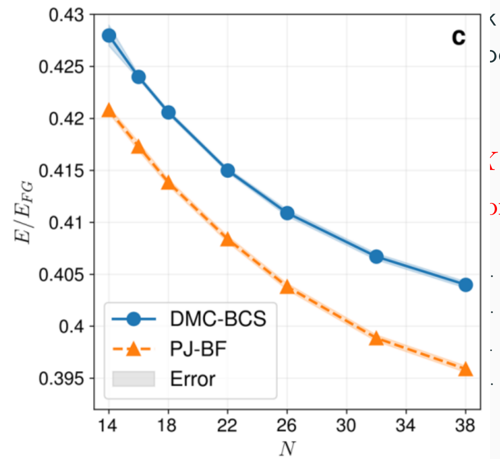
architecture - crea[...] [...]ocation

that are already w[...]

[...]$)$

[...]$\mathrm{of}^2(P) = \mathrm{Det}(P)$





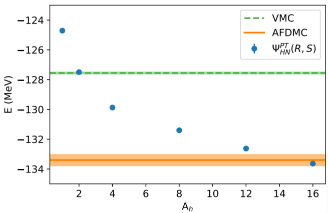
$\phi(x_1, x_N)$
$\phi(x_2, x_N)$
$\vdots$
0

J. Kim, G. Pescia, B. Fore, N. Nys, G. Carleo, S. Gandolfi, M. Hjorth-Jensen, and A. Lovato, Communications Physics 7, 148 (2024)

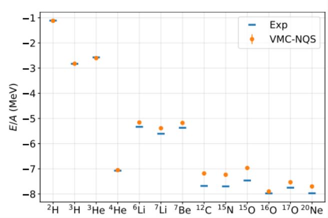
A prominent example of an **antisymmetric wavefunction** is the **Hidden Nucleons architecture**. This extension of the slater determinant allows much more flexibility.

$$\Psi_{HN}(X) \equiv \begin{vmatrix} \phi_v(X) & \chi_v(X_h) \\ \chi_h(X) & J_h(X_h) \end{vmatrix},$$

Flexibility can be enhanced by incorporating a symmetric Jastrow like terms.



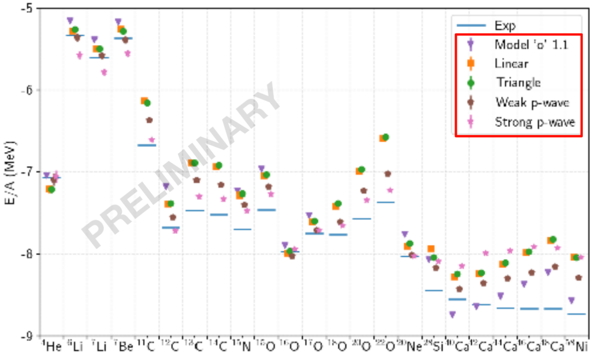
A. Lovato et al., Phys. Rev. R 4, 043178 (2022)



A. Lovato et al. (2024)

B. Fore, JK, et al., in prep.

RESULTS: MEDIUM-MASS NUCLEI

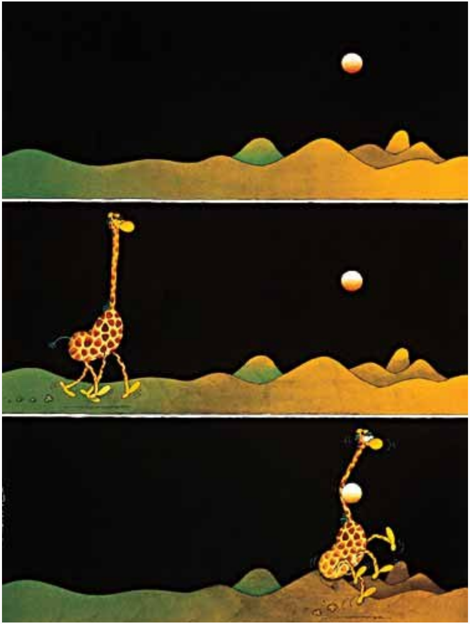


Different LO pionless EFT Hamiltonians

Neural Quantum State (NQS) Codes (ChatGPT)

