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NUCLEI
Nuclear Computational Low-Energy Initiative

Efficient emulators for three-body scattering using eigenvector continuation

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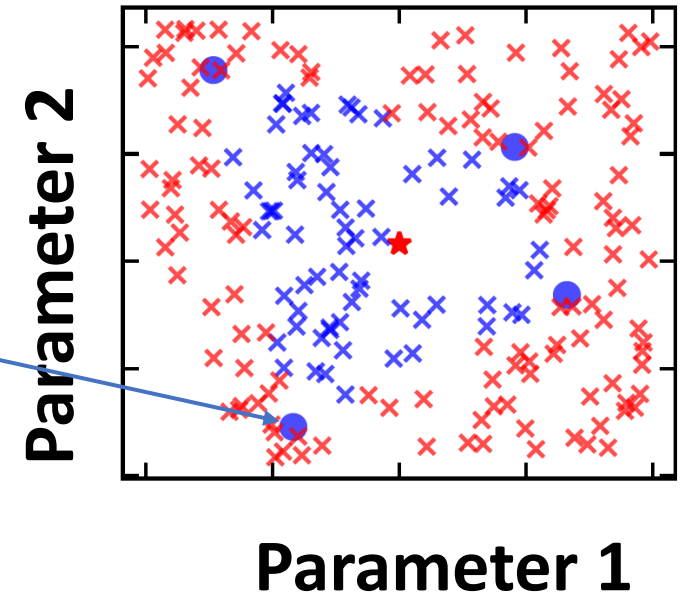
Collaborators: R.J. Furnstahl, A.J. Garcia, P.J. Millican

Outline

- Introduction on emulators
- Eigenvector-Continuation (EC) emulators for nuclear structure calculations
- EC emulators for two-body scatterings
- EC emulators for three-body scatterings
- Generalizations, including a connection with ab initio scattering and reaction calculation
- Summary and outlook

Emulator

- Model fitting/error propagation → solving the model at many points in its parameter space
- A bottleneck issue: high computational cost for solving models
- Need efficient and accurate emulators for models (train the emulators using **training points** and then make predictions at other points)
- Applications in nuclear physics:
  - Many-body bound-state calculations
  - Few-body scattering and reactions calculations
    - **Fitting Chiral three-nucleon interactions to the proton-deuteron scattering data**
    - **Data fittings involving deuteron-nucleus scattering and reactions, e.g., A(d,p)B and A(d,n)B**



EC emulators for bound state calculations

D. Frame, et.al., *Eigenvector continuation with subspace learning*, *Phys.Rev.Lett.* **121**, 032501 (2018) [1711.07090](1711.07090)

$$\hat{H}(\boldsymbol{\theta}) = \hat{T} + \hat{V}(\boldsymbol{\theta})$$ depending on $\boldsymbol{\theta}$

$$\hat{H}(\boldsymbol{\theta}_i) \rightarrow |\psi_{\rm gs}(\boldsymbol{\theta}_i)\rangle$$ $|\psi_{\rm gs}(\boldsymbol{\theta}_i)\rangle$ live in a low-dimension Hilbert space

Construct emulators based on variational calculation method

S. König, et.al., *Eigenvector Continuation as an Efficient and Accurate Emulator for Uncertainty Quantification*, *Phys. Lett. B* ***810****, 135814 (2020)* [1909.08446](1909.08446) **;** A. Ekström and G. Hagen, *Global sensitivity analysis of bulk properties of an atomic nucleus, Phys.Rev.Lett.* **123**, 252501 (2019) [1910.02922](1910.02922)

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

$$\delta\left[\langle\psi_{\rm trial}|\hat{H}(\boldsymbol{\theta})|\psi_{\rm trial}\rangle - \lambda(\langle\psi_{\rm trial}|\psi_{\rm trial}\rangle - 1)\right] = 0$$

Ground state energy

Ground state WF

$$\sum_k (H_{jk} - \lambda N_{jk}) c_k = 0$$

$$H_{ij}(\boldsymbol{\theta}) \equiv \langle\psi_{\rm gs}(\boldsymbol{\theta}_i)|\hat{H}(\boldsymbol{\theta})|\psi_{\rm gs}(\boldsymbol{\theta}_j)\rangle$$

$$N_{ij}(\boldsymbol{\theta}) \equiv \langle\psi_{\rm gs}(\boldsymbol{\theta}_j)|\psi_{\rm gs}(\boldsymbol{\theta}_i)\rangle$$

N_b-dim linear algebra→ fast emulator calculations

Emulators for two-body scattering based on Kohn variational method

R. J. Furnstahl, A. J. Garcia, P. J. Millican, and XZ, *PLB* ***809,*** *135719 (2020) [2007.03635]*

There exists a functional: $\beta\left[|\psi_{\rm trial}\rangle\right] = \tau_{\rm trial} - 2\mu\langle\psi_{\rm trial}|\widehat{H}(\boldsymbol{\theta}) - E|\psi_{\rm trial}\rangle$ μ as the reduced mass

with an asymptotic condition $r\psi_{\rm trial}(r) \overset{r\to\infty}{\longrightarrow} \sin(pr - \ell\pi/2)/p + \tau_{\rm trial}\cos(pr - \ell\pi/2)$

With the exact scattering WF ➡ $\beta\left[|\psi_{\rm exact}\rangle\right] = \frac{1}{p}[\tan\delta_\ell(E)]_{\rm exact} \equiv \tau_{\rm exact}$

Plugging a trial WF gives $\delta\beta\left[|\psi_{\rm exact}\rangle\right] = 0 + O\left[(\delta|\psi\rangle)^2\right]$

