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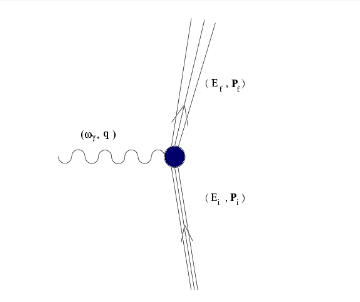
Inelastic Reactions - The Nuclear Response Function

Nir Barnea

Aug. 31, 2026, MITP-JGU, Mainz

Electro-weak Reactions

EW reactions



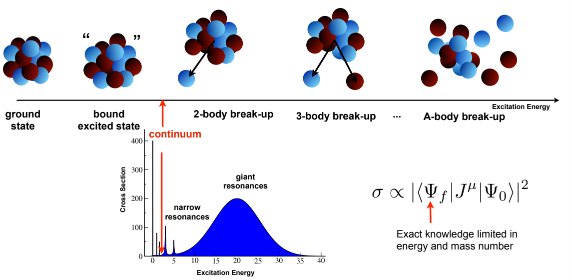
- Study of nuclear structure
- Study of SM / Behind SM physics
- Input for Astrophysics
- A crucial test for the nuclear theory kinematic regimes not accessible by elastic reactions
- Probing of underlying degrees of freedom
- Analysis of high energy experiments with nuclear targets

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)

Integral transforms

The nuclear response function

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

Integral transform with kernel $K(\omega, \sigma)$

$$\boxed{\mathcal{L}(\sigma) \equiv \int d\omega K(\omega, \sigma) R(\omega)}$$

Some manipulations

$$\begin{aligned}
\mathcal{L}(\sigma) &= \sum\!\!\!\!\!\!\!\int d\Psi_f K(E_f - E_0, \sigma) |\langle \Psi_f \mid \hat{\Theta} \mid \Psi_0 \rangle|^2 \\
&= \sum\!\!\!\!\!\!\!\int d\Psi_f \langle \Psi_0 \mid \hat{\Theta}^\dagger \mid \Psi_f \rangle \langle \Psi_f \mid K(\hat{H} - E_0, \sigma) \hat{\Theta} \mid \Psi_0 \rangle
\end{aligned}$$

Closure

$$\boxed{\mathcal{L}(\sigma) = \langle \Psi_0 | \hat{\Theta}^\dagger K(\hat{H} - E_0, \sigma) \hat{\Theta} | \Psi_0 \rangle}$$

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The Lorentz Integral transform (LIT) method

The Lorentz kernel

$$\boxed{K(\omega,\sigma) = \frac{1}{(\omega-\sigma)^2+\Gamma^2}}$$

The LIT

$$\boxed{\mathcal{L}(\sigma) = \langle\Psi_0|\hat{\Theta}^\dagger \frac{1}{(\hat{H}-E_0-\sigma)^2+\Gamma^2}\hat{\Theta}|\Psi_0\rangle}$$

Can also be written as

$$\mathcal{L}(\sigma) = \underbrace{\langle\Psi_0 \mid \hat{\Theta}^\dagger \frac{1}{\hat{H}-E_0-\sigma-i\Gamma}}_{\langle\tilde{\Psi}|}\underbrace{\frac{1}{\hat{H}-E_0-\sigma+i\Gamma}\hat{\Theta} \mid \Psi_0\rangle}_{|\tilde{\Psi}\rangle}$$

Hence,

$$\boxed{\begin{gathered}\mathcal{L}(\sigma) = \langle\tilde{\Psi}(\sigma) \mid \tilde{\Psi}(\sigma)\rangle \\ (H-E_0-\sigma+i\Gamma)|\tilde{\Psi}(\sigma)\rangle = \hat{\Theta}|\Psi_0\rangle\end{gathered}}$$

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The LIT method

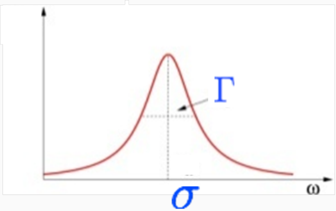
Efros, Leidemann, Orlandini, PLB 238, 130 (1994)

- The Response function

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

- The Lorentz Integral Transform (LIT)

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



- The LIT equation

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

Short summary

- 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

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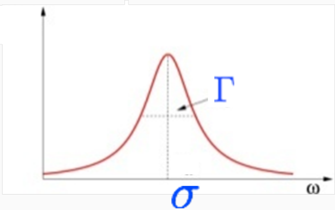

