Nuclear continuum states and their emulators

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FRIB-TA Program: Theoretical Justifications and Motivations for Early High-Profile FRIB Experiments
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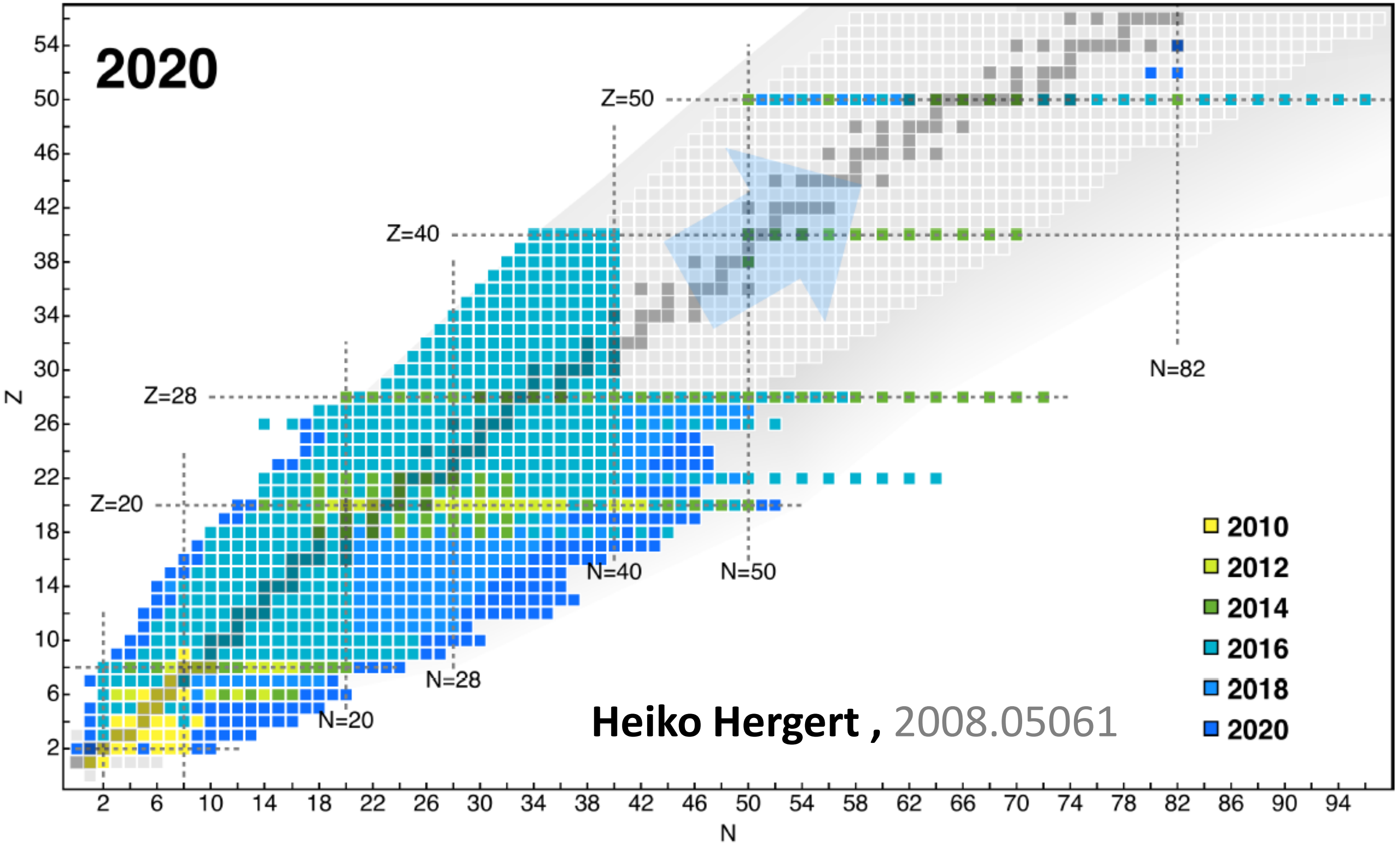
Outline

- Drip-line nuclei in the cluster picture: core plus neutrons
- Emulators for continuum states
- Takeaway points

Motivations

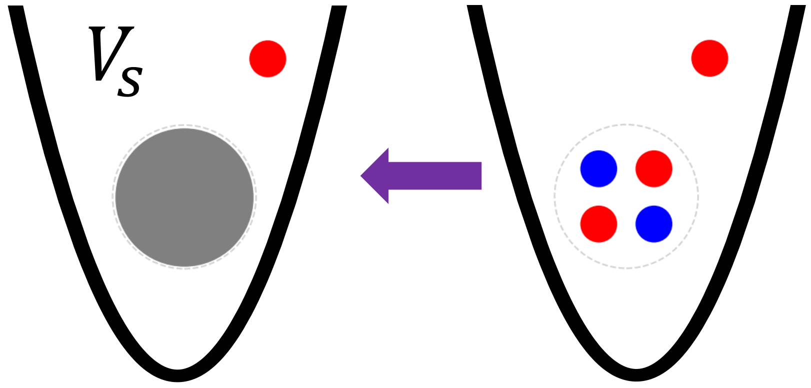
- Nuclear astrophysics
- Understanding nuclei near drip-lines
- Interpretating direct-reaction data

How to take advantage of the progress made in ab initio structure calculations for computing **continuum states**?

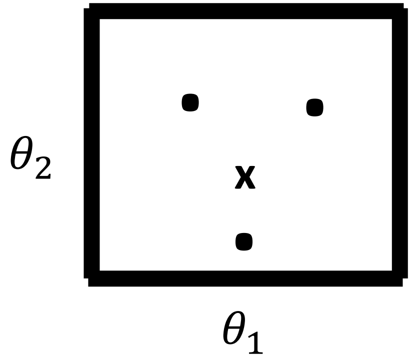


Heiko Hergert , 2008.05061

Calibrating macroscopic (cluster) theories against microscopic calculations



Parameter space ($\boldsymbol{\theta}$)



Emulators for fast interpolation

Continuum

Trap them within calculations

Bound State

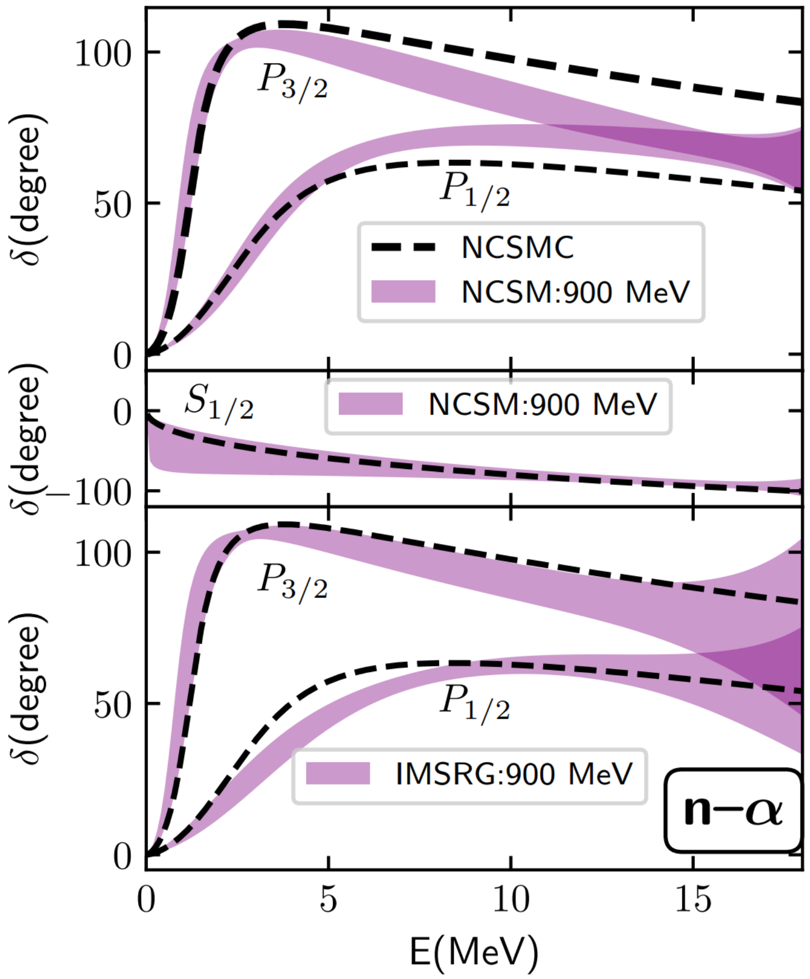
Constrain EFT (or model on V_s) → compute scattering, reactions, resonances

