Eigenvector Continuation Emulators for Chiral EFT

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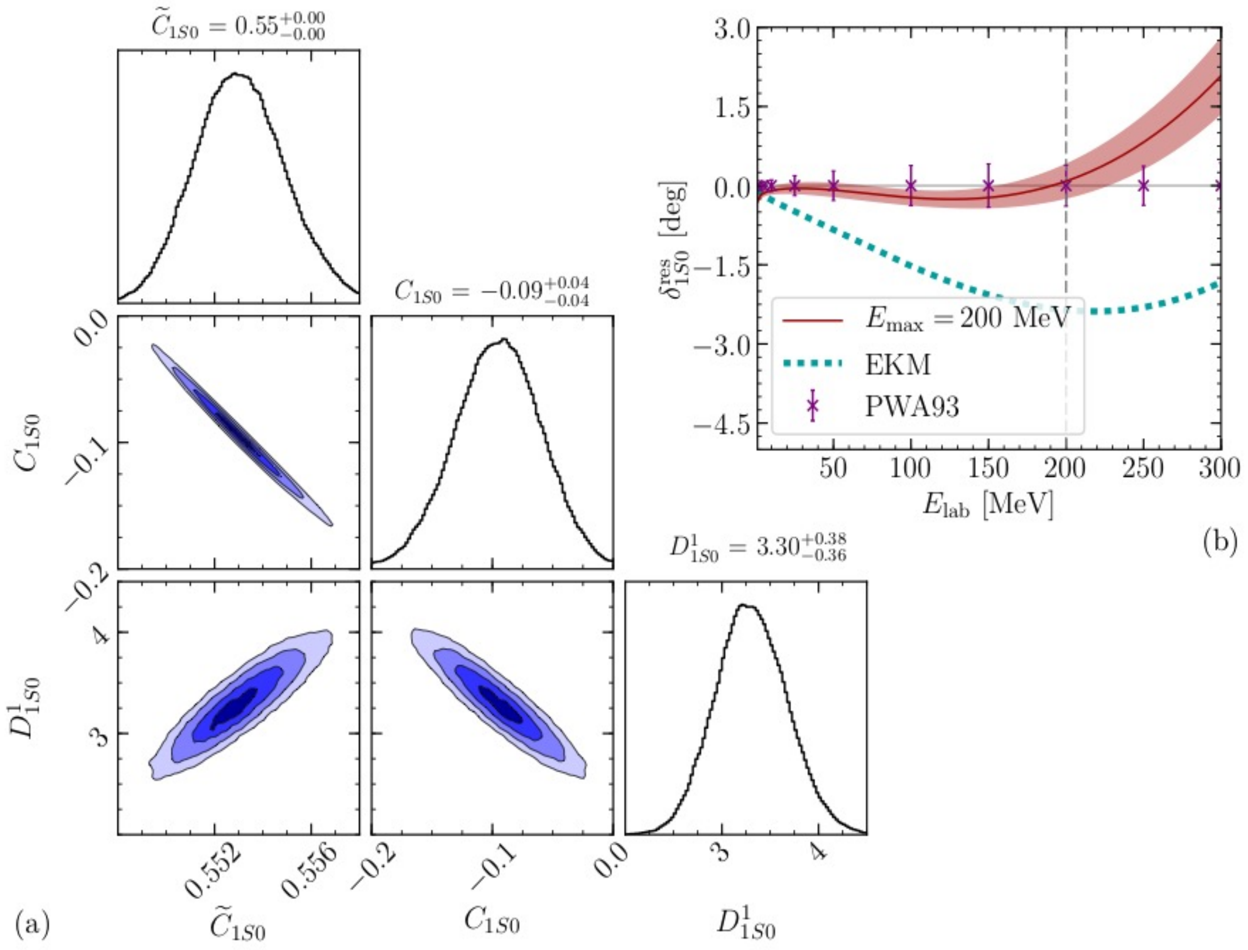
J.A. Melendez, C. Drischler, ajg, R.J. Furnstahl, and Xilin Zhang,
arXiv: 2106.15608 , Phys. Lett. B 821, 136608 (2021)

