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Light nuclear scattering from neural quantum states via stable minimum principles

Yukari Yamauchi

In collaboration with **Scott Lawrence** (LANL)

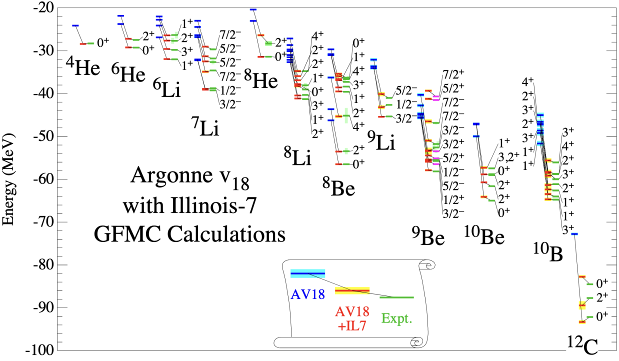
May 18th, 2026

INT workshop "Nuclear Hamiltonians for Advancing Nuclear Physics and Beyond"

Nuclear reactions for nuclear interactions

Scattering processes for determining nuclear interactions

For example, Argonne potentials via **nucleon-nucleon scattering** (+deuteron binding),



[J. Carlson, S.Gandolfi, F. Pederiva, Steven C. Pieper, R. Schiavilla, K.E. Schmidt, R.B. Wiringa. arXiv:1412.3081]

More examples: for chiral interactions

nucleon-deuteron scattering

Few- and many-nucleon systems with semilocal coordinate-space regularized chiral two- and three-body forces

E. Epelbaum,[1] J. Golak,[2] K. Hebeler,[3] T. Hüther,[3] H. Kamada,[4] H. Krebs,[1] P. Maris,[5] Ulf-G. Meißner,[6,7,8] A. Nogga,[7] R. Roth,[3] R. Skibiński,[2] K. Topolnicki,[2] J.P. Vary,[5] K. Vobig,[3] and H. Witała[2]
(LENPIC Collaboration)

neutron-alpha scattering

Chiral Three-Nucleon Interactions in Light Nuclei, Neutron-α Scattering, and Neutron Matter

J. E. Lynn,[1,*] I. Tews,[2,3] J. Carlson,[1] S. Gandolfi,[1] A. Gezerlis,[4] K. E. Schmidt,[5] and A. Schwenk[2,3]

and many more!!!

Scattering with 5 or more dynamical nucleons still look challenging...

Outline

1. **Stable minimum principles for scattering states**

   "When loss gets smaller, you approach the correct answer"

2. **Neural scattering states**
   - neutron - proton
   - neutron - deuteron (elastic and inelastic)

3. **Emulator without emulating: Interaction-dependent NQS**

Scattering states

Scattering via eigenstates with known energy:

$$\left(-\frac{\nabla_x^2}{2M}+V(x)\right)\psi(x)=\frac{k^2}{2M}\psi(x)$$

decomposed into

$$\psi=e^{ikx}+\frac{e^{ikr}}{r}f(\theta,\phi)+O(r^{-2})$$

Scattering states encode the S-matrix $\hat{S}$:

$$\langle k,\theta,\phi|\hat{S}|k,0,0\rangle=f(\theta,\phi)$$

Scattering states are not normalizable:

$$\int dx\ |\psi|^2\to\infty$$

History

Variational principles for scattering states have been studied for decades:

- Kohn (1948)

$$L[\psi] = \int dx\ \psi^* \left(E - \hat{H}\right) \psi$$

- Kato (1951)

$$L[\psi, \rho] = \int dx\ \rho^{-1}\ \psi^* \left(E - \hat{H}\right)^\dagger \left(E - \hat{H}\right) \psi$$

- Darewych, Pooran, and Sokoloff (1978-1980)

$$L[\psi] = \int dx\ \left|\left(E - \hat{H}\right) \psi\right|$$

, total of 18 citations so far

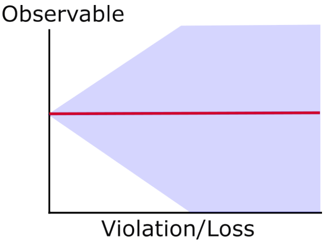
A minimum principle

For example, how about the inner product of the "Schrodinger's violation"?