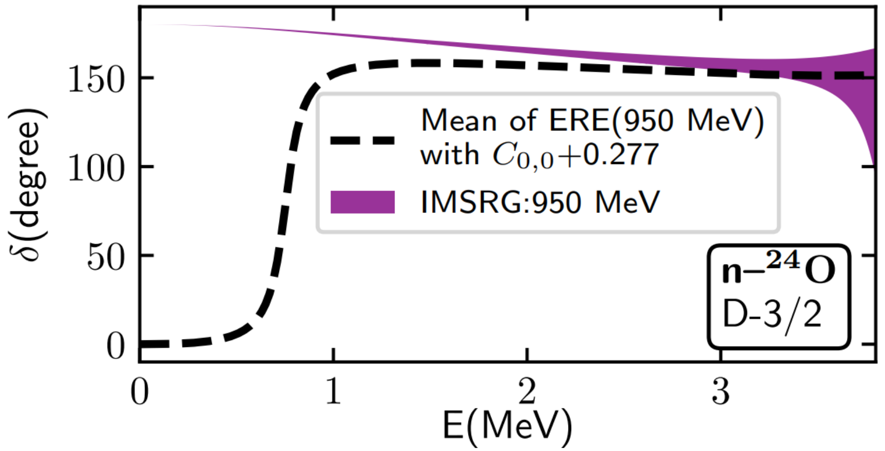
For **two-body** scattering: $(\boldsymbol{E}, \boldsymbol{\omega_T}) \rightarrow \boldsymbol{\delta_l(E)}$

XZ, PRC.101.051602(R) (2020) [1905.05275]

Early results

How to get this scattering info. experimentally? p-O, d-O scattering measurements?





NCSM: no-core shell model, IMSRG: in-medium similarity renormalization group, Dashed line: NCSM+continuum

XZ et.al., PRL 125, 112503 (2020) [2004.13575]

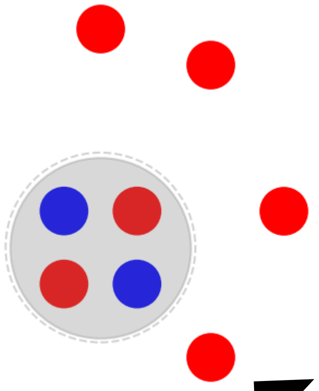
Towards dripline (e.g., He, O and Ca)

Exp.

Many-body

using traps

V_{cn}, V_{cnn}



Need to solve **3 and higher-** body systems many times

- Gamow-shell model
- MC methods
- **Emulators!**

Driven by ab initio perspective, but experimental information (e.g., threshold) could be combined → Experimental design

Takeaway points

- Core + n and core+2n are within reach in short term: including UQ from underlying NN interaction
- Any measurements about this type of systems will be valuable for developing cluster theory
- Binding energy, resonance location and width, or even scattering information, e.g., for (d,p), will be helpful
- Theory prior + experiments could be important for getting physics out of small-beam-intensity experiments?
- If so, emulators could help couple these the two sides

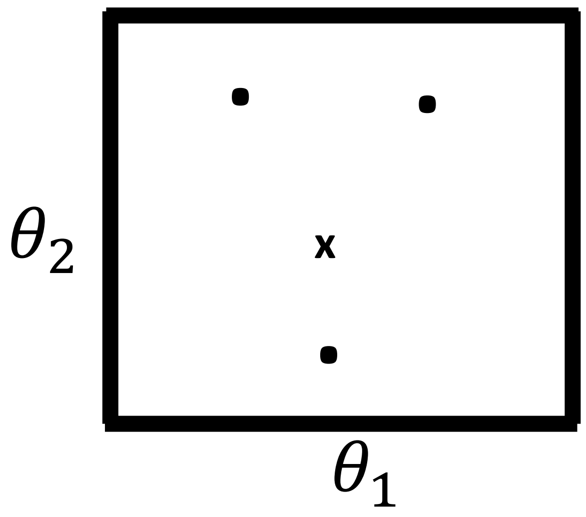
Emulators and their applications

Emulators enable fast and accurate interpolation and extrapolation of model **outputs** in the **input** parameter space

- Model calibrations and error propagation (in Bayesian statistics)
  - Chiral (e.g., three-body) interactions to exp. data (e.g., $N - d$ scattering)
  - Error propagations for many-body calculations

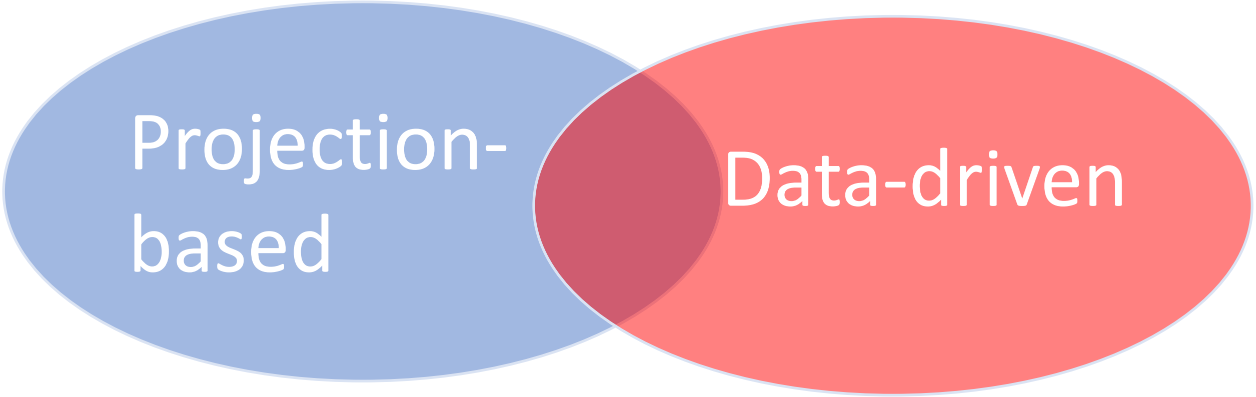
- New calculations
  - Calibrating macroscopic (cluster) theories against microscopic calculations
  - Extrapolations from feasible calculations→ infeasible regions

Parameter space ($\boldsymbol{\theta}$)



Emulators

"Eigenvector continuation with subspace learning"
Dillon Frame et. al., *Phys.Rev.Lett.* 121 (2018) 3, 032501, 1711.07090



- Reduced basis method (RBM); also known as eigenvector continuation (EC) in nuclear physics
- Intrusive
- but includes more physics, requires less training data, and has better extrapolation

$$\boldsymbol{\psi}(\boldsymbol{\theta}) = \sum_{i=1}^{N_b} C_i(\boldsymbol{\theta})\, \boldsymbol{\psi}(\boldsymbol{\theta}_i)$$

- Machine learning (ML): Gaussian process and neural networks
- nonintrusive
- agnostic of physics and requires more training data

"BUQEYE Guide to Projection-Based Emulators in Nuclear Physics," C. Drischler, J.A. Melendez, R.J. Furnstahl, A.J. Garcia, and XZ, 2212.04912
"Training and projecting: A reduced basis method emulator for many-body physics," Edgard Bonilla, Pablo Giuliani, Kyle Godbey, Dean Lee, *Phys.Rev.C* 106 (2022) 5, 054322, 2203.05284
"Model reduction methods for nuclear emulators, " J.A. Melendez, C. Drischler, R.J. Furnstahl, A.J. Garcia, XZ, 2203.05528

RBM/EC emulators for nuclear continuum states

$$[E - H(\boldsymbol{\theta})]|\psi(\boldsymbol{\theta})\rangle = 0 \quad \text{for a given } E$$

"Efficient emulators for scattering using eigenvector continuation,"R. J. Furnstahl, A. J. Garcia, P. J. Millican, and XZ, PLB **809,** 135719 (2020) [2007.03635]

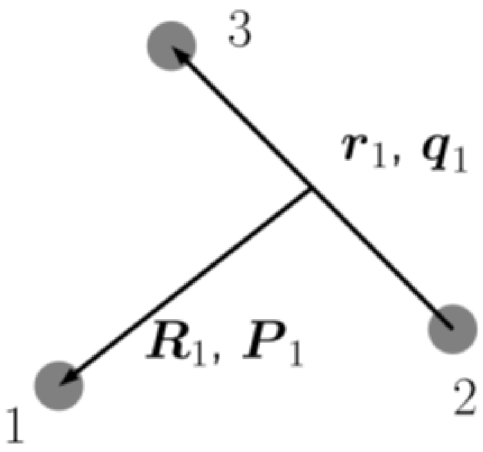
- Developed RBM emulator for two-body scatterings based on variational principle for scattering
- Systems with and without Coulomb interaction
- Complex optical potential
- General partial waves (or without pw decomp.)
- Need to deal with Kohn anomalous singularities

$$|\psi_t\rangle = \sum_{i=1}^{N_b} c_i |\psi_{\rm gs}(\boldsymbol{\theta}_i)\rangle$$