- **General-purpose NQS / VMC frameworks**
  - **NetKet** (Python, JAX)
    Spin, Bose/Fermi; RBM, CNN, scalable VMC
  - **NeuralQuantumStates.jl** (Julia)
    Early Julia-based NQS; pedagogical and research-oriented
- **Quantum chemistry–focused NQS**
  - **PauliNet** (Python, PyTorch)
    Fermi w.f. with explicit physical priors (Slater, Jastrow)
  - **FermiNet** (Python, JAX)
    Electronic structure
  - **DeepErwin** (Python, TensorFlow/JAX)
    Deep-learning-based variational ansatz for molecules
- **Hybrid quantum / differentiable programming libraries**
  - **PennyLane** (Python)
    NQS-like variational w.f. and differentiable quantum models
  - **TorchQuantum** (Python, PyTorch)
    Neural-network-driven quantum state representations

What about reactions?



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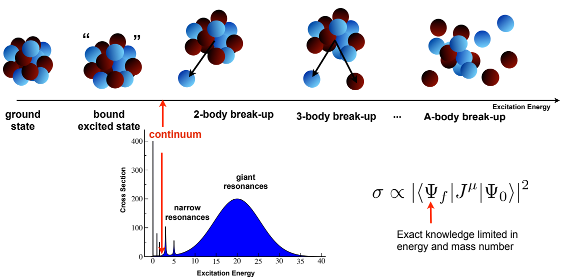
The EW interaction Hamiltonian: $\hat{H}_{EW} = \int dx \hat{A}_\mu(x)\hat{J}^\mu(x)$

Example - the photo-absorption **cross-section**

$$\sigma(\omega) = 4\pi^2\alpha\omega \sum_J [\mathcal{R}_{E_J}(\omega) + \mathcal{R}_{M_J}(\omega)]$$

$$\mathcal{R}_\Theta(\omega) = \sum\!\!\!\!\!\!\int_f |\langle\Psi_f|\hat{\Theta}|\Psi_0\rangle|^2\delta(E_f - E_0 - \omega)$$



The Lorentz Integral Transform (LIT)

The Lorentz Integral Transform method

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- Response in continuum

$$\mathcal{R}(\omega) = \sum\!\!\!\!\!\!\int_f |\langle \Psi_f | \hat{\Theta} | \Psi_0 \rangle|^2 \delta(E_f - E_0 - \omega)$$

- Lorentz integral transform (LIT) method

$$\mathcal{L}(\sigma, \Gamma) = \int d\omega \frac{\mathcal{R}(\omega)}{(\sigma - \omega)^2 + \Gamma^2} = \langle \tilde{\Psi} | \tilde{\Psi} \rangle$$

V. Efros, W. Leidemann, G. Orlandini, PLB 238, 130 (1994)

- The LIT equation

$$(H - E_0 - \sigma + i\Gamma)|\tilde{\Psi}\rangle = \hat{\Theta}|\Psi_0\rangle$$

The LIT:

- The LIT equation is a Schrödinger equation with a **source**
- $|\tilde{\Psi}\rangle$ has bound-state asymptotic behavior
- $\mathcal{R}(\omega)$ is obtained inverting the LIT

- Response in continuum

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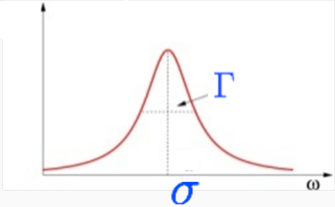

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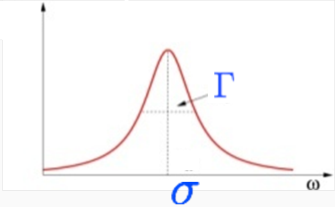
V. Efros, W. Leidemann, G. Orlandini, PLB 238, 130 (1994)

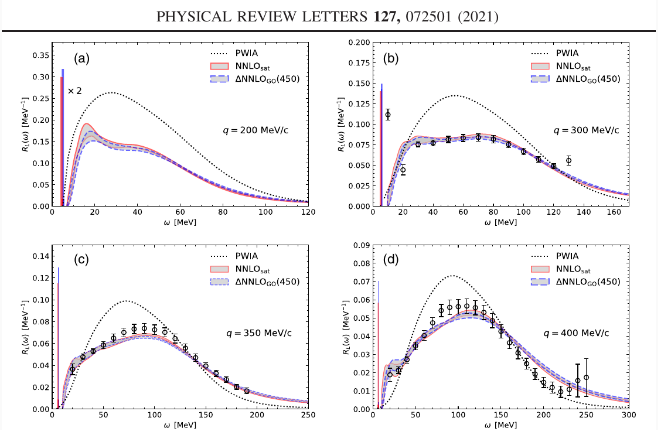


The LIT:

- The LIT equation is a Schrödinger equation with a **source**
- $|\tilde{\Psi}\rangle$ has bound-state asymptotic behavior
- $\mathcal{R}(\omega)$ is obtained inverting the LIT

The CC-LIT method

Longitudinal response of ^{40}Ca



J. E. Sobczyk, B. Acharya, S. Bacca, and G. Hagen

- **The LIT variational principle**
- **The convergence lemma**
- **The H_{LIT} ground state gap**
- **The fidelity and the accuracy of the LIT**

The LIT equation

$$(\hat{H}-z)|\tilde{\Psi}\rangle = |R\rangle \qquad ; \qquad |R\rangle \equiv \hat{\Theta}|\Psi_0\rangle,$$

Here $z = E_0 + \sigma - i\Gamma$.

Lemma:

The solution $\tilde{\Psi}$ is unique, and minimizes the functional

$$\mathcal{I}[\tilde{\Psi}] = \left|(\hat{H}-z)|\tilde{\Psi}\rangle - |R\rangle\right|^2$$

Proof:

If $|\tilde{\Psi}_0\rangle$ is the exact LIT WF then $\mathcal{I}[\tilde{\Psi}_0] = 0$.
Otherwise, for $|\tilde{\Psi}\rangle = |\tilde{\Psi}_0 + \delta\tilde{\Psi}\rangle$ one has

$$\mathcal{I}[\tilde{\Psi}] = \left|(\hat{H}-z)|\tilde{\Psi}_0 + \delta\tilde{\Psi}\rangle - |R\rangle\right|^2$$
$$= |(\hat{H}-z)|\delta\tilde{\Psi}\rangle|^2 \geq \Gamma^2\langle\delta\tilde{\Psi}|\delta\tilde{\Psi}\rangle|^2 \geq 0.$$

V. Efros, W. Leidemann, and G .Orlandini, PLB **238**, 130 (1994).

The convergence lemma

Lemma: The relative accuracy of the LIT function $\mathcal{L}$ is given by

$$\left|\frac{\Delta\mathcal{L}}{\mathcal{L}}\right| = \mathcal{O}\left(\frac{\sqrt{\mathcal{I}[\tilde{\Psi}]}}{\Gamma\sqrt{\mathcal{L}}}\right) \quad ; \quad \Delta\mathcal{L} = \langle\tilde{\Psi}|\tilde{\Psi}\rangle - \langle\tilde{\Psi}_0|\tilde{\Psi}_0\rangle$$

In the limit $\Gamma \to 0$, $\sigma \approx \omega$, and $\mathcal{L} \to (\pi/\Gamma)\mathcal{R}$,

Hence, we may further suggest that

$$\left|\frac{\Delta\mathcal{R}}{\mathcal{R}}\right| = \mathcal{O}\left(\sqrt{\frac{\mathcal{I}[\tilde{\Psi}]}{\Gamma\mathcal{R}}}\right)$$

Implication:

For a desired relative accuracy in $\mathcal{R}$, we need to calculate $\mathcal{I}$ with a precision proportional to Γ.

The LIT Hamiltonian

Given the **LIT** equation

$$(\hat{H} - z)|\tilde{\Psi}\rangle = |R\rangle \qquad ; \qquad |R\rangle \equiv \hat{\Theta}|\Psi_0\rangle,$$

we introduce the LIT Hamiltonian:

$$H_{LIT} \equiv (\hat{H} - z^*)(1 - \hat{P}_R)(\hat{H} - z) \qquad ; \qquad \hat{P}_R = \frac{|R\rangle\langle R|}{\langle R|R\rangle}$$

Observations:

- H_{LIT} is Hermitian
- The LIT w.f. $|\tilde{\Psi}\rangle$ minimizes H_{LIT}
- $|\tilde{\Psi}\rangle$ is the zero energy eigenstates of H_{LIT}
- The spectrum of H_{LIT} has a gap above the ground state.

