Emulators for Open Quantum Systems

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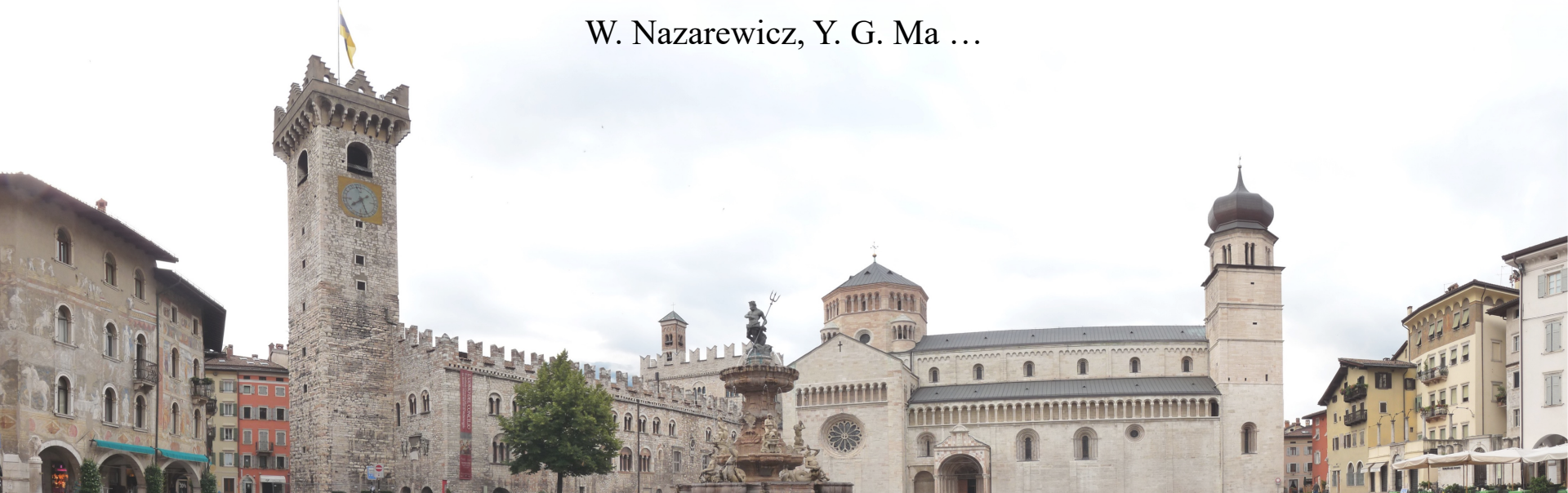
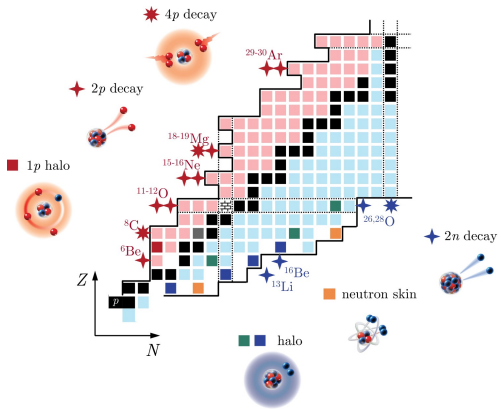
Collaborators: R. Y. Cheng, Z. C. Xu, K. Godbey, X. L. Zhang,
W. Nazarewicz, Y. G. Ma …

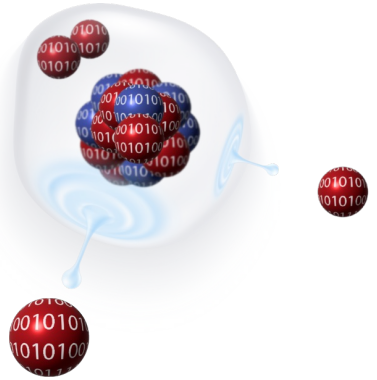


Outline

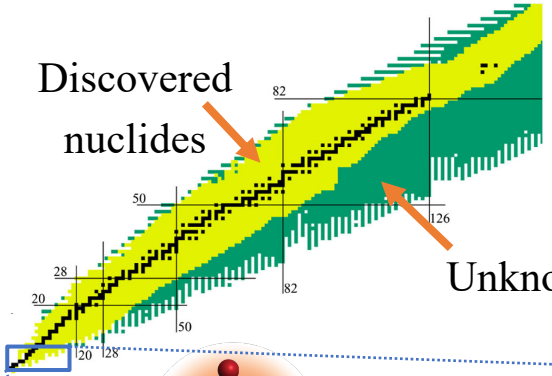
- Introduction
  - Open quantum systems (OQSs)
  - Theoretical developments and challenges



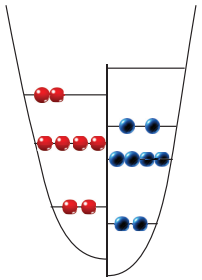
- Emulators for OQSs (resonances)
  - Response function
  - Resonance energy/width
  - Continuum coupling & asymptotic observable