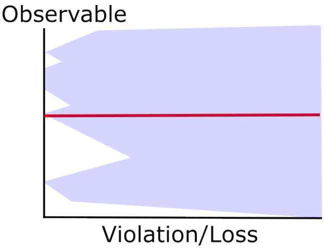
$$L_2[\tilde{\psi}] \equiv \left|\left| \left(E - \hat{H} \right) \psi \right|\right|_2 = \int dx \ \left| \left(E - \hat{H} \right) \psi \right|^2$$

It's great since $L_2 = 0$ when ψ is exactly the scattering state.

However!! "$L_2 = 0$ at exact scattering states" is not enough!!!



Stable principle (Good)



Unstable principle (Bad)

A stable minimum principle[1]

Considered by Darewych, Pooran, and Sokoloff (1978-1980).

$$L_1[\tilde{\psi}] \equiv \left|\left|\left(E - \hat{H}\right)\psi\right|\right|_1 = \int dx \;\left|\left(E - \hat{H}\right)\psi\right|$$

This loss is stable — How? For any $g(x)$ (follows from Hölder):

$$\int dx \;|f| \geq ||g||_\infty^{-1} \left|\int dx \; fg\right| \;, \quad ||g||_\infty \equiv \sup_x |g|$$

Given an exact (ψ) and approximate ($\tilde{\psi}$) state, for $\phi = \tilde{\psi} - \psi$:

$$\left|\left|\left(E - \hat{H}\right)\tilde{\psi}\right|\right|_1 = \left|\left|\left(E - \hat{H}\right)\phi\right|\right|_1 \geq ||\xi||_\infty^{-1} \left|\int dx \; \xi^* \left(E - \hat{H}\right)\phi\right|$$

By choosing an exact scattering state as ξ with energy E,

$$2M \, ||\xi||_\infty^{-1} \left|\left|\left(E - \hat{H}\right)\psi\right|\right|_1 \geq \oint_{R\to\infty} \xi^* \nabla_r \phi - \phi \nabla_r \xi^*$$

[1] S.Lawrence and Y. Yamauchi. arXiv:2605.17139

Stability theorem for partial-wave amplitudes

Some integral of the error at $r \to \infty$ is bounded by the loss

$$2M \, ||\xi||_\infty^{-1} \left|\left| \left(E - \hat{H}\right) \psi \right|\right|_1 \geq \oint_{R\to\infty} \xi^* \nabla_r \phi - \phi \nabla_r \xi^*$$

With a proper choice of ξ, one can bound the error in asymptotic behavior.

For example: partial-wave amplitudes f_l in

$$\psi = e^{ikx} + \frac{e^{ikr}}{r} f(\theta) + O(r^{-2}) \, , \quad f = \sum_{l=0}^{\infty} (2l+1) f_l P_l(\cos\theta)$$

the bound is

$$\left| f_l - \tilde{f}_l \right| \leq \frac{M}{2\pi(2l+1)} \, ||\xi||_\infty \left|\left| \left(E - \hat{H}\right) \tilde{\psi} \right|\right|$$

for the true amplitudes f_l and approximate amplitudes $\tilde{f}_l$.

Stability theorem for cross sections

Again using

$$2M\,||\xi||_{\infty}^{-1}\left|\left|\left(E-\hat{H}\right)\psi\right|\right|_{1}\geq\oint_{R\to\infty}\xi^{*}\nabla_{r}\phi-\phi\nabla_{r}\xi^{*}$$

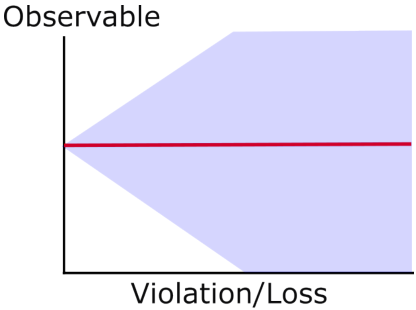
for cross sections:

$$\tilde{\sigma}-2\sqrt{\tilde{\sigma}}C+C^{2}\leq\sigma\leq\tilde{\sigma}+2\sqrt{\tilde{\sigma}}C$$
$$\text{with}\quad C=\frac{1}{2\sqrt{\pi}}M\Xi\left|\left|\left(E-\hat{H}\right)\psi\right|\right|_{1}$$

for the true cross section σ and approximate cross section $\tilde{\sigma}$.