For emulators, construct $|\psi_{\rm trial}\rangle = \sum_{i=1}^{N_b} c_i|\psi_E(\boldsymbol{\theta}_i)\rangle$ out of the WFs at training points

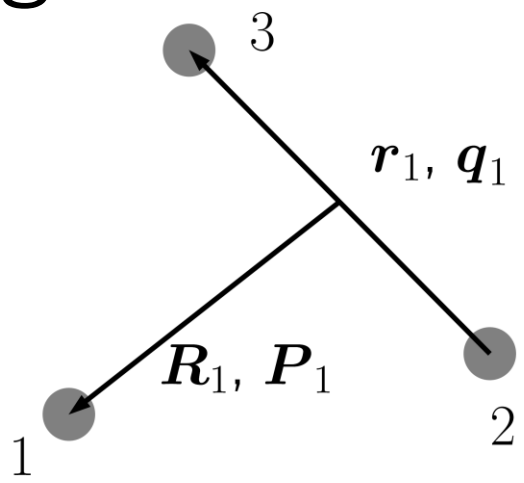
At the stationary point, c_i staisifies $\sum_{i=1}^{N_b}\left(\Delta U^{\intercal} + \Delta U\right)_{ij} c_j = \tau_i - \lambda$

$$\Delta U_{ij} \equiv 2\mu\langle\psi_E(\boldsymbol{\theta}_i)|\widehat{H}(\boldsymbol{\theta}) - E|\psi_E(\boldsymbol{\theta}_j)\rangle$$

- τ_i is related to the phase shift of the ith training point
- λ is a Lagrange multiplier
- ΔU_{ij} integral vanishes outside the strong interaction range

N_b-dim linear algebra→ fast emulator calculations

Generalization to three-body scattering: below breakup threshold (S wave)



For three identical spin-0 bosons, $H = T_r + T_R + V_{2-body} + V_{3-body}$

Suppose V_{2-body} gives a two-body (dimer) bound state ϕ_b

Compute the boson-dimer scattering. The scattering WF

$$\Psi(\boldsymbol{r_1}, \boldsymbol{R_1}) \xrightarrow{R_1 \to \infty} \phi_b(\boldsymbol{r_1}) \frac{1}{\sqrt{v}} [-e^{-iP_1R_1} + S\, e^{iP_1R_1}]$$

The functional estimates the scattering S-matrix:

$$\beta[\Psi_{\text{trial}}] = S_{\text{trial}} - \frac{1}{3i} \langle \Psi_{\text{trial}} | \hat{H}(\boldsymbol{\theta}) - E | \Psi_{\text{trial}} \rangle$$

The two-body emulator can be generalized to emulate $H(\theta)$ with **varying V_{3-body} but with V_{2-body} fixed**

Separable V_{2-body}, e.g., $V_{23} = \lambda |g\rangle\langle g|$

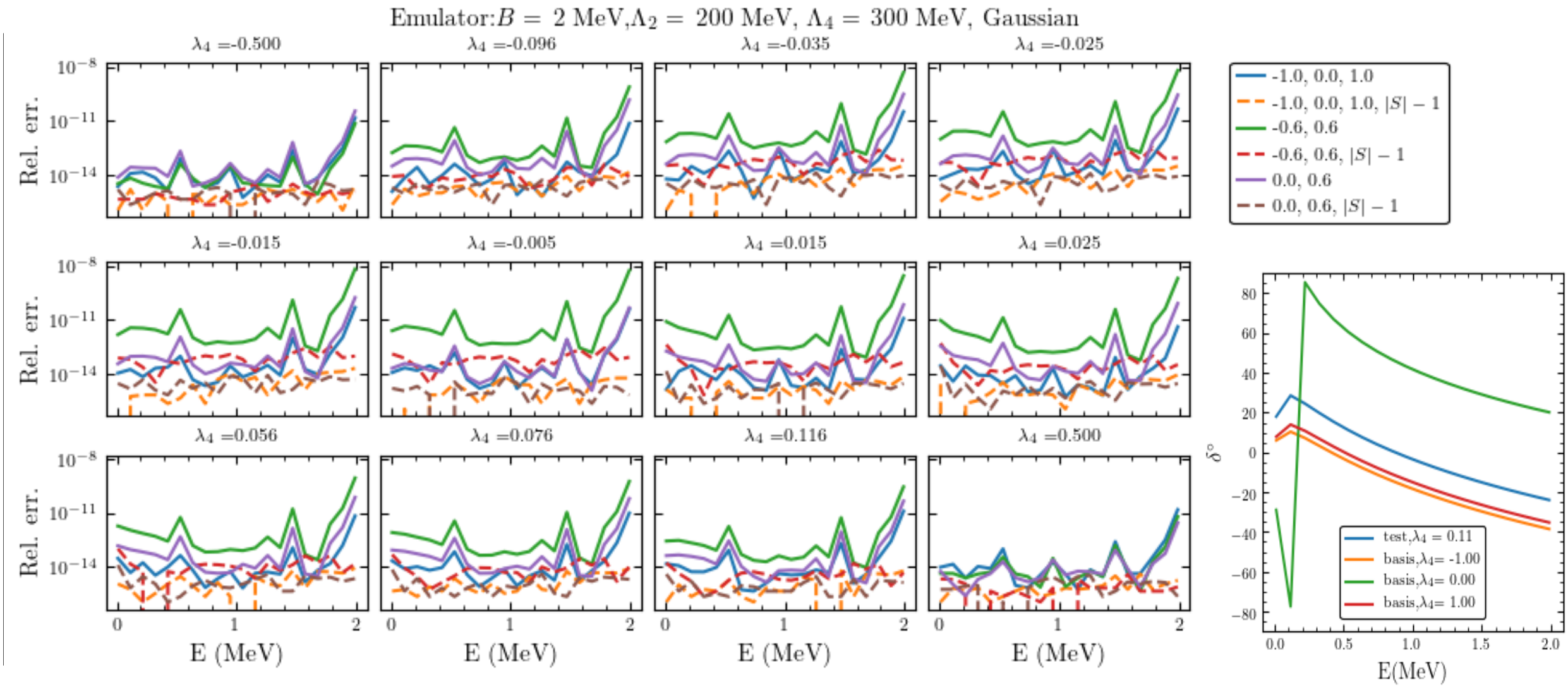
$$\langle \boldsymbol{q}_1 | g \rangle \propto e^{-q_1^2/(2\Lambda^2)}$$

