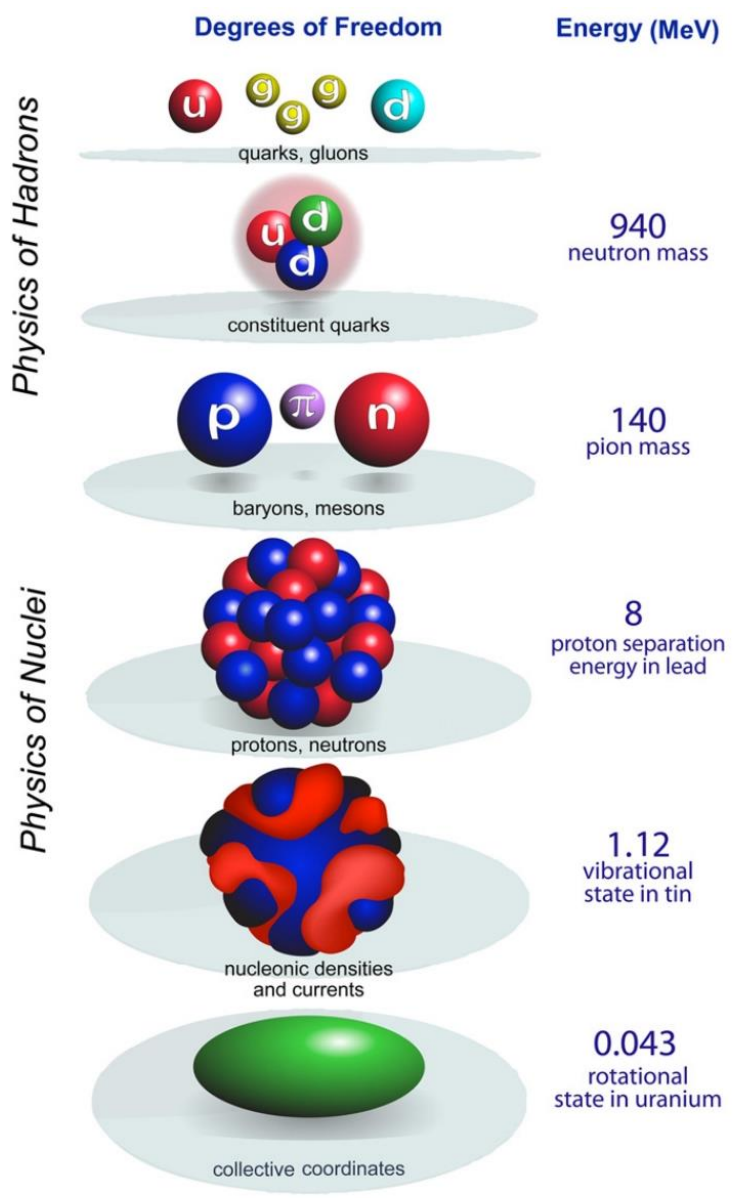
A novel method for extracting and emulating continuum physics of finite quantum systems

Xilin Zhang

Facility for Rare Isotope Beams

Michigan State University

Recent Progress in Many-Body Theories (RPMBT22), Kasuga Campus, University of Tsukuba, Japan, Sep. 2024



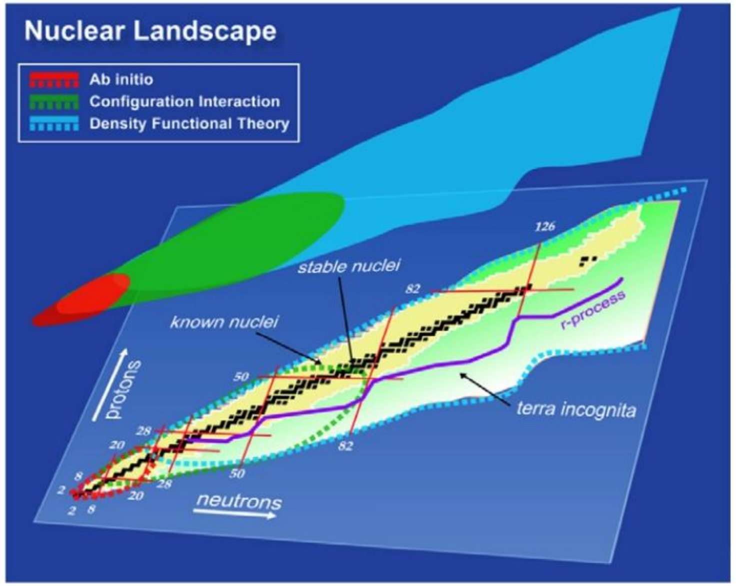
Low-energy nuclear theory

- Nucleons as basic degrees of freedom

- Interactions w/ complex structures and uncertainties

- Systematic expansion of the interactions

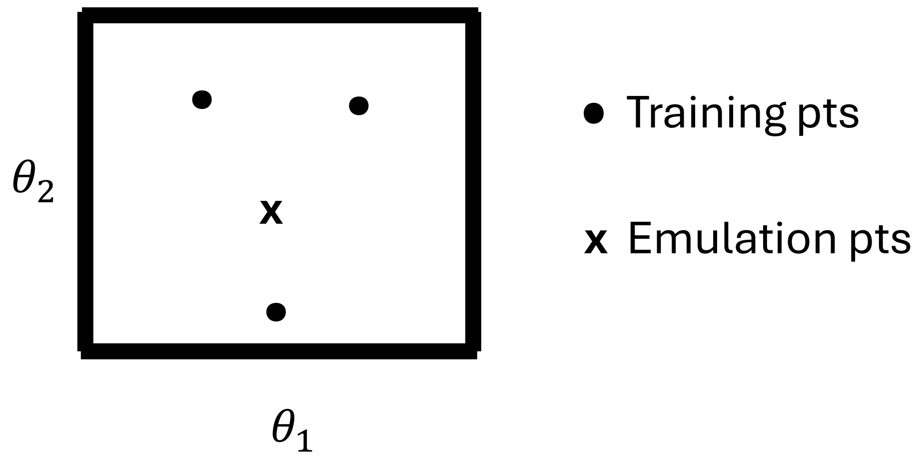
- Many-body calculations: discrete bound and continuum states (e.g., responses and scatterings)



From RJ Furnstahl and K Hebeler, Rep. Prog. Phys. 76 (2013) 126301

Two topics to be covered

- Fast interpolation of the expensive computations in the input parameter space
- Extracting the continuum physics from bound-state-like calculations



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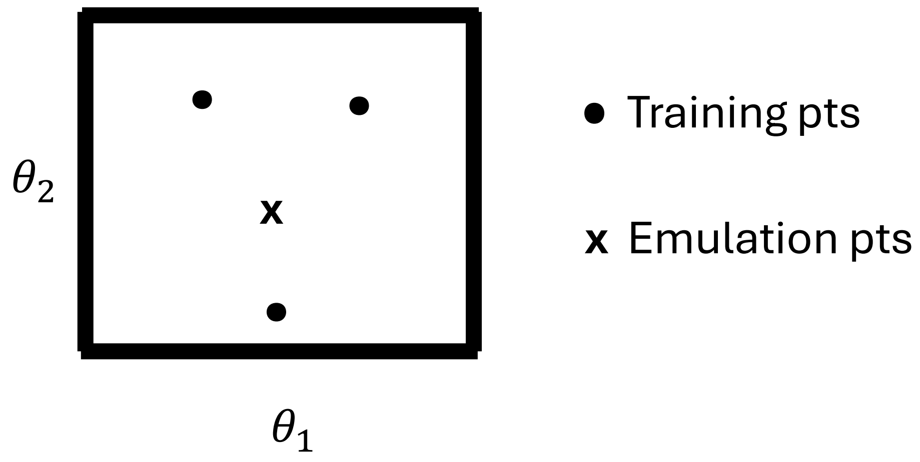
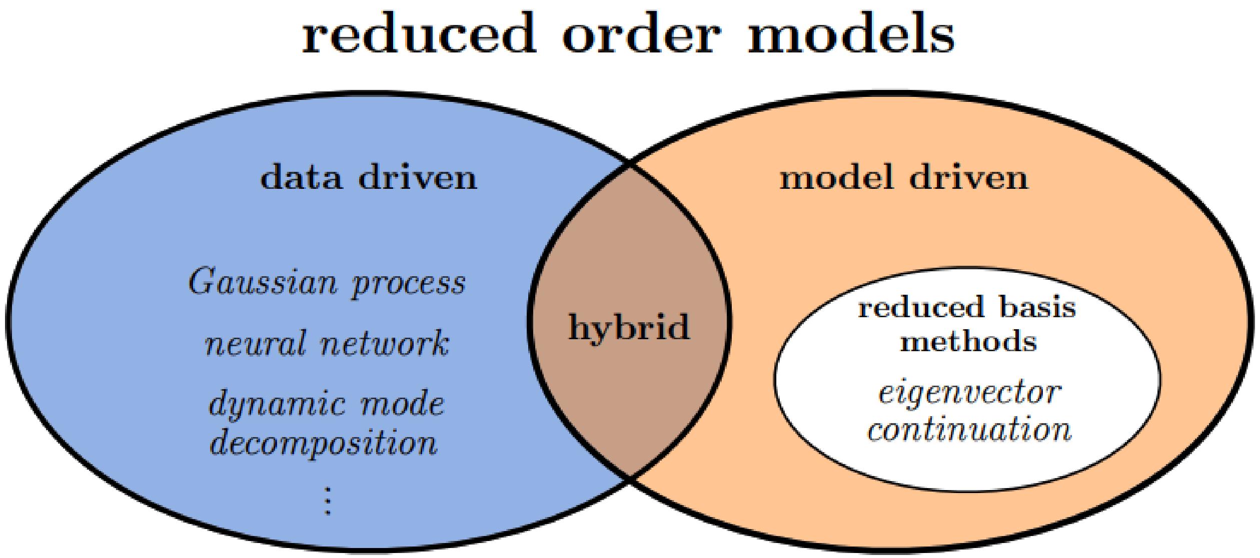


Mostly based on this recent paper:
A non-Hermitian quantum mechanics approach for extracting and emulating continuum physics based on bound-state-like calculations, **X.Z.** [2408.03309]

Outline

- Emulators in general
- Emulators in quantum physics
- Continuum states of finite quantum systems
    - Computational challenges
    - Complex-energy emulator as a solution
    - Emulation in input parameters
- Summary

Emulators: two main types and their hybrid



2310.19419

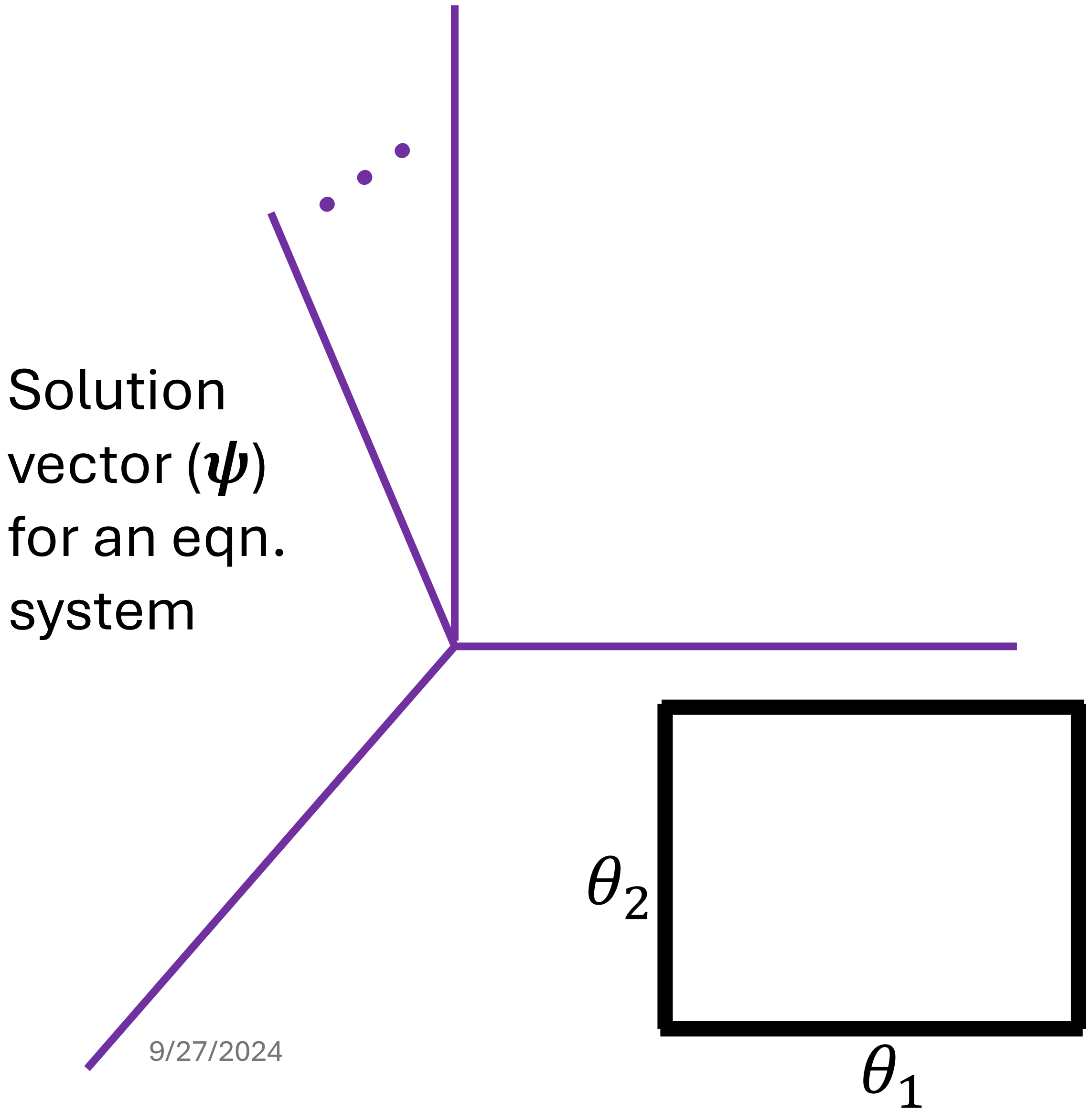
Colloquium: Eigenvector continuation and projection-based emulators

Thomas Duguet, Andreas Ekström, Richard J. Furnstahl, Sebastian König, and Dean Lee
Rev. Mod. Phys. **96**, 031002 – Published 14 August 2024

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

Model driven: Reduced basis method (RBM)



