Recent developments in the emulations of quantum continuum states

Xilin Zhang **(MSU/FRIB)**

LECM LOW ENERGY COMMUNITY MEETING
Low Energy Community Meeting 2022

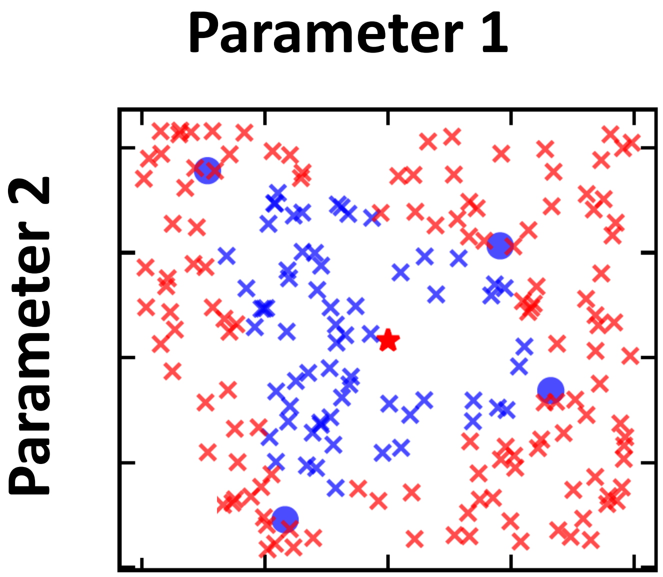
Argonne National Laboratory &
Online, August 2022

Outline

- Motivations
- Recent developments of continuum-state emulators
- My ongoing study on emulation in energy’s complex plane
- Summary and outlook

Motivations for reduced basis method/eigenvector continuation (RBM/EC) emulators

- Fast interpolations and extrapolations in theory parameter space (e.g., NN interactions)
- Rapid exploration of the parameter space
- Mediators between expensive calculations and users (potentially impact workflow)
- **In addition**, they enable continuum-state calculations using bound-state calculation methods



RBM/EC emulators for bound states

D. Frame, et.al.,, Phys.Rev.Lett. **121**, 032501 (2018)
S. König, et.al., Phys. Lett. B **810**, 135814 (2020)
A. Ekström and G. Hagen, Phys.Rev.Lett. **123** , 252501 (2019)

$$\mathcal{F}_{\boldsymbol{\theta}}[\psi_t] = \langle \psi_t | \widehat{H}(\boldsymbol{\theta}) | \psi_t \rangle$$

Variational method for estimating E_{gs}

$$\widehat{H}(\boldsymbol{\theta}_i) \;\rightarrow\; |\psi_{\mathrm{gs}}(\boldsymbol{\theta}_i)\rangle$$

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

Extremely efficient way to construct ψ_t

$$\delta\big[\mathcal{F}_{\boldsymbol{\theta}}[\psi_t] - \lambda(\langle \psi_t | \psi_t \rangle - 1)\big] = 0$$

N_b-dim linear algebra→ fast emulators

J.A. Melendez, C. Drischler, R.J. Furnstahl, A.J. Garcia, XZ, 2203.05528
Edgard Bonilla, Pablo Giuliani, Kyle Godbey, Dean Lee 2203.05284

EC ≈ RBM in the field of model reduction

Continuum-state emulators at a given energy

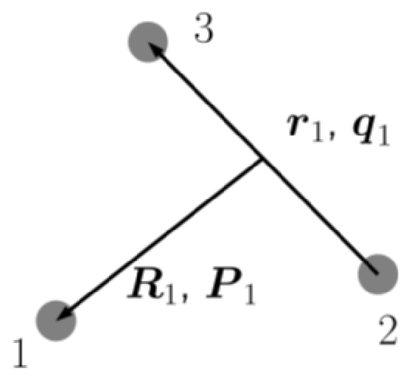
R. J. Furnstahl, A. J. Garcia, P. J. Millican, and XZ, PLB **809**, 135719 (2020) [2007.03635]