Separable V_{3-body}: $V_4 = \lambda_4 |g_4\rangle\langle g_4|$

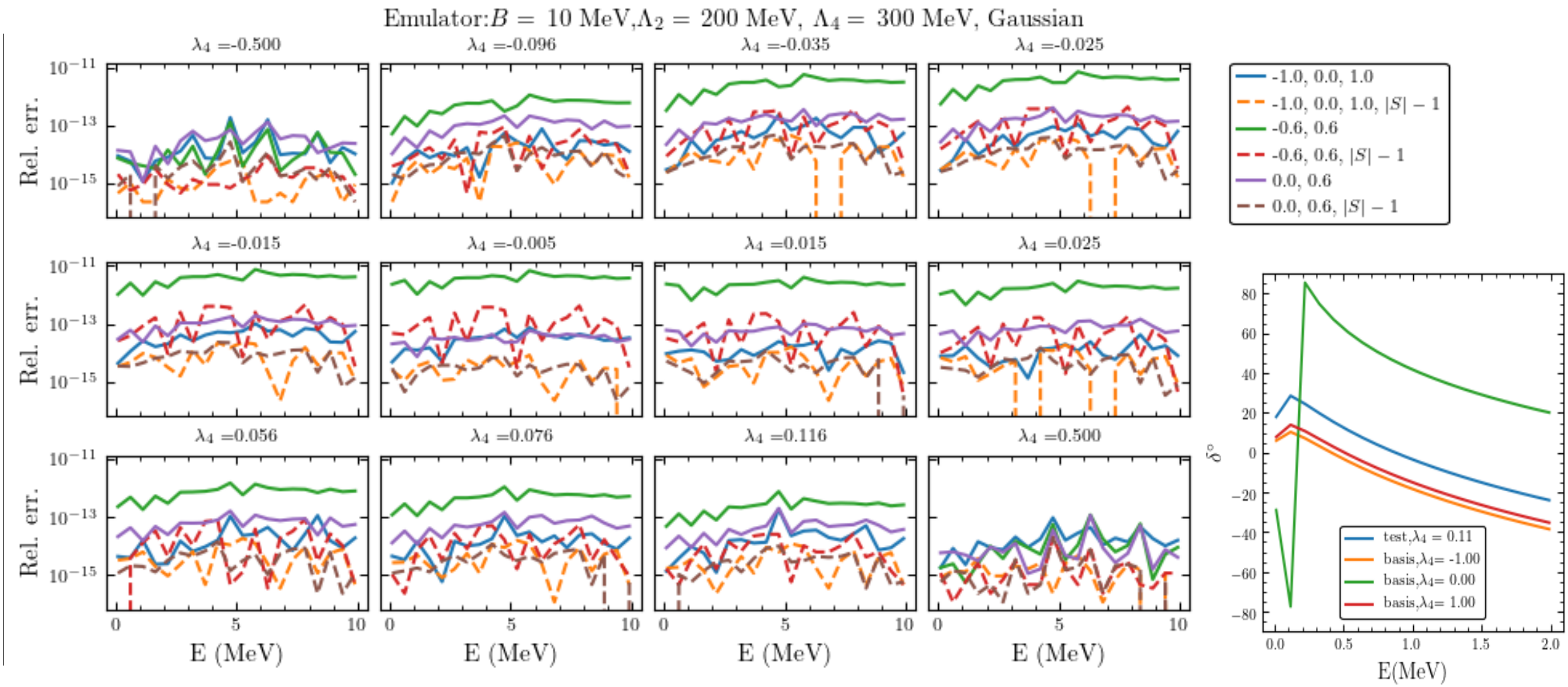
$$\langle \boldsymbol{P_1 q_1} | g_4 \rangle \propto e^{-(q_1^2 + \frac{3}{4}P_1^2)/(2\Lambda_4^2)}$$