Remarks

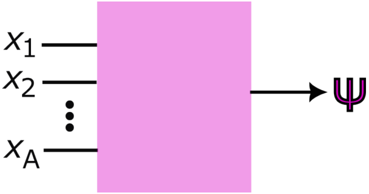
- Theorems provide a linear constraint, great.
- The theorems generalize to cases with the Coulomb interaction and momentum-dependent interactions.
- The theorems generalize to multi-particle scattering processes.
- $||\xi||_\infty$ depends on interactions.
  - for 1-dim, see our paper
  - for weak potentials, Bardsley, Gerjuoy, and Sukumar (1972)
  - For nuclear interactions, an open problem (as far as I know)



2. Neural scattering states

Neural quantum states

We parametrize a wavefunction with neural networks[2]:



and train the weights via a loss function $L[\psi(x;\alpha)]$ according to its gradient

$$\alpha \to \alpha - \epsilon \frac{\partial L[\tilde{\psi}(x;\alpha)]}{\partial \alpha} \;, \quad \epsilon = \text{learning rate}$$

The method has been applied to

- nuclear ground states, responses
- a lot more outside nuclear Physics

[2] G.Carleo and M.Troyer. arXiv:1606.02318

For nuclear ground states

$$L[\tilde{\psi}(x;\alpha)] = \langle\tilde{\psi}|\hat{H}|\tilde{\psi}\rangle / \langle\tilde{\psi}|\tilde{\psi}\rangle$$

Distilling the essential elements of nuclear binding via neural-network quantum states

Alex Gnech,[1,2] Bryce Fore,[3] and Alessandro Lovato[2,3,4]

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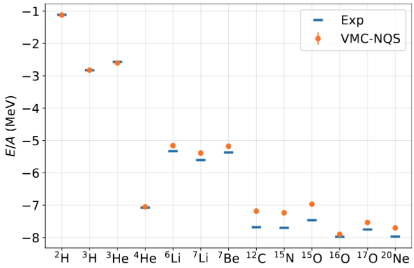
(Dated: September 1, 2023)



using potential based on pionless EFT [R. Schiavilla, L. Girlanda, A. Gnech, A. Kievsky, A. Lovato, L. E. Marcucci, M. Piarulli, and M. Viviani, arXiv:2102.02327]

Neural scattering states (2-body case)

Parametrize the scattering state for fixed incoming state e^{ikx}:

$$\tilde{\psi}(\vec{x}) = e^{ikx} + \tilde{\psi}_{\rm bulk} + \tilde{\psi}_{\rm out}\ , \quad \vec{x} = \vec{x}_1 - \vec{x}_2$$

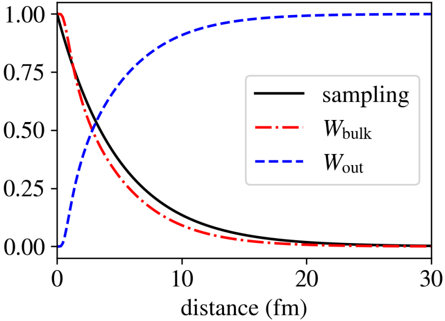
with

$$\tilde{\psi}_{\rm bulk}(r,\theta,\phi) = {\rm MLP}(r,\theta,\phi)\ W_{\rm bulk}(r)$$

$$\tilde{\psi}_{\rm out}(r,\theta,\phi) = \left(f(\theta,\phi)\frac{e^{ikr}}{r} + \frac{\Delta_\Omega f(\theta,\phi)}{2ik}\frac{e^{ikr}}{r^2} \right)\ W_{\rm out}(r)$$