Phase shifts for nucleon-nucleon (NN) scattering with UQ

- Full sampling for Bayesian UQ can be expensive using direct calculations

- Alternative: sample from a previously trained computer model

- <u>Linear</u> parameter dependence in χEFT allows for fast calculations



Wesolowski et al., J. Phys. G 46, 045102 (2019)

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Chiral EFT potentials for NN scattering

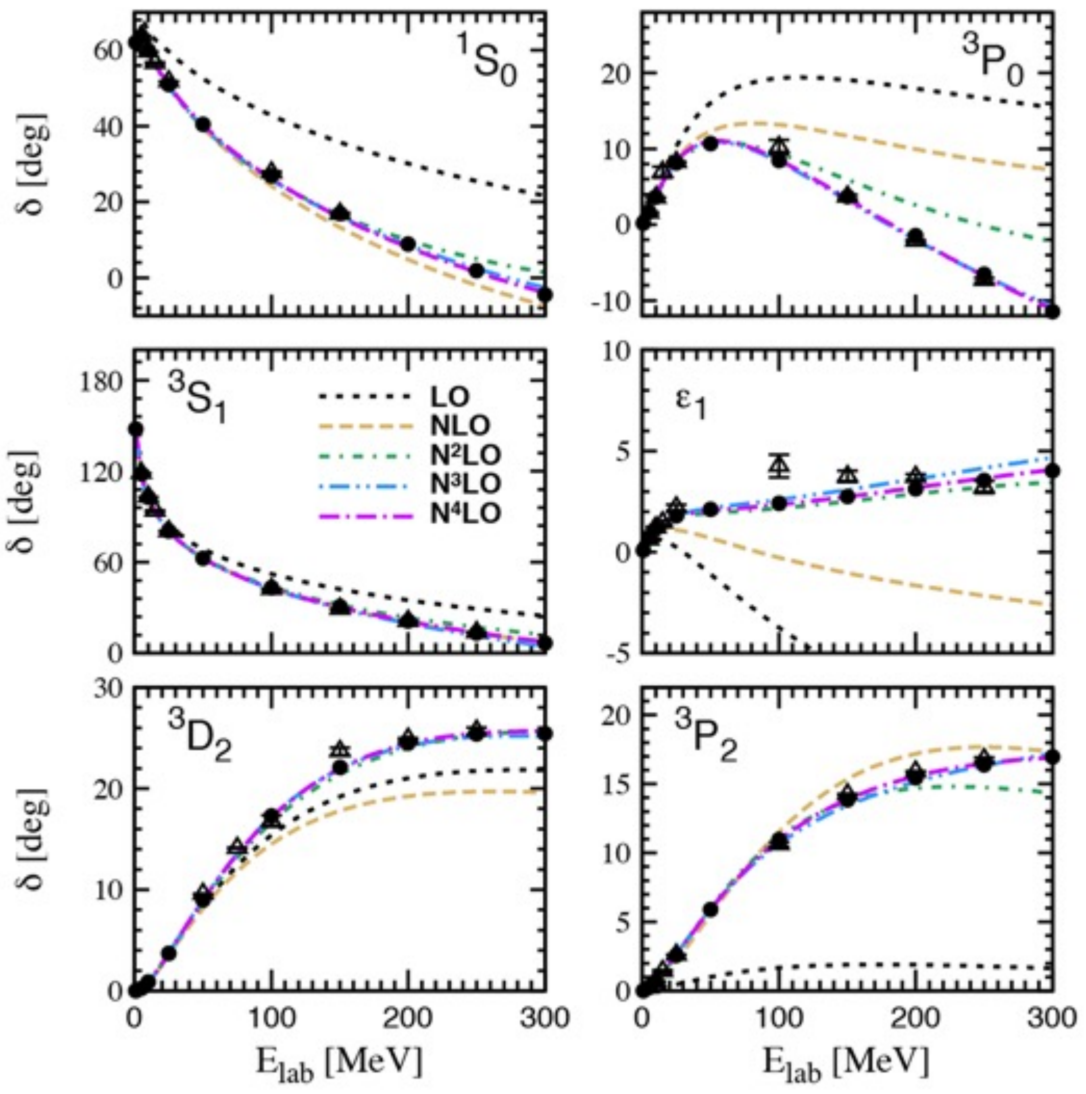
P. Reinert et al., Eur. Phys. J B 54, 86 (2018)