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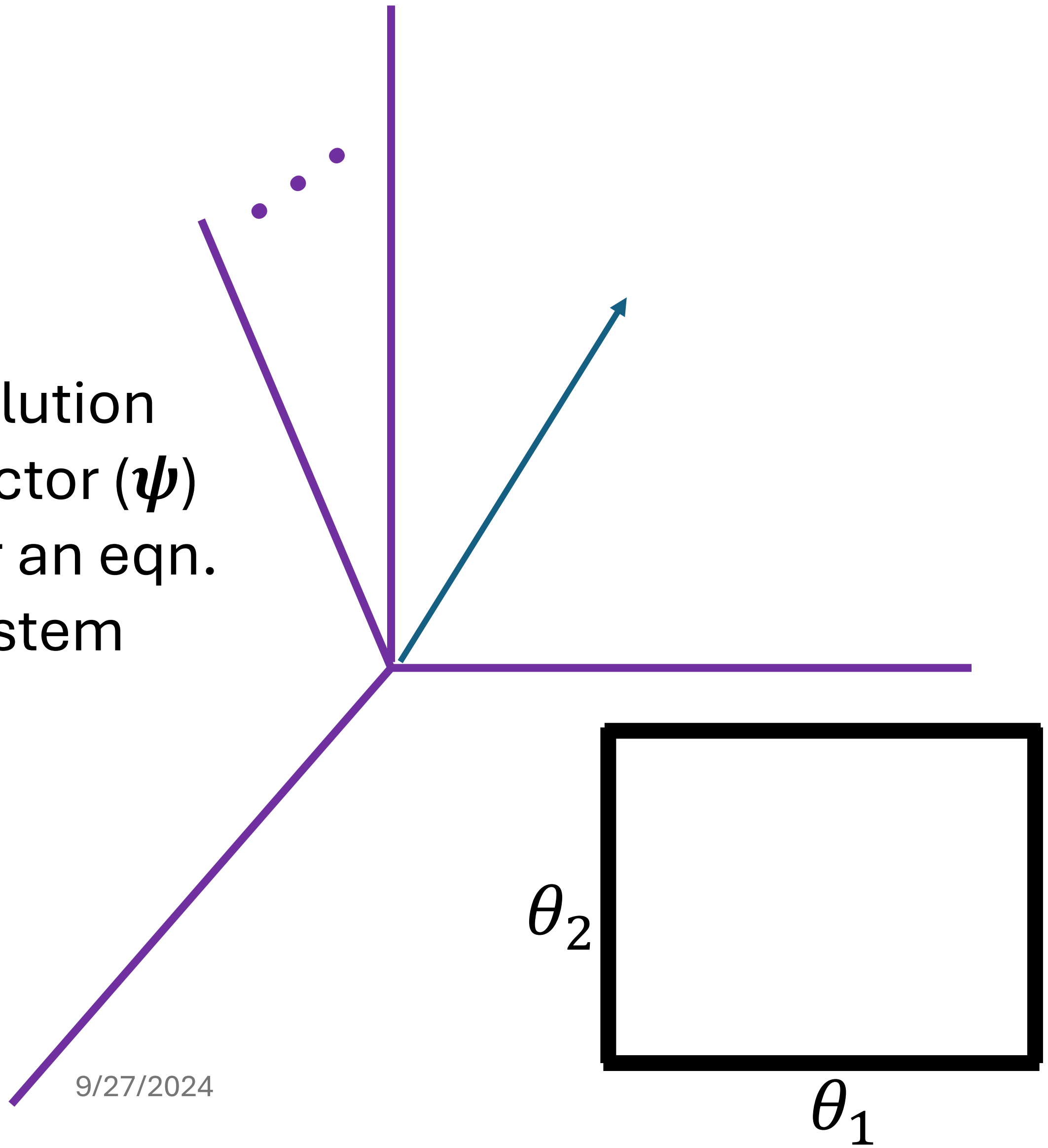
Solution vector ($\boldsymbol{\psi}$) for an eqn. system



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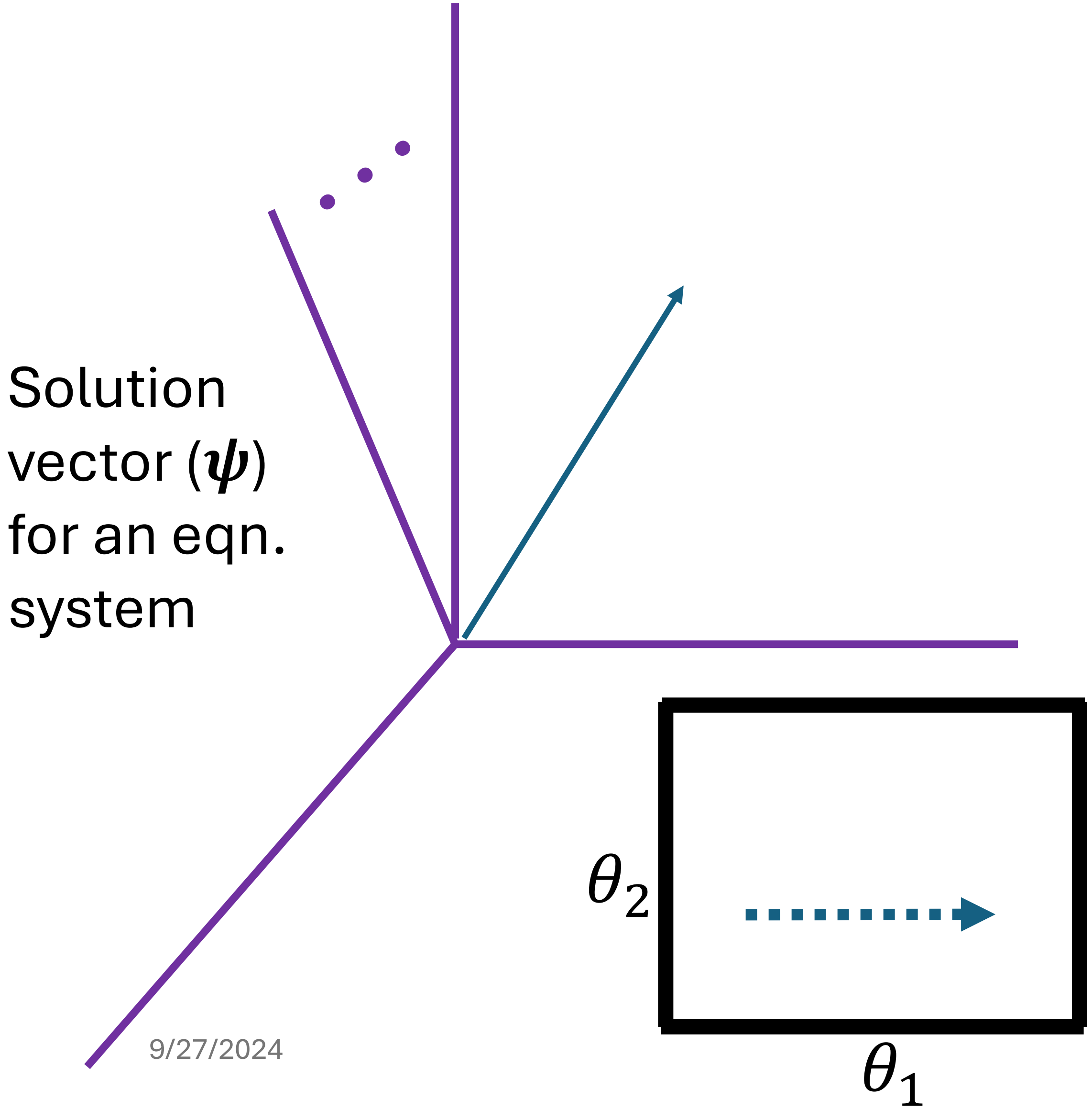

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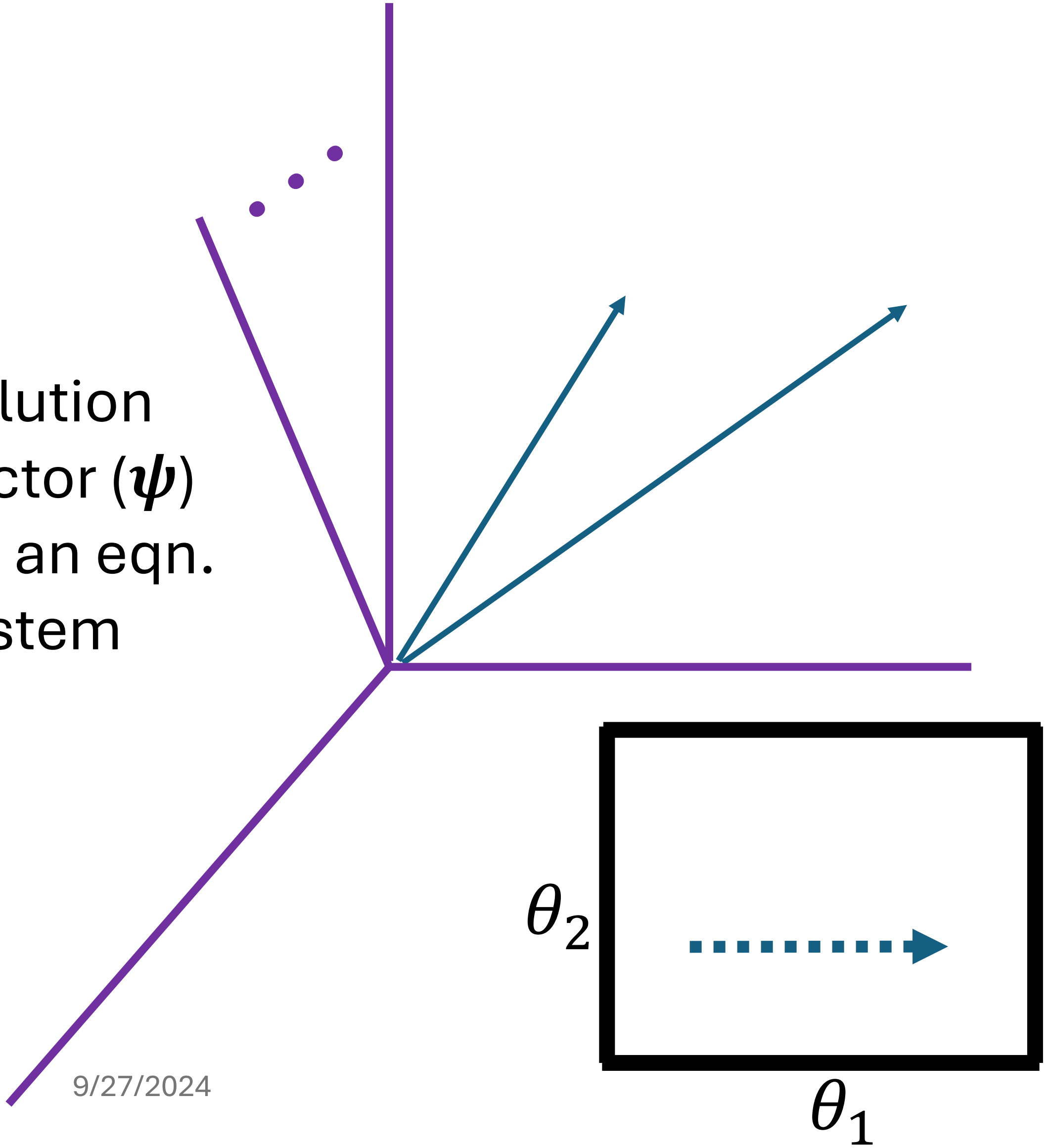

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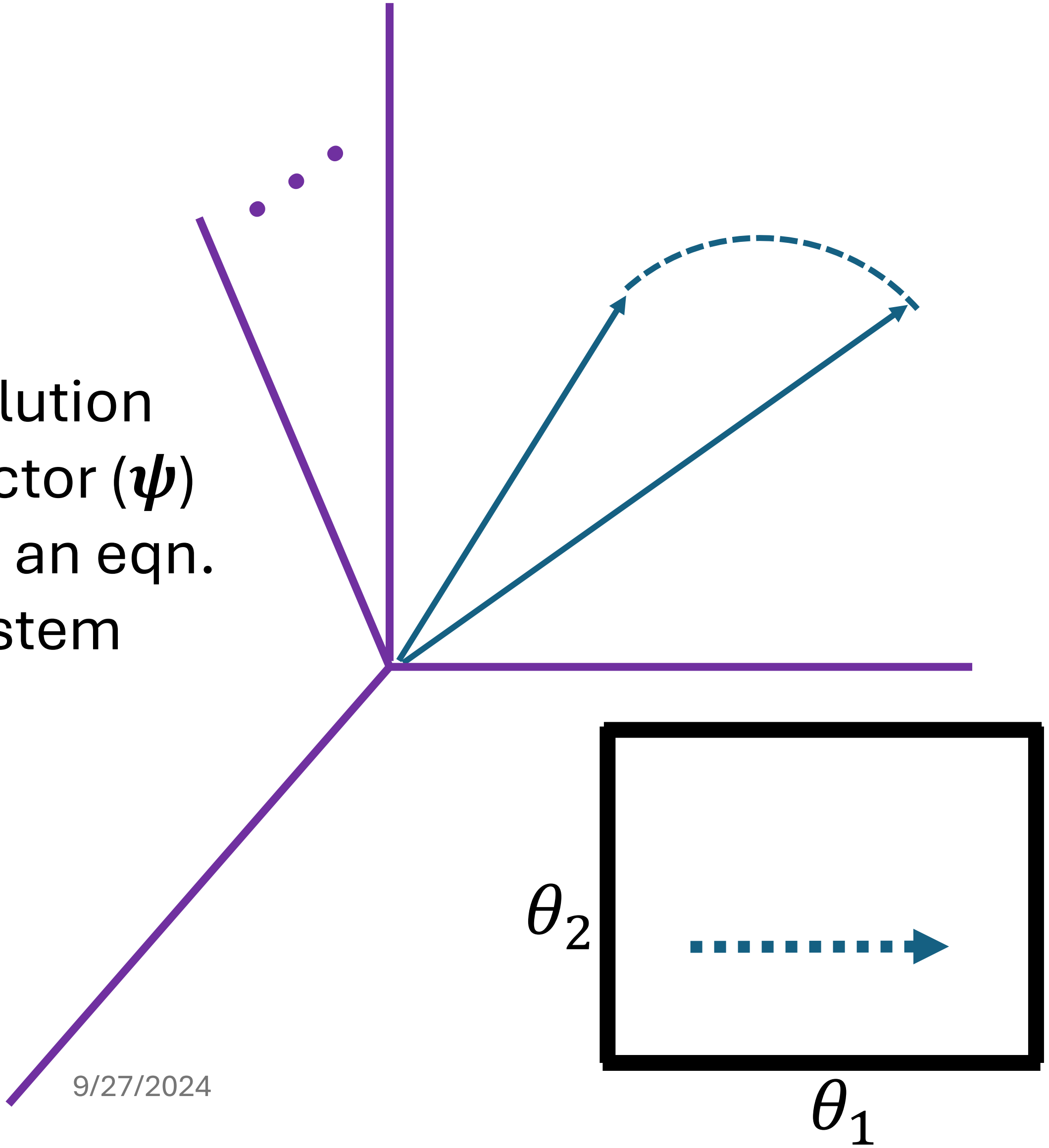