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- **Nuclear polarizability**

  $\Rightarrow$ energy-dependent sum rule of a response function:

$$S = \int_0^\infty d\omega \, \mathcal{R}(\omega) \, g(\omega)$$

- Calculate S directly without explicitly solving $\mathcal{R}(\omega)$.
- Using a compact basis

$$S_M = \sum_{n \neq 0}^{M} |\langle N_m | \hat{\Theta} | N_0 \rangle|^2 g(E_m - E_0)$$

- If $g(\omega)$ is **well behaved** S_M converges rather fast.
- If $|\mathcal{L}(\sigma) - \mathcal{L}_M(\sigma)| \leq \varepsilon_M$, then

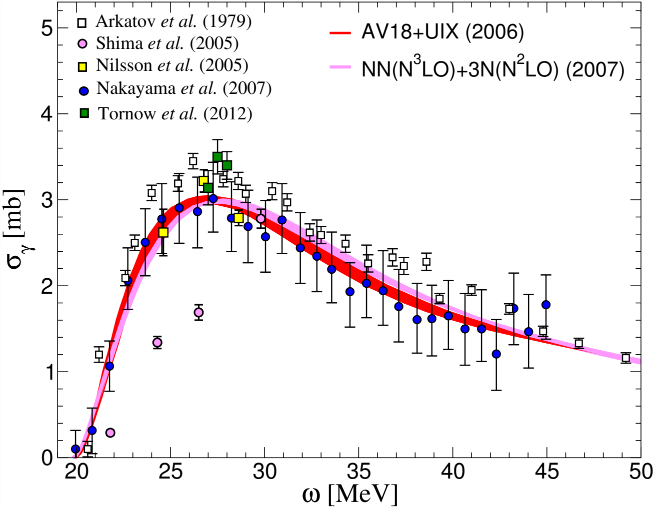
$$|S - S_M| \leq \varepsilon_M \int d\sigma \, |h(\sigma, \Gamma)|$$

$$g(\omega) = \frac{\Gamma}{\pi} \int d\sigma \frac{h(\sigma, \Gamma)}{(\omega - \sigma)^2 + \Gamma^2}$$

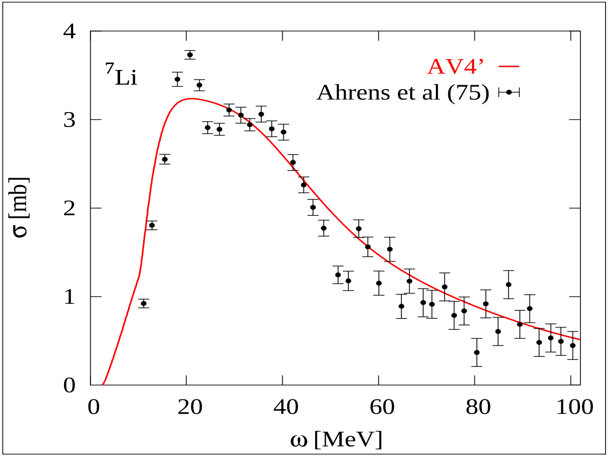
Nevo-Dinur, Barnea, Ji, Bacca, PRC **89**, 064317 (2014)

^{4}He photoabsorption cross-section

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



^{7}Li photoabsorption cross-section $\sigma_\gamma(\omega)$

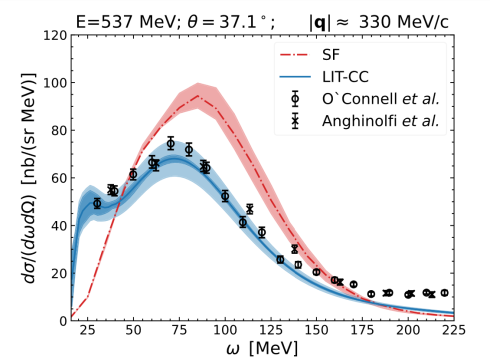


Bacca, Arenhövel, Barnea, Leidemann, and Orlandini
Phys. Lett. B **603** (2004)

Coupled Cluster LIT - CCLIT

The CC-LIT method

^{16}O(e,e') differential cross-section



Acharya, Sobczyk, Bacca, Hagen, Jiang, PRL 134, 202501 (2025)