- Here: SMS semi-local momentum-space regularized potential
- Candidate for full Bayesian UQ using emulators
- Can take advantage of linearity between matrix elements and LECs:

$$V = \boxed{C_0} V^{(0)} + \boxed{C_2} V^{(2)} + \boxed{C_4} V^{(4)}$$

→ only calculate matrix elements once!

- Test emulators on neutron-proton *scattering* at cutoff $\Lambda = 450\, MeV$



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Emulating the Lippmann-Schwinger (LS) equation

LS equation: Sets of parameters: K-matrix formulation:

$$K(\vec{a}) = V(\vec{a}) + V(\vec{a})\, G_0(E_q)\, K(\vec{a}) \rightarrow \{\vec{a}_i\} \rightarrow K_\ell(E_q) = -\tan\delta_\ell(E_q)$$

$$E_q = q^2/2\mu$$

Newton variational principle (NVP):

$$\tilde{K}(\vec{\beta}) = \sum_{i=1}^{n_t} \beta_i K_i \longrightarrow \mathcal{K}[\tilde{K}] = V + VG_0\tilde{K} + \tilde{K}G_0V - \tilde{K}G_0\tilde{K} + \tilde{K}G_0VG_0\tilde{K}$$

$$\mathcal{K}[K_{\text{exact}} + \delta K] = K_{\text{exact}} + (\delta K)^2$$

Implementation:

$$\langle\phi'|\mathcal{K}(\vec{a},\vec{\beta})|\phi\rangle = \langle\phi'|V(\vec{a})|\phi\rangle + \vec{\beta}^T\vec{m}(\vec{a}) - \frac{1}{2}\vec{\beta}^T M(\vec{a})\vec{\beta}$$

J. A. Melendez et al., Phys. Lett. B 821, 136608 (2021)

$$\frac{d\mathcal{K}}{d\vec{\beta}} = 0 \rightarrow \langle\phi'|\mathcal{K}(\vec{a},\vec{\beta})|\phi\rangle \approx \langle\phi'|V(\vec{a})|\phi\rangle + \frac{1}{2}\vec{m}^T M^{-1}(\vec{a})\,\vec{m}$$

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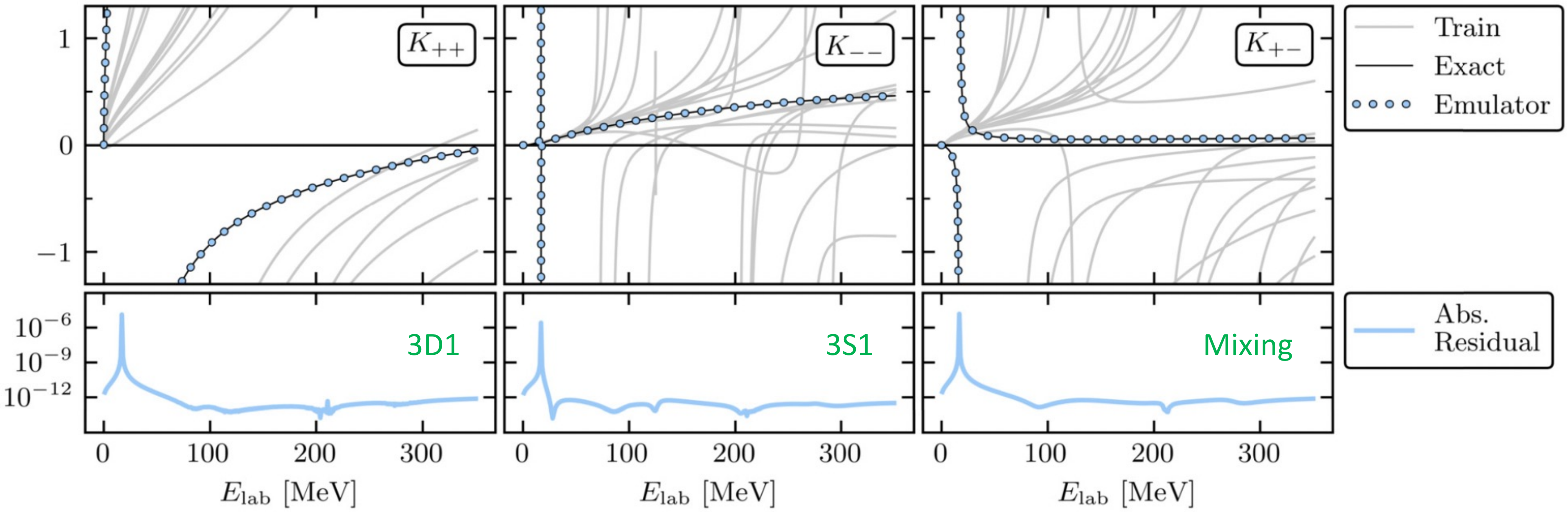
NVP emulation: SMS chiral potential