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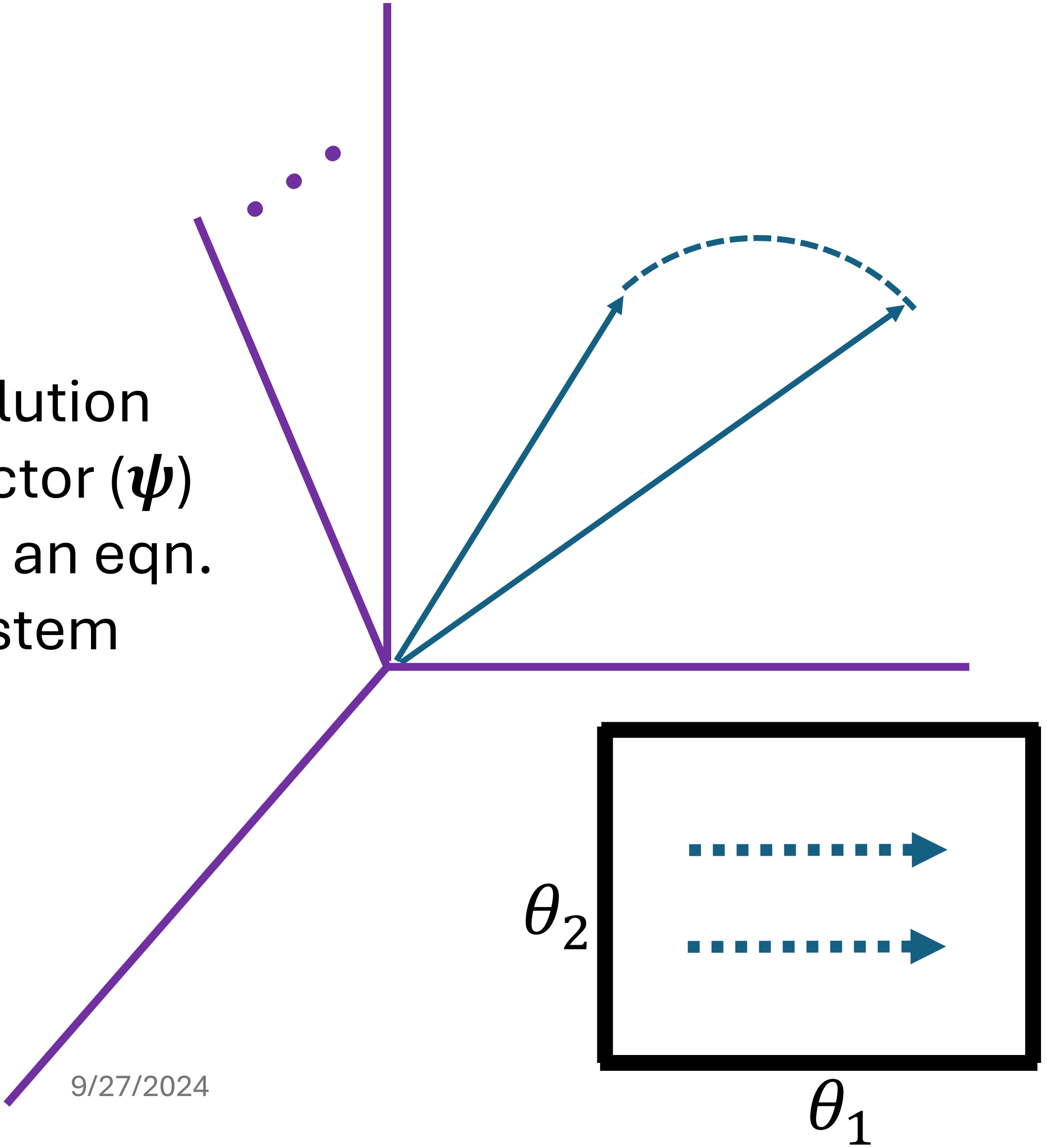

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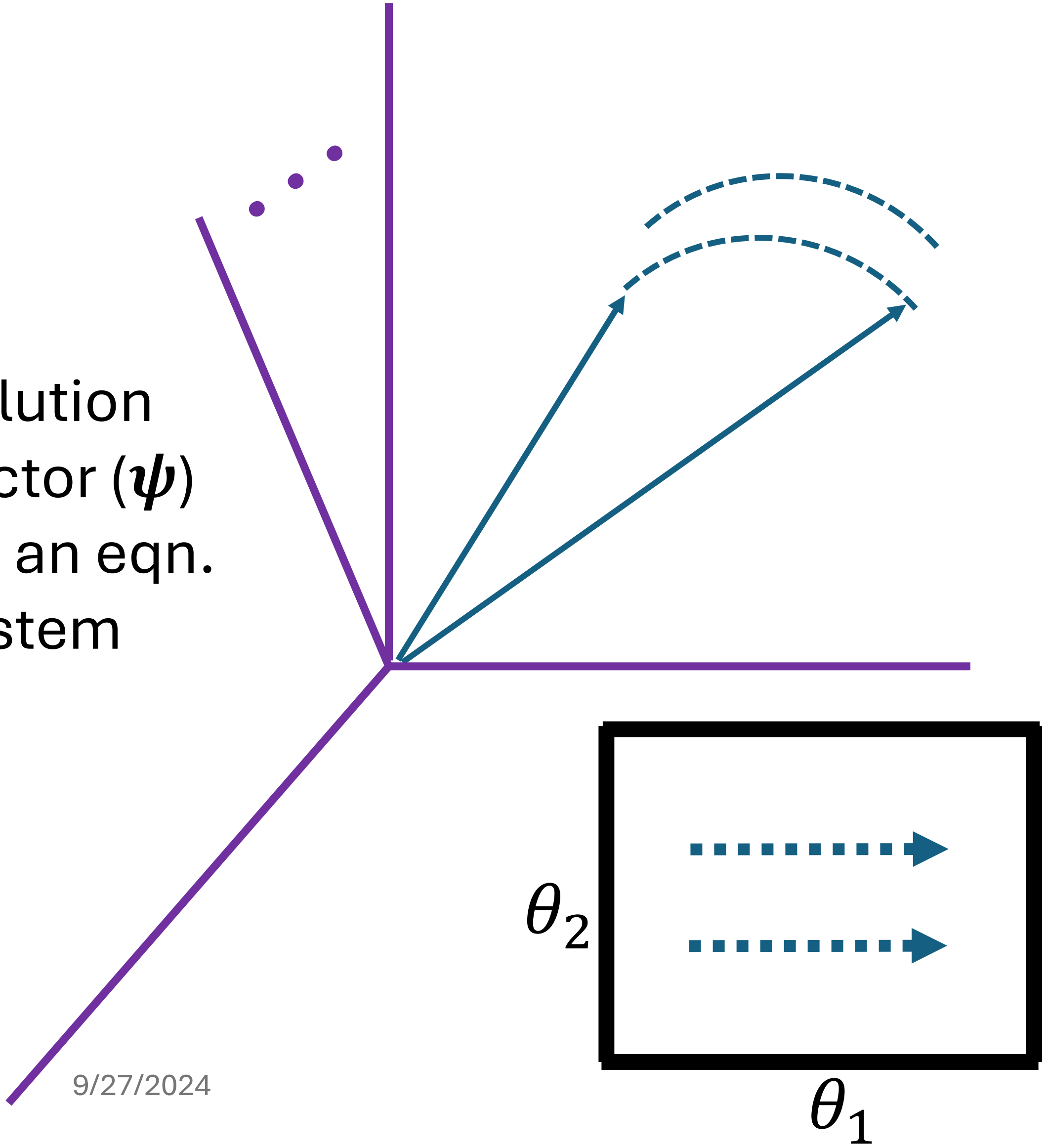

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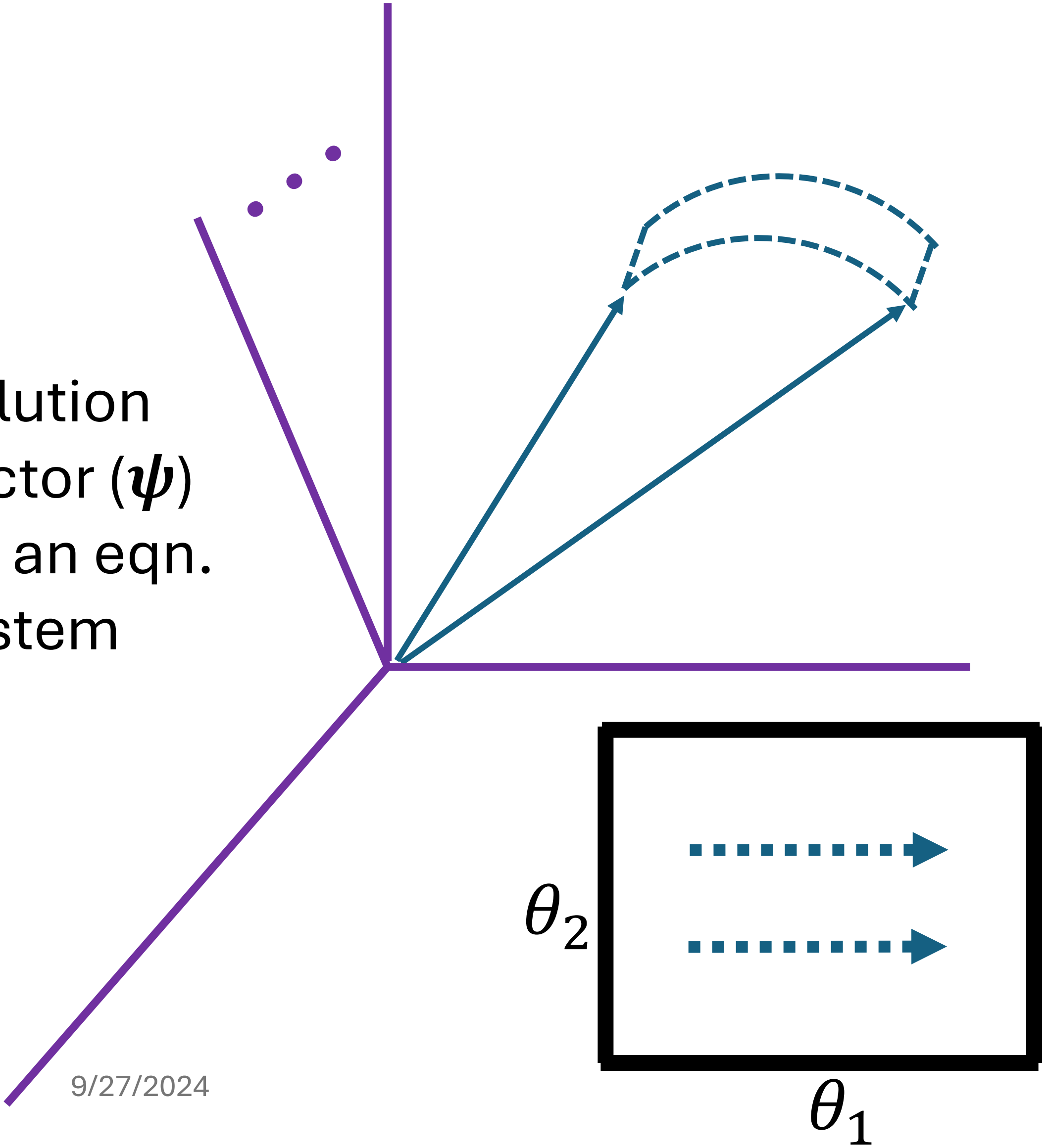

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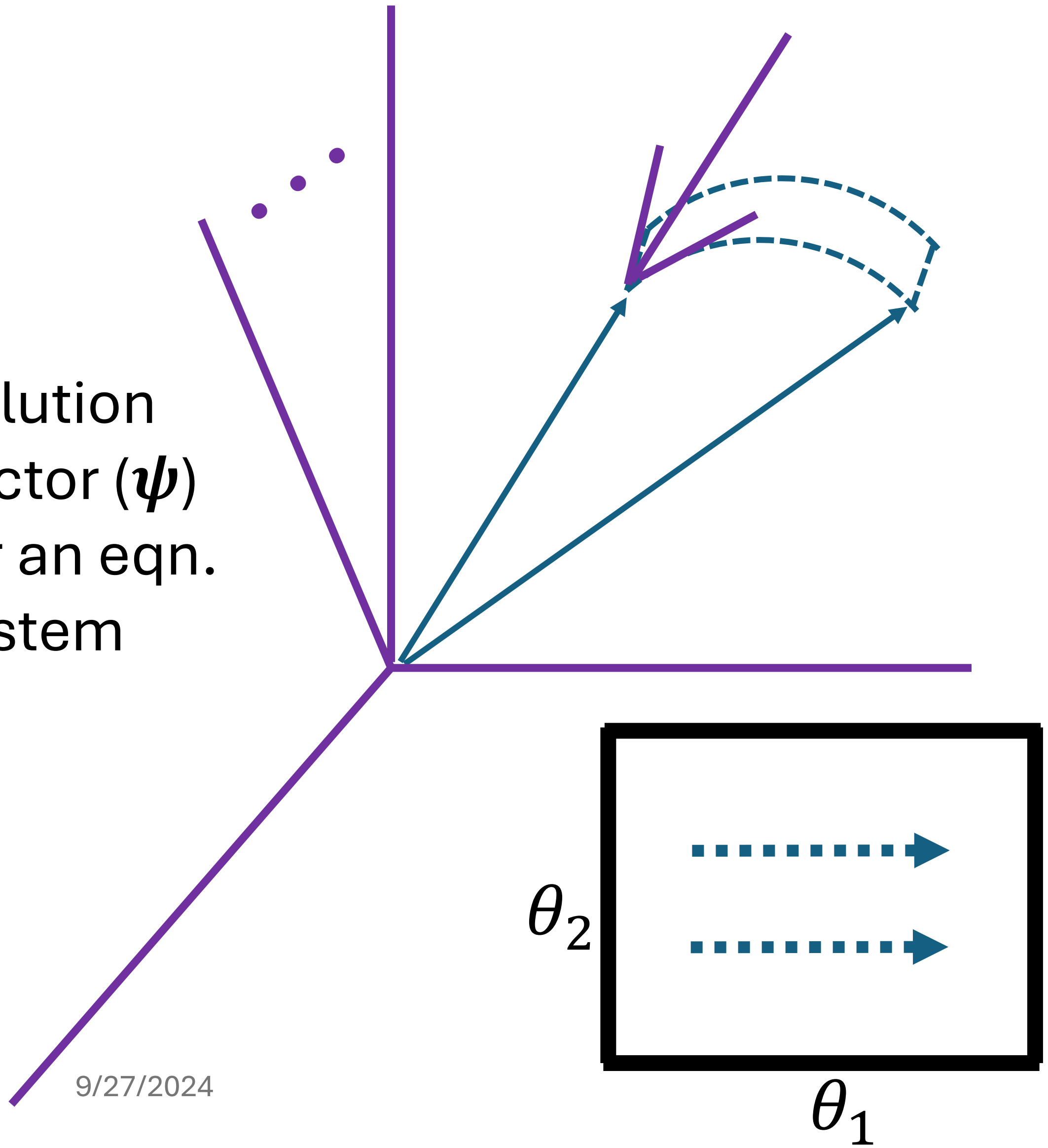