Combine the variational approach for two-body scattering with the EC concept

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

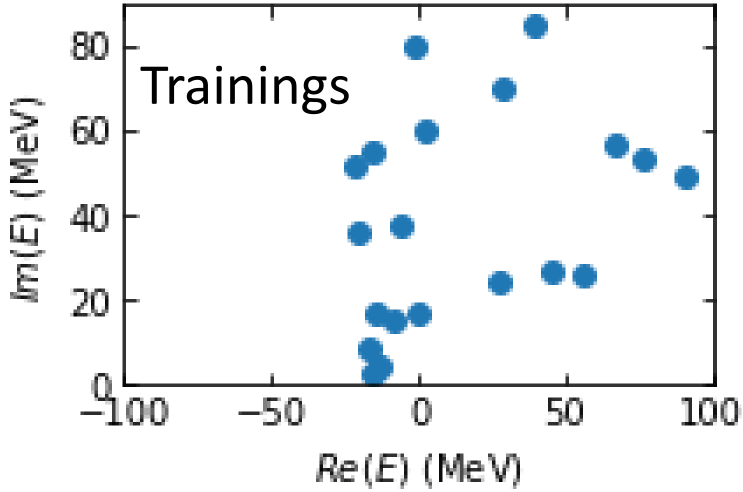
"Fast emulation of quantum three-body scattering",
XZ and R.J. Furnstahl, Phys. Rev. C 105, 064004 (2022), 2110.04269

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



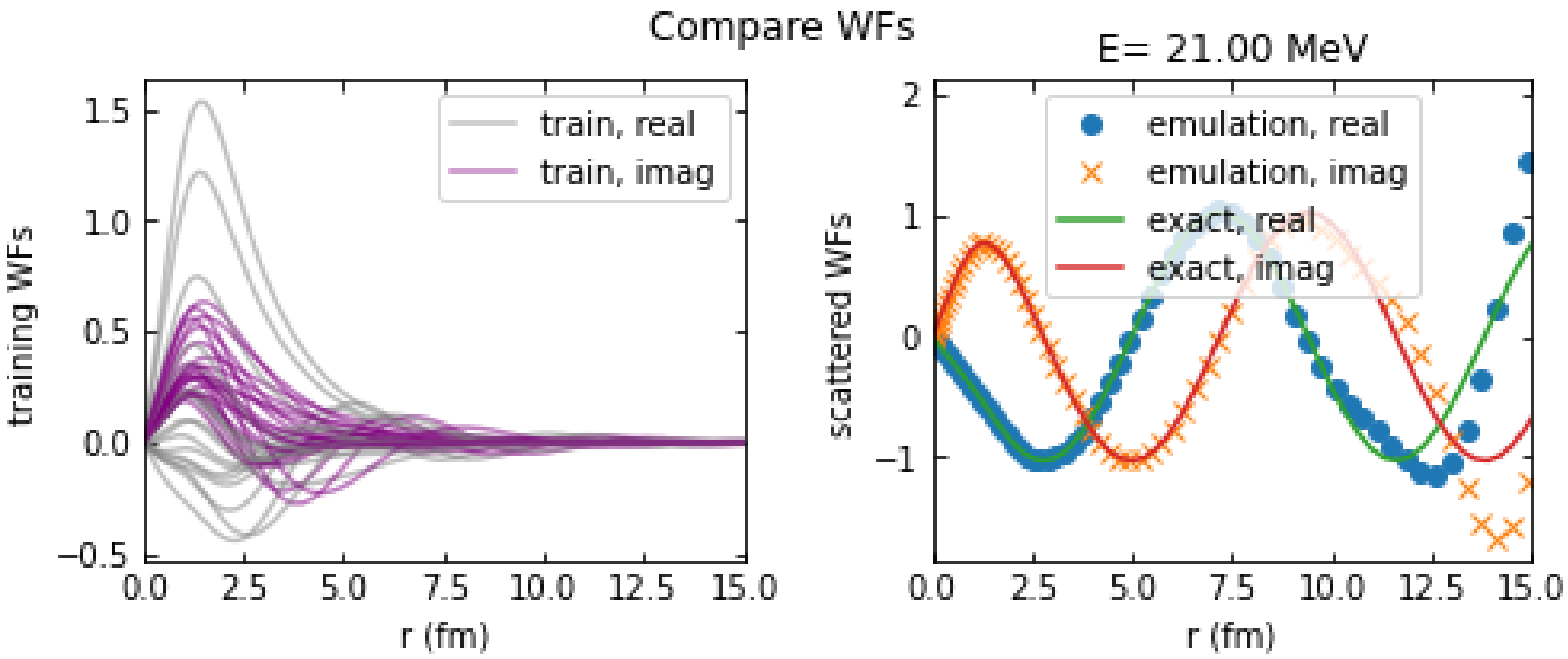
These studies require the same real energy for trainings and emulations.