D. Bai & Z. Ren (2021); C. Drischler, et. al., (2021); J.A. Melende et.al., (2021); D. Bai (2022)…

Recent results

“Fast emulation of quantum **three-body** scattering”, XZ and R.J. Furnstahl, Phys. Rev. C 105, 064004 (2022), 2110.04269

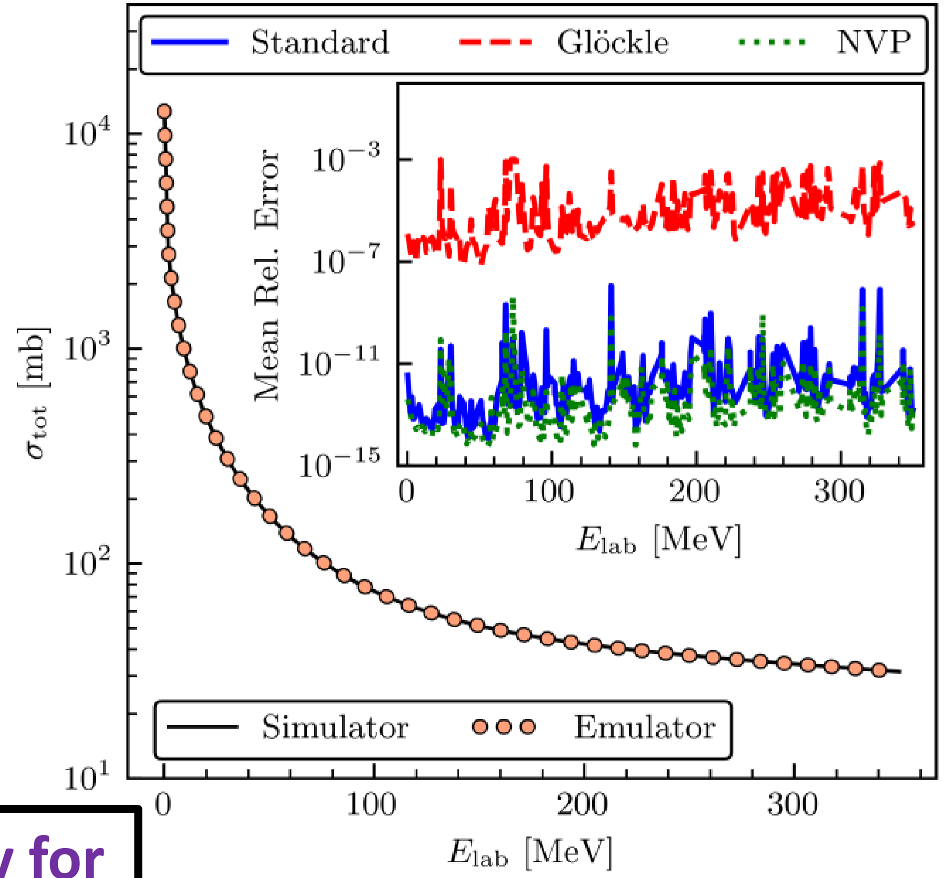


EC emulators	S relative error	Time	Memory
linear[a]	10^{-14} to 10^{-13}	ms	< MB
nonlinear-1	10^{-6} to 10^{-5}	ms	MB
nonlinear-2	10^{-4}	ms	10s MB

In contrast, the costs of full realistic calculations are 10^3s

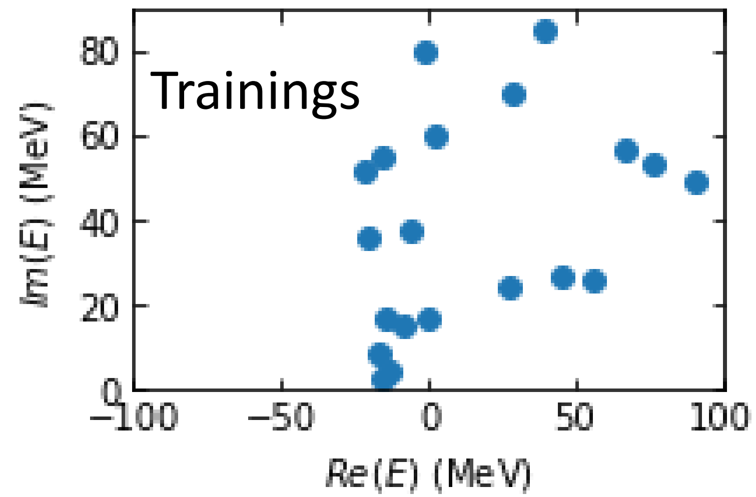
$n-p$ coupled-channel

“Wave function-based emulation for nucleon-nucleon scattering in momentum space,” A.J. Garcia, C. Drischler, R.J. Furnstahl, J.A. Melendez, XZ (2301.05093)



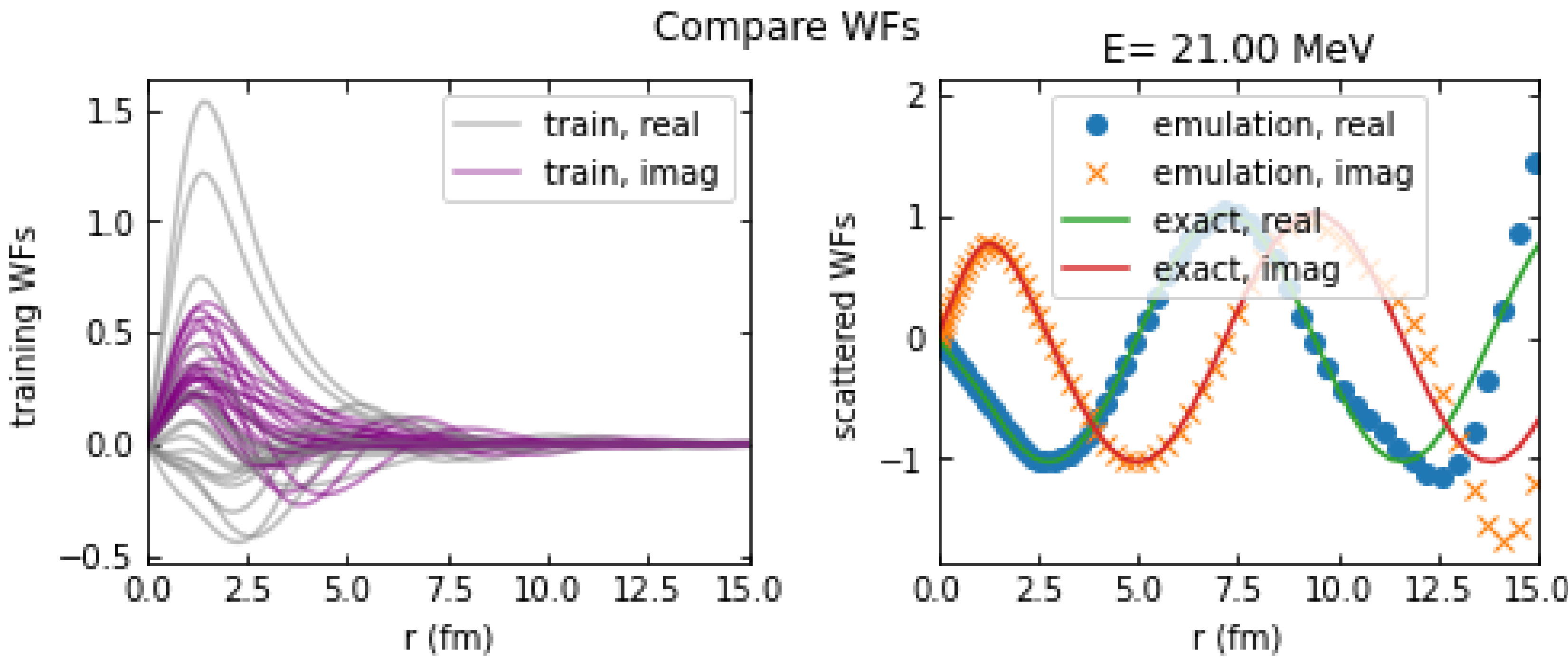
These studies require the same real energy for trainings and emulations.