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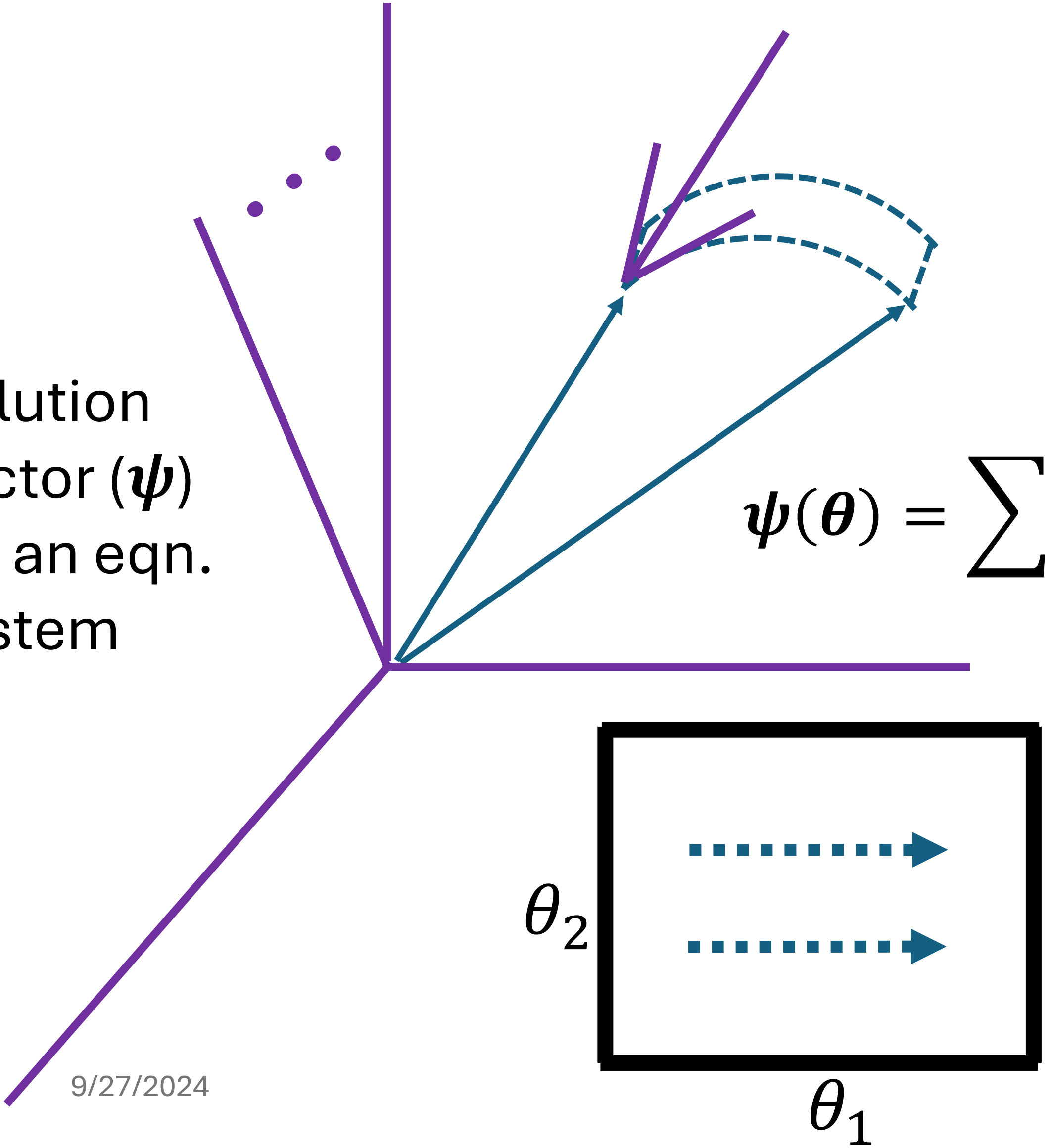

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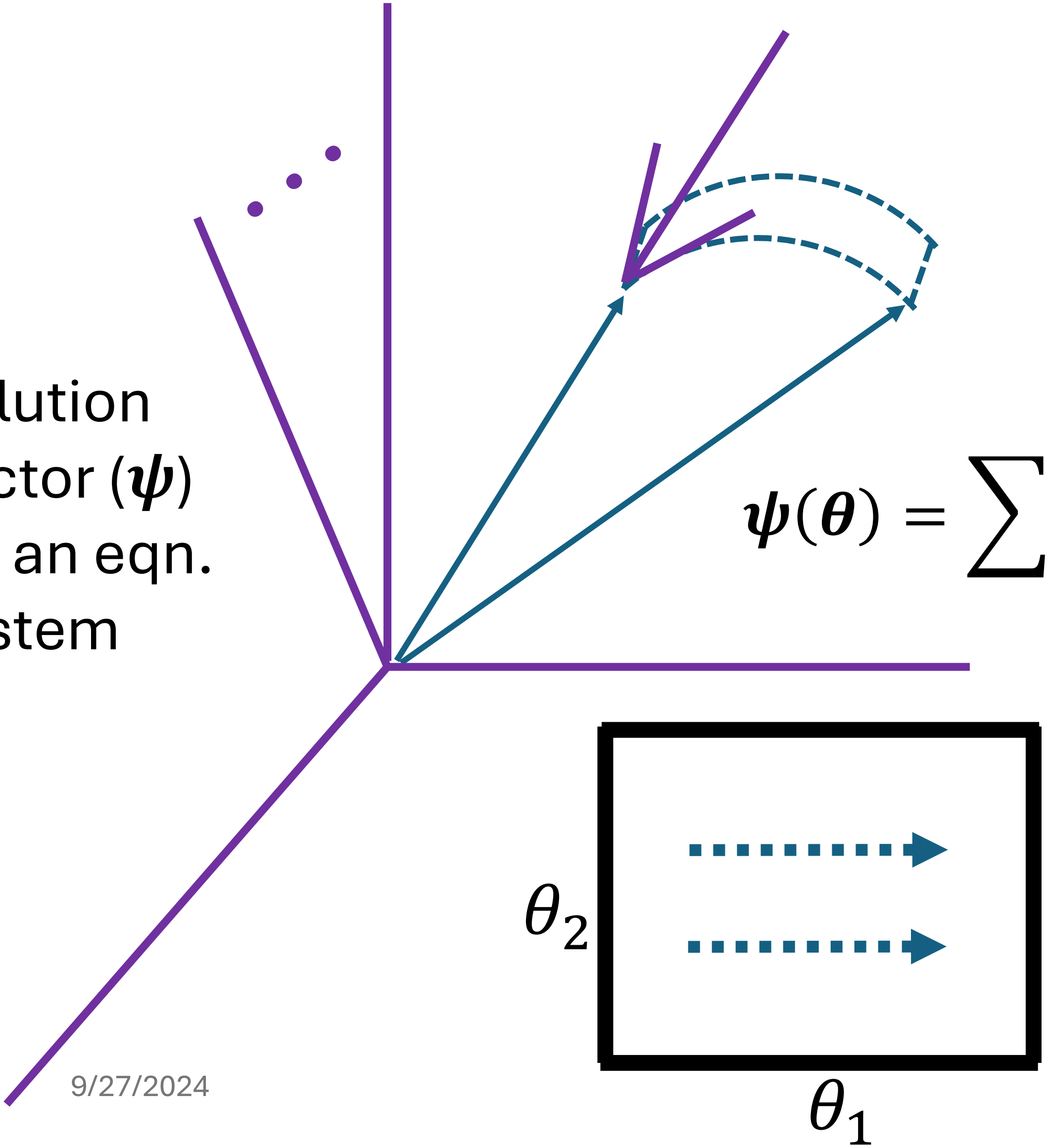

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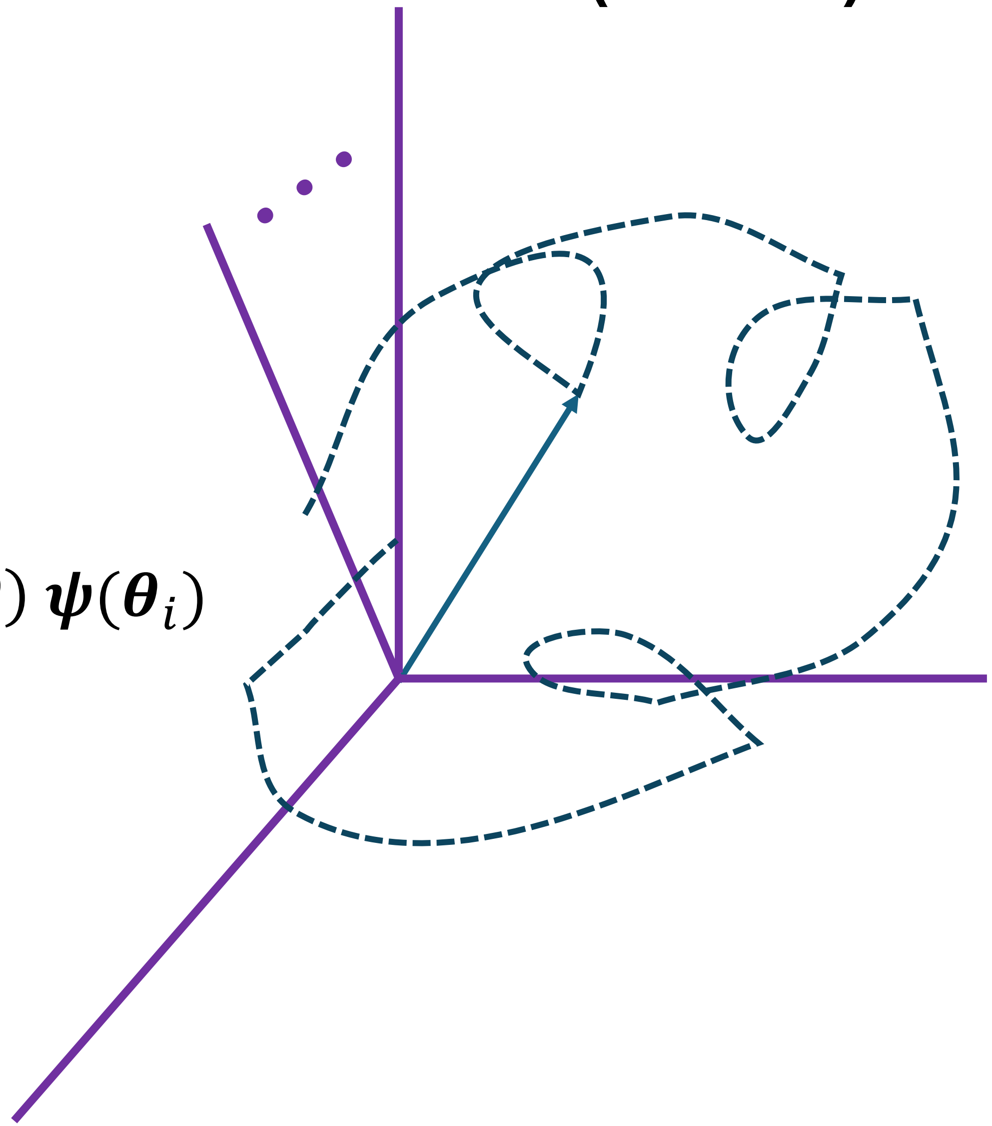

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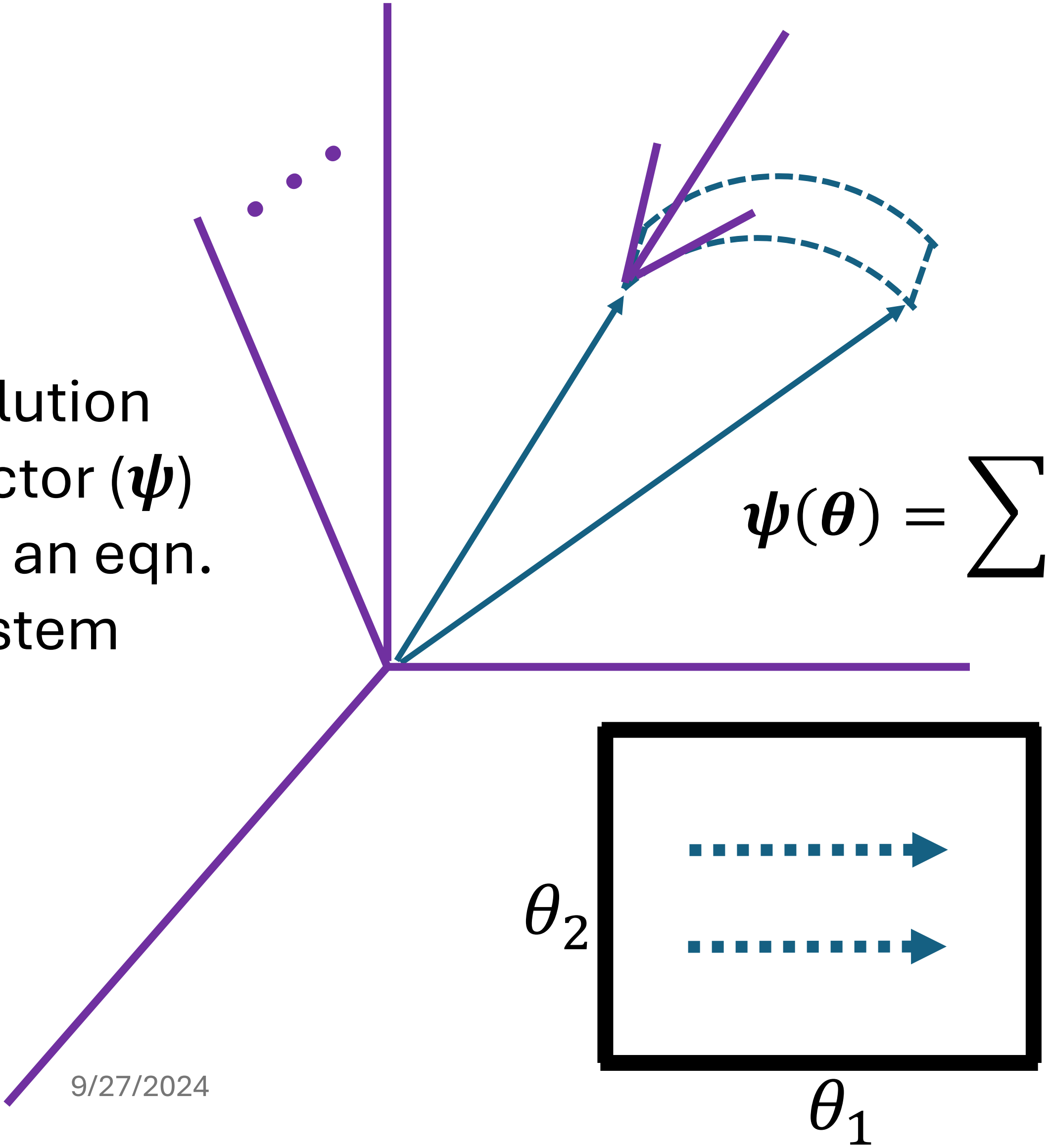