Mass as nucleon mass

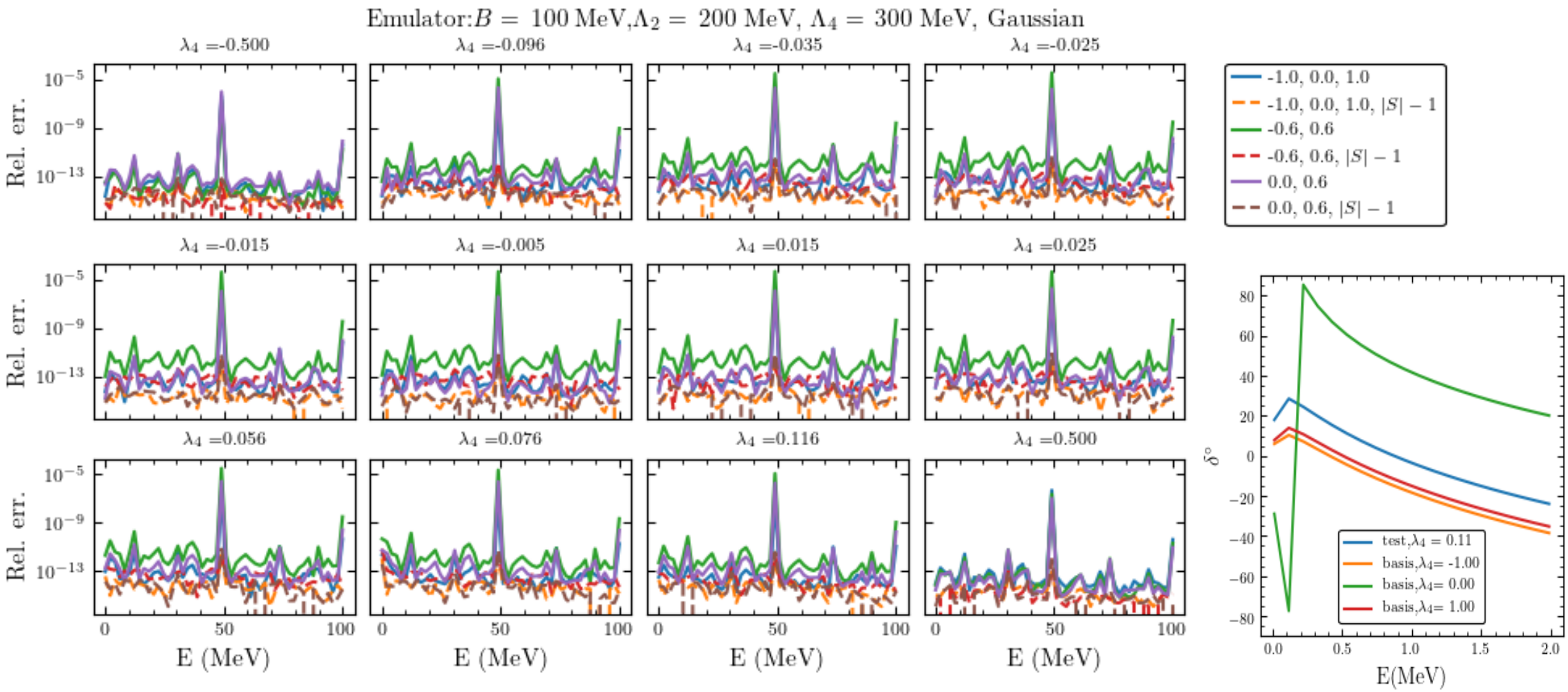
Vary 3-body potential strength λ_4



Vary 3-body potential strength λ_4



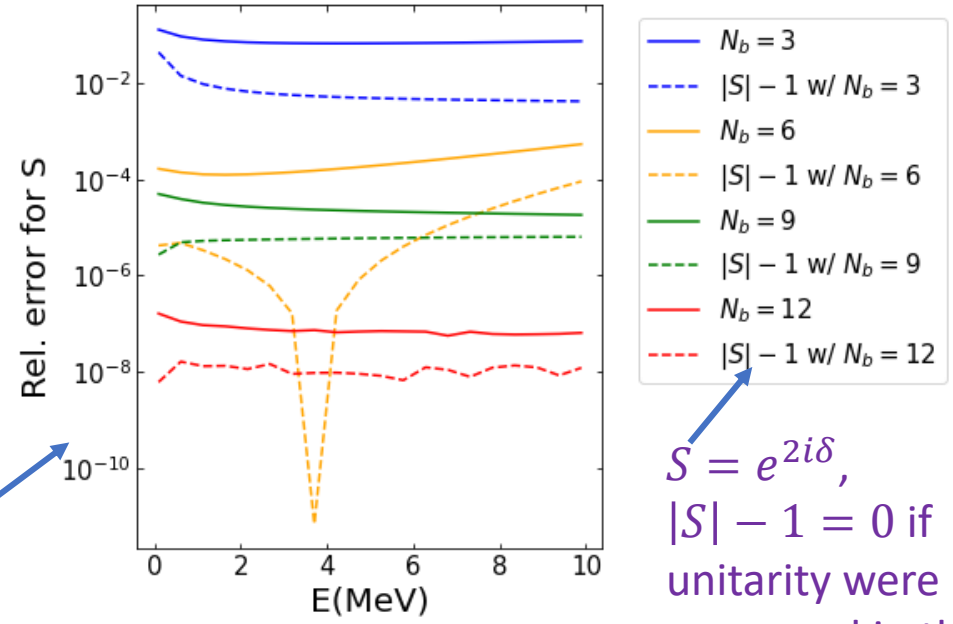
Vary 3-body potential strength λ_4



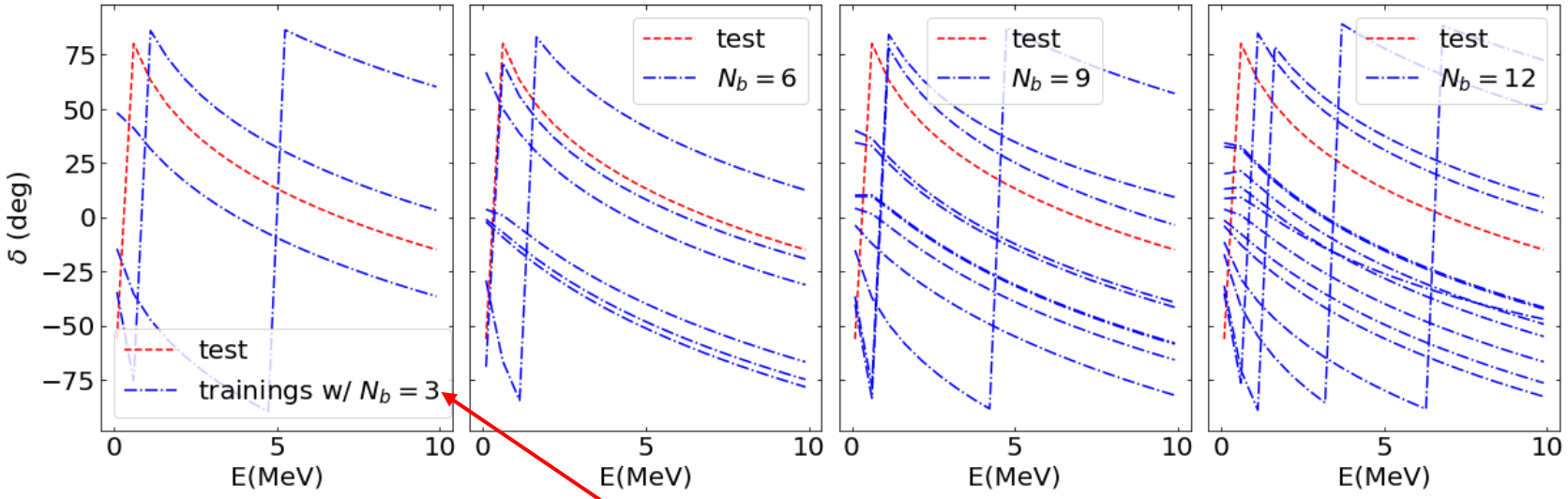
Vary both λ_4 and range Λ_4

Fix V_{2-body} ($\Lambda = 200$ MeV) to get dimer binding energy at 10 MeV