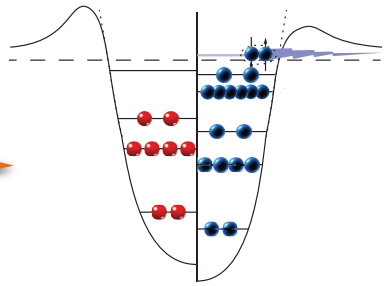
Rich phenomena towards the dripline

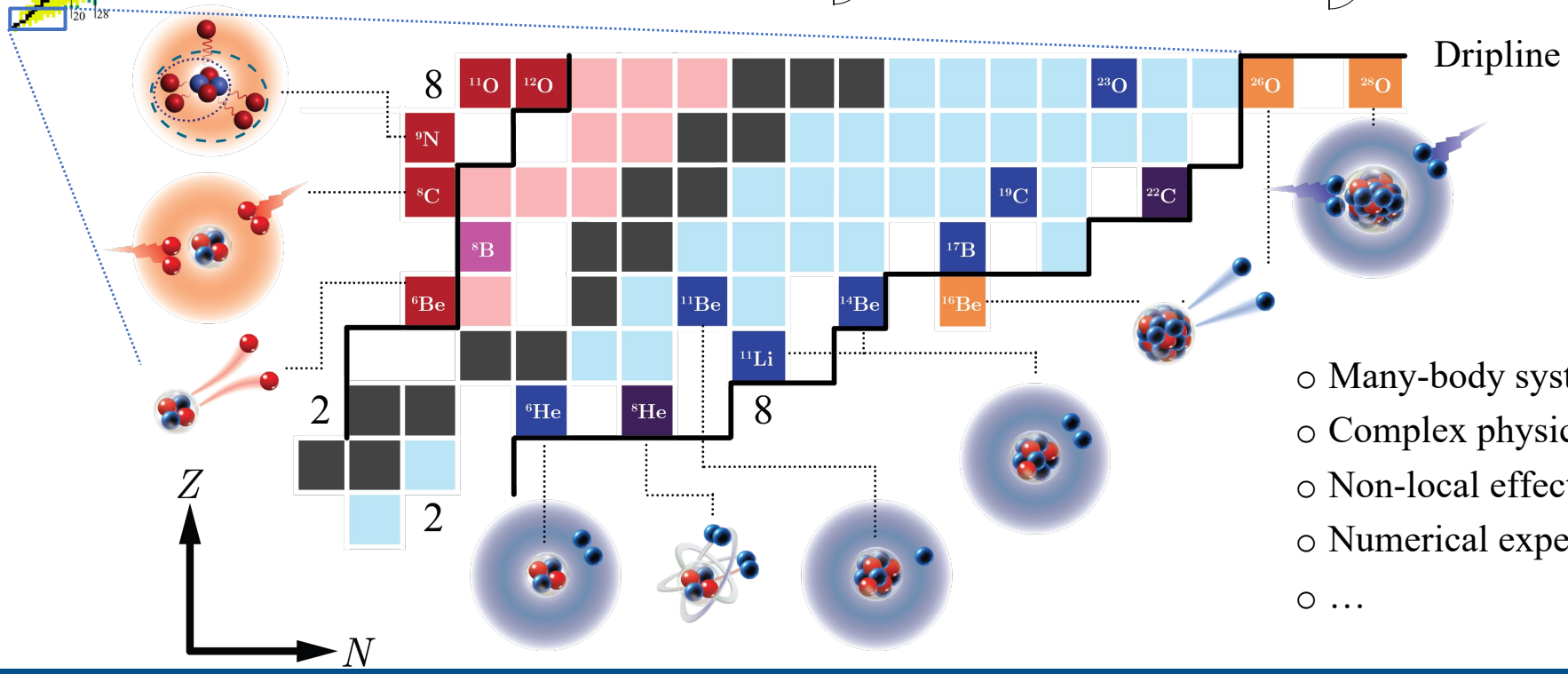


Closed quantum system



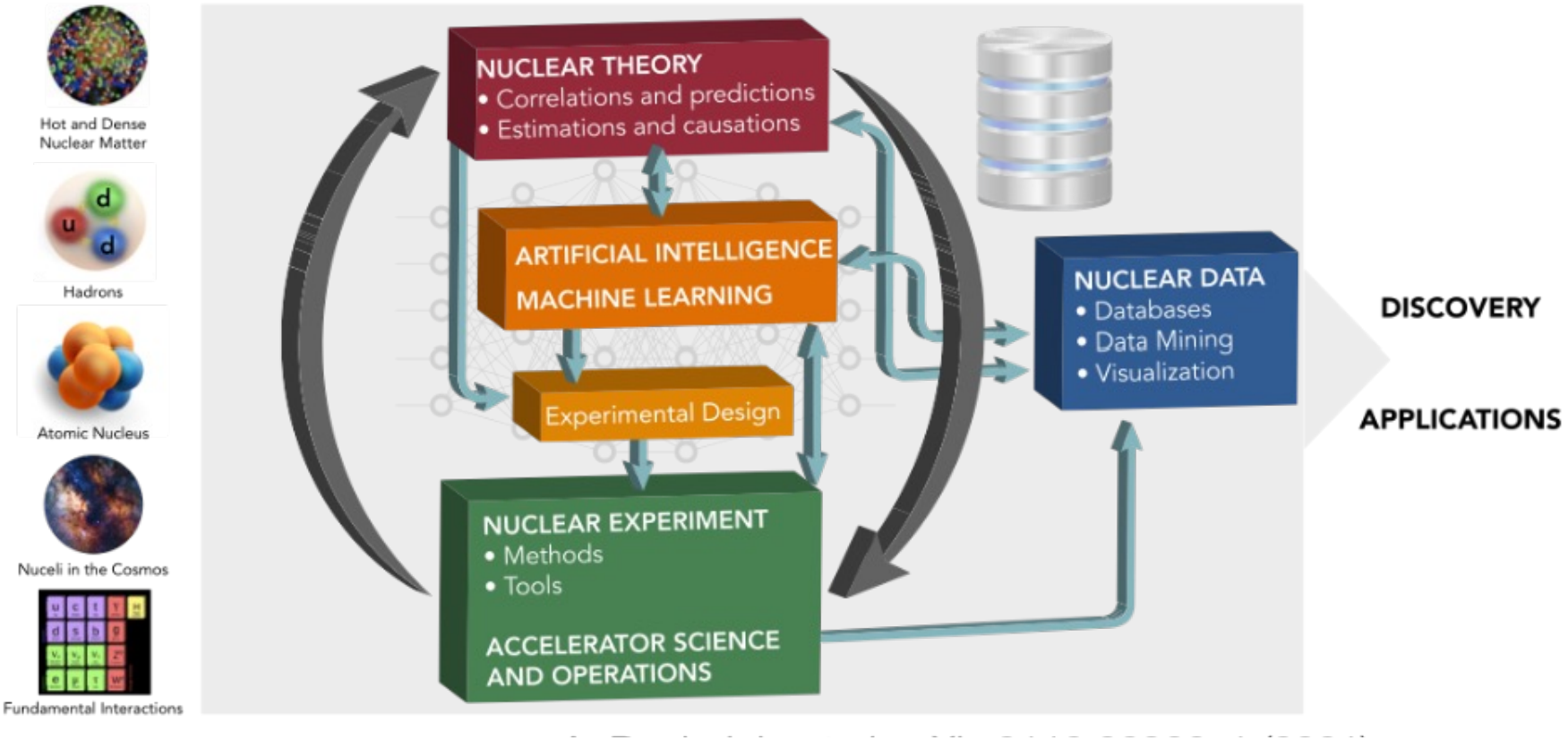
Open quantum system





- Many-body systems
- Complex physics
- Non-local effect
- Numerical expenses
- …