Parametrization of f:

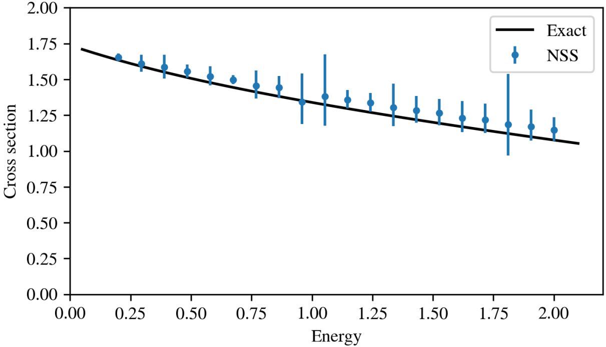
- Spherical harmonics
- Neural networks



To start: hard-sphere potential scattering[3]

In 3-dimension

$$V(r) = V_0 \; H(r_0 - r), \quad M = V_0 = r_0 = 1$$

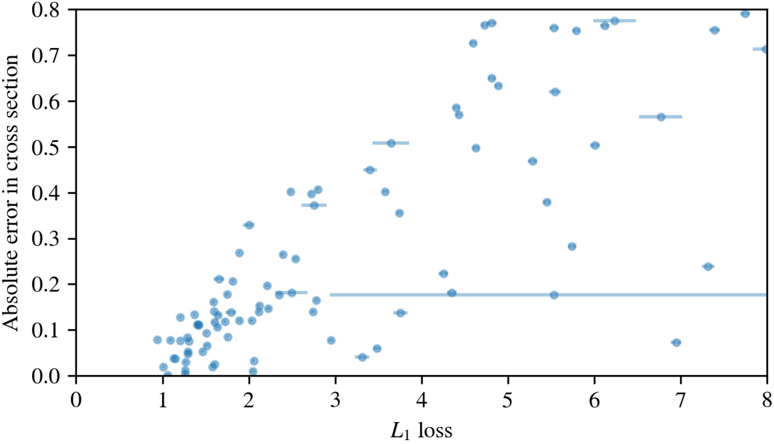


Error is computed by

$$\left| \sqrt{\sigma} - \sqrt{\tilde{\sigma}} \right| \leq \frac{M}{2\sqrt{\pi}} \, ||\xi||_\infty \, L[\tilde{\psi}]$$

[3] S. Lawrence and Y. Yamauchi. "Light nuclear scattering from neural quantum states"

Error in cross section vs L_1 loss



Neural scattering states: proton-neutron scattering

Via Argonne v_6' potential[4]:

$$\equiv [1, \sigma_i \cdot \sigma_j, S_{ij}] \otimes [1, \tau_i \cdot \tau_j] \ , \quad S_{ij} = (\sigma_i \cdot \hat{r}) \otimes (\sigma_j \cdot \hat{r}) - 3\sigma_i \cdot \sigma_j$$

The scattering state is now 4-component:

$$\tilde{\psi}(\vec{x}_p, \vec{x}_n) = e^{ikx}(u_p \otimes u_n) + \tilde{\psi}_{\text{bulk}} + \tilde{\psi}_{\text{out}}$$

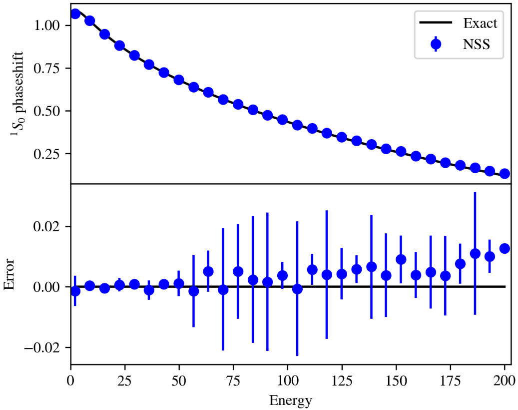
with incoming spins u_p, n_n of proton and neutron.