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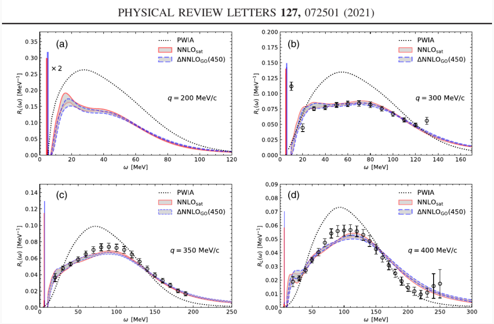
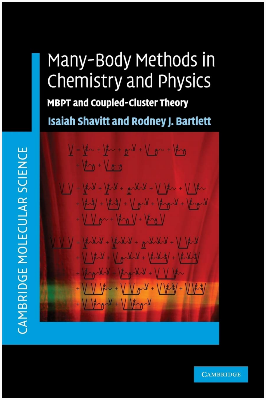
The CC-LIT method

Longitudinal response of ^{40}Ca



Sobczyk, Acharya, Bacca, Hagen, PRL 127, 072501 (2021)



Topical Review

R. J. Bartlett and M. Musial
Coupled cluster theory in quantum chemistry
Rev. Mod. Phys. **79**, 291 (2007).

Motivation

Application of the CC method to study inelastic reactions on medium size nuclei, $A \geq 10$.

Problem

The basic LIT formalism is incompatible with the CC method.
The expression $L = \langle\tilde{\psi}|\tilde{\psi}\rangle$ contains an infinite number of diagrams !

The Coupled Cluster method

- The CC transformation

$$\boxed{H \longrightarrow \bar{H} = \exp(-T)\hat{H}\exp(T)}$$

- The CC operator

$$T = T_1 + T_2 + \ldots + T_n$$

- given by

$$T_1 = \sum_{i\,a} t_i^a \hat{a}^\dagger \hat{i}$$

$$T_2 = \frac{1}{4}\sum_{ij\,ab} t_{ij}^{ab} \hat{a}^\dagger \hat{b}^\dagger \hat{j}\hat{i}$$

- The CC amplitudes are fixed by

$$\langle \Phi_{ij\ldots}^{ab\ldots} | \bar{H} | \Phi_0 \rangle = 0$$

- Ground state energy

$$E_0 = \langle \Phi_0 | \bar{H} | \Phi_0 \rangle$$

The Coupled Cluster method

The eigenvectors

$$H|\mu\rangle = E_\mu|\mu\rangle$$

are mapped into right and left eigenvectors

$$\begin{aligned} |\mu\rangle &\longrightarrow |\mu_R\rangle = \exp(-T)|\mu\rangle \\ \langle\mu| &\longrightarrow \langle\mu_L| = \langle\mu|\exp(T) \end{aligned}$$

Specifically

$$|0_R\rangle = |\Phi_0\rangle \qquad \langle 0_L| = \langle\Phi_0|(1+\Lambda)$$

Closure

$$\sum_\mu |\mu\rangle\langle\mu| = \sum_\mu \exp(-T)|\mu_R\rangle\langle\mu_L|\exp(+T) = \sum_\mu |\mu_R\rangle\langle\mu_L| = 1$$

Coupled Cluster formulation of the LIT

- Start from the response

$$R(\omega) = \sum_f \langle 0|\hat{\Theta}^\dagger|f\rangle\langle f|\hat{\Theta}|0\rangle\delta(E_f - E_i - \omega)$$

- Perform the LIT

$$L(\sigma,\Gamma) = \langle 0|\hat{\Theta}^\dagger \frac{1}{H - E_0 - \sigma - i\Gamma}\frac{1}{H - E_0 - \sigma + i\Gamma}\hat{\Theta}|0\rangle$$

- Apply the CC transformation

$$\boxed{L(\sigma,\Gamma) = \langle 0_L|\bar{\Theta}^\dagger \frac{1}{\bar{H} - E_0 - \sigma - i\Gamma}\frac{1}{\bar{H} - E_0 - \sigma + i\Gamma}\bar{\Theta}|0_R\rangle}$$

where

$$\bar{\Theta} = \exp(-T)\hat{\Theta}\exp(T)$$

$$\bar{\Theta}^\dagger = \exp(-T)\hat{\Theta}^\dagger\exp(T)$$

Coupled Cluster formulation of the LIT

- Define $z = E_0 + \sigma + i\Gamma$
- Rewrite the LIT as

$$L(\sigma,\Gamma) = \frac{1}{2\Gamma}\langle 0_L|\bar{\Theta}^\dagger \left(\frac{1}{\bar{H}-z} - \frac{1}{\bar{H}-z^*}\right)\bar{\Theta}|0_R\rangle$$