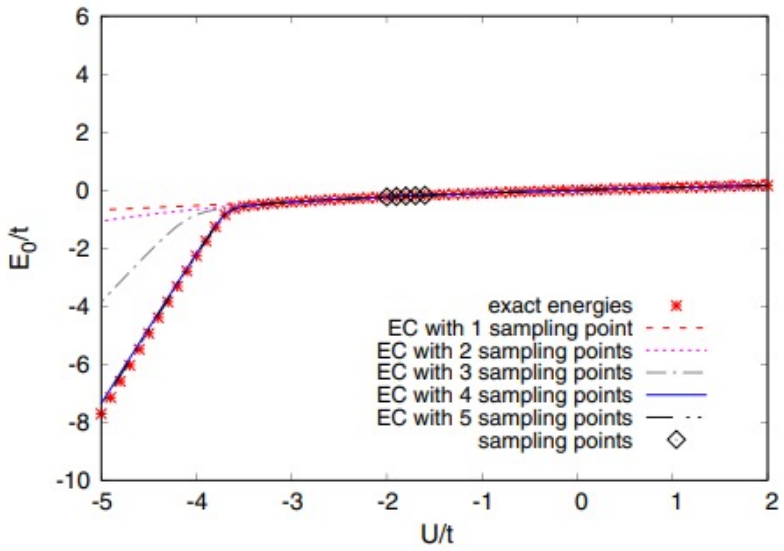
Demand of machine learning



A. Boehnlein *et al.*, Rev. Mod. Phys. 94, 031003 (2022)

Emulator for bound system

Eigenvector continuation (EC)

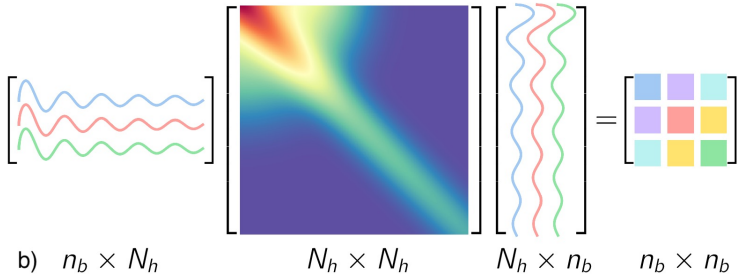


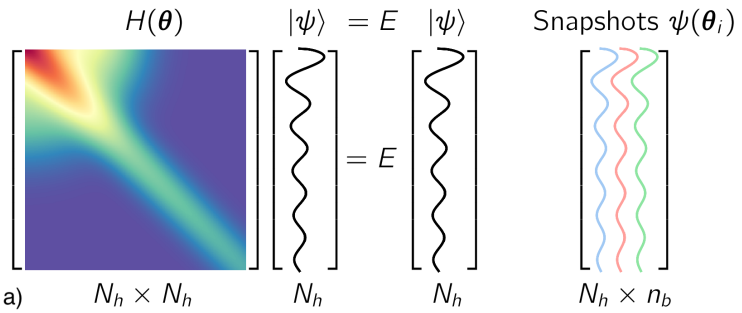
D. Frame *et al.*, Phys. Rev. Lett. 121, 032501 (2018)
T. Duguet *et al.*, Rev. Mod. Phys. 96, 031002 (2024)

- Eigenvalues can be extrapolated very well
- Information learned by the eigenvector changes
- Requirement: the continuity of the eigenvector

Flowchart

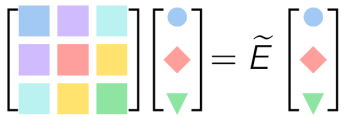
Projection (after orthonormalizing snapshots)





Emulation ($E \approx \widetilde{E}$)

$$\widetilde{H}(\boldsymbol{\theta})\ \vec{\beta} = \widetilde{E}\widetilde{N}\vec{\beta}$$