- Emulation of 3S1-3D1 coupled channel
- Basis size of 12 at $\mathrm{N^4LO+}$

Dealing with anomalies/singularities: C. Drischler et al., arXiv: 2108.08269 (2021)



J. A. Melendez et al., Phys. Lett. B 821, 136608 (2021)

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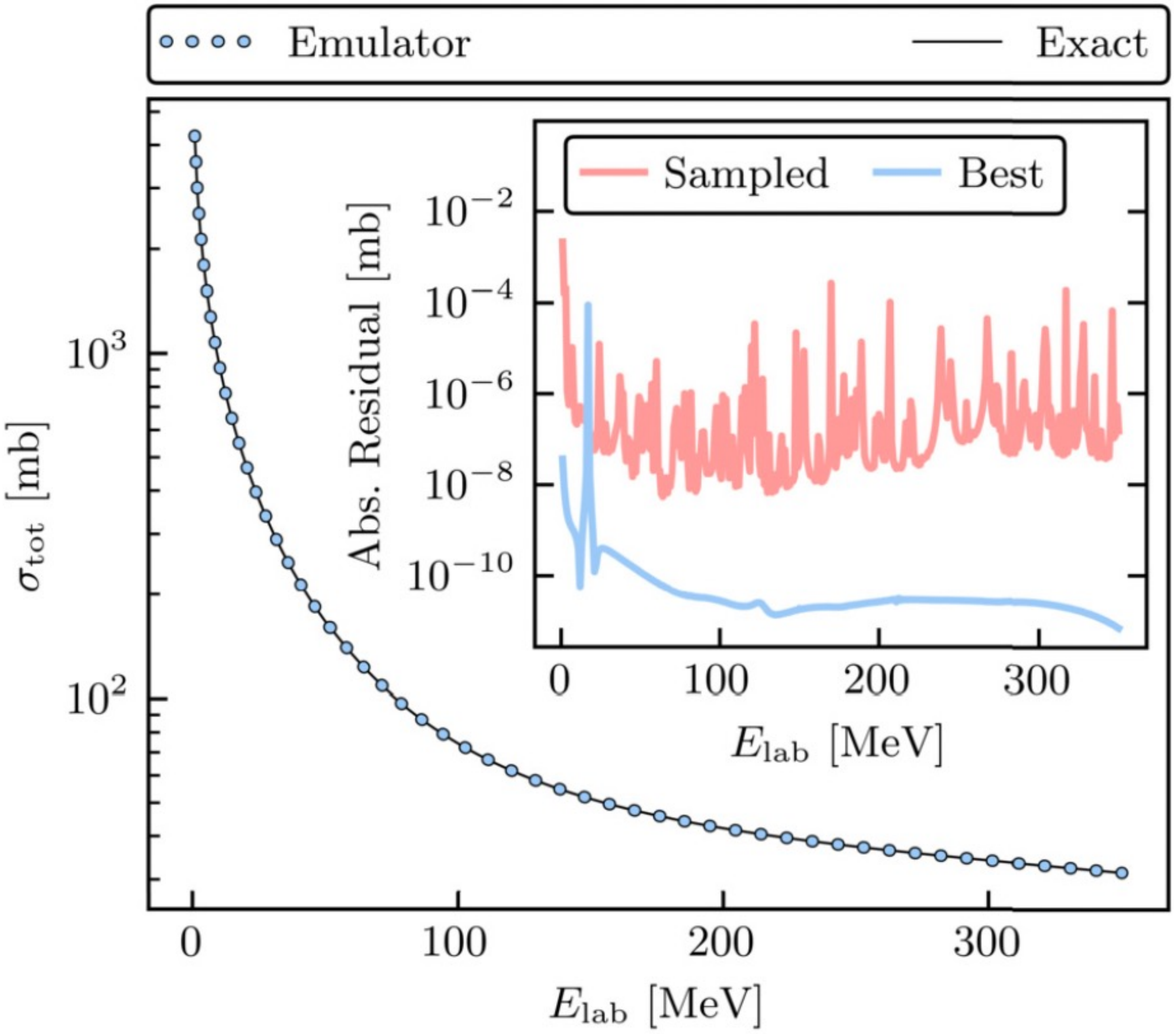
NVP emulation: SMS chiral potential