Emulation in E-complex plane: two-nucleon examples

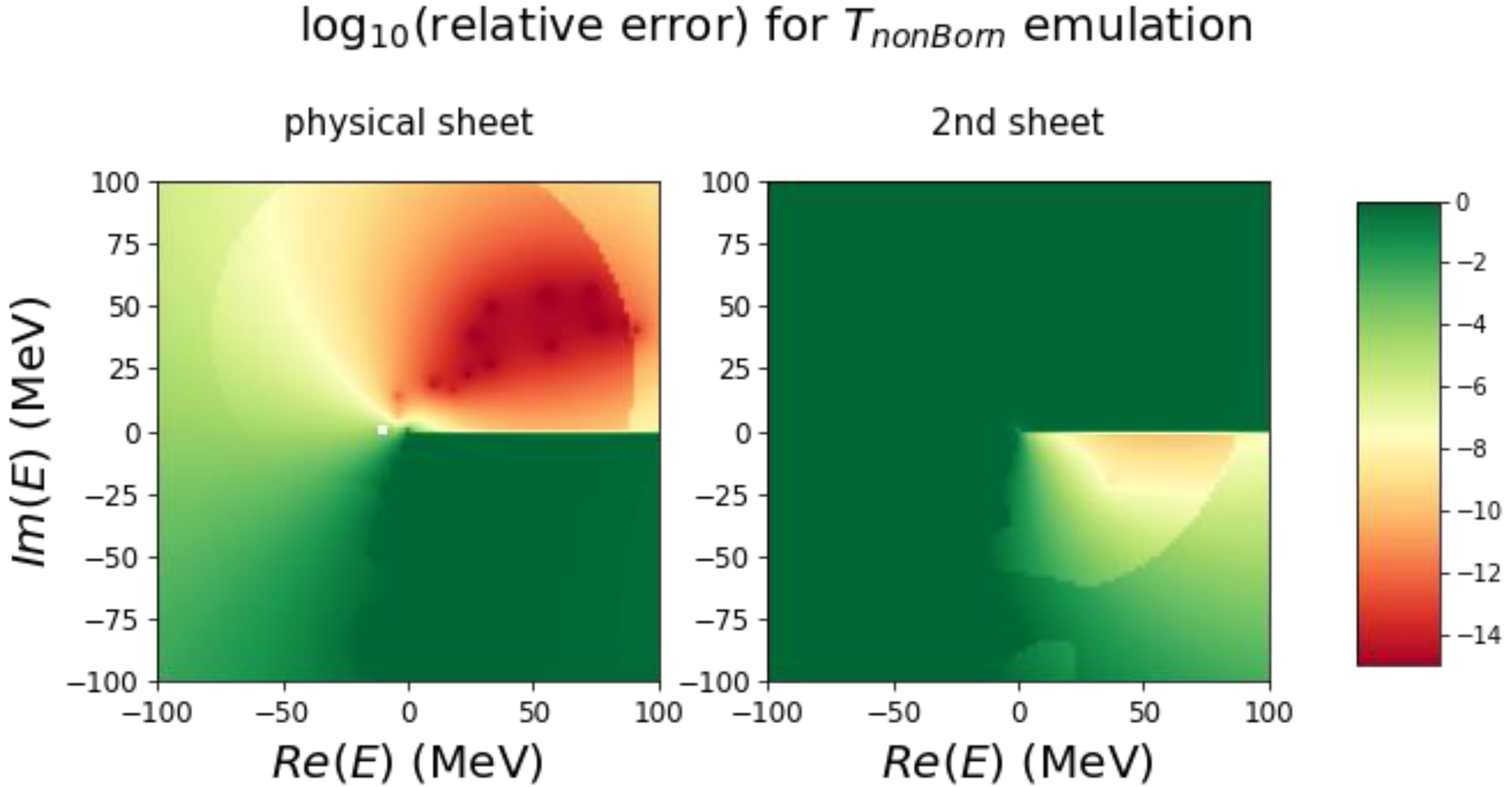


- Training wave functions (WFs) are localized
- Bound state methods for trainings

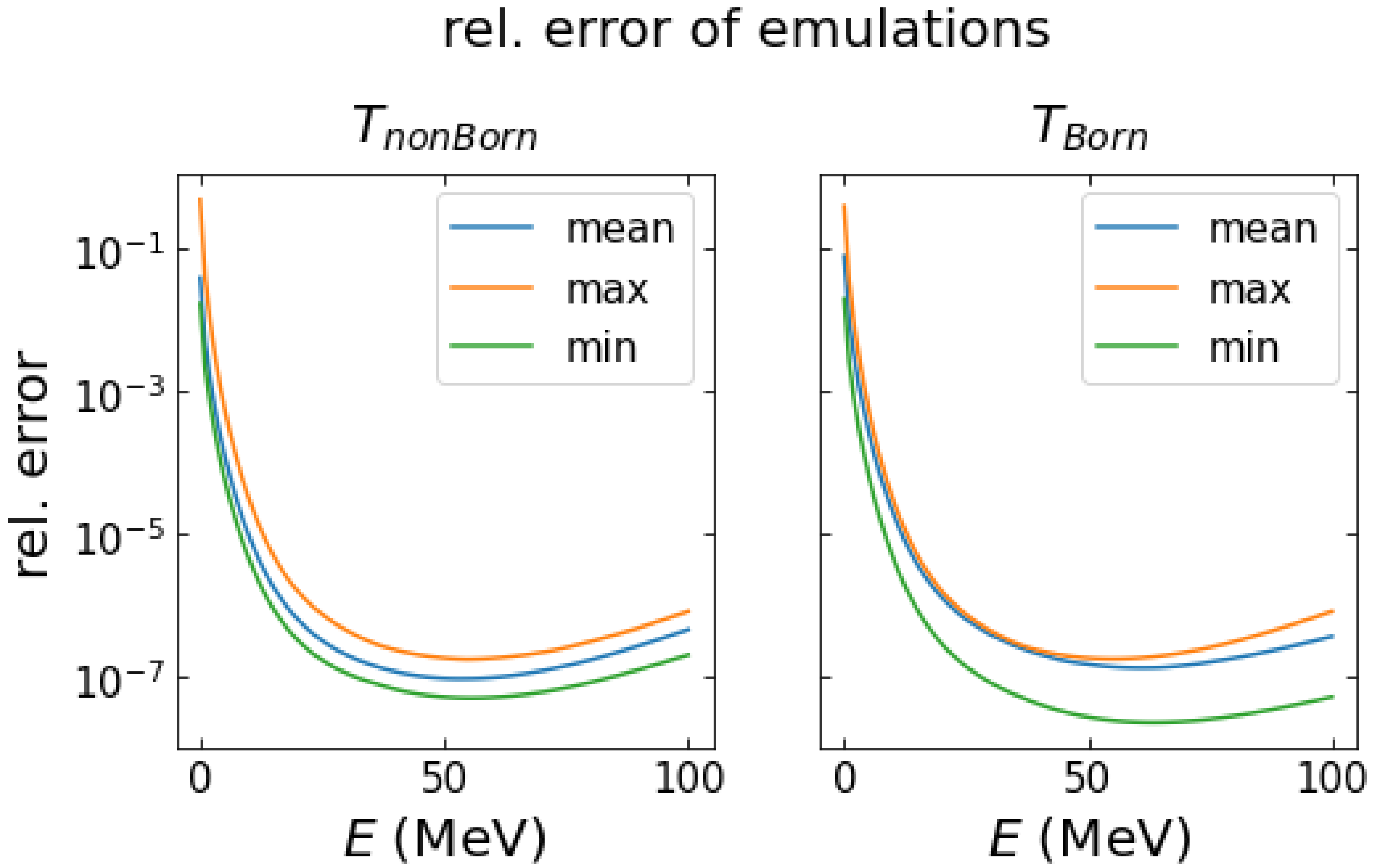
- Emulations → continuum states
- Compute continuum states based on structure solvers
- Allows emulations for other parameters



Emulation in E-complex plane: two-body in s-wave



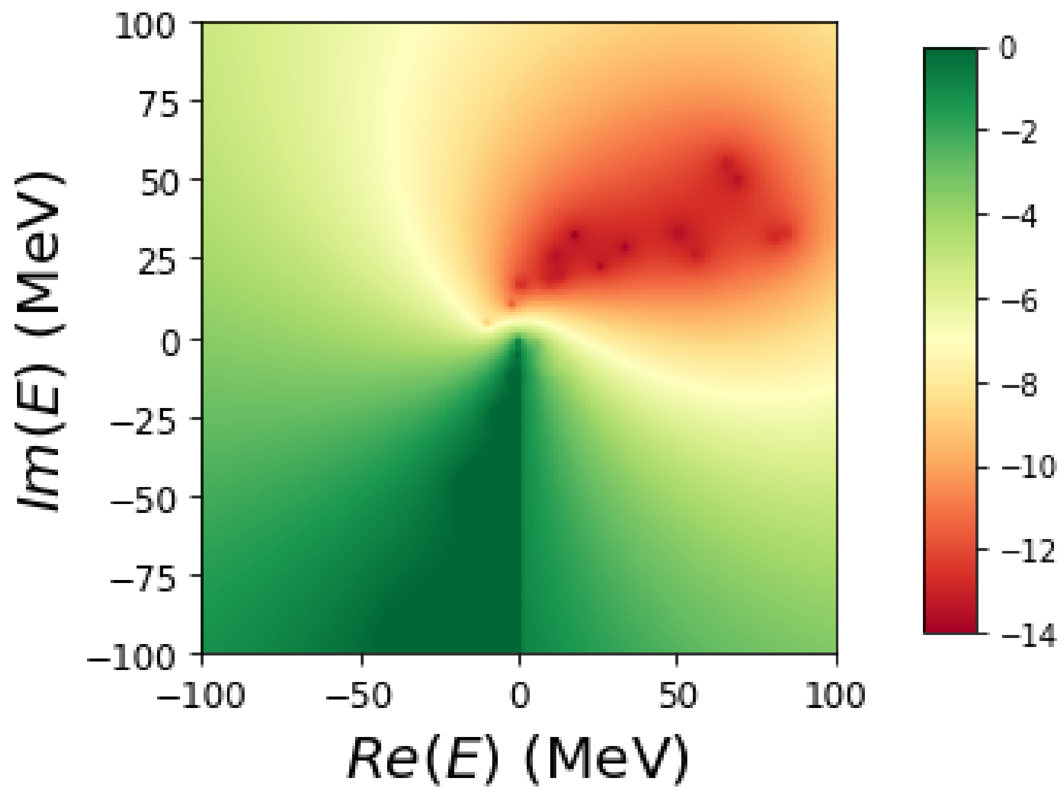
Emulation in E-complex plane: two-body in s-wave