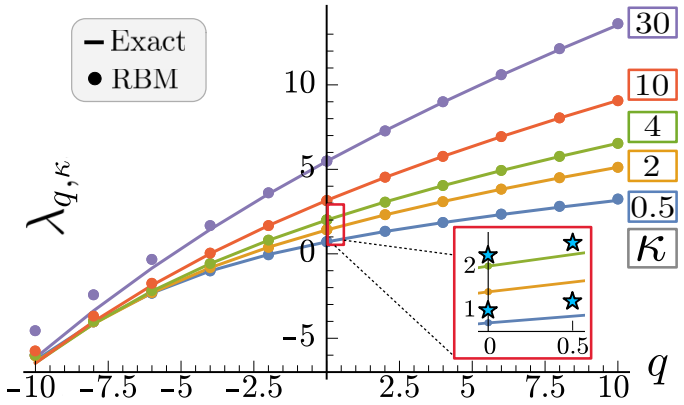


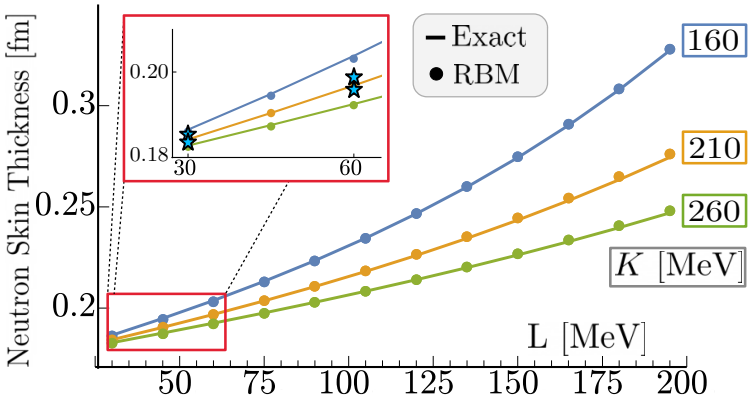
$(\widetilde{N} = \mathbb{1})$

c) All size-n_b operations

Emulator for bound many-body system

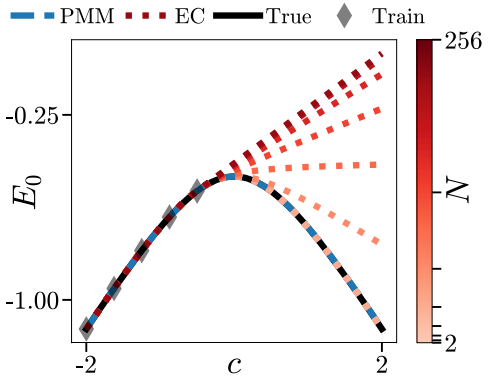
Reduce basis method (model driven)



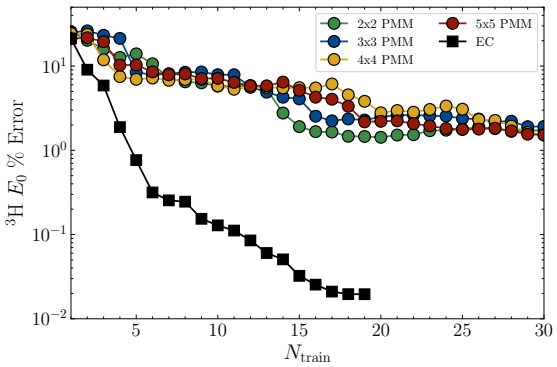


E. Bonilla *et al.*, Phys. Rev. C 106, 054322 (2022)

Parametric matrix models (hybrid)



P. Cook *et al.*, Nat. Commun. 16, 5929 (2025)

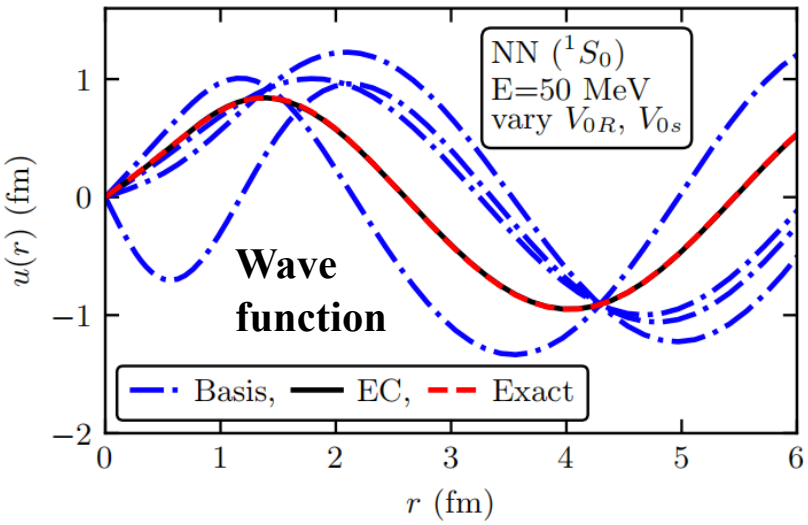


See Prof. Schwenk's talk

R. Curry *et al.*, arXiv:2510.15860 (2025)

Emulator for reaction

EC for for scattering

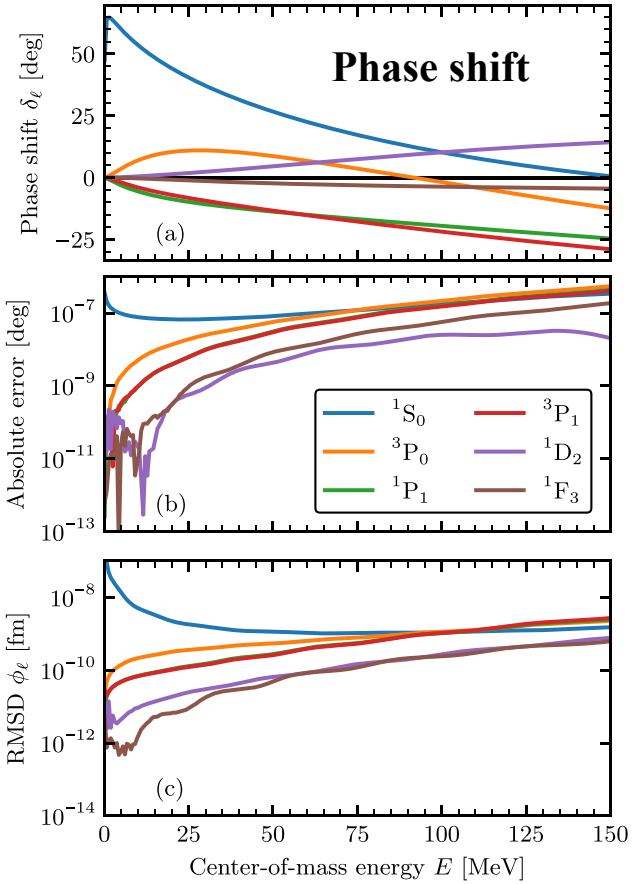


See Prof. Furnstahl's talk

- Successfully preproduce wave function, phase shift
- Different from resonance prediction, E is pre-known