FIDELITY and the LIT accuracy

The Lorentz Integral Transform is obtained from the solution of the inhomogeneous equation:

$$\underbrace{(\hat{H} - z)\,|\tilde{\Psi}\rangle}_{|L\rangle} = \underbrace{\hat{O}\,|\Psi_0\rangle}_{|R\rangle}$$

We solve the LIT equation maximizing the **FIDELITY**

$$\boxed{\mathcal{F} = \frac{\langle L|R\rangle\langle R|L\rangle}{\langle L|L\rangle\langle R|R\rangle}}$$

Upper bounds on the LIT uncertainty:

$$\Delta\mathcal{L}(\omega_0, \Gamma) \le \mathcal{D}\,\frac{\mathcal{N}^{-1}||R\rangle|}{\Gamma}\sqrt{\frac{1-\mathcal{F}}{\mathcal{F}}},$$

where

$$\mathcal{D} = \min\left(\left|(1 - P_R)|\tilde{\Psi}\rangle\right|, \left|(1 - P_R)\frac{H}{\sqrt{\sigma^2 + \Gamma^2}}|\tilde{\Psi}\rangle\right|\right)$$

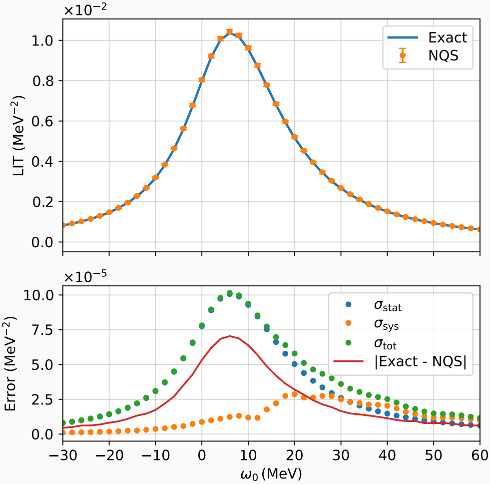
NNLIT

Key Idea:

A variational Monte Carlo framework to compute dynamical nuclear response functions

- Neural-network quantum states (NQS)
- Lorentz Integral Transform (LIT)
- Both ground state Ψ_0 and LIT state $\tilde{\Psi}$ represented by NQS
- Optimized via the neural net

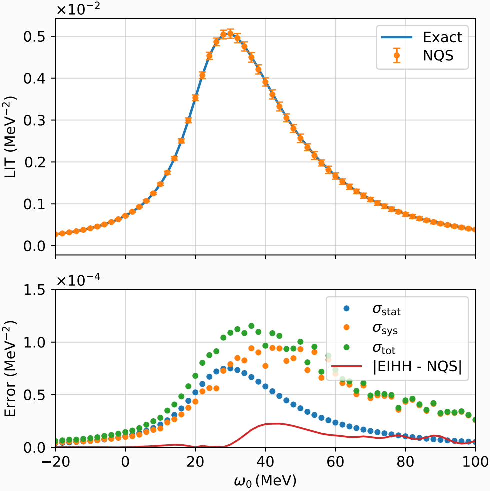
- Avoids explicit treatment of continuum states
- Compact representation
- Efficient scaling with particle number
- Rigorous upper bounds for systematic errors derived



- **Upper panel:** LIT of the ^{2}H photo-absorption dipole response
- $\Gamma = 10$ MeV

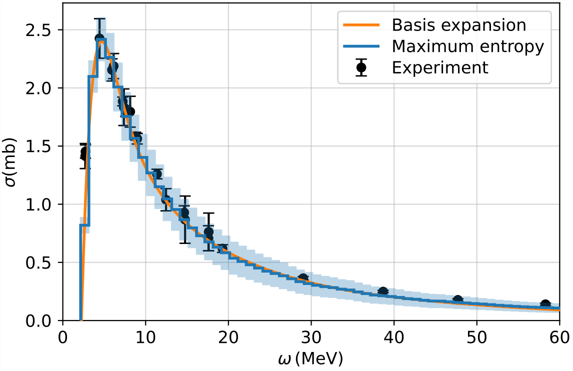
- **Lower panel:** NQS errors
- Statistical - MC sampling
- Systematic - LIT error-bound lemma
- Total - sum of the two