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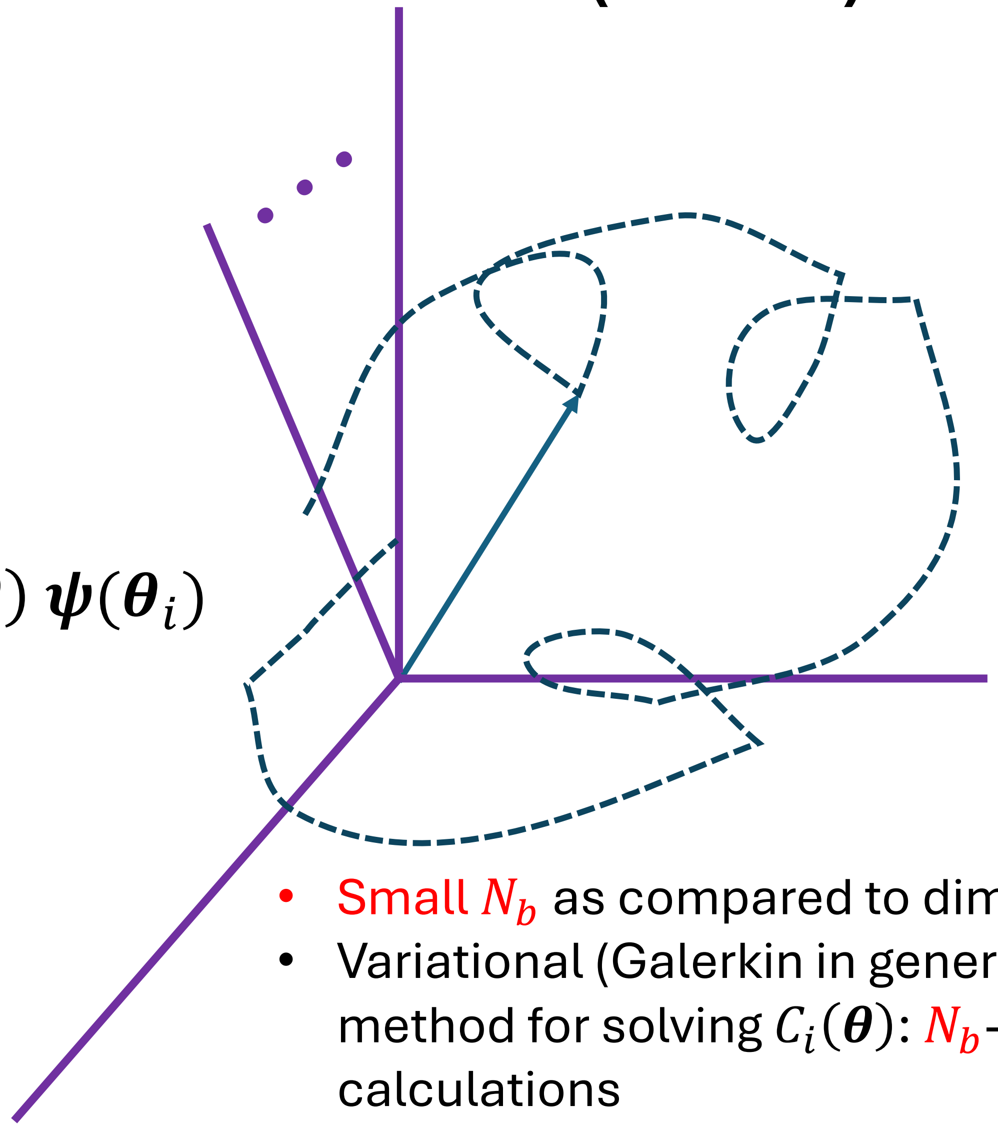
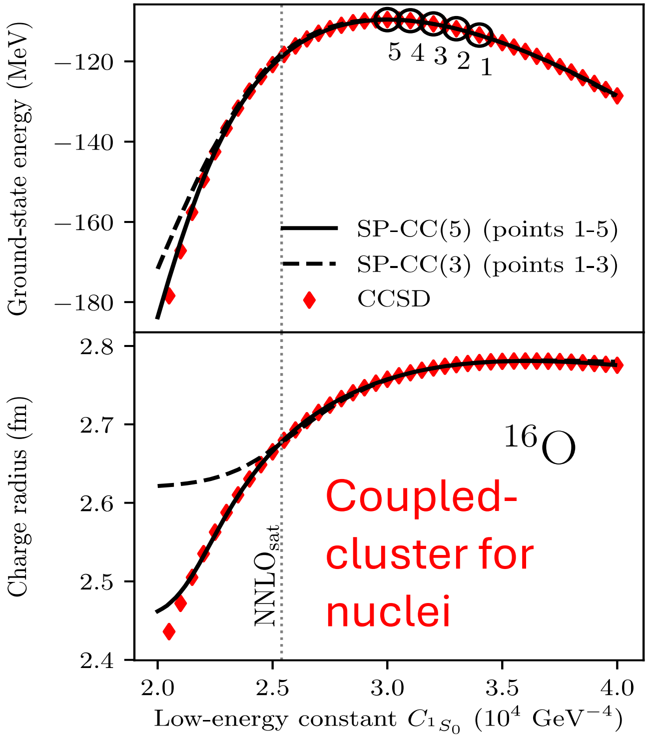


- Small N_b as compared to dim($\boldsymbol{\psi}$)
- Variational (Galerkin in general) method for solving $C_i(\boldsymbol{\theta})$: N_b-dim calculations
- $\rightarrow f(\boldsymbol{\theta})$ fast

RBM emulators for finite quantum systems

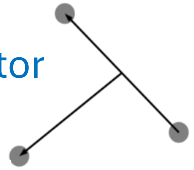
A. Ekström and G. Hagen
Global sensitivity analysis of bulk properties of an atomic nucleus
Phys.Rev.Lett. 123 (2019) 25, 252501, 1910.02922

"about 1 Million samples in 16-dim space, 20 years calculation → 1 hour on a standard laptop."



XZ and R. Furnstahl
Fast emulation of quantum three-body scattering
Phys.Rev.C 105 (2022) 6, 064004, 2110.04269

Real-E emulator



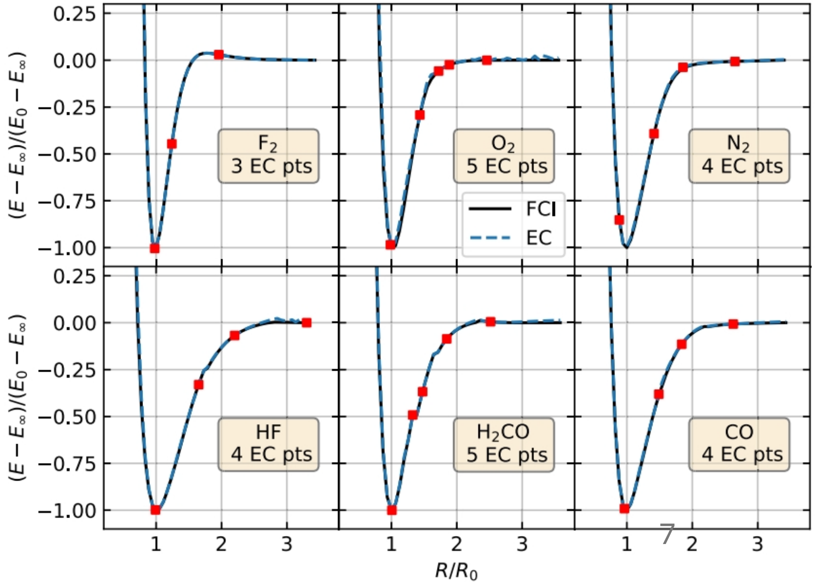
EC emulators	S relative error	Time	Memory
linear[a]	10^{-14} to 10^{-13}	ms	< MB
nonlinear-1	10^{-6} to 10^{-5}	ms	MB
nonlinear-2	10^{-4}	ms	10s MB

A typical full computation: 10^3 s

Pablo Giuliani, Kyle Godbey, Edgard Bonilla, Frederi Viens, Jorge Piekarewicz
Bayes goes fast: Uncertainty Quantification for a Covariant Energy Density Functional emulated by the Reduced Basis Method, Front. Phys. 10, 54524, 2209.13039

Mejuto-Zaera, C., and A. F. Kemper
Quantum eigenvector continuation for chemistry applications
Electron. Struct. 5, 045007 (2023)

Energy surface→



Continuum physics of finite quantum systems: a difficulty due to infinite space-time volume

- Before dim. reduction, how to perform H → $[H]$ matrix for computing $\left\langle \tilde{S} \middle| \frac{1}{E-H} \middle| S \right\rangle \equiv R(E)?$
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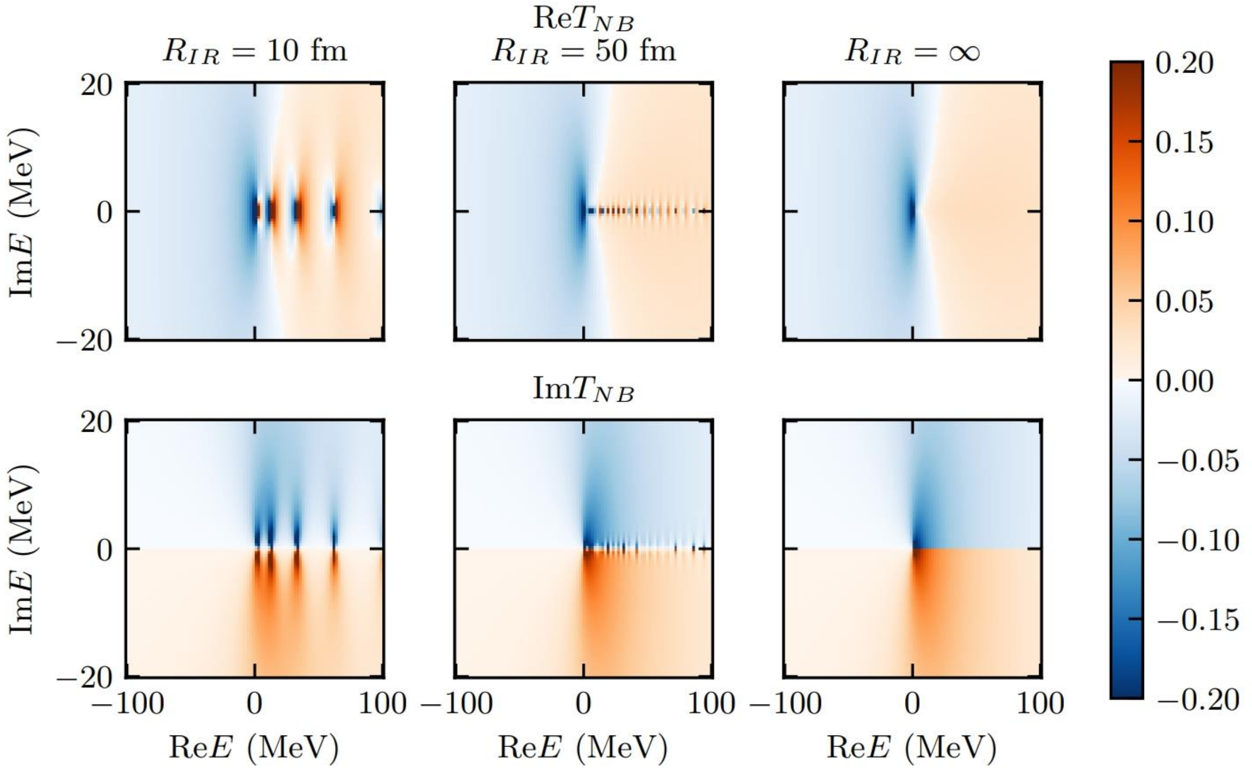

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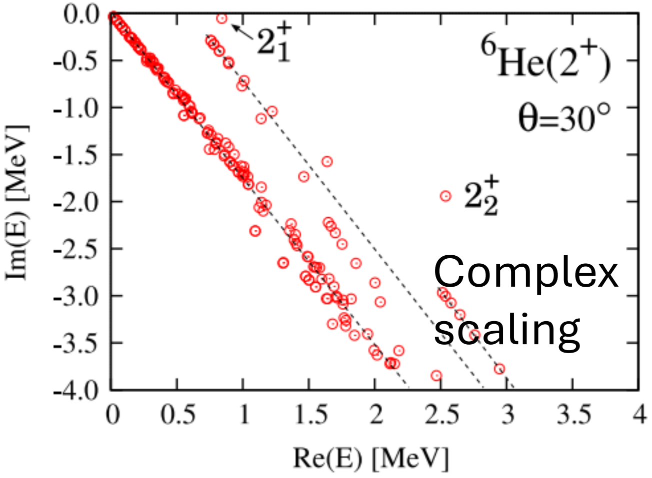
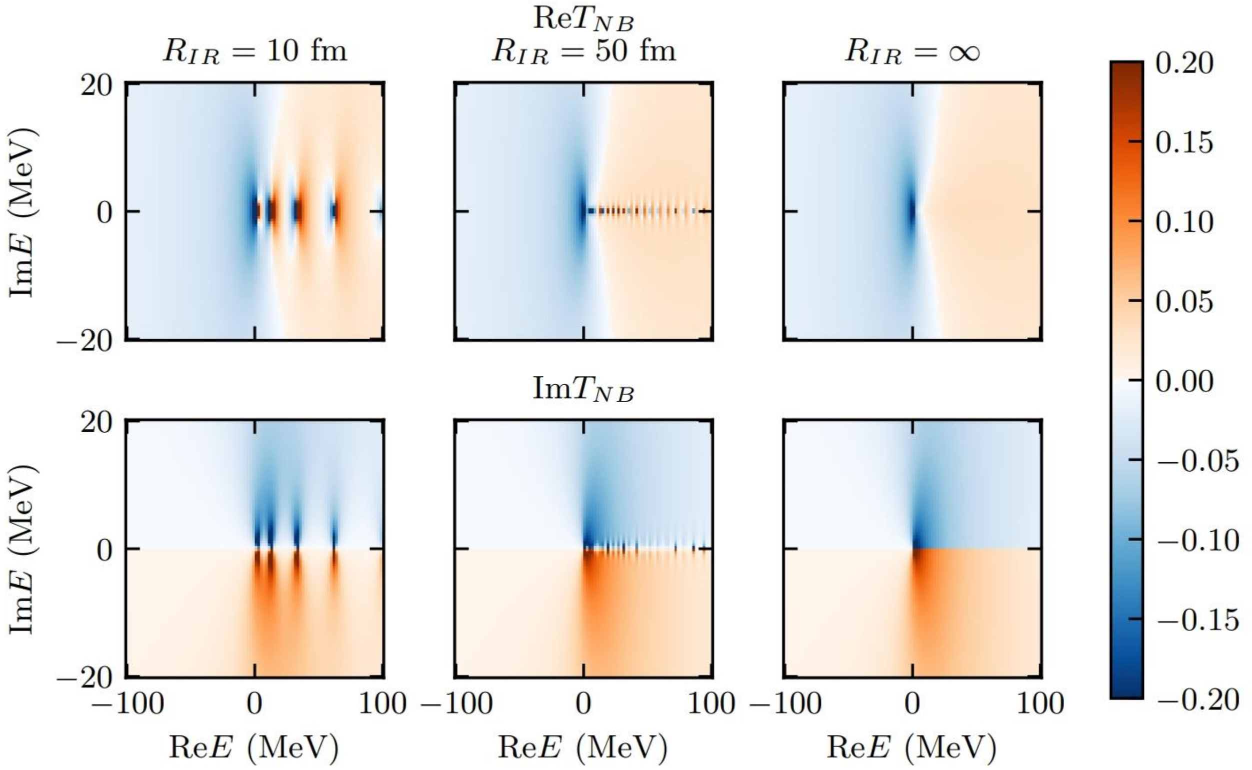