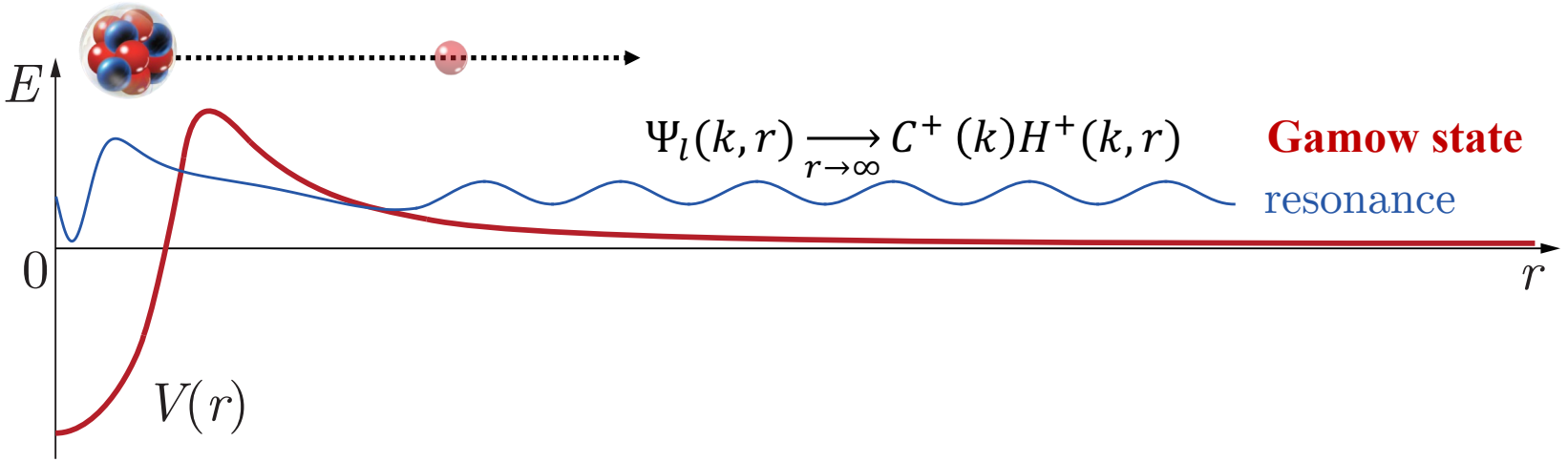
R. Furnstahl *et al.*, Phys. Lett. B 809, 135719 (2020)

Greedy emulators for 2b scattering



J. M. Maldonado *et al.*, Phys. Rev. C 112, 024002 (2025)

Challenges in resonance predictions

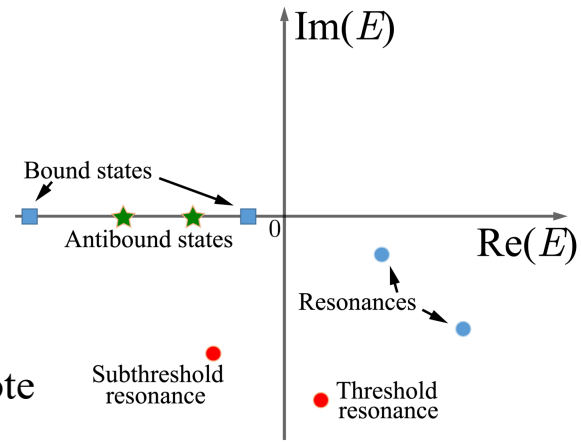


Complex Schrödinger equation

$$\hat{H}\Psi = \tilde{E}\Psi \text{ , where } \tilde{E} = E_R - i\frac{\Gamma}{2}$$

$$\Psi(t) = e^{-i\frac{\hat{H}}{\hbar}t}\Psi(0) = e^{-i\frac{E_R t}{\hbar} - \frac{\Gamma t}{2\hbar}}\Psi(0)$$