The emulator's relative errors using different training sets



$S = e^{2i\delta}$, $|S| - 1 = 0$ if unitarity were preserved in the emulators

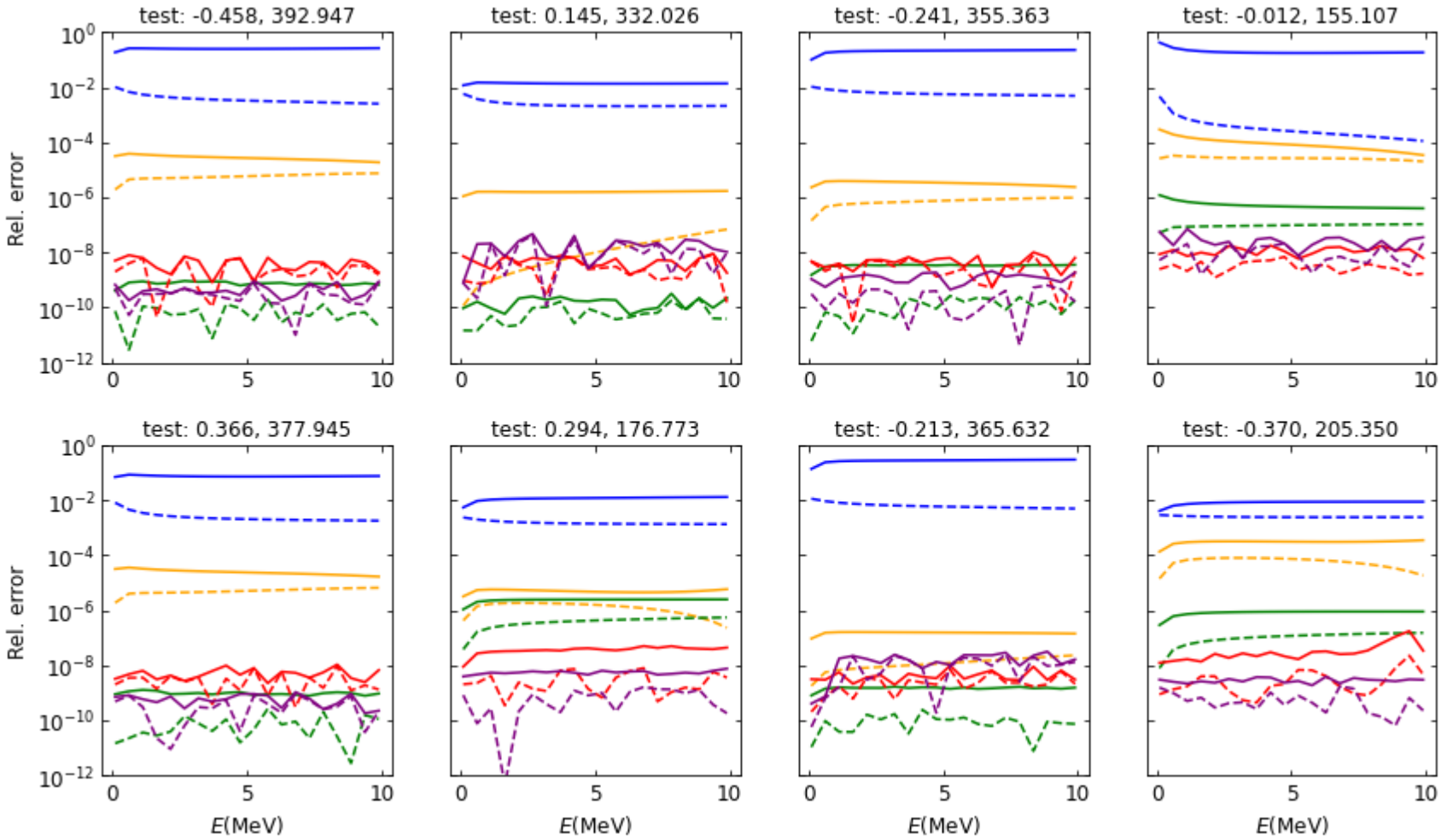


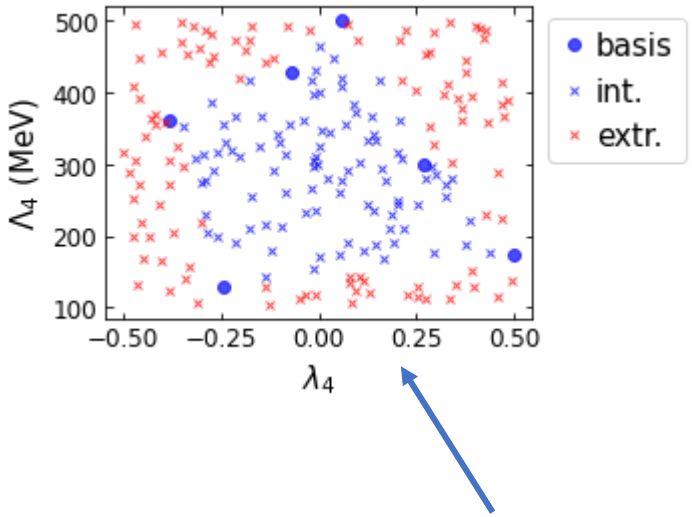
The number of training points is N_b.