Neural network:

- $\tilde{\psi}_{\text{bulk}}$: with MLP (output 8 real numbers)
- $\tilde{\psi}_{\text{out}}$: with spherical harmonics up to d-wave

[4] R. B. Wiringa and Steven C. Pieper, arXiv:0207050[nucl-th]

Neural scattering states: proton-neutron scattering



Error bar estimated from the violation of unitarity:

$$1 + 2ikf = e^{2i\delta}$$

We also got cross sections very well.

Neutron - Deuteron scattering in elastic regime

This is still effectively a two-body problem, with complications:

- antisymmetrizing two neutrons
- deal with approximate deuteron state

The incoming state:

$$\psi_{\text{in}} = e^{ik(z_{1p}-z_2)} u_n \otimes \Psi_{d,s_{\text{in}}}(\vec{x}_1 - \vec{x}_p) - \{1 \leftrightarrow 2\} \ , \quad \vec{x}_{1p} = \frac{M_p \vec{x}_p + M_n \vec{x}_1}{M_p + M_n}$$

The outgoing state:

$$\psi_{\text{out}} = \frac{e^{ikr}}{r} f_s(\theta, \phi) \otimes \Psi_{d,s}(\vec{x}_1 - \vec{x}_p) W_{\text{out}} - \{1 \leftrightarrow 2\}, \quad r = |\vec{x}_{1p} - \vec{x}_2|$$

(Only s-wave included in f, so $O(r^{-2})$ term vanishes)

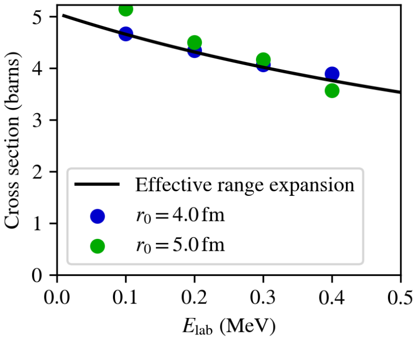
Neutron - Deuteron scattering in elastic regime

With the approximate deuteron wavefunction:

$$(E_d - \hat{H})\Psi_d \neq 0,\ L_1 \to \infty$$

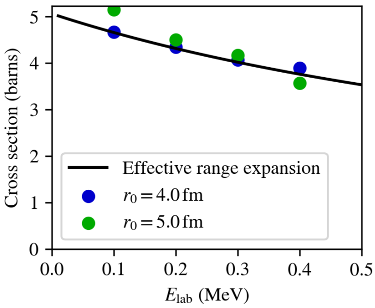
The game is not over!!!! $L_1 < \infty$ by dropping the terms $(E_d - \hat{H})\Psi_d$

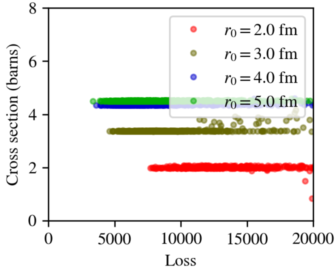
$$(E - \hat{H})\psi_{\text{in}} = \left[\frac{k^2}{2M} + E_d - \left(-\frac{\nabla^2_{n-d}}{2M} + \hat{V}_{n-d} - \frac{\nabla^2_d}{2M} + \hat{V}_d\right)\psi_{\text{in}}\right]$$

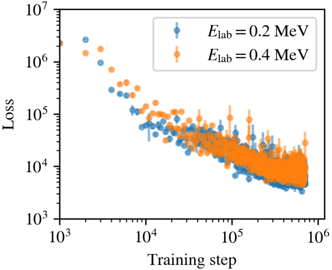


r_0: patameter in ψ_{bulk}, determining the rate of exponential decay

Neutron - Deuteron scattering in elastic regime







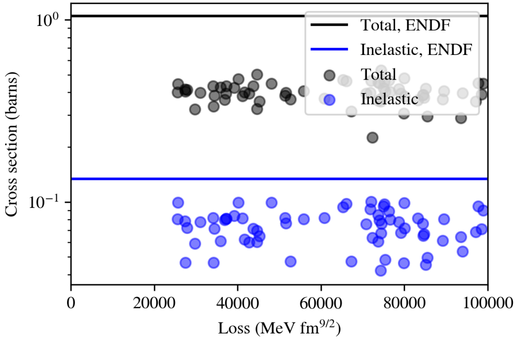
Neutron - Deuteron scattering in inelastic regime