T. Myo et al. / Progress in Particle and Nuclear Physics 79 (2014) 1–56



- Non-Hermitian quantum mechanics: change integration contour, complex-scaling, Berggren basis
- (1) no unphysical real-E poles, (2) threshold behavior systematically improvable, (3) physical poles on the same Riemann sheet (res. as an eigenstate)

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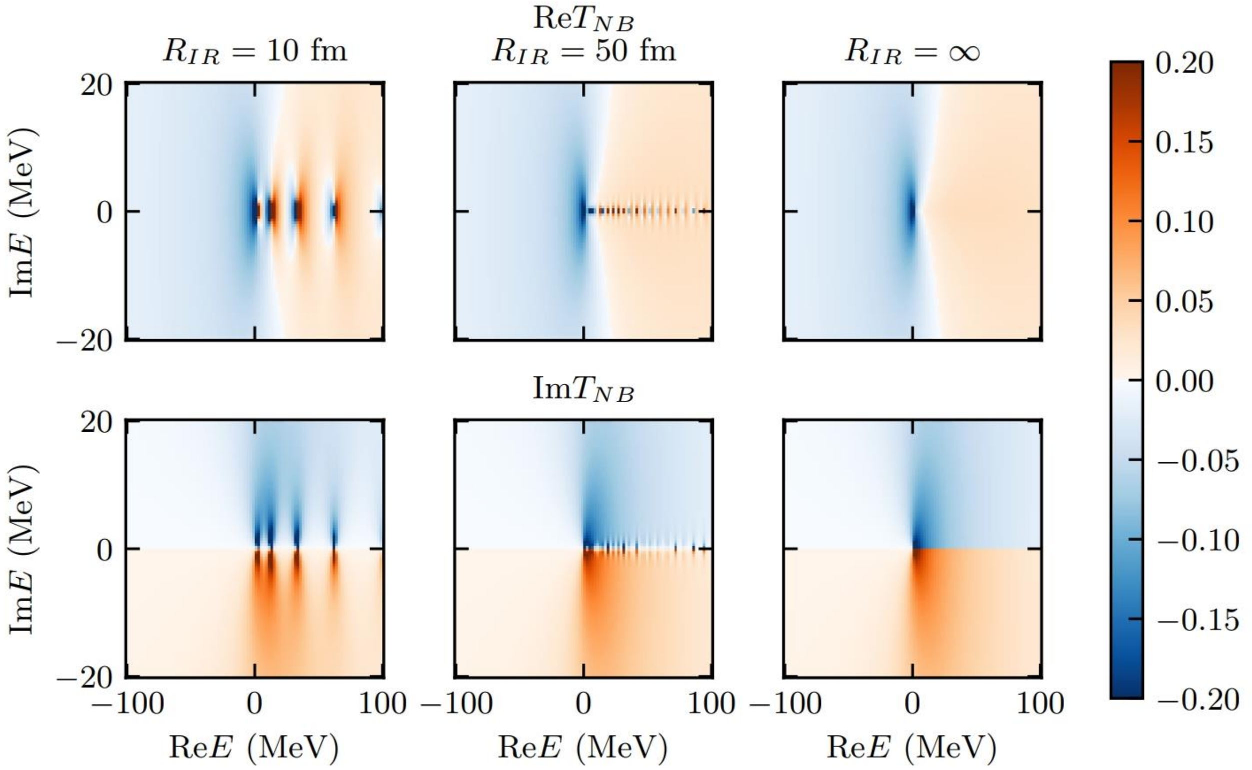

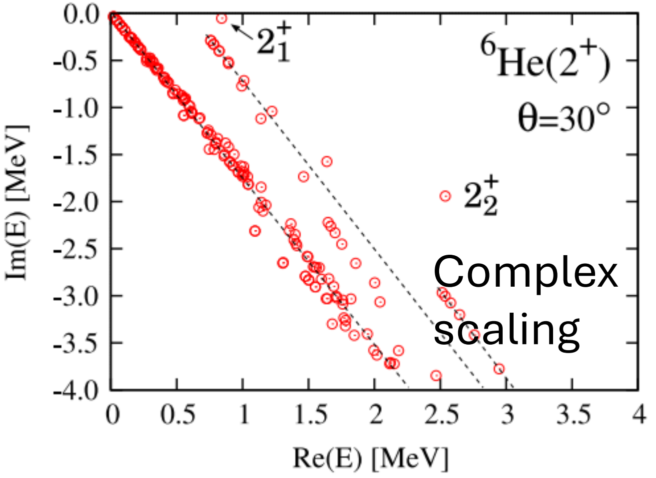

A "desperate" prescription:
$R(E + i\delta) \approx R(E)$
w/ real E and finite δ

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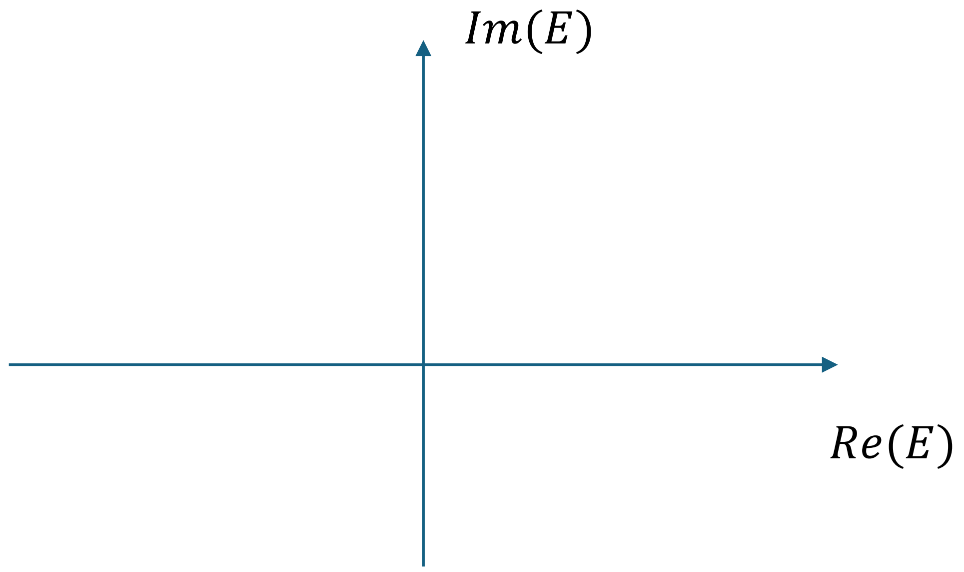
Complex-E emulator for continuum



Complex-E emulator for continuum

- $[E - H(\boldsymbol{\theta})]|\psi(\boldsymbol{\theta})\rangle = |S\rangle$ for complex E is a bound-state-like problem

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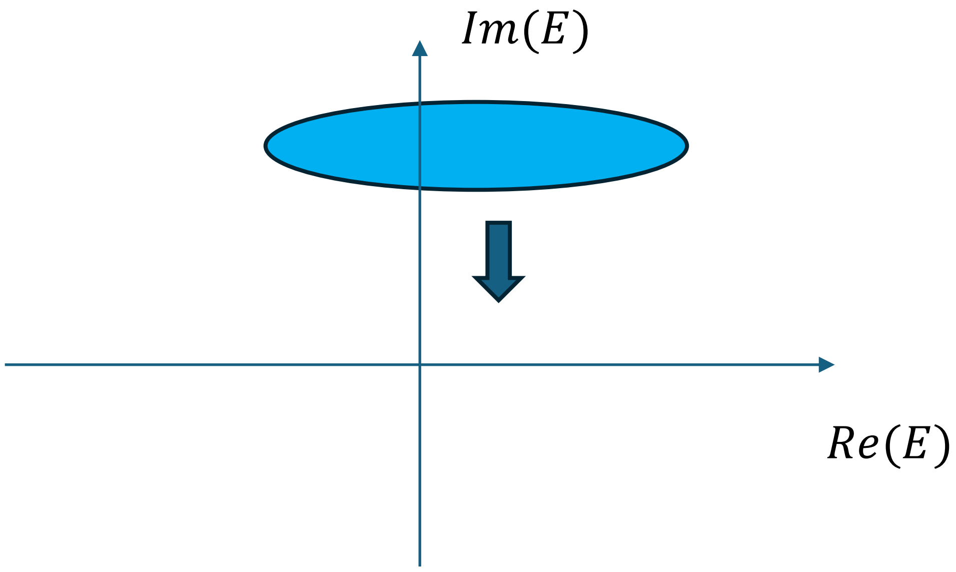

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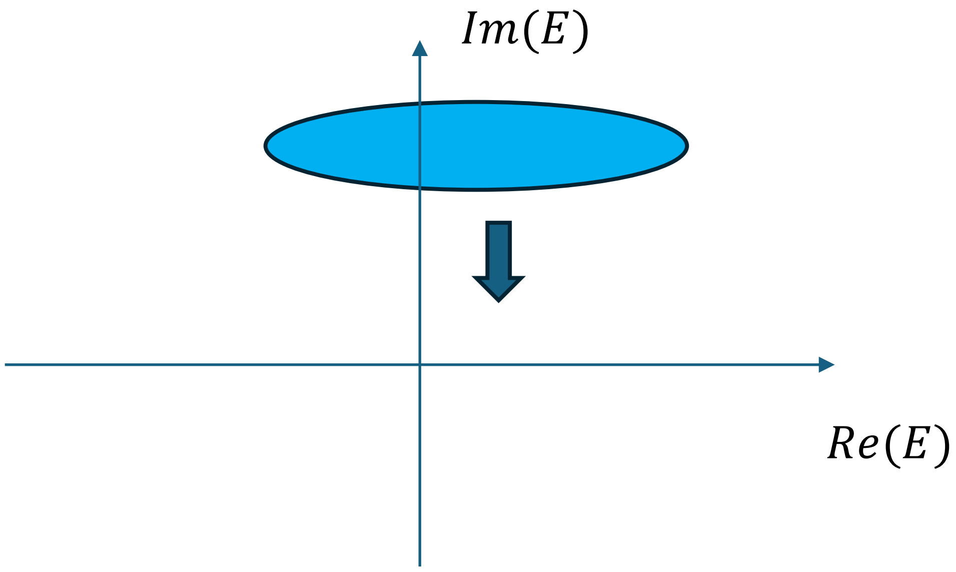

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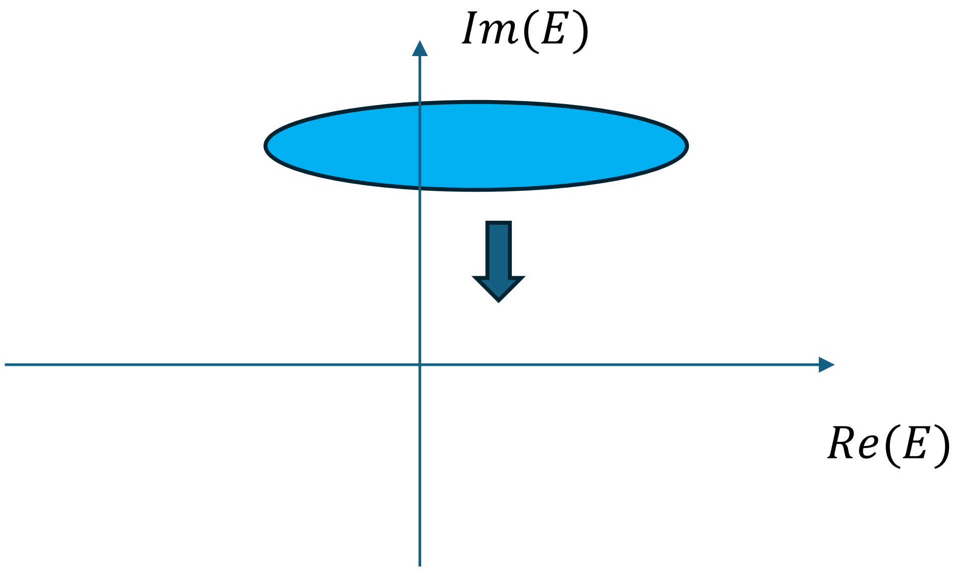

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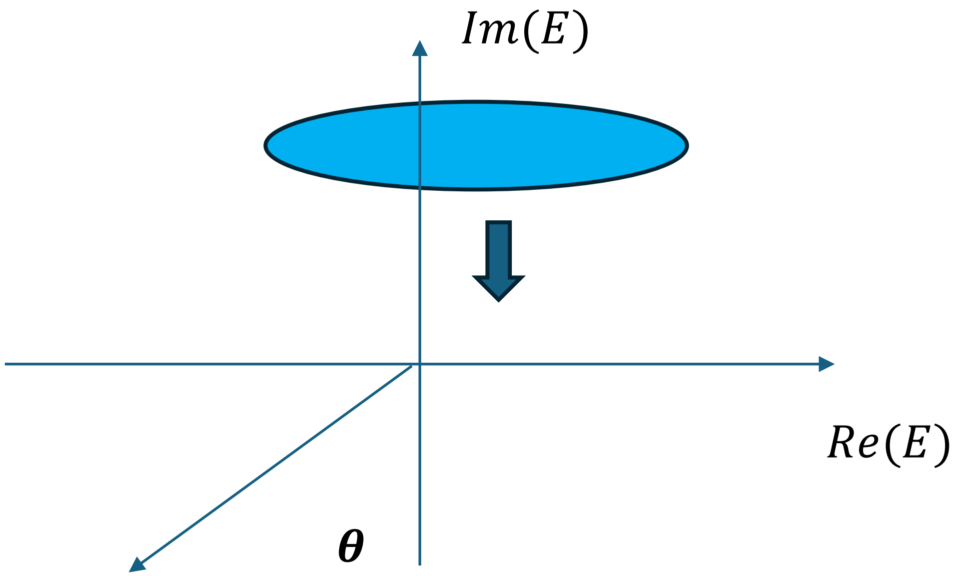

