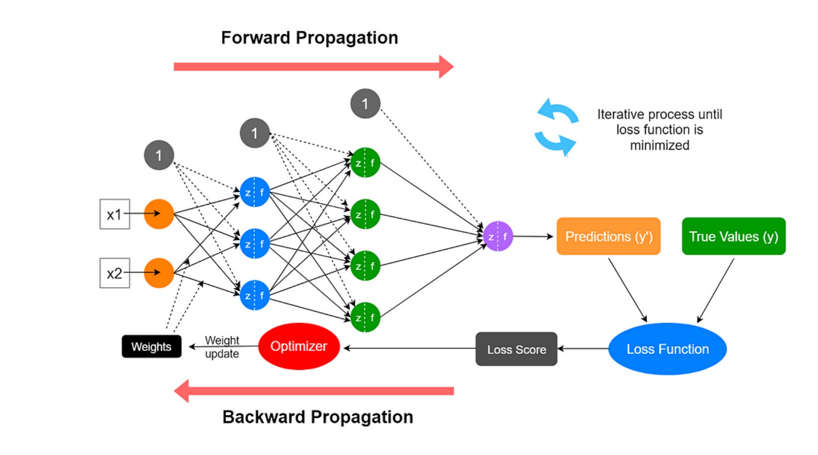
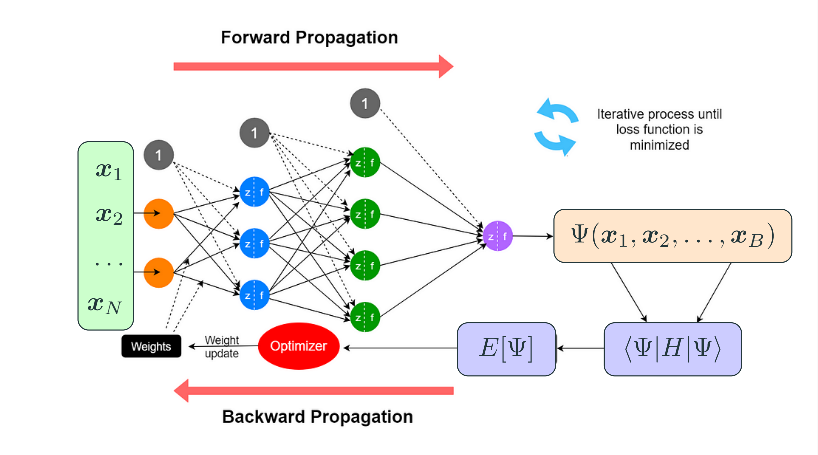
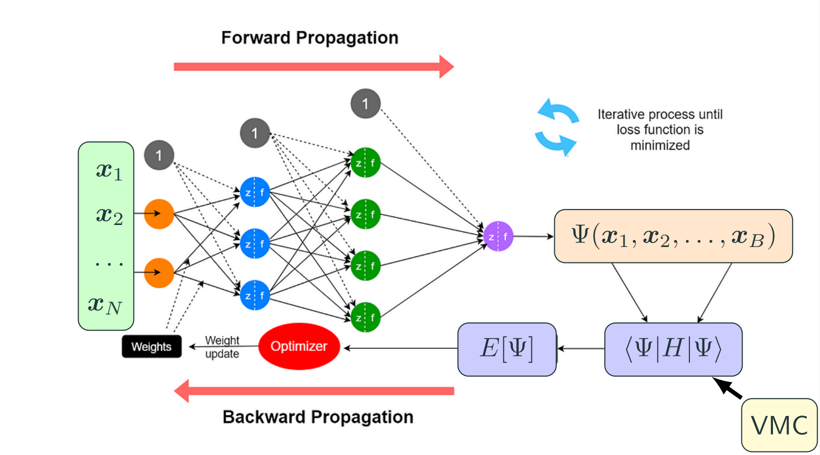
Nuclear Responses with Neural-Network Quantum States

Nir Barnea

EMMI Workshop, January 18-24, 2026
Hirschegg


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
$\cdots$
x_N
1
1
1
z f
$\Psi(x_1, x_2, \ldots, x_B)$
$\langle\Psi|H|\Psi\rangle$
$E[\Psi]$
Optimizer
Weight update
Weights
Backward Propagation


Forward Propagation
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x_1
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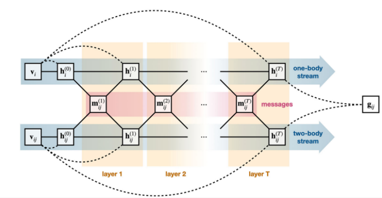
Weights
Weight update
Optimizer
$E[\Psi]$
$\langle\Psi|H|\Psi\rangle$
VMC
Backward Propagation

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 …

…)