Phase shifts of one test point and a series of sets of training points (picked using Latin Hypercube sampling)

Vary both λ_4 and range Λ_4

Relative errors at more test points



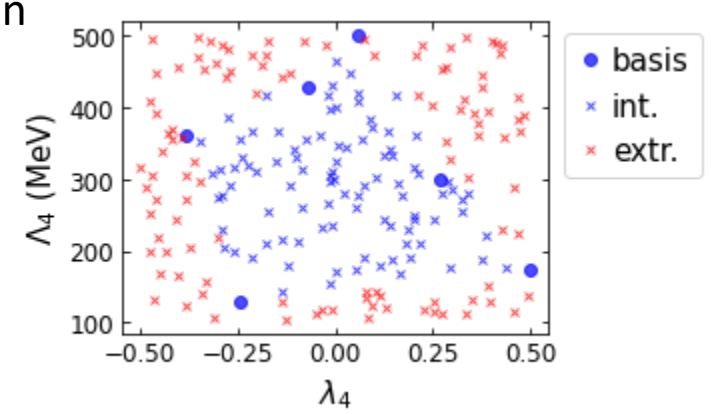


- The blue dots: one training-point set
- Crosses are test points

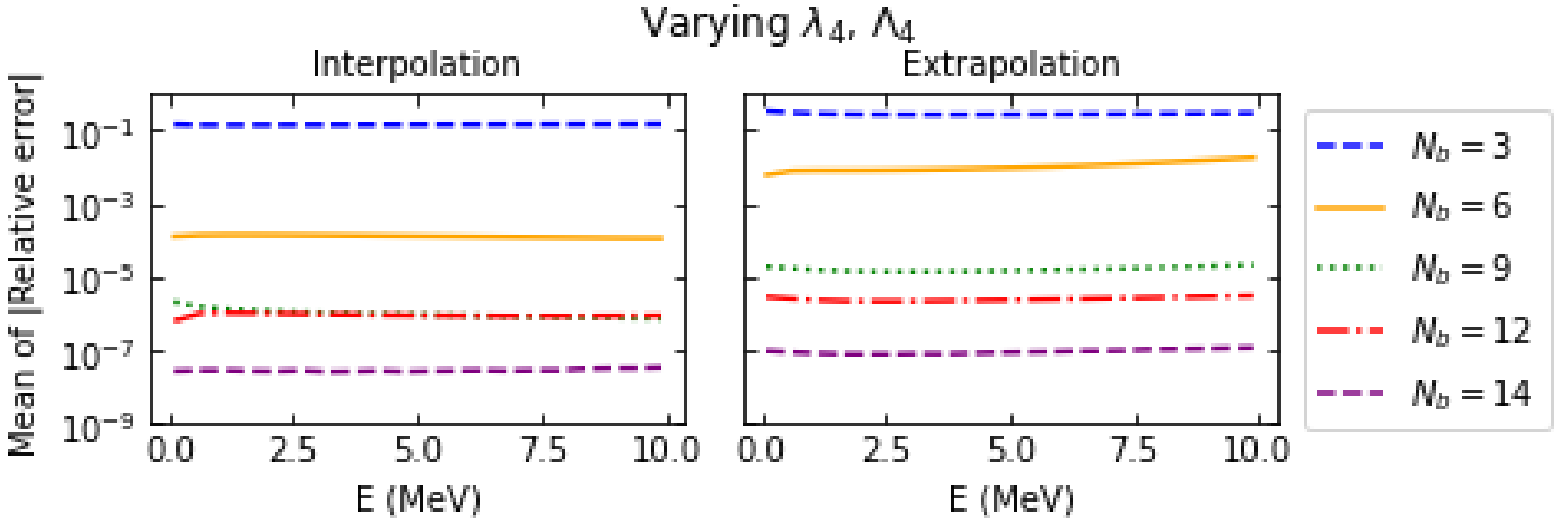
With $N_b = 6$, the relative errors become 10^{-4} at most