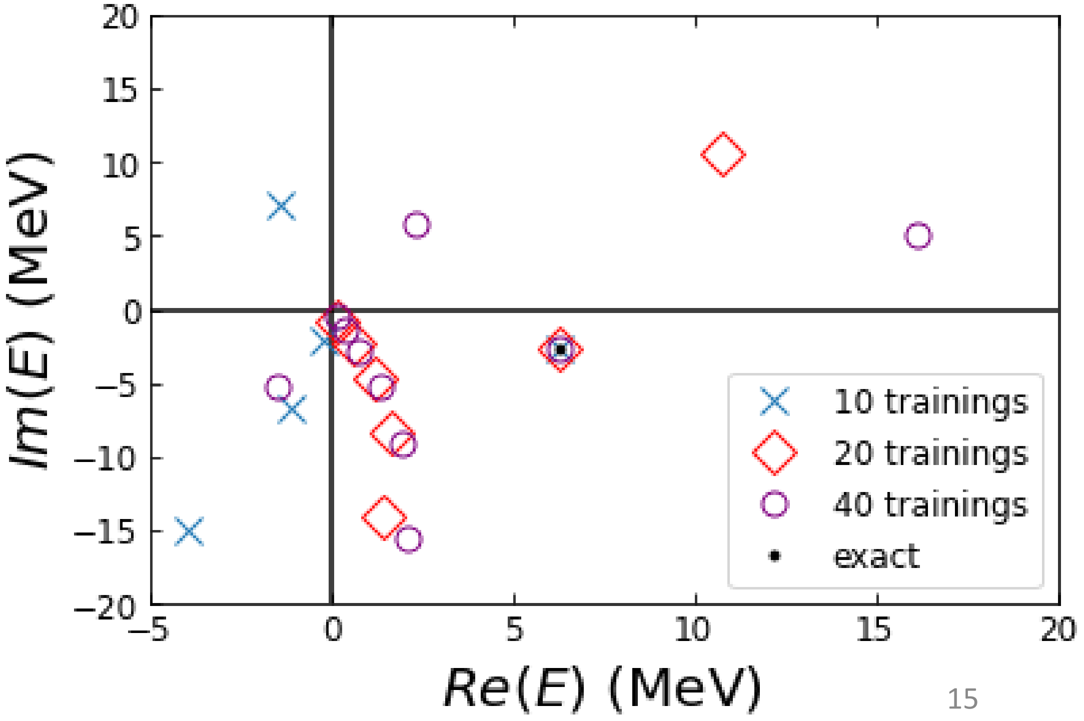
10 training points in 4-dim space: E_{in}, $Re(E)$, $Im(E)$, potential strength

Emulation in E-complex plane: two-body in p-wave

log$_{10}$(relative error) for $T_{nonBorn}$ emulation



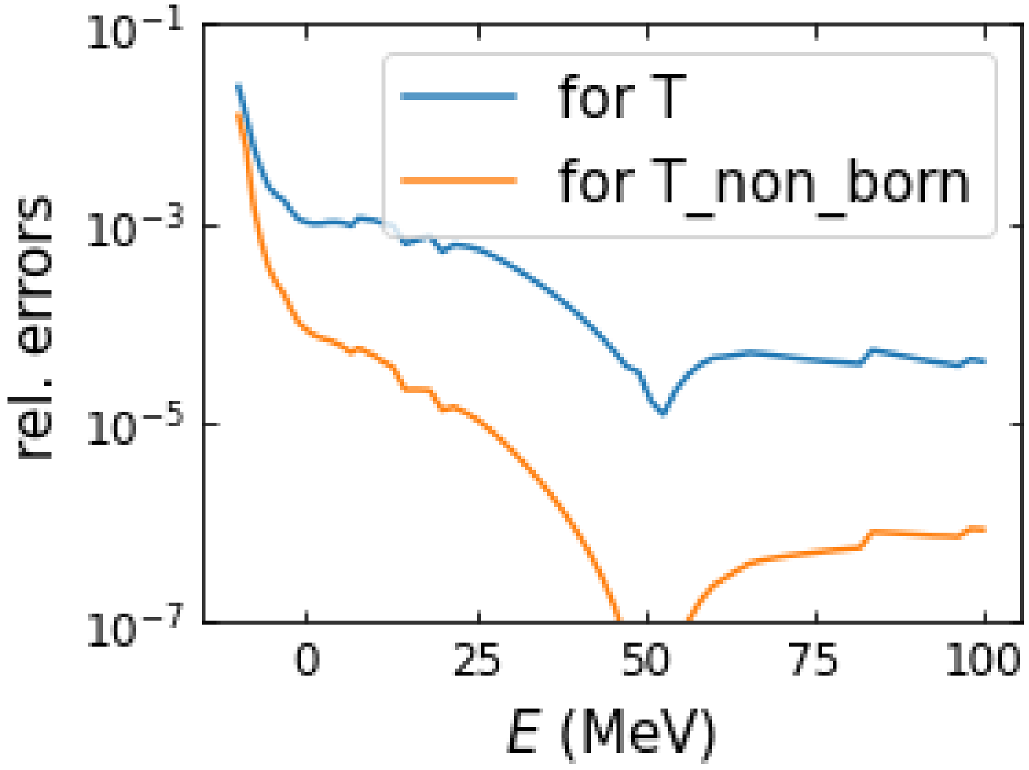
- Emulation → fast identifications of bound state and resonances
- The poles correspond to the complex eigenvalues of a complex symmetrical H (full H projected to training-solution subspace)



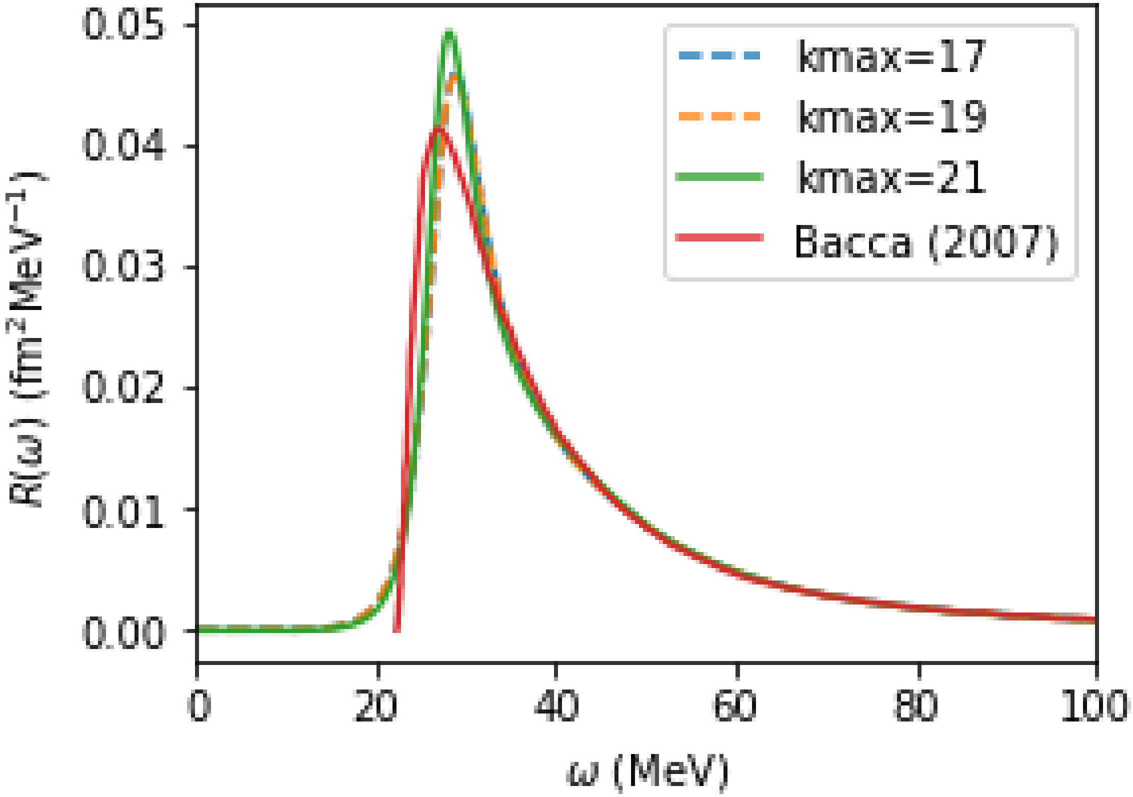
Preliminary results

With **Bijaya Acharya** and **Alex Gnech** (also experimenting with BIGSTICK, thanks to **Calvin Johnson**)