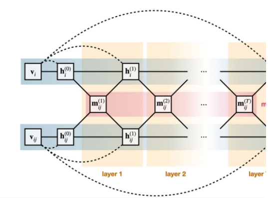
… $f^2(P) = \mathrm{Det}(P)$

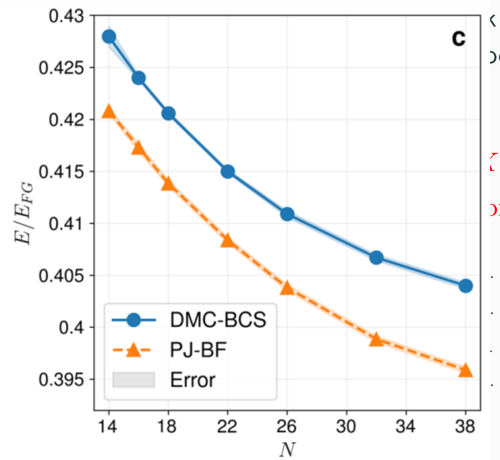
$\phi(x_1, x_N)$

$\phi(x_2, x_N)$

$\vdots$

0





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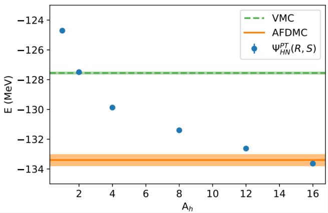
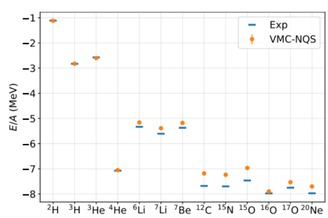
A prominent example of an **antisymmetric wavefunction** is the **Hidden Nucleons architecture**. This extension of the slater determinant allows much more flexibility.

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

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



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

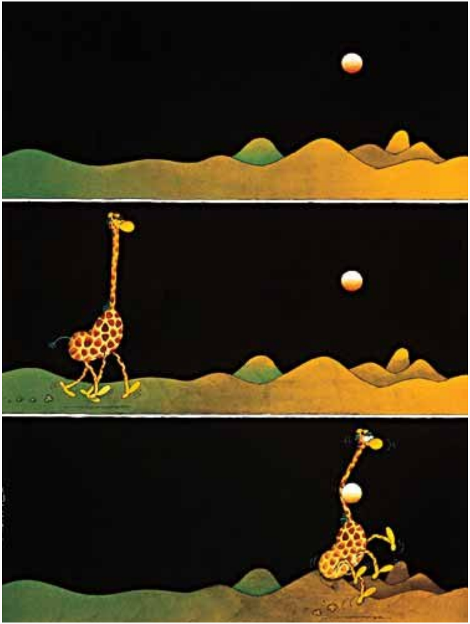


A. Lovato et al. (2024)

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?

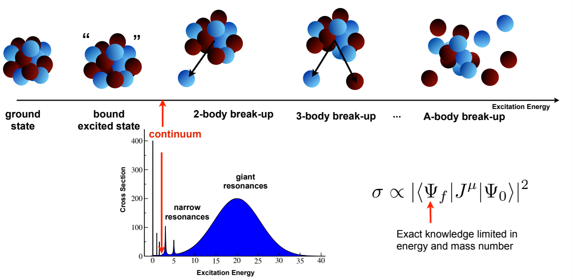


The EW interaction Hamiltonian: $\hat{H}_{EW} = \int d\boldsymbol{x} \hat{A}_\mu(\boldsymbol{x}) \hat{J}^\mu(\boldsymbol{x})$

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

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

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



The Lorentz Integral Transform (LIT)

- 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

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

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

The Lorentz Integral Transform method

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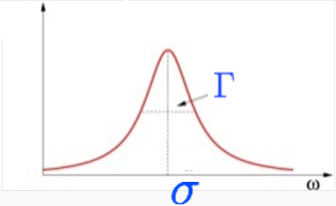

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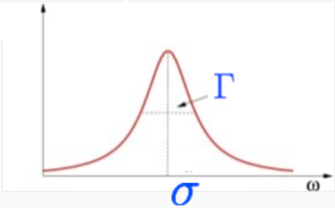


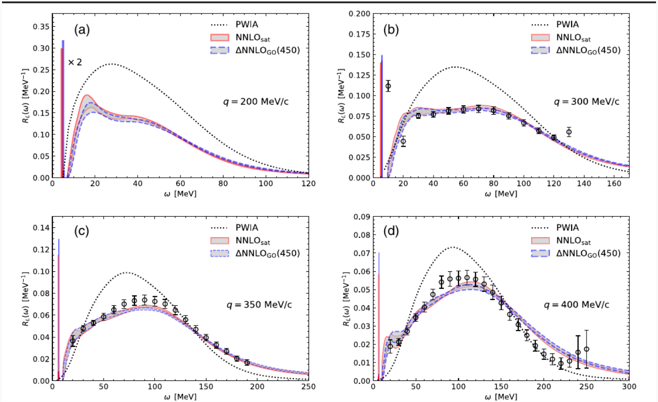
The LIT:

- 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

PHYSICAL REVIEW LETTERS **127,** 072501 (2021)



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

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

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

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

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

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.