- It is evident that the solution of the CCLIT equation

$$\boxed{(\bar{H}-z)|\widetilde{\Phi}_R(z)\rangle = \bar{\Theta}|0_R\rangle}$$

- leads directly to the transform

$$L(z) = \frac{1}{2\Gamma}\{\langle 0_L|\bar{\Theta}^\dagger|\widetilde{\Phi}_R(z)\rangle - \langle 0_L|\bar{\Theta}^\dagger|\widetilde{\Phi}_R(z^*)\rangle\}$$

- or setting $|\widetilde{\Phi}_R(z)\rangle = R(z)|\Phi_0\rangle$

$$\boxed{L(z) = \frac{1}{2\Gamma}\left[\langle\Phi_0|(1+\Lambda)\bar{\Theta}^\dagger R(z)|\Phi_0\rangle - \langle\Phi_0|(1+\Lambda)\bar{\Theta}^\dagger R(z^*)|\Phi_0\rangle\right]}$$

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The equation of motivation (EOM) method

- Assume a solution in the form,

$$|\widetilde{\Phi}_R(z)\rangle = R(z)|\Phi_0\rangle = \left(R_0 + \sum_{ia} R_i^a \hat{a}^\dagger \hat{i} + \sum_{ij\,ab} R_{ij}^{ab} \hat{a}^\dagger \hat{b}^\dagger \hat{j} \hat{i} + \ldots \right) |\Phi_0\rangle$$

- Substituting $|\widetilde{\Phi}\rangle$ in the CCLIT equation,

$$(\bar{H} - z)R(z)|\Phi_0\rangle = \bar{\Theta}|\Phi_0\rangle$$

- subtracting the relation

$$R(z)\bar{H}|\Phi_0\rangle = E_0 R(z)|\Phi_0\rangle$$

- we get the **CCLIT equation**

$$\boxed{[\bar{H}, R(z)]|\Phi_0\rangle = (z - E_0)R(z)|\Phi_0\rangle + \bar{\Theta}|\Phi_0\rangle}$$

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$$(\bar{H} - z)R(z)|\Phi_0\rangle = \bar{\Theta}|\Phi_0\rangle$$

- subtracting the relation

$$R(z)\bar{H}|\Phi_0\rangle = E_0 R(z)|\Phi_0\rangle$$

- we get the **CCLIT equation**

$$\boxed{[\bar{H}, R(z)]|\Phi_0\rangle = (z - E_0)R(z)|\Phi_0\rangle + \bar{\Theta}|\Phi_0\rangle}$$

- This is just the **CC-EOM** equation with a source term!

The equation of motivation (EOM) method

- Assume a solution in the form,

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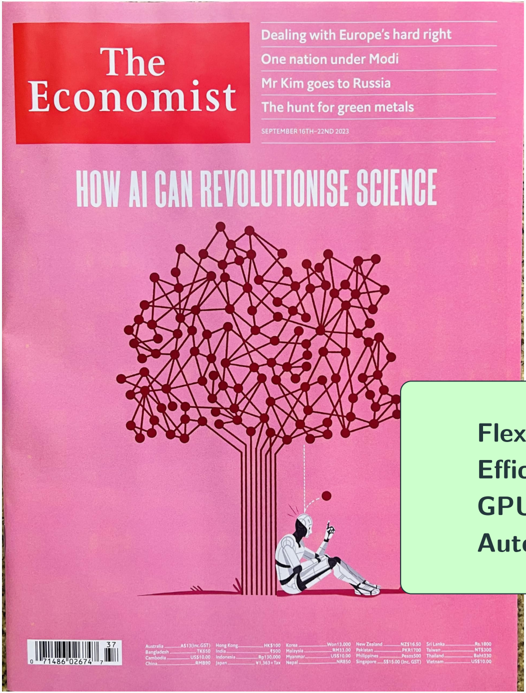
Neural network