- Observable: Total cross section for partial waves up to $j = 20$
- Sampling: randomly chose values in an interval of [-5, 5]
- Errors: consistent for cutoffs $\Lambda = 400 - 550\,\mathrm{MeV}$
- **<u>Negligible</u>** compared to other uncertainties
- Timing: Speed up of > 300x compared to exact calculation
- >1000x if mesh size is doubled



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Eigenvector continuation (EC) for scattering

Hamiltonian:

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

Sets of parameters:

$$\{(\boldsymbol{\theta})_i\}$$

K-matrix formulation:

$$\mathcal{K}_\ell(E) = \tan\delta_\ell(E)$$

Kohn variational principle (KVP):

S-wave: $\ell = 0$

$p \equiv \sqrt{2\mu E}$

R. J. Furnstahl et al., Phys. Lett. B 809, 135719 (2020)

$$|\psi_{trial}\rangle \xrightarrow[r\to\infty]{} \frac{1}{p}\sin(pr) + \frac{[\mathcal{K}_0(E)]_{trial}}{p}\cos(pr)$$

$$\delta\beta\big[|\psi_{trial}\rangle\big] = \delta\left[\frac{[\mathcal{K}_0(E)]_{trial}}{p} - \frac{2\mu}{\hbar^2}\langle\psi_{trial}|\hat{H}(\boldsymbol{\theta}) - E|\psi_{trial}\rangle\right] = 0 \;\longrightarrow\; \beta\big[|\psi_{exact}\rangle\big] = \frac{[\mathcal{K}_0(E)]_{exact}}{p}$$

EC implementation:

$$|\psi_{trial}\rangle = \sum_{i=1}^{N_b} c_i|\psi_E(\boldsymbol{\theta}_i)\rangle \;\longrightarrow\; \sum_j \left(\Delta U^T + \Delta U\right)_{ij} c_j = \sum_j \Delta\tilde{U}_{ij}c_j = \frac{\mathcal{K}_0^{(i)}(E)}{p} - \lambda$$

$$\Delta U_{ij} \equiv \frac{2\mu}{\hbar^2}\iint dk\,dp\,\psi_E(p;\theta_i)\left[V(k,p;\theta) - V_j(k,p)\right]\psi_E(k;\theta_j)$$