Complex energy plane



Challenges

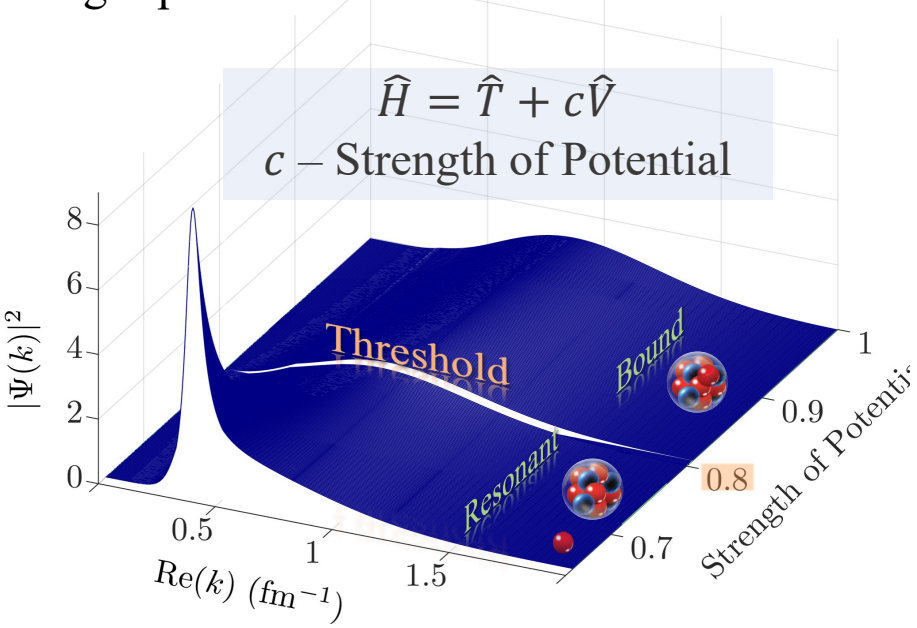
a) Complex physics

b) Easily impacted by the environment and asymptote

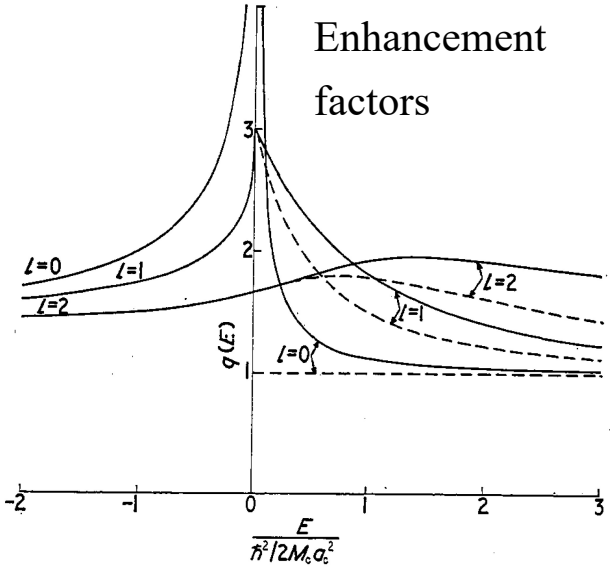
c) Large computational expenses

Challenges in resonance predictions

Single-particle wave function



Wigner cusp



F. C. Barker, Proc. Phys. Soc. 84, 681 (1964)

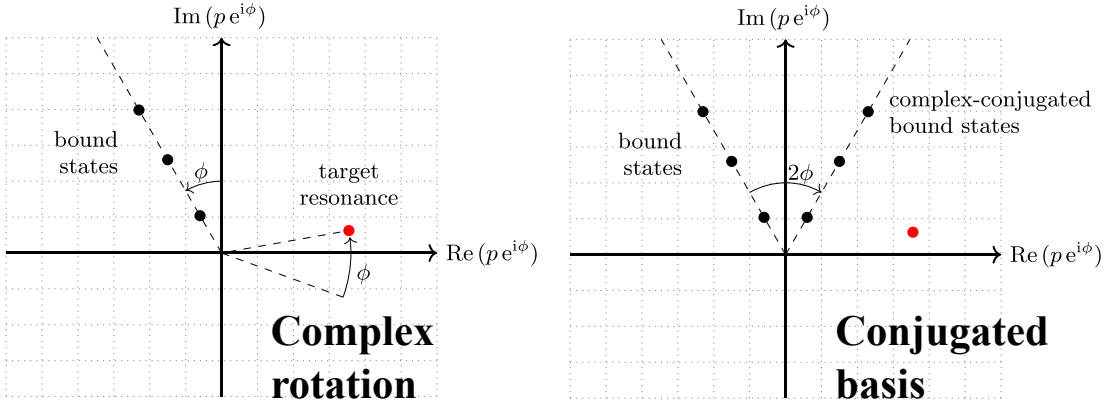
Challenges to overcome for emulators

a) Predict the energy and width at the same time

b) Short-range structure vs long-range observables

c) Discontinuity in wave functions and observables

Complex-augmented eigenvector continuation



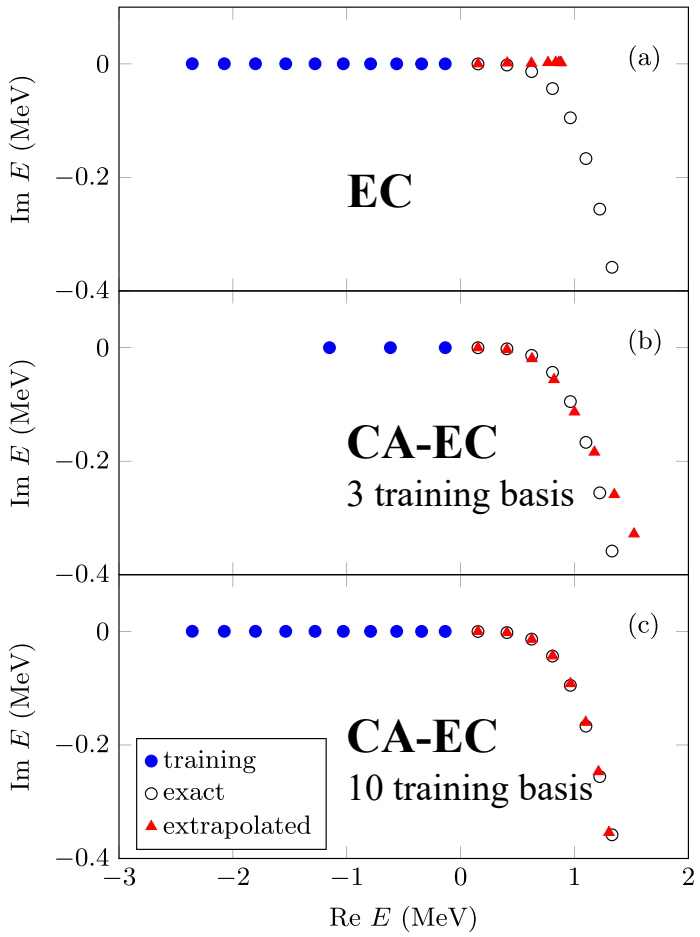
Rotate the complex plane $\quad H^+(k,r) \underset{r\to\infty}{\longrightarrow} e^{+ikr}$

$$H_{\mathrm{EC}} \left|\psi\left(c_*\right)\right\rangle_{\mathrm{EC}} = E\left(c_*\right)_{\mathrm{EC}} N_{\mathrm{EC}} \left|\psi\left(c_*\right)\right\rangle_{\mathrm{EC}} .$$

where

$$\left(H_{\mathrm{EC}}\right)_{ij} = \left\langle\psi\left(c_i\right)\right| H\left(c_*\right) \left|\psi\left(c_j\right)\right\rangle ,$$
$$\left(N_{\mathrm{EC}}\right)_{ij} = \left\langle\psi\left(c_i\right) \mid \psi\left(c_j\right)\right\rangle .$$

N. Yapa *et al.*, Phys. Rev. C 107, 064316 (2023)



N. Yapa *et al.*, Phys. Rev. C 111, 064318 (2025)

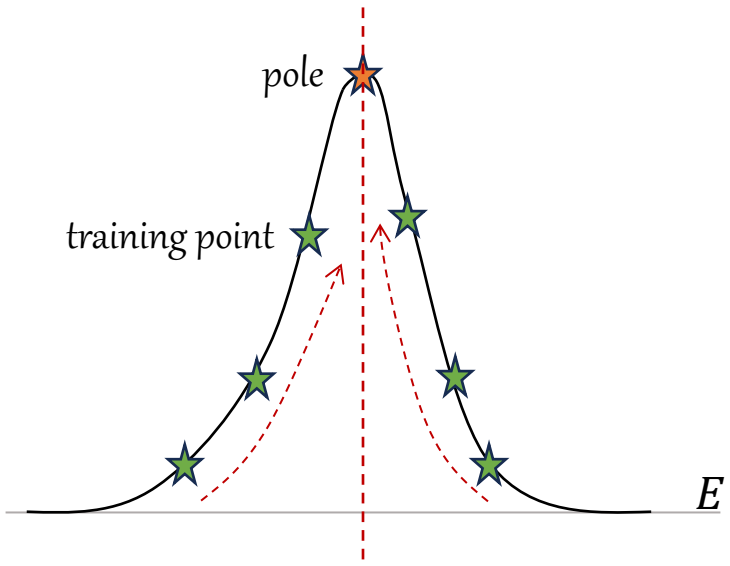
Emulator for response function

- Response function

$$R(E) \equiv \langle S' | \frac{1}{E - H} | S \rangle$$

Accumulated effect from all eigen states

(bound states, resonances, and continuum)