$$\psi = \psi_{\text{in}} + \psi_{\text{bulk}} + \psi_{\text{out,el}} + \psi_{\text{out,inel}}$$

with

$$\psi_{\text{out,inel}} = \frac{e^{ikr}}{r^{5/2}} \left[f^{(0)}_{\text{inel}} + r^{-1} f^{(1)}_{\text{inel}} + r^{-2} f^{(2)}_{\text{inel}} \right]$$

Then the Schrodinger violation is $O(r^{-13/2})$, so L_1 converges.
At 10 MeV neutron energy



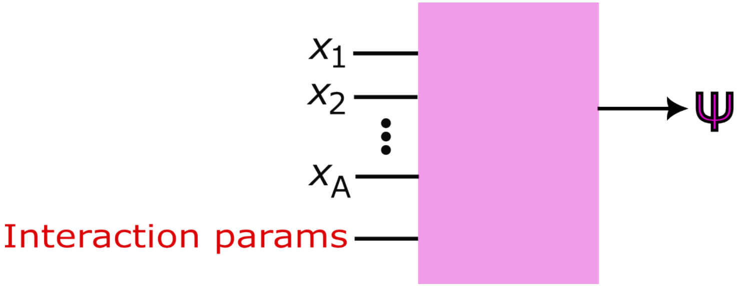
3. Emulator without emulating: Interaction-dependent NQS/NSS

Interaction-dependent neural quantum states[5]

In our work, each run of n-d simulations took $\sim$ 10 GPU hours.

What if we need computations for thousands of parameter sets??

We can "emulate" without emulating in a straightforward manner



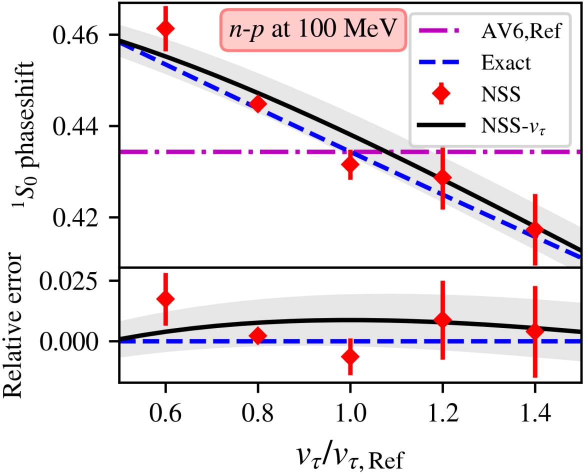
Importantly

For any set of parameters
The solution is protected by the stable minimum principles

[5] G. King, S.Lawrence, R. Somasundaram, I. Tews, Y. Yamauchi. *In preparation*

Case study with neutron-proton scattering

$$L_1[\tilde{\psi}(x, p; \alpha)] \equiv = \int dp \int dx \ \left| \left(E - \hat{H}\right) \psi \right|$$



To summarize

- We have established a set of stable minimum principles for scattering states.
- We have applied NSS method to n-p and n-d with Argonne v_6'
- Interaction-dependent NQS/NSS has the potential to serve as error-proven emulators.

Next

- Use chiral interactions, including 3N.
- Applications to neutron - α, deuteron - triton, ...
- On ML side, explore more flexible NN architecture and improve the optimization/training scheme
- Calibrate chiral interactions with scattering processes

Questions to you

1. What scattering/reaction processes are most critical for calibrating nuclear Hamiltonians?
2. In performing scattering calculations, what are the formalisms/systematics in nuclear Hamiltonians that people still debate over?
3. Our NSS method is developed for systems of nucleons–can such a method be built for other systems?

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