Accuracy

blue crosses: interpolation
red ones: extrapolations

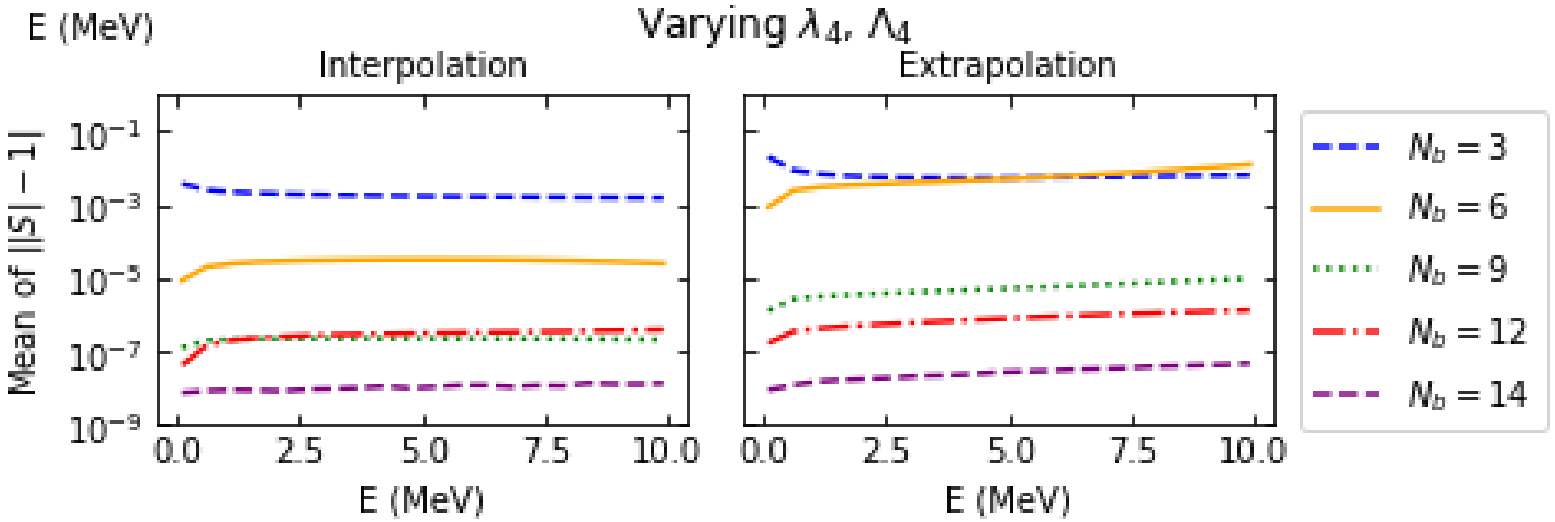


Randomly sample 200 test points



$|S| - 1$ (emulator's violation of unitarity) gives a conservative estimate of the emulators' errors

Larger errors for the extrapolation points due to a few test points with large errors at $\Lambda_4 \approx 100$ MeV



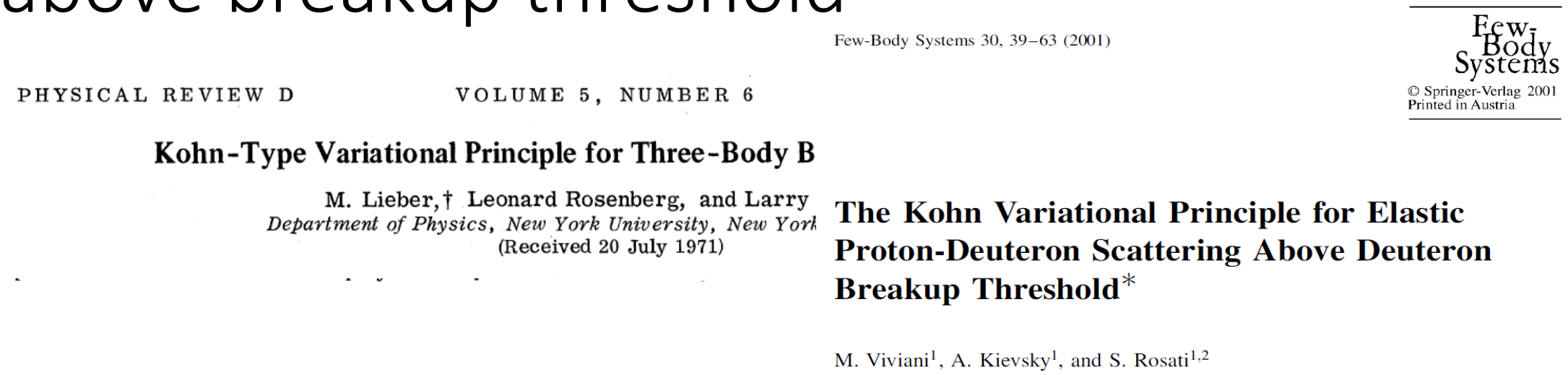
Efficiency

	Full calculation	EC-emulator
Computing time (in seconds) per scattering energy on a laptop	3 (10^3 for realistic calculations)	0.01 (10^{-3} for N_b-dim linear algebra)

- Simplified full calculations
- Typical cost of a realistic calculation: **hours**
- The emulator cost is from computing ΔU (the N_b-dim linear algebra cost is much smaller)
- If only varying λ_4, ΔU cost is eliminated. The emulator cost (the linear algebra) is 10^{-3} s (on a laptop). **This low cost applies to realistic calculations.**
- The above scenario → fitting Chiral three-nucleon interactions to proton-deuteron scattering data
- In general, the potential's parametric dependence can be linearized to reduce the ΔU-cost. (exploring new ideas)