NQS-EIHH ^{4}He LIT Benchmark



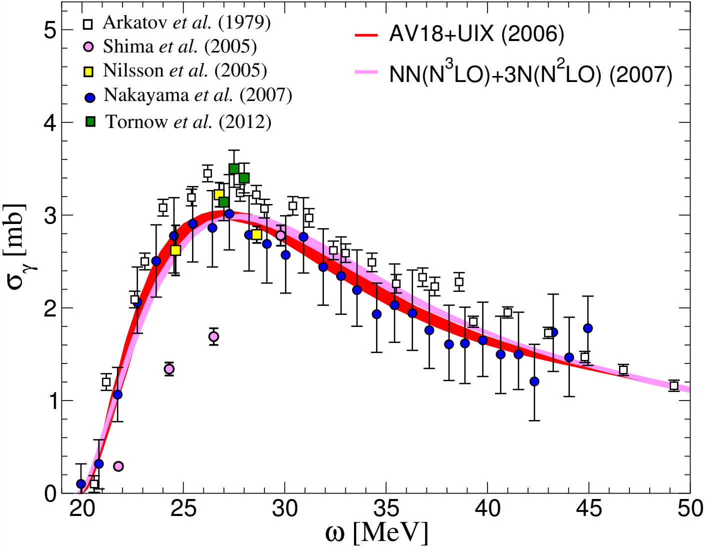
- **Upper panel:** LIT of the ^{4}He photo-absorption dipole response
- $\Gamma = 10$ MeV
- **Lower panel:** NQS errors
- Statistical - MC sampling
- Systematic - LIT error-bound lemma
- Total - sum of the two

- Pionless EFT inspired potential [A]
- Excellent accuracy at the LIT level
- Inversion - Basis expansion + regulation, Maximum entropy
- Error bars - sys+stat+inver



[A] R. Schiavilla, et. al., Phys. Rev. C 103, 054003 (2021).

$$\sigma_\gamma(\omega) = 4\pi^2 \alpha\omega \mathcal{R}_{D1}(\omega)$$



^{4}He photoabsorption, E. Parnas, et al. (PRL 2026)

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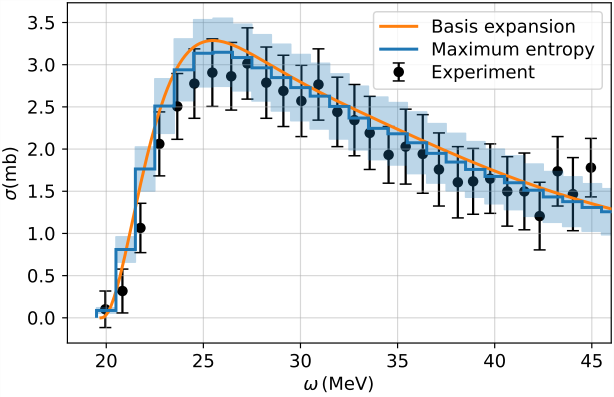
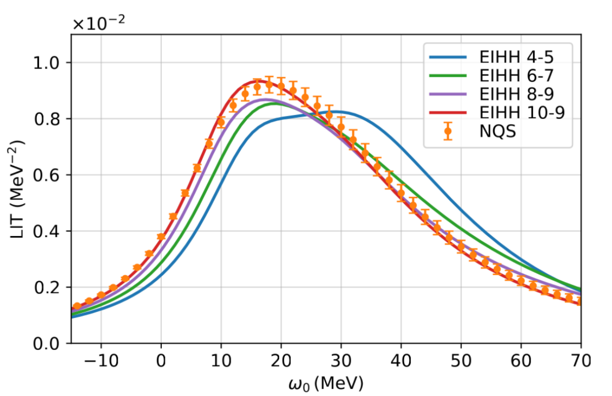
- Pionless EFT inspired potential [A]
- Comparison with highly accurate EIHH calculations
- LIT reproduced at percent-level accuracy
- Photoabsorption cross-section:
  - Good agreement with the experimental data



^{6}Li photoabsorption cross-section $\sigma_\gamma(\omega)$



Comparison between NLIT and EIHH

EIHH - Effective Interction Hyperspherical Harmonics method

Summary

Conclusions and Outlook

- **NQS+LIT** provides an accurate and scalable framework for nuclear responses
- Robust propagation of statistical and systematic uncertainties
- **Successful** description of ^{2}H and ^{4}He photoabsorption data
- Outlook:
  - Extension to nuclei with $A \leq 20$
  - Improved interactions (local χEFT)
  - Exclusive reactions
  - Applications beyond nuclear physics (atoms, molecules)

Questions

- How difficult is the generalization for non central forces?
- How good will this method work for **hard** potentials?
- What is the interplay between **human wisdom** and **artifical intelligence**?
- What is the correct form of the wave-function?
- Should we optimize the energy or the wave-function?
- How to deal with excited states in general?
- ....

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Thank you !