Emulating particle-dimer scatterings in 3-dim space: E_{in}, $Re(E)$, $Im(E)$



He-4 E1 response function



Takeaway points

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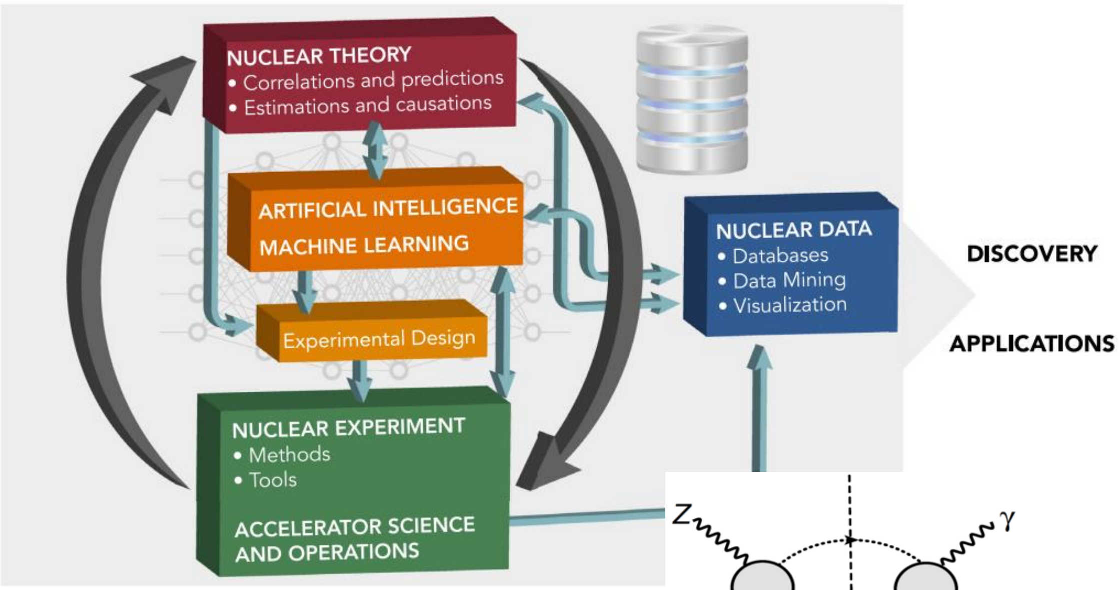
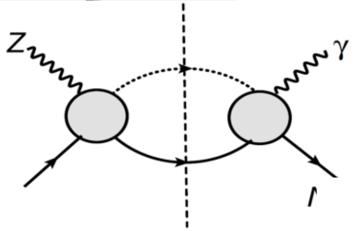
- Any measurements about this type of systems will be valuable for developing the cluster theory
- Binding energy, resonance location and width, or even scattering information, e.g., for (d,p) will be helpful
- Theory prior + data could be important for getting physics out of small-beam-intensity experiments?
- **If so, emulators could help couple theories with experiments**
- The complex-E emulation approach aims to expand ab initio continuum state calculations **and their emulators (**including scattering amplitude, response function, and even optical potentials)
- It can also be a useful solver for the cluster theory





Impacts on other areas

- Hadronic physics: few-body continuum emulators, fast resonance identifications. They are important for Jlab, colliders (heavy quark systems)
- Fundamental symmetry: neutrino-nucleus (for neutrino oscillation experiments), two-boson processes in radiative correction to weak decay, neutrinoless double-beta decay,,,

Back up

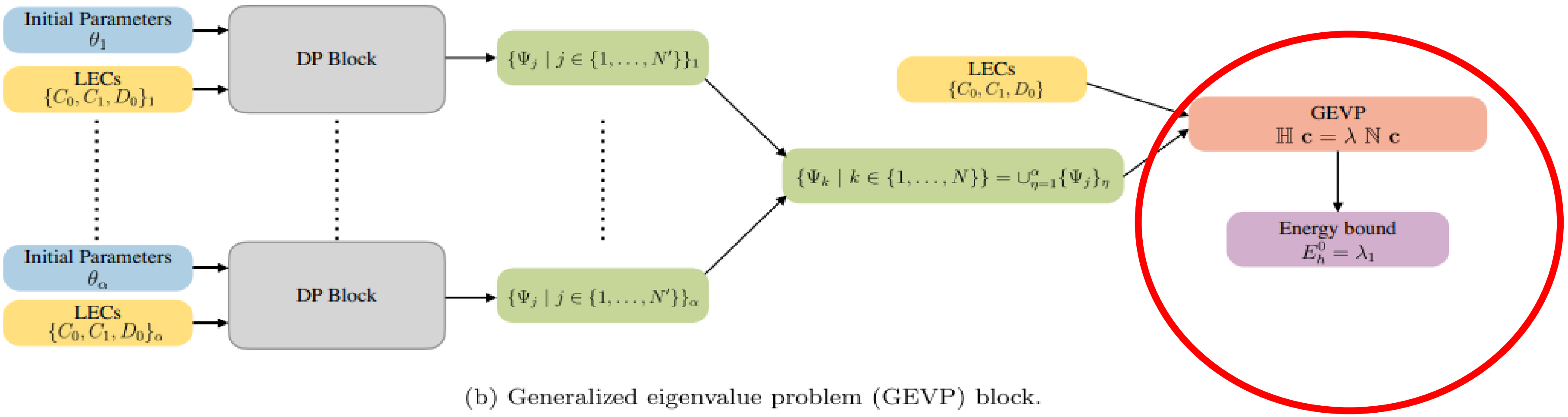
Emulators for calibrating nucleonic theory with Lattice QCD simulations

PHYSICAL REVIEW D **105,** 074508 (2022)

Finite-volume pionless effective field theory for few-nucleon systems with differentiable programming