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

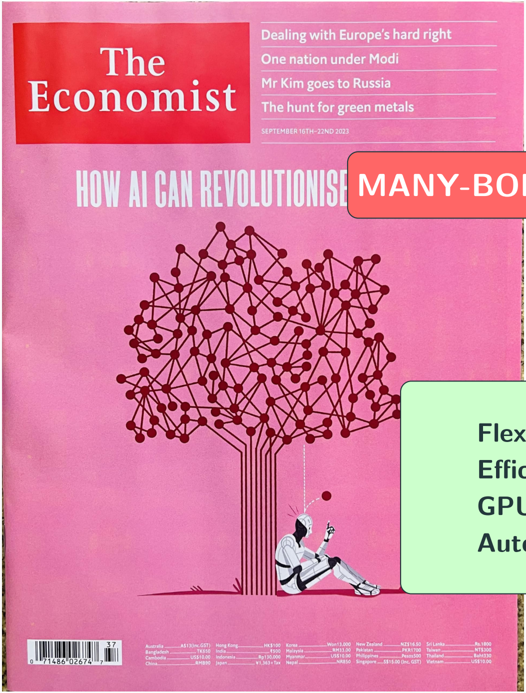


Flexible Model

Efficient Minimization

GPU Tech

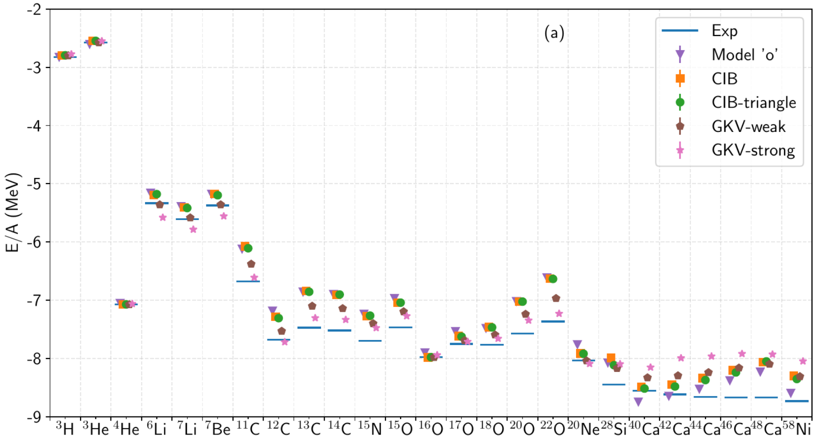
Automatic Differentiation



MANY-BODY THEORY?

- Flexible Model
- Efficient Minimization
- GPU Tech
- Automatic Differentiation

Jane's Talk (Thu. 27/08)



Fore, Kim, Lovato, Tropiano, Arxiv 2607.09223

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?

NNLIT

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- **The LIT variational principle**
  Loss function
- **The convergence Lemma**
  Controlled accuracy
- **The H_{LIT} ground state gap**
  For fun ...
- **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

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

we introduce the LIT Hamiltonian:

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

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

E. Parnas, et al. (PRL 2026)

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**

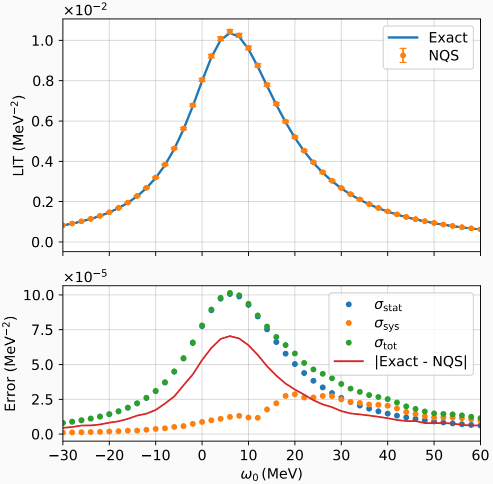
$$\boxed{\mathcal{F} = \frac{\langle L|R\rangle\langle R|L\rangle}{\langle L|L\rangle\langle R|R\rangle}}$$

Upper bounds on the LIT uncertainty:

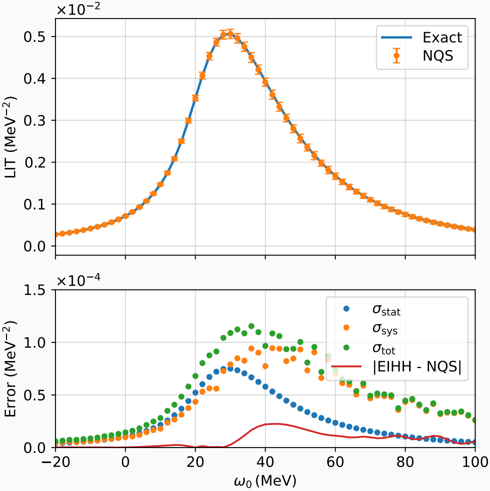
$$\Delta\mathcal{L}(\sigma, \Gamma) \leq \mathcal{D}\,\frac{\mathcal{N}^{-1}||R\rangle|}{\Gamma}\sqrt{\frac{1-\mathcal{F}}{\mathcal{F}}},$$

where

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



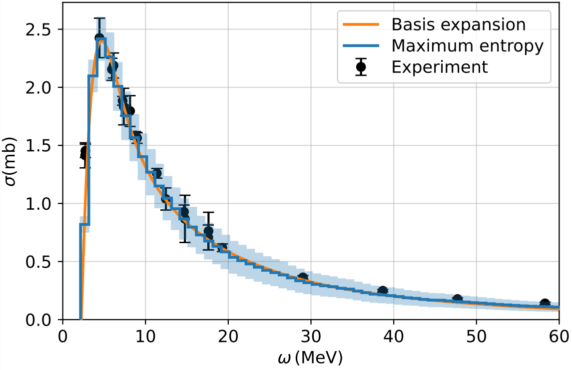
- **UPPER PANEL:**
  LIT of the ^{2}H photo-absorption dipole response
- $\Gamma = 10$ MeV
- **LOWER PANEL:**
  NQS errors
- Statistical - MC sampling
- Systematic - LIT error-bound lemma
- Total - sum of the two



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

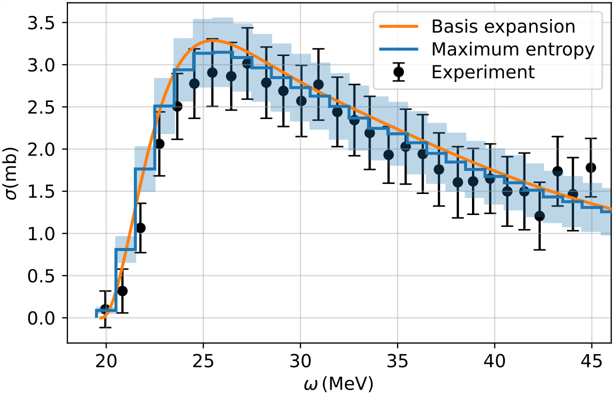
- **LOWER PANEL:**
  NQS errors
- Statistical - MC sampling
- Systematic - LIT error-bound lemma
- Total - sum of the two

- 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).

- 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 $\sigma_\gamma(\omega)$

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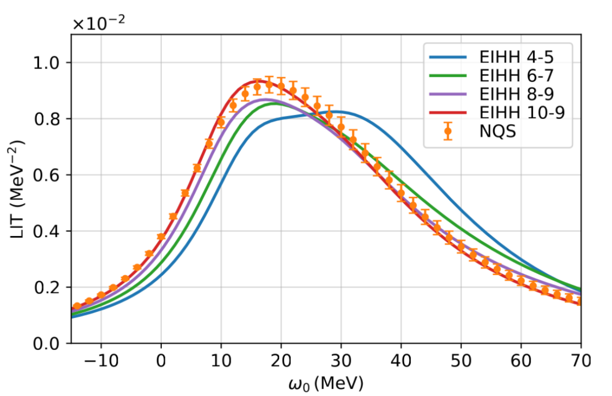


Comparison between NLIT and EIHH

EIHH - Effective Interction Hyperspherical Harmonics method

Can we improve the kernel?

Get better results at the same costs?

Fourier analysis

The LIT is a transform with a **convolution kernel**

$$L(\sigma) = \int d\omega \, K(\sigma - \omega) \, R(\omega) = (K * R)(\sigma)$$

Considering the Fourier transform $\mathcal{F}$

$$\widetilde{f}(k) = \mathcal{F}[f](k) = \int d\omega \, f(\omega) \, e^{-ik\omega}$$

The **convolution theorem** turns the LIT into a product, with formal inversion

$$\boxed{R(\omega) = \mathcal{F}^{-1}\left[\frac{\widetilde{L}(k)}{\widetilde{K}(k)}\right](\omega)}$$