Flowchart

1. Choose complex energies

$$|\Psi_n^{\mathrm{RB}}\rangle = \frac{1}{E_n - H} |S\rangle$$

2. Training basis

$$E_n \to E_n + i\epsilon_n$$

3. Project $[H]$ to subspace, obtaining $[\widetilde{H}]$

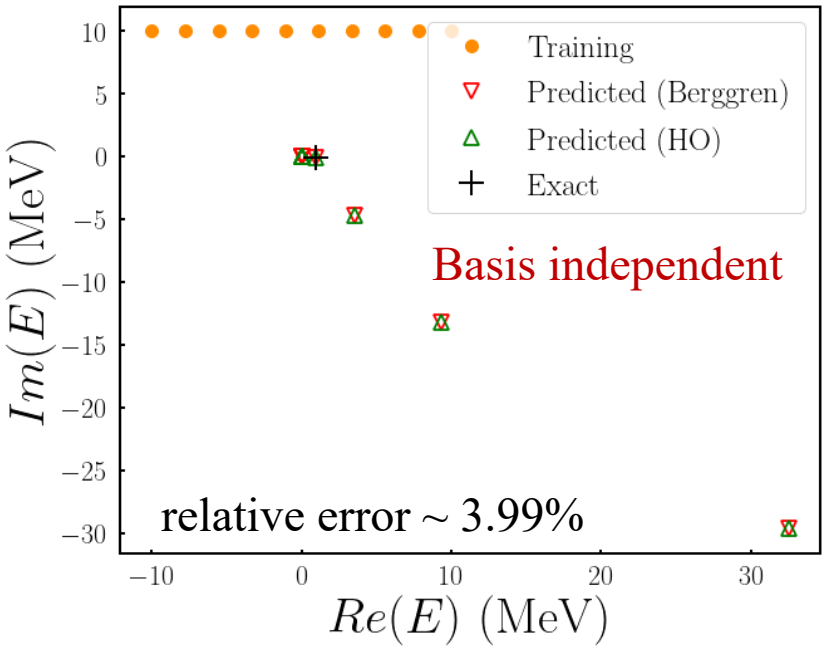
4. Solve eigenvalues E_i^{eig} of $[\widetilde{H}]$

5. Compute $R(E)$ using E_i^{eig}

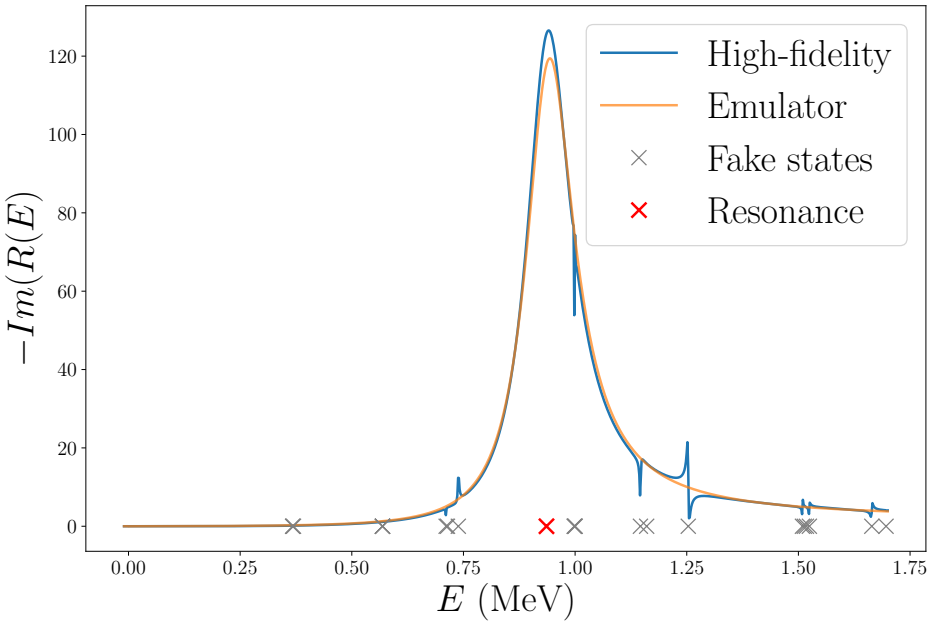
Collaboration with X. L. Zhang

Emulator for response function

Eigen values



Response function



R. Y. Cheng *et al.*, in preparation

- Why does it work?