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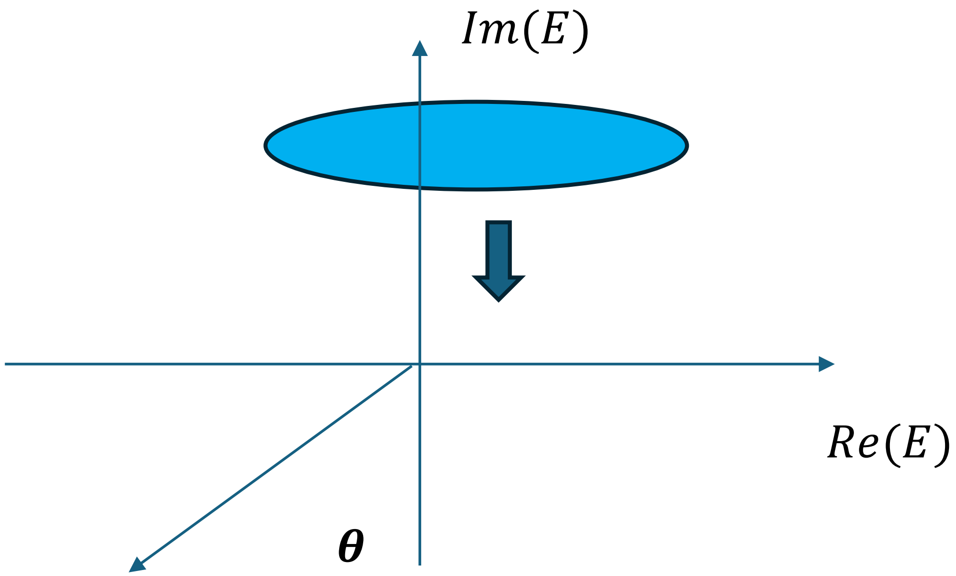

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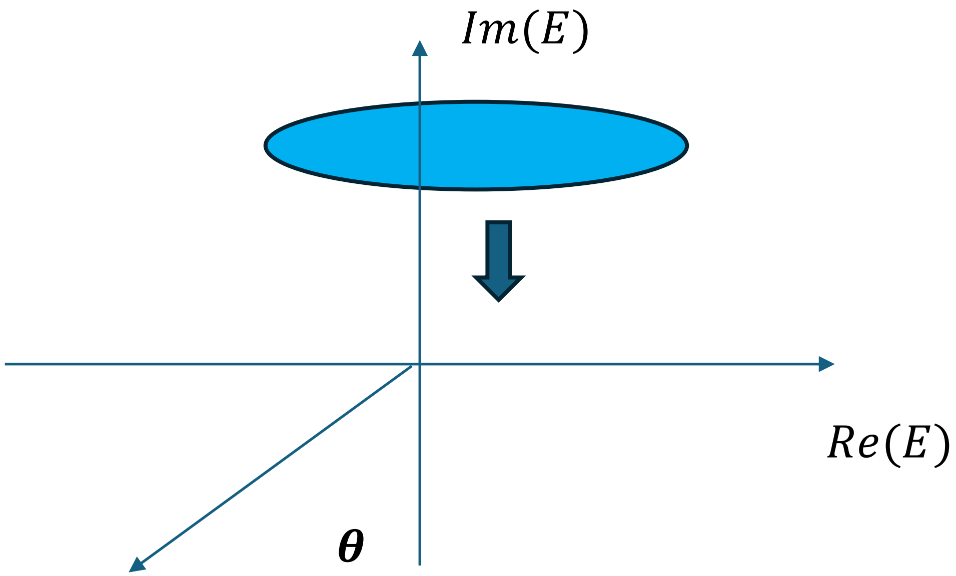
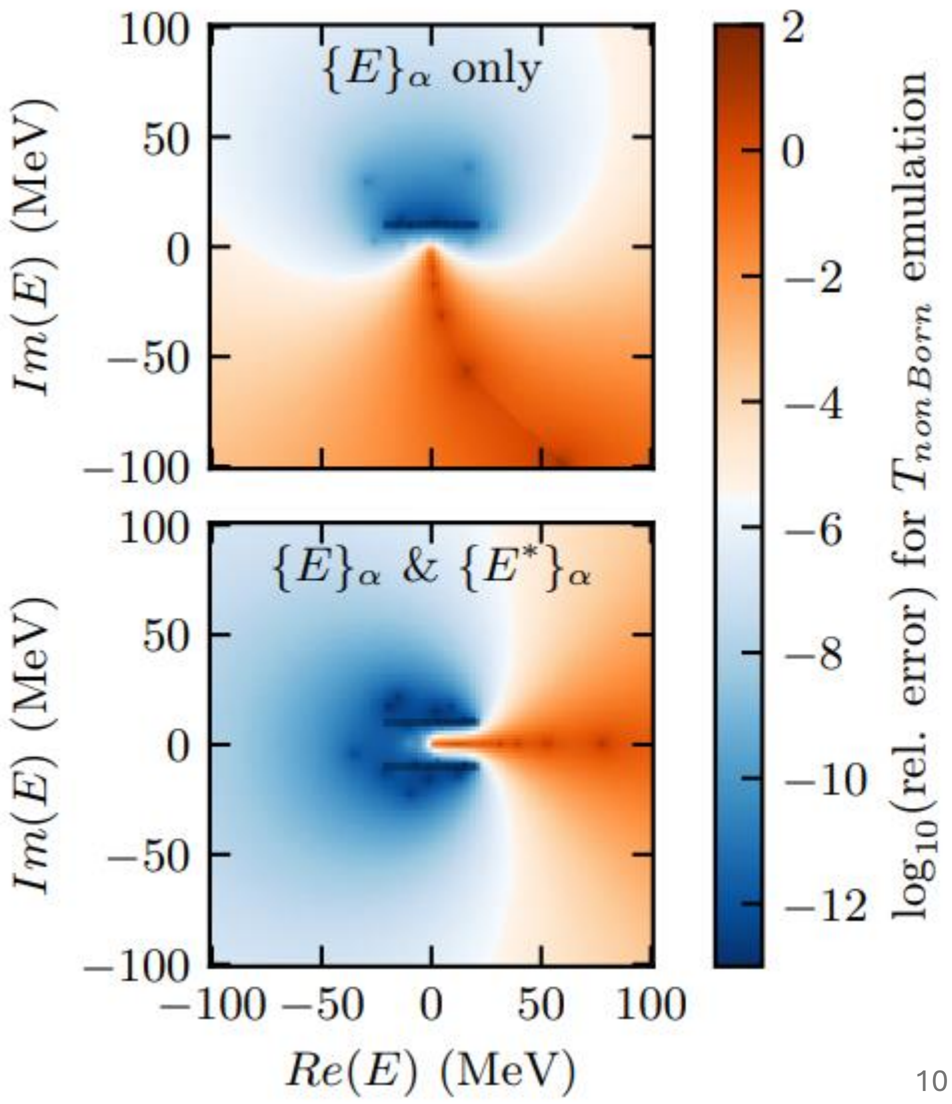


A non-Hermitian quantum mechanics approach for extracting and emulating continuum physics based on bound-state-like calculations, **X.Z.** 2408.03309

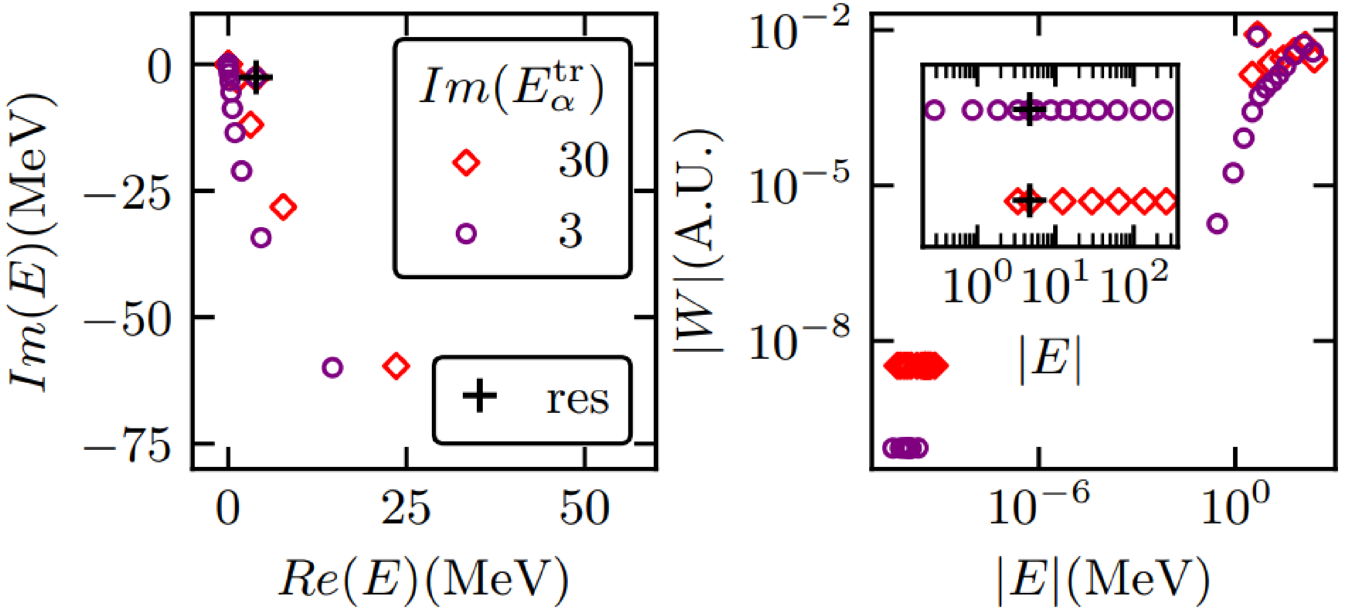
Complex-E emulator for continuum: basics

- Two-body model (like NN)
- The error plot for $R(E)$ is shown
- The arrangement of training points can make $[H]$'s eigenvalues complex in general or real only
- The former is good for continuum
- The latter is good for discrete spectrum
- Note emulating both spectrum (excited states and resonances) and observables



Complex-E emulator for continuum: basics

- Spectrum: physical states + discretized branch cuts
- The BC poles exponentially clustered towards the branch point/singularity
- The concept of effective dim



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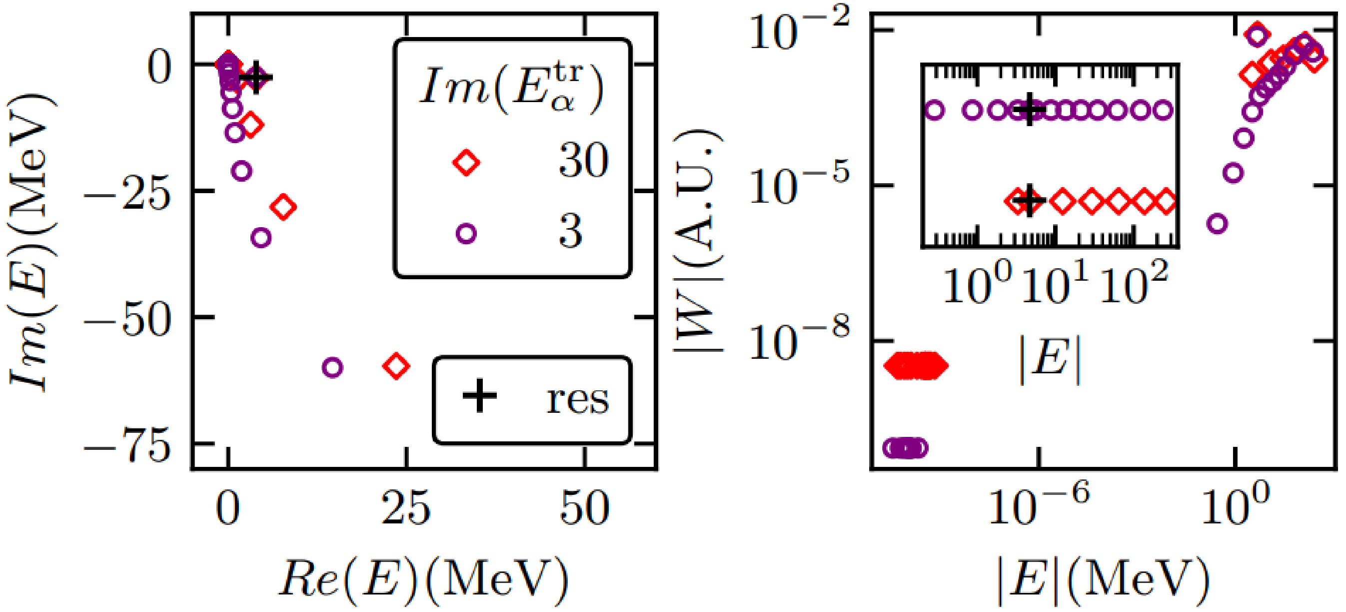
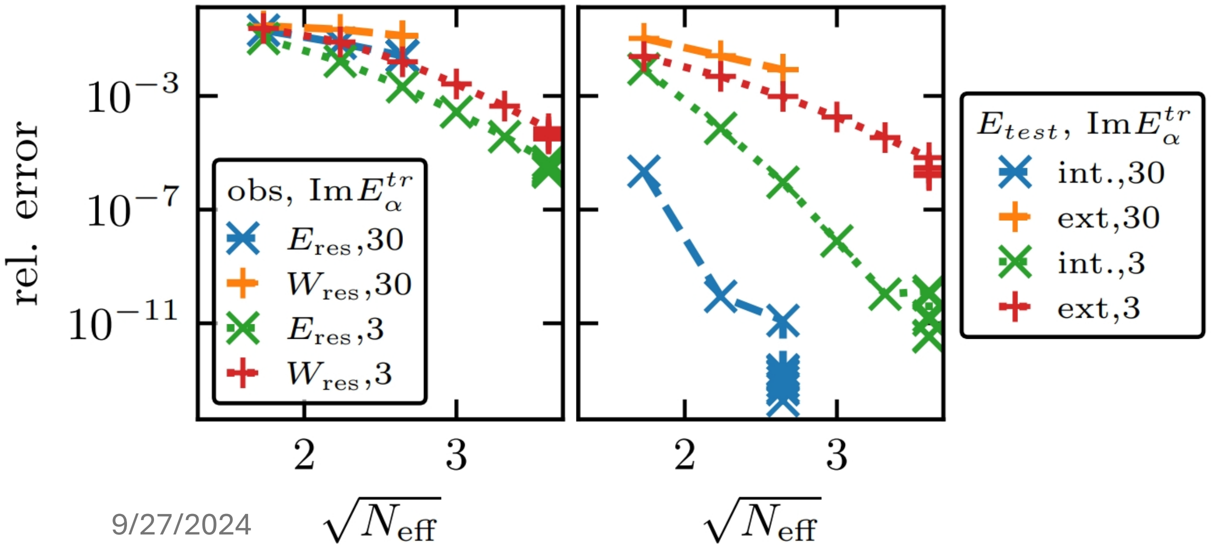