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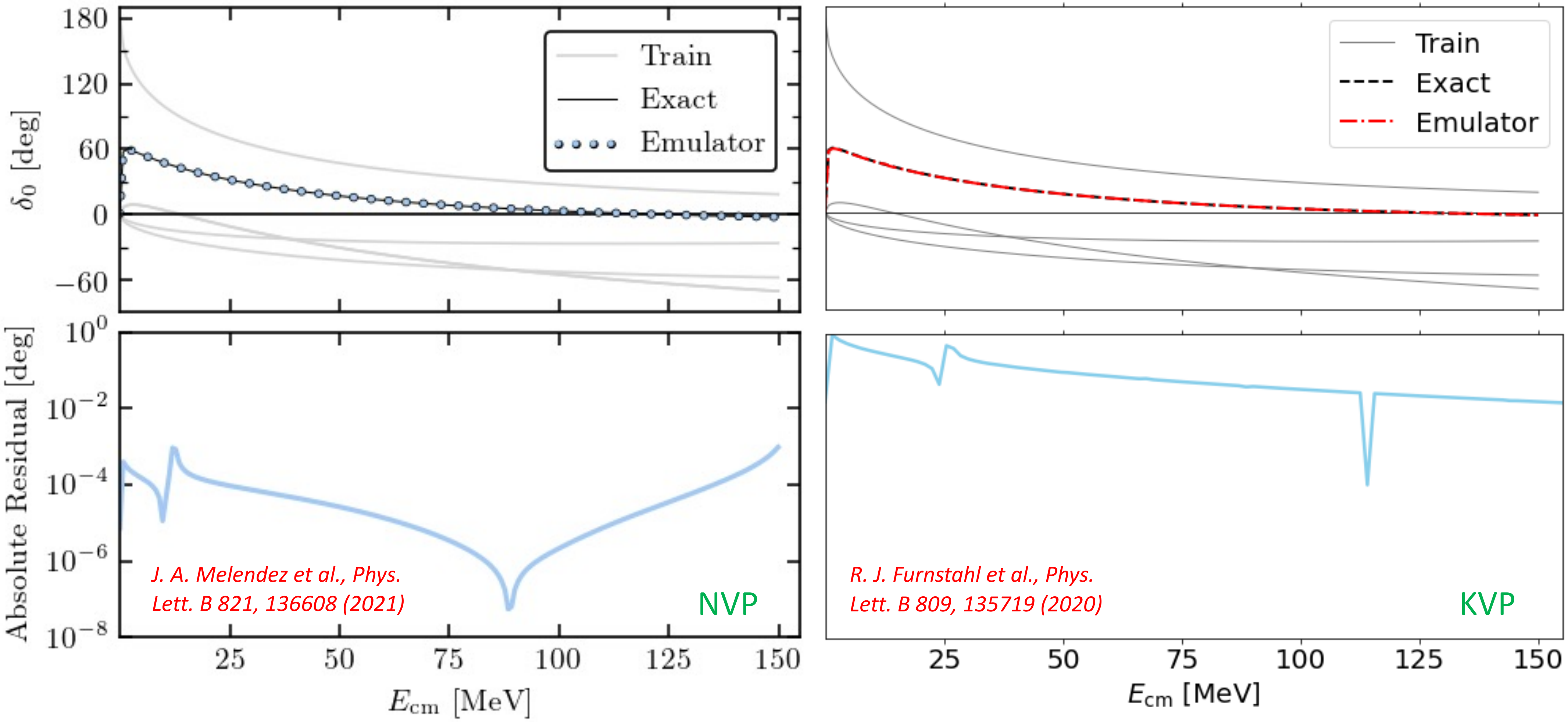
Comparing both methods: Minnesota potential

$$V(r) = V_{0R} e^{-\kappa_R r^2} + V_{0s} e^{-\kappa_s r^2}$$

$$V_{0R} = 200.0\,\text{MeV} \quad k_R = 1.487\,\text{fm}^{-2}$$
$$V_{0s} = -91.85\,\text{MeV} \quad k_s = 0.465\,\text{fm}^{-2}$$