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:

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

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:

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

where

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

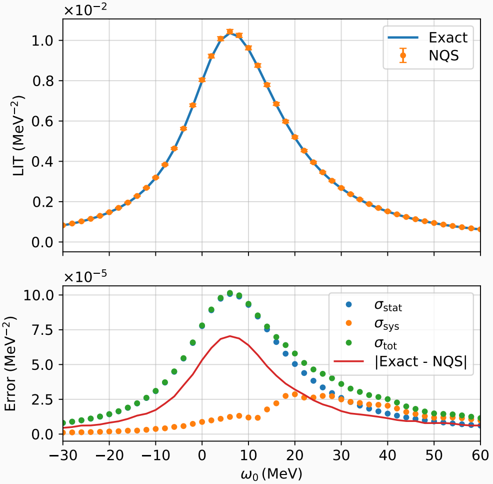
NNLIT

Key Idea:

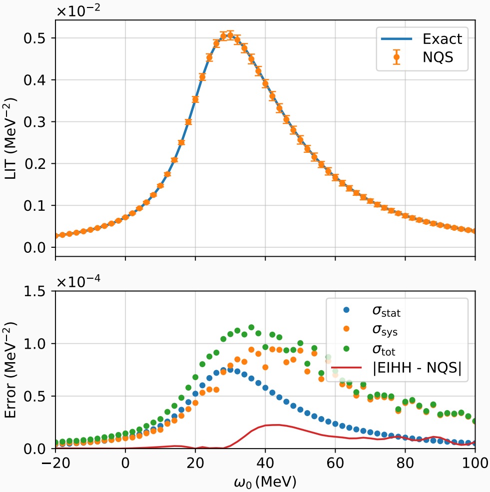
A variational Monte Carlo framework to compute dynamical nuclear response functions

- 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



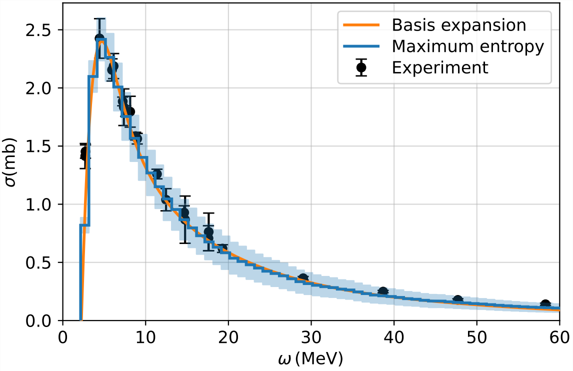
- **Upper panel:** LIT of the ^{2}H photo-absorption dipole response
- $\Gamma = 10$ MeV
- **Lower panel:** NQS errors
- Statistical - MC sampling
- Systematic - LIT error-bound lemma
- Total - sum of the two



- **Upper panel:** LIT of the ^{4}He photo-absorption dipole response
- $\Gamma = 10$ MeV

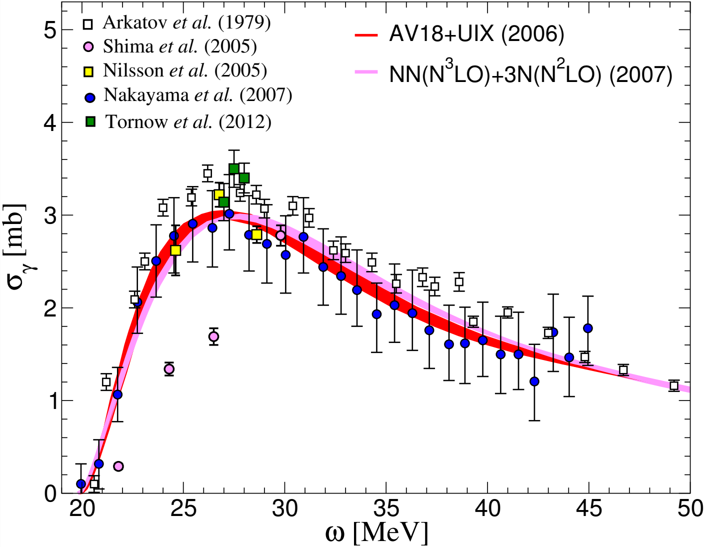
- **Lower panel:** NQS errors
- Statistical - MC sampling
- Systematic - LIT error-bound lemma
- Total - sum of the two

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



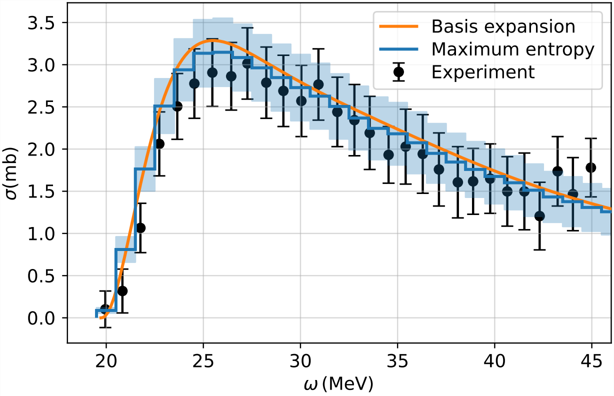
[A] R. Schiavilla, et. al., Phys. Rev. C 103, 054003 (2021).

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



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

- 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



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)
  - Applications beyond nuclear physics (atoms, molecules)

Collaboration

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Thank you !