Generalization to varying two-body interactions

Generalization to three-body scattering: above breakup threshold



PHYSICAL REVIEW D VOLUME 5, NUMBER 6

Kohn-Type Variational Principle for Three-Body B

M. Lieber,† Leonard Rosenberg, and Larry
Department of Physics, New York University, New York
(Received 20 July 1971)

Few-Body Systems 30, 39–63 (2001)

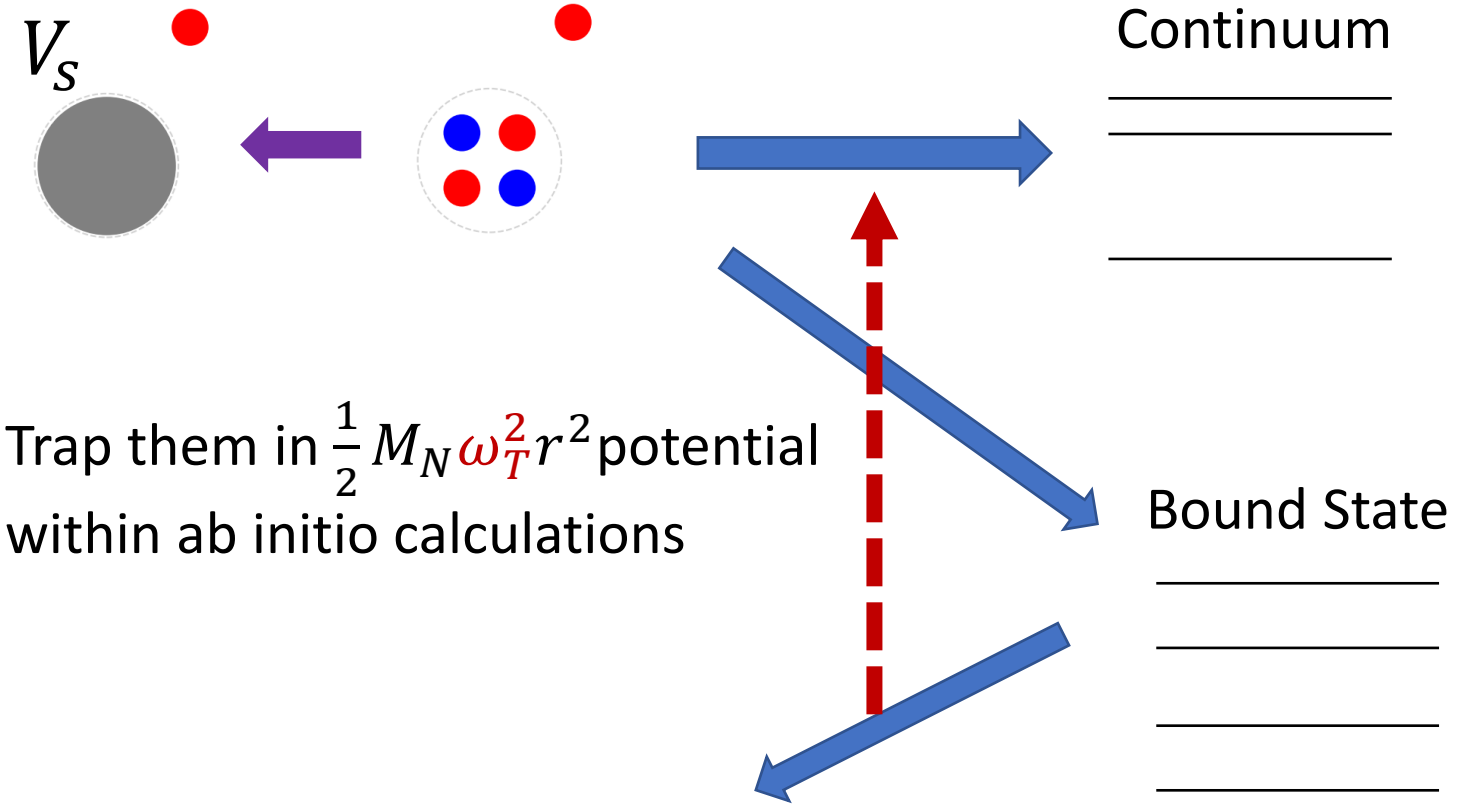
Few-Body Systems

The Kohn Variational Principle for Elastic Proton-Deuteron Scattering Above Deuteron Breakup Threshold*

M. Viviani[1], A. Kievsky[1], and S. Rosati[1,2]

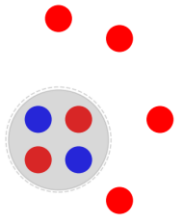
Generalization for fitting 3-N interaction to Lattice QCD calculations

Ab initio scattering/reaction calculations based on computer experiment



Trap them in $\frac{1}{2} M_N \omega_T^2 r^2$ potential within ab initio calculations

Constrain EFT (or model on V_s)
→ compute scattering and reaction



For two-body scattering:
XZ, PRC.101.051602(R) (2020) [1905.05275]; XZ et.al., PRL 125, 112503 (2020) [2004.13575]

How about ^{13}C + n **?**

- Parallel studies in LQCD generalizing the Luscher method to 3-hadron (more analytical understanding)
- Computer experiment strategy (Faddeev + **data analysis tools** for 3-cluster) → V_{cn}, V_{cnn}
- Emulators for higher body-solvers, e.g., Gamow-shell model calculations

Summary and outlook

- EC emulators for the three-body scatterings are accurate and efficient
- Currently working on the emulators with varying V_{2-body}
- Reducing the cost of computing ΔU when the potential's parametric dependence is nonlinear
- Generalizations to reactions above the break-up threshold
- Implementations with realistic three-body calculations (both NN and nuclear calculations)
- Connection to discrete-spectrum calculations