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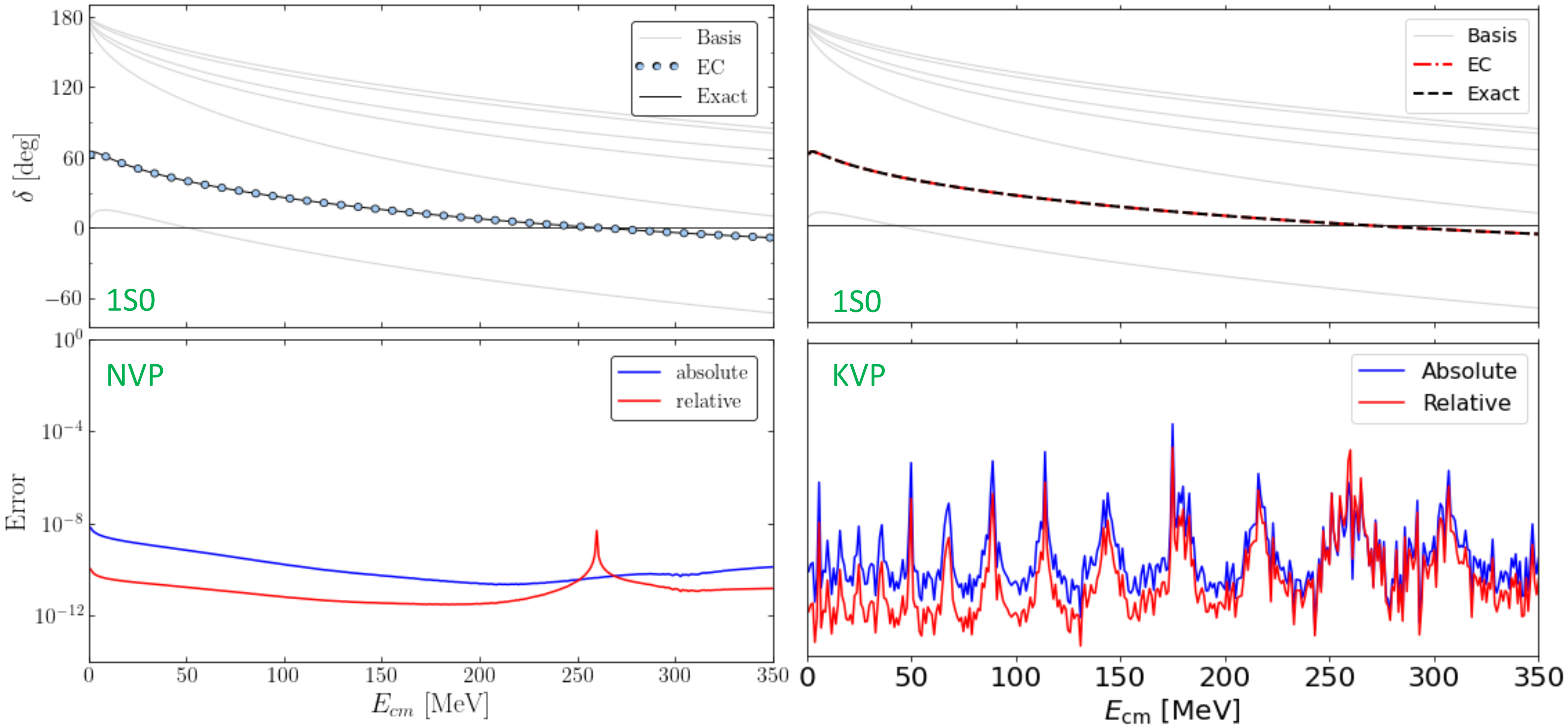
Comparing both methods: SMS chiral potential



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Summary

- NVP provides a general method of creating emulators for scattering
- Wave functions are not required for emulation of two-body scattering observables!
- Preliminary results show that NVP and KVP have similar accuracy

Ongoing work

- Understand sensitivity of LECs
- Compare NVP and KVP emulation of observables
- Compare timing between NVP and KVP
- EC applications to three-body scattering (Xilin Zhang)
- What else can be emulated?

Thank you!