arXiv: 2202.03530

Xiangkai Sun, William Detmold, Di Luo, and Phiala E. Shanahan

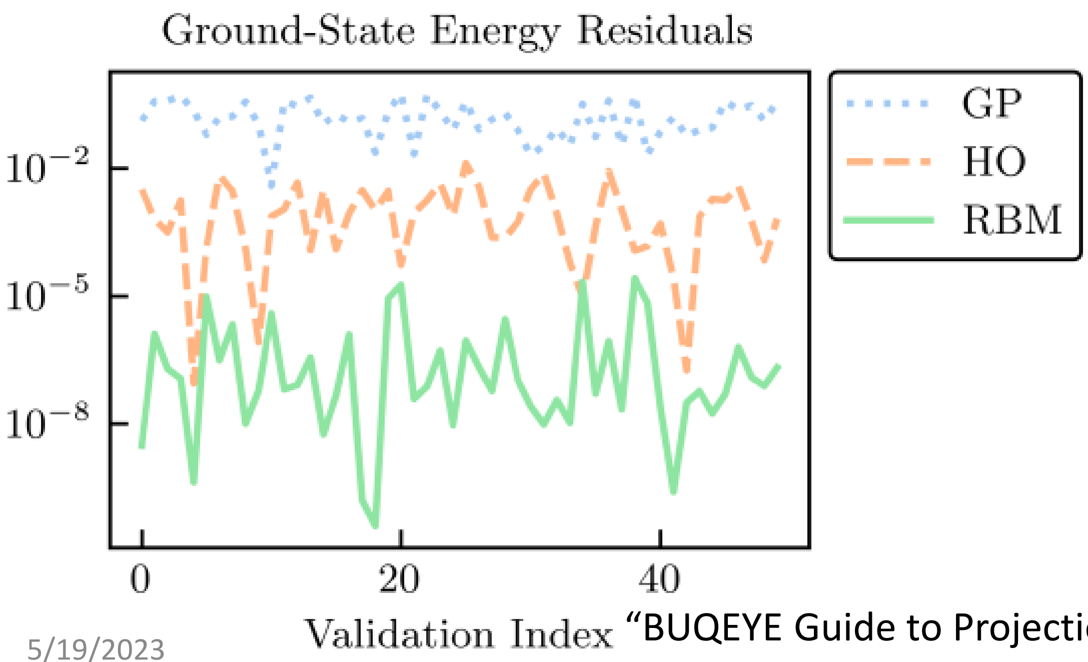


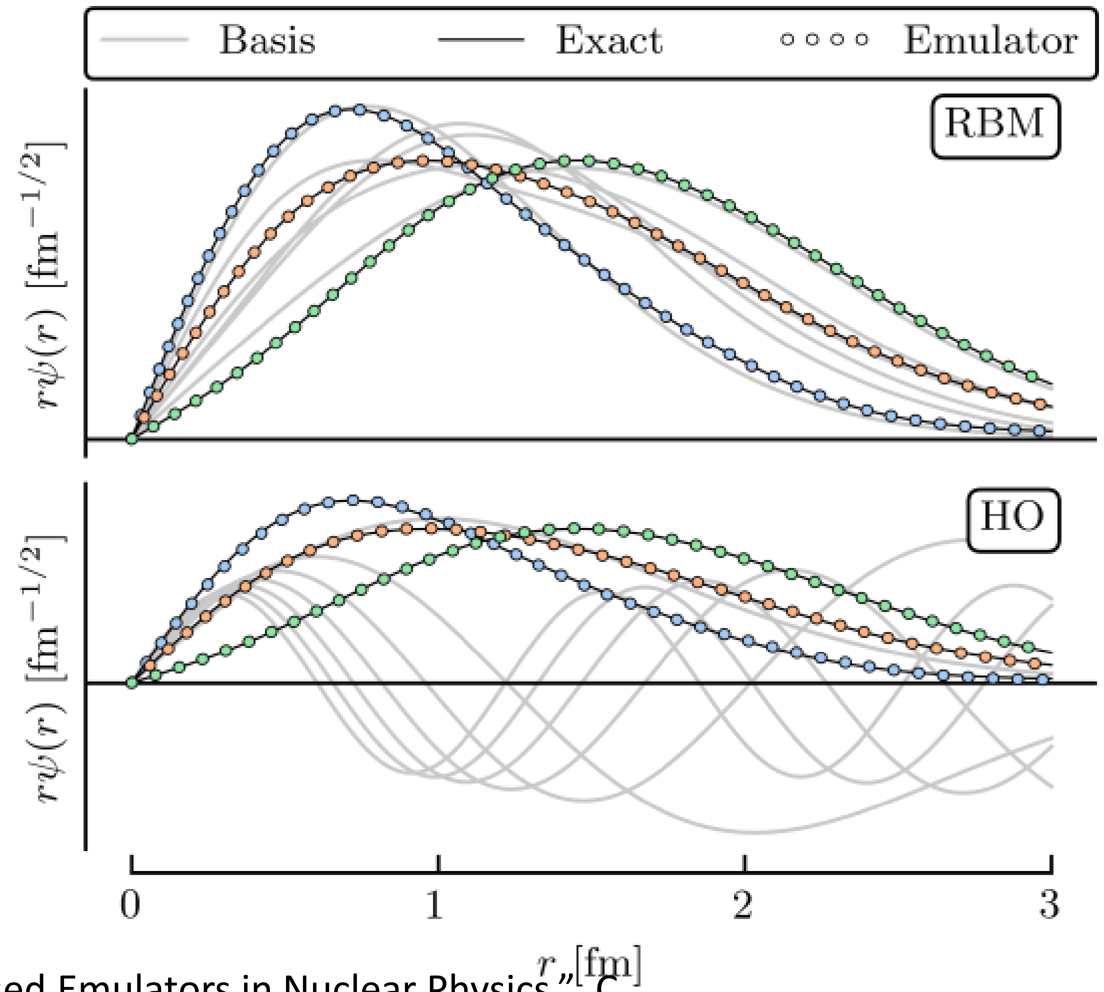
(b) Generalized eigenvalue problem (GEVP) block.

A toy-model: bound state emulator

$$V(r;\boldsymbol{\theta}) = V_{\mathrm{HO}}(r) + \sum_{n=1}^{3} \theta_n \exp(-r^2/\sigma_n^2),$$