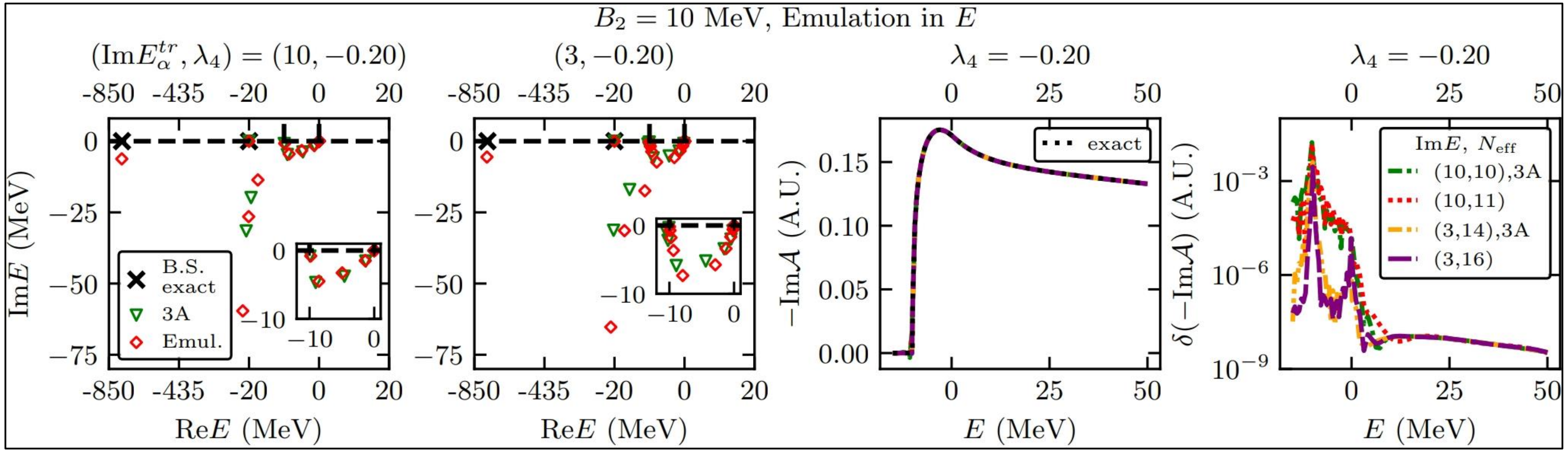


- Error exponentially decreases w/ $\sqrt{N_{eff}}$
- Seen in the optimal rational approx. of functions with branch points (L. N. Trefethen et.al., since ~2018)

Complex-E emulator for continuum: three-body

Two and three-body interactions with couplings λ, λ_4 (see 2110.04269)

3A: AAA rational approximation due to Trefethen et.al.



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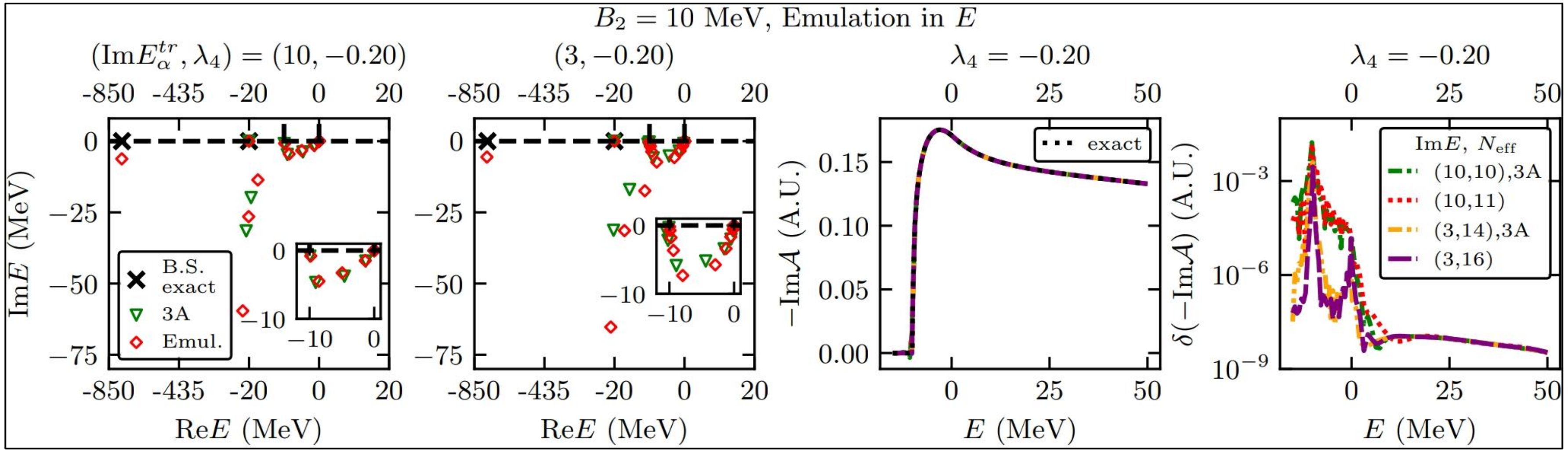

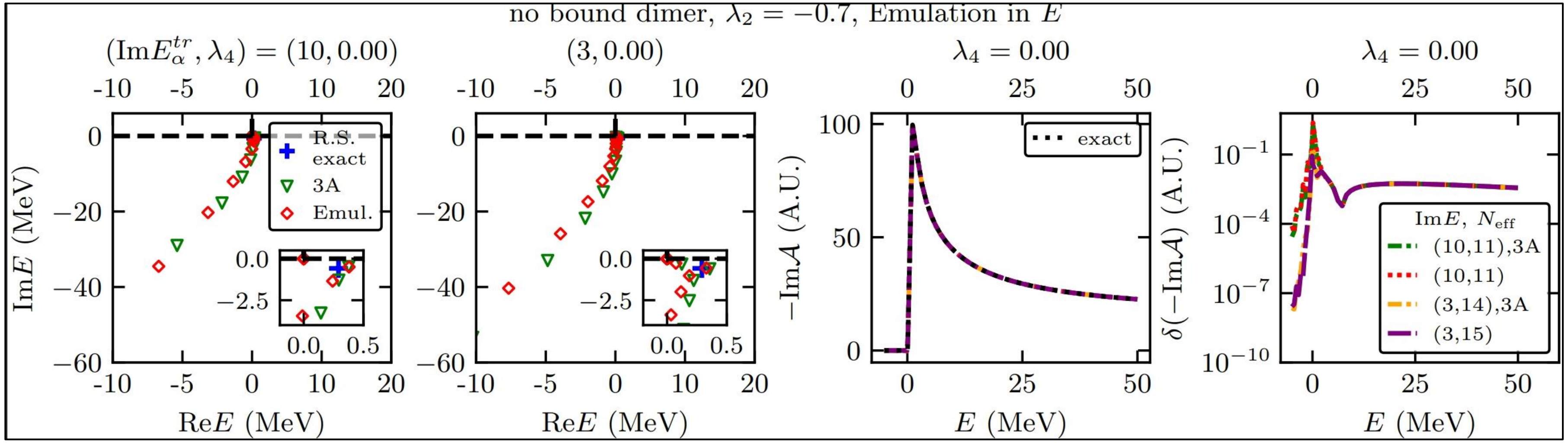

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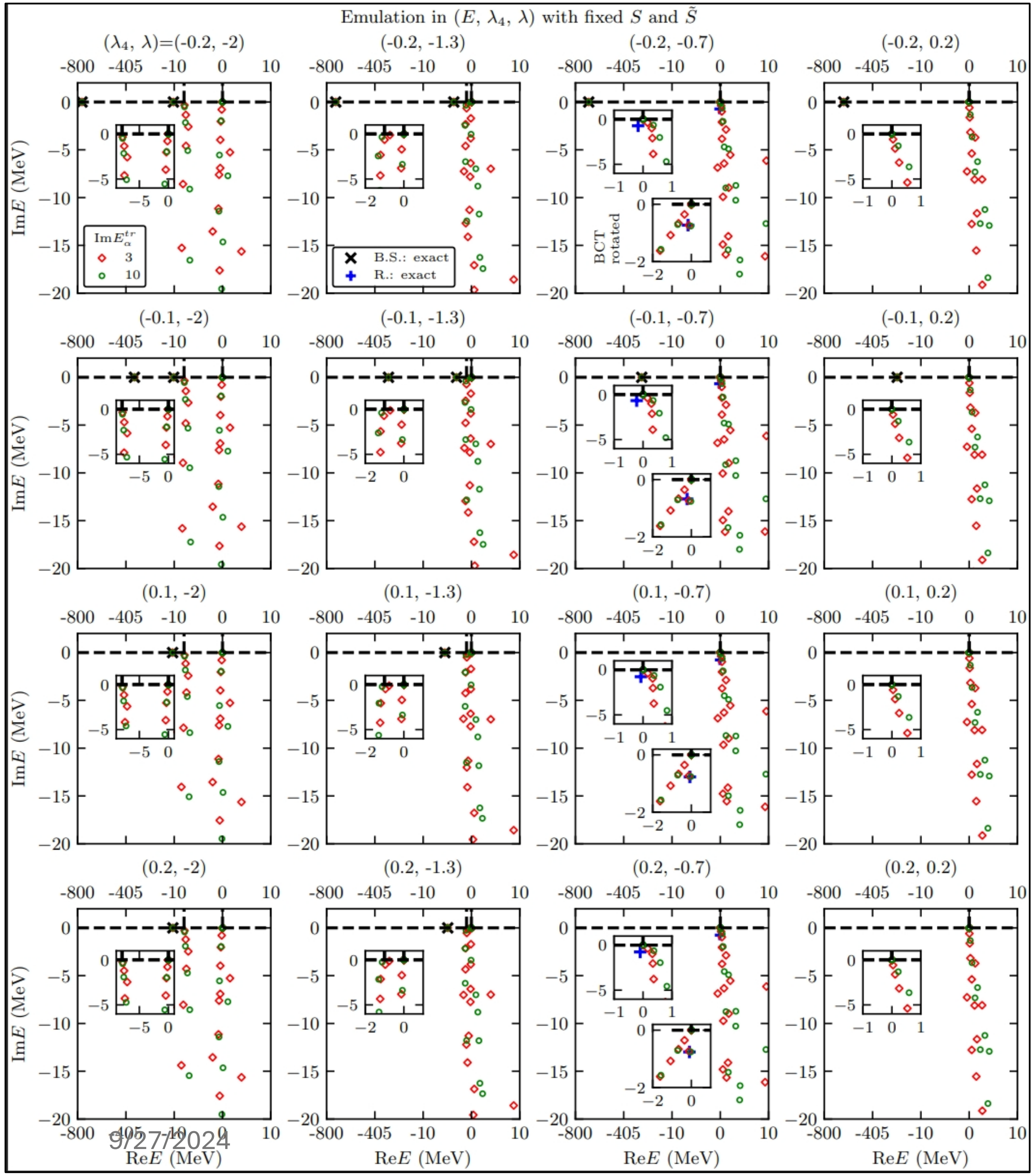
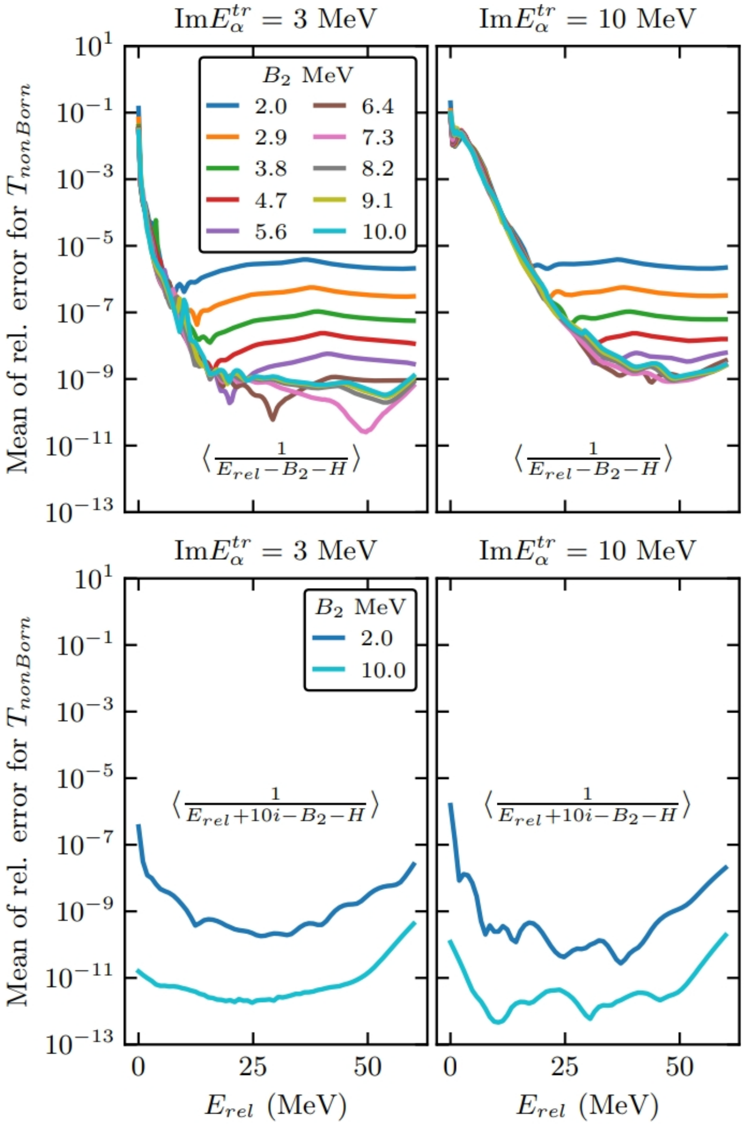
Emulating spectrum



Emulating amplitudes



Summary

- RBM emulators are being actively developed in nuclear theory
- Emulating Schrodinger equation in energy's complex plane → NHQM approach for extracting continuum physics from bound-state calculations
- The extraction can be emulated in the input parameter space
- Many other applications: linear response in density functional theory, coupling with other NHQM methods, and etc