Continuum-state emulators in energy's complex plane: two-body examples



- Emulate in E's complex plane
- Training wave functions (WFs) are localized

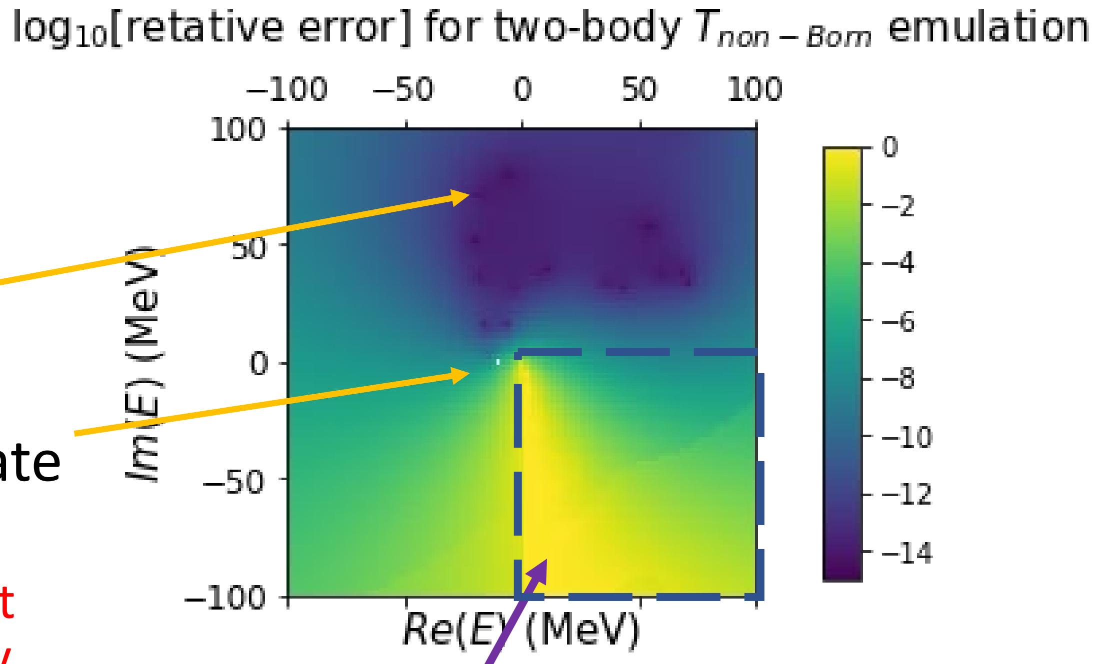
- Bound state methods for trainings
- Emulations → continuum
- Also allows emulations for other parameters