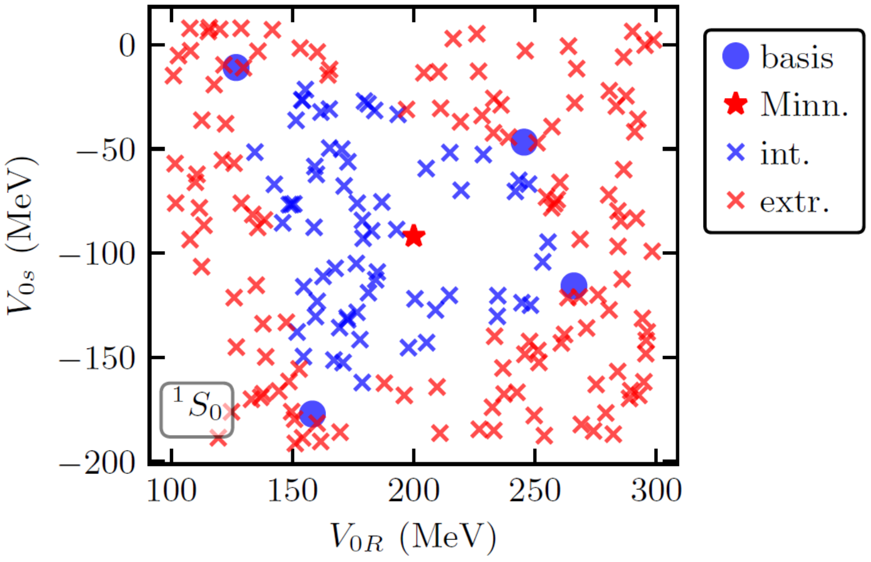
6 training points in 3-dim space

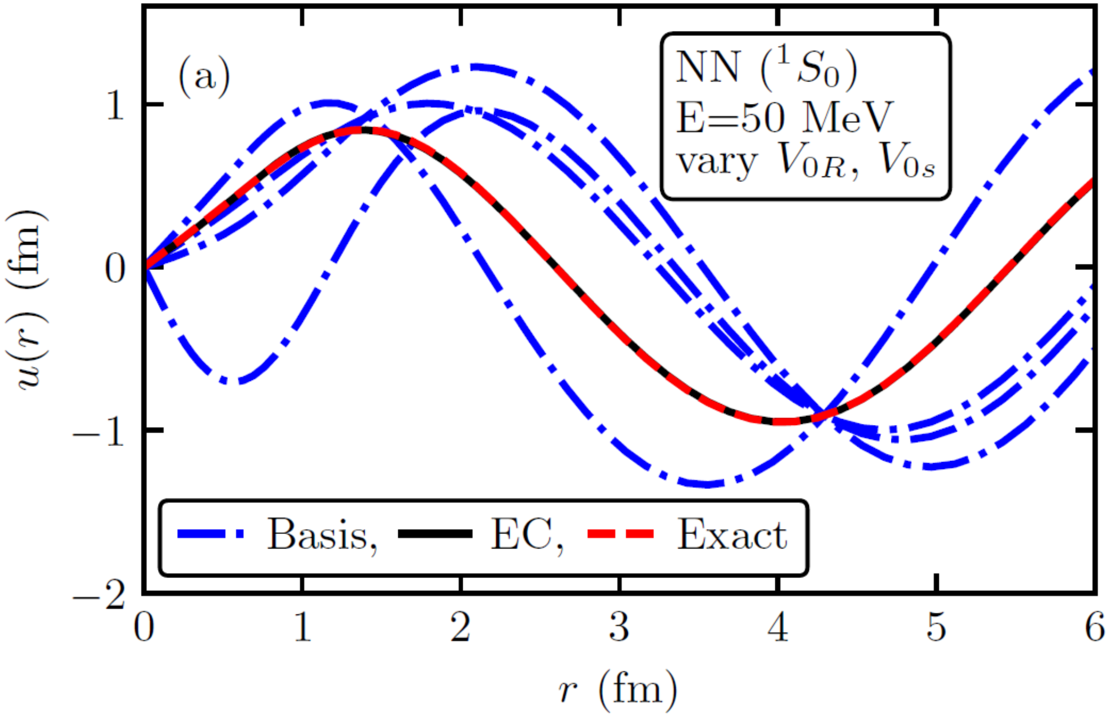


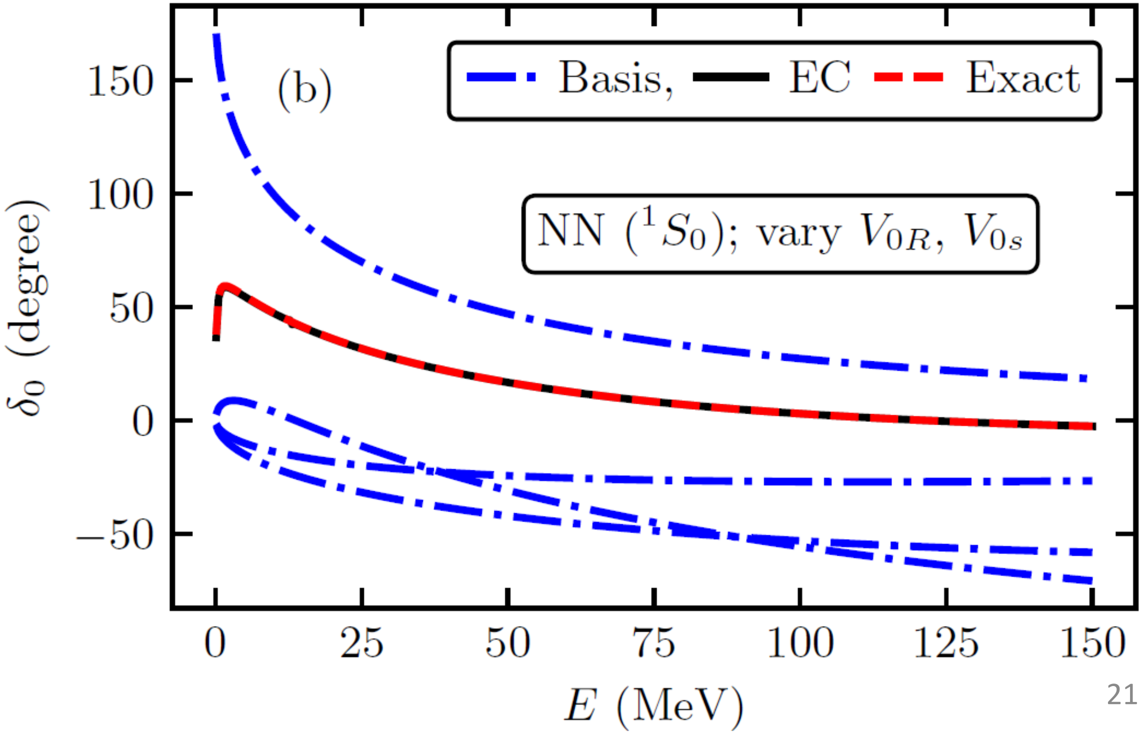


“BUQEYE Guide to Projection-Based Emulators in Nuclear Physics,” C. Drischler, **J.A. Melendez**, R.J. Furnstahl, A.J. Garcia, and XZ, 2212.04912

Tests of the emulators: NN scattering

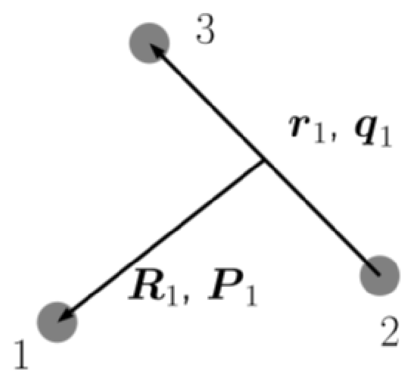




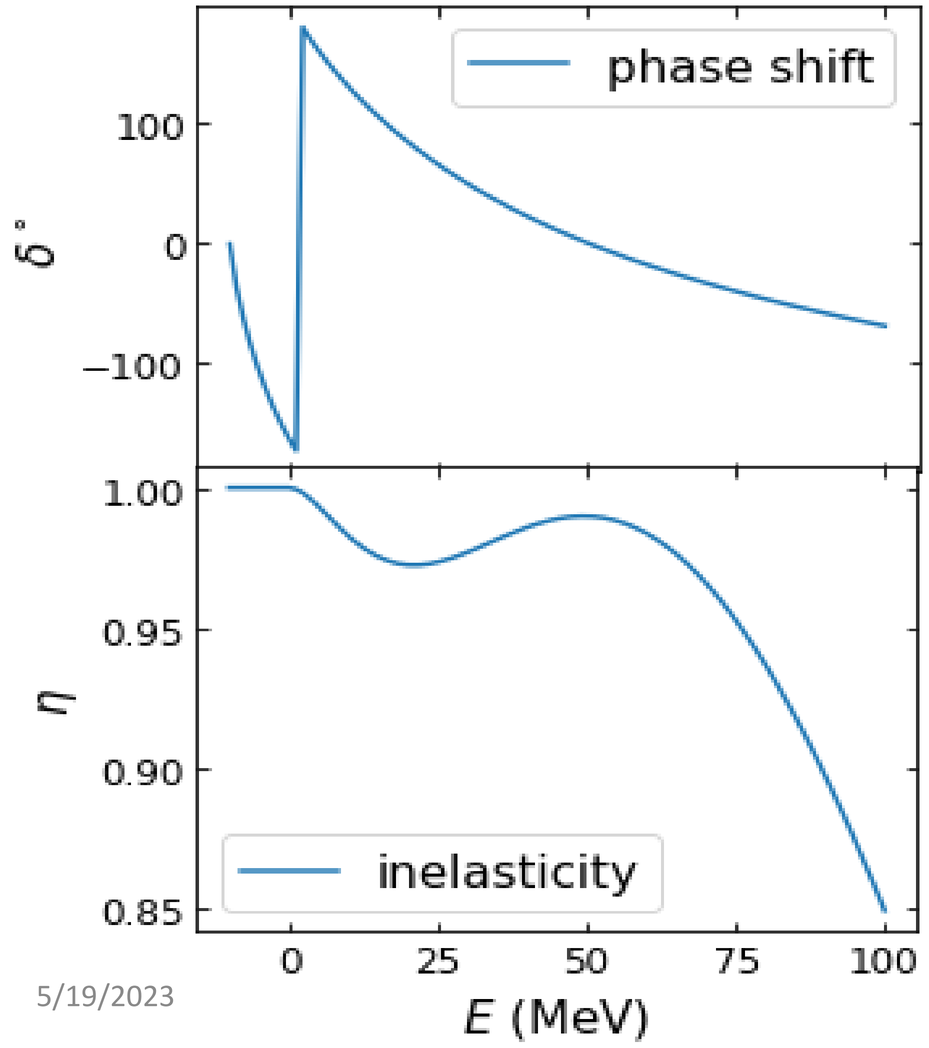


$$V_{^1S_0}(r) \equiv V_{0R} e^{-\kappa_R r^2} + V_{0s} e^{-\kappa_s r^2}$$

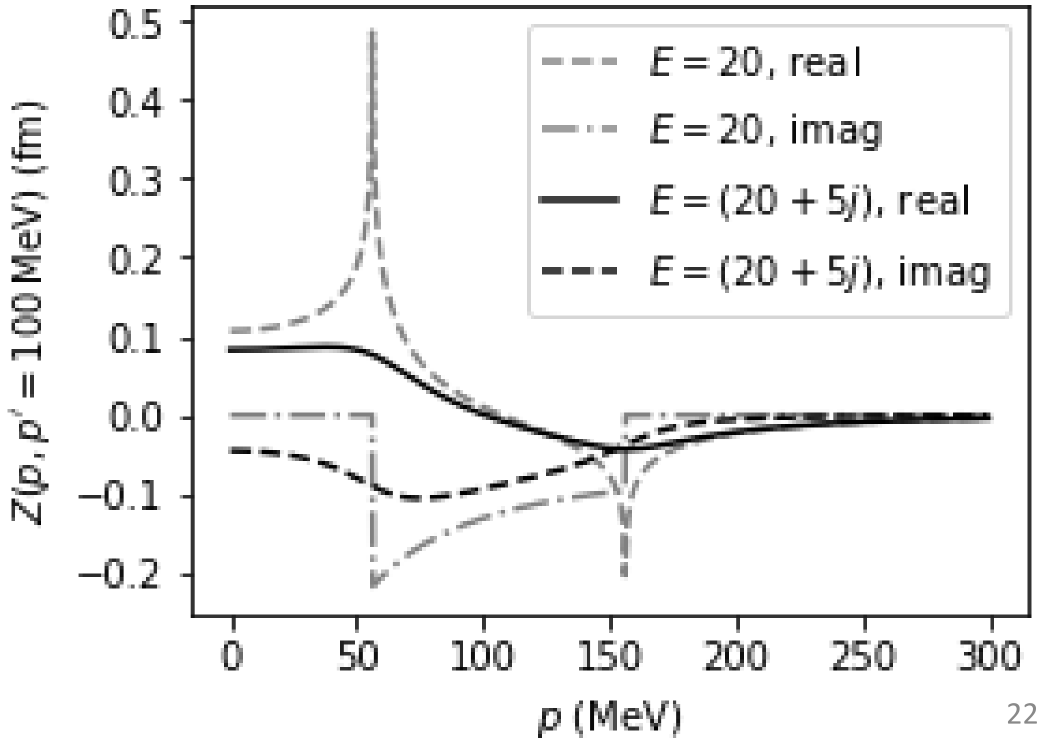
Three-boson scattering



Full calculations:



The challenge for direct continuum calculations:



Even broader impacts