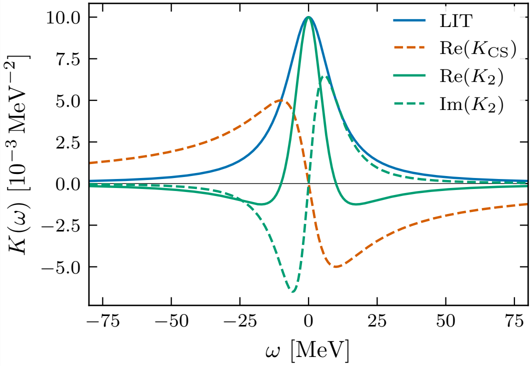
Comments:

- Ill-posed - The error in $\widetilde{L}(k)$ are amplified by $1/|\widetilde{K}(k)|$.
- Stability of the inversion is governed by the tail of $|\widetilde{K}(k)|$ at large k.

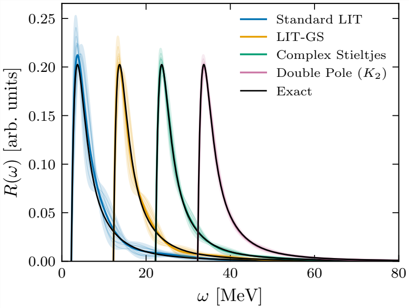
Different kernels that can be constructed from **solutions of the LIT equation**

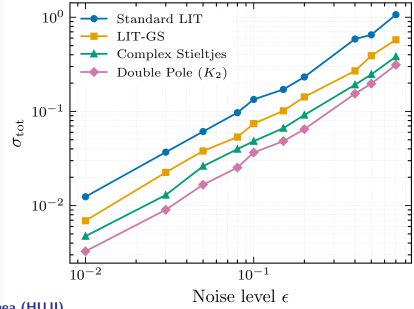
Here $|\Phi\rangle = \hat{O}|\Psi_0\rangle$ stands to the rhs of the LIT equation.

Kernel	$K(\omega;\sigma,\Gamma)$	Computed as	$\widetilde{K}(k)$
Standard LIT	$\frac{1}{(\omega-\sigma)^2+\Gamma^2}$	$\langle\tilde{\Psi}(\sigma)\|\tilde{\Psi}(\sigma)\rangle$	$\frac{\pi}{\Gamma}\, e^{-\Gamma\|k\|}$
LIT-GS	$\frac{1}{(\omega-\sigma)^2+\Gamma^2}$	$-\frac{1}{\Gamma}\,\mathrm{Im}\langle\Phi\|\tilde{\Psi}(\sigma)\rangle$	$\frac{\pi}{\Gamma}\, e^{-\Gamma\|k\|}$
Comp. Stieltjes	$-\frac{1}{\Gamma}\,\frac{1}{\omega-\sigma+i\Gamma}$	$-\frac{1}{\Gamma}\langle\Phi\|\tilde{\Psi}(\sigma)\rangle$	$\frac{2\pi i}{\Gamma}\, e^{-\Gamma k}\,\Theta(k)$
Double-pole K_2	$\frac{1}{(\omega-\sigma+i\Gamma)^2}$	$\langle\tilde{\Psi}(\sigma,-\Gamma)\|\tilde{\Psi}(\sigma,\Gamma)\rangle$	$2\pi k\, e^{-\Gamma k}\,\Theta(k)$



- $K(\omega - \sigma)$ at $\sigma = 0$
- $\Gamma = 10$ MeV.
- The standard LIT kernel coincides with $\mathrm{Im}\{K_{CS}\}$.
- $\mathrm{Re}\{K_{CS}\}$ - antisymmetric and carries sign information absent from the LIT.
- K_2 has narrower central structure, and an antisymmetric imaginary part.





Noise model:

$$\tilde{\Psi}(r_j) \;\rightarrow\; \tilde{\Psi}(r_j)\left[1 + \epsilon\,\eta_j + i\,\epsilon\,\eta'_j\right]$$

- Inverted $R(\omega)$ from 10 independent realizations at noise level $\epsilon = 0.2$.
- Thin lines - individual realizations
- Thick line - mean
- band - $\pm 2\sigma$ spread.
- **LOWER PANEL:** Integrated standard deviation σ_{tot} of the inverted response.

Summary

Conclusions and Outlook

- **LIT** provides a useful framework for nuclear responses
- Applied with **HH**, **NCSM**, and **CC**
- see talks by Sobczyk, El Batchy

- **NQS+LIT** 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

Thank you !