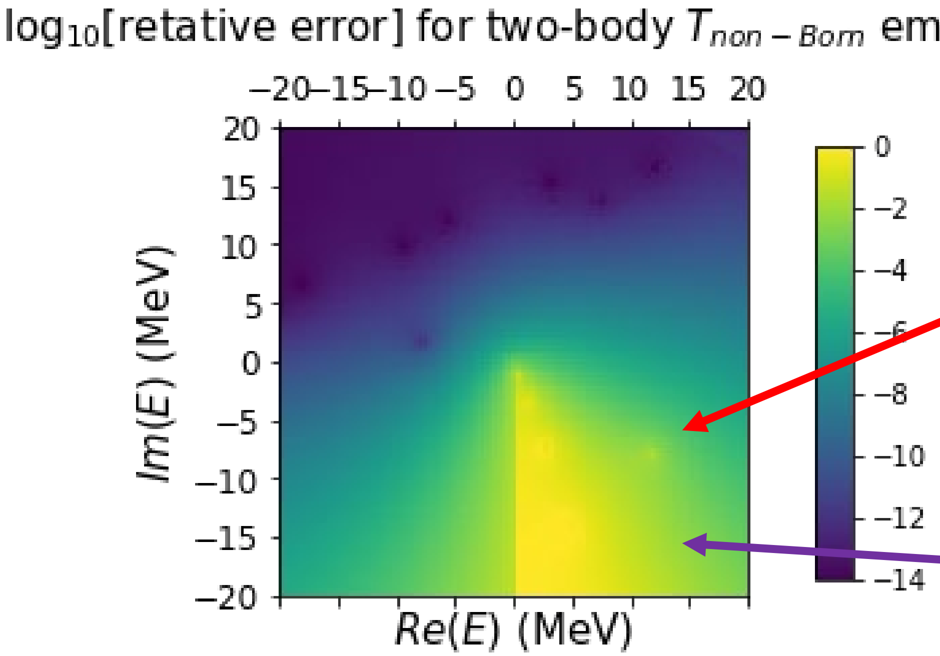
Continuum-state emulators in energy's complex plane: two-body examples

- Emulation → fast identifications of bound state and resonances

S-wave



P-wave



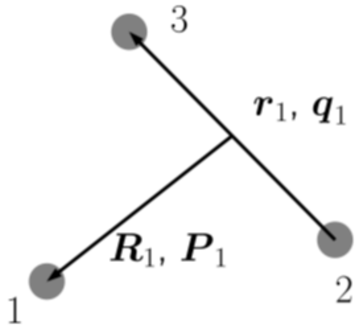
Trainings

Bound state

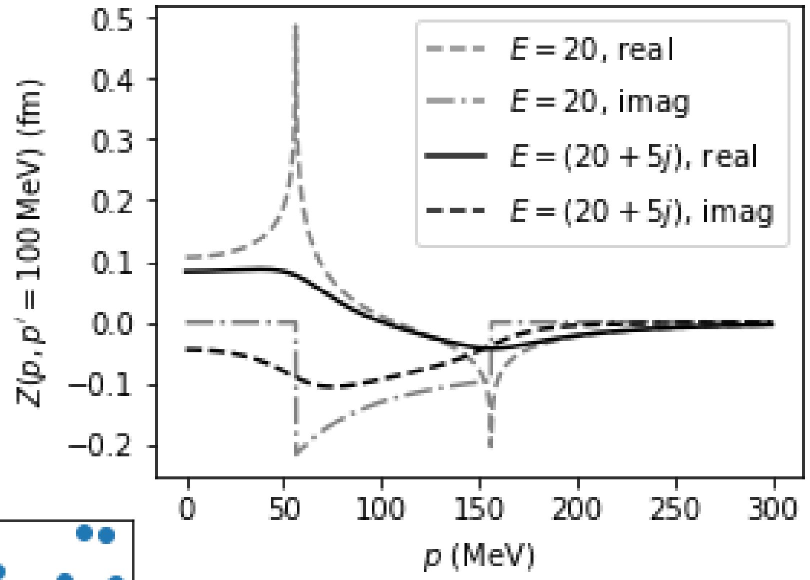
- Resonance at $12 - 8i$ MeV
- Emul. rel. error for the location is 10^{-4}

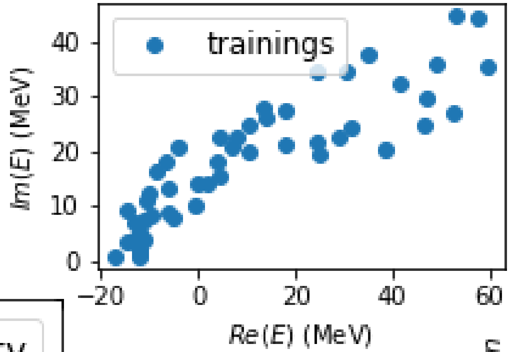
The 4^{th} quadrant is on the 2^{nd} Riemann sheet; others on the physical sheet

Three-boson scattering (preliminary results)

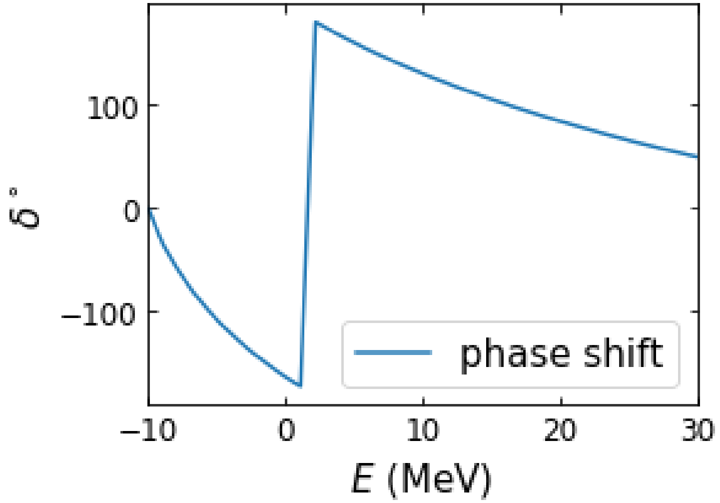


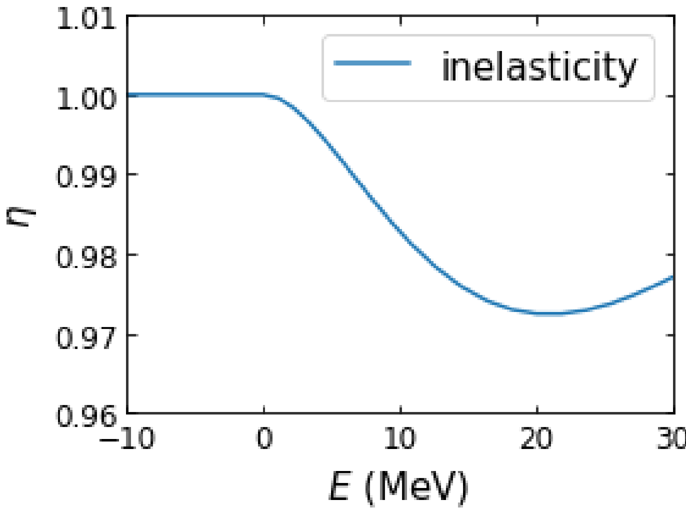
The challenge for direct continuum calculations:



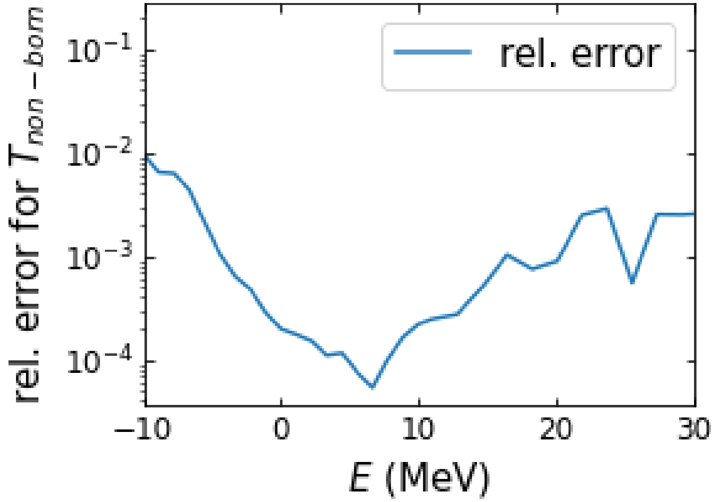


Full calculations:





Emulation errors



Summary and outlook

- RBM/EC is applicable for emulating continuum states in energy's complex plane **and** Hamiltonian parameter space
- Emulations enable continuum-state calculations based on bound-state calculation methods **and** parameter-space exploration
- Currently testing the idea for three-body break-up process; and for many-body continuum states (with Bijaya Acharya at ORNL)
- Also exploring emulations for hadronic-reaction modeling (with Satoshi Nakamura at USTC)