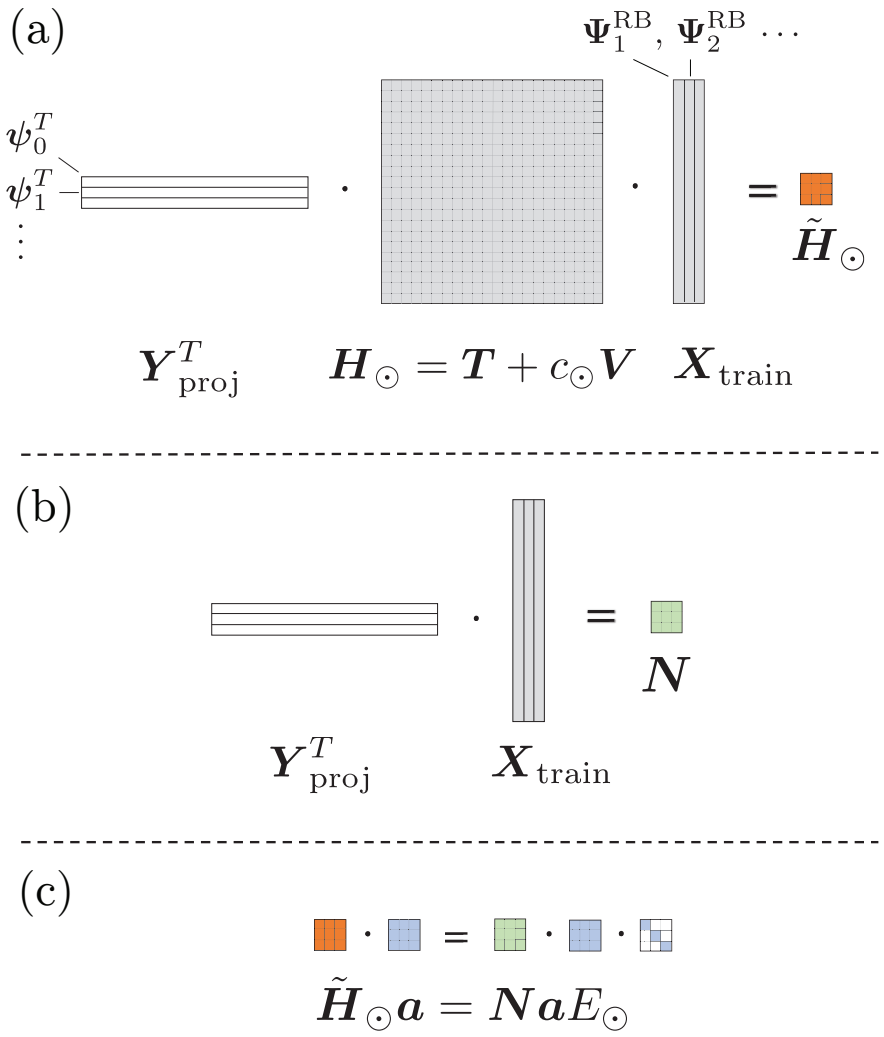
$$|\Psi_n^{\mathrm{RB}}\rangle = \frac{1}{E_n - H}|S\rangle$$

Filter

Upper panel of complex plane

Localized wave function

Reduce basis method (RBM)



- **Training basis**

  Eigenvectors at the *n*-th parameter

$$H_n \Psi_n^{\mathrm{RB}} = E_n \Psi_n^{\mathrm{RB}}$$

  Solve in the high-fidelity space

- **Target wavefunction**

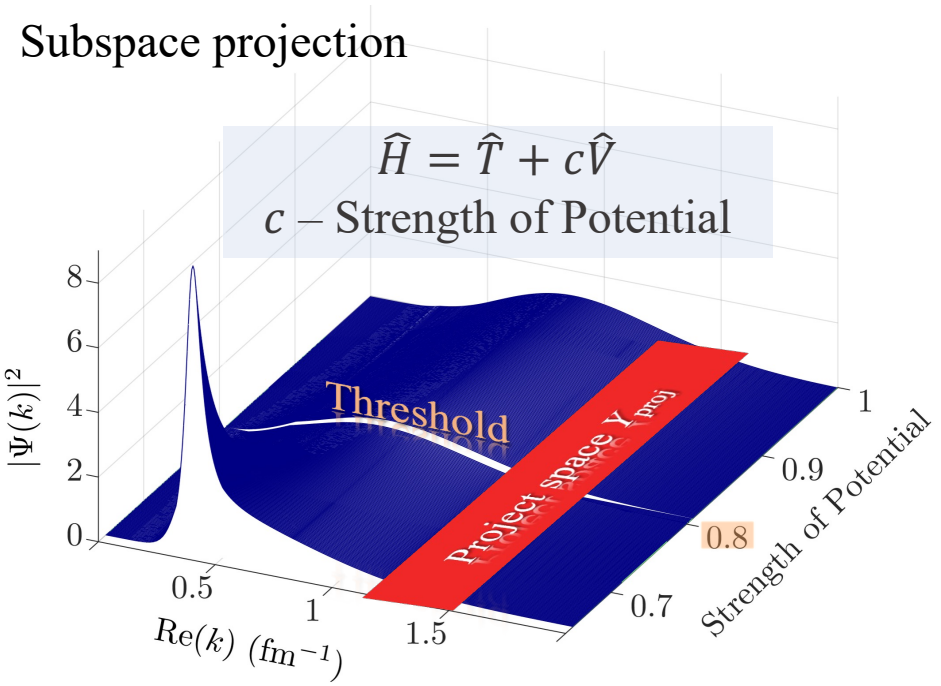
$$H_\odot \Psi_\odot^{\mathbf{Int}} = E_\odot \Psi_\odot^{\mathbf{Int}}$$

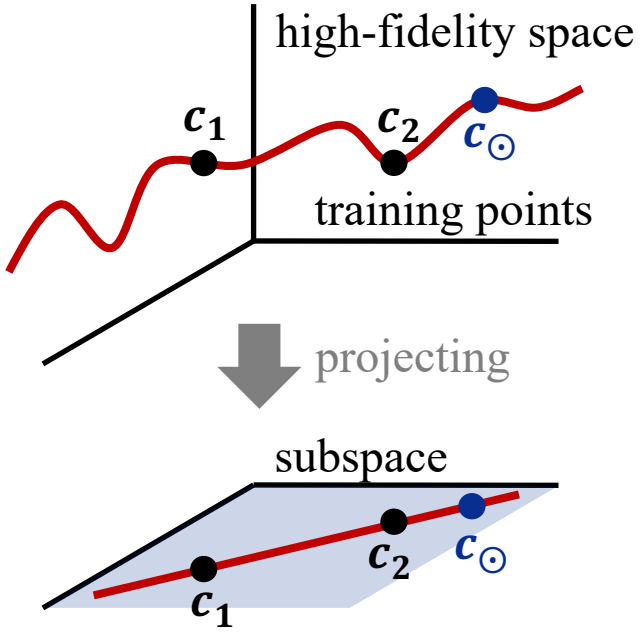
$$\Psi_\odot^{\mathbf{Int}} \approx \sum_{n=0}^{N_b-1} a_n \Psi_n^{\mathrm{RB}} = X_{\mathrm{train}} \cdot a$$

Hint:
system should vary smoothly with parameters

Collaboration with K. Godbey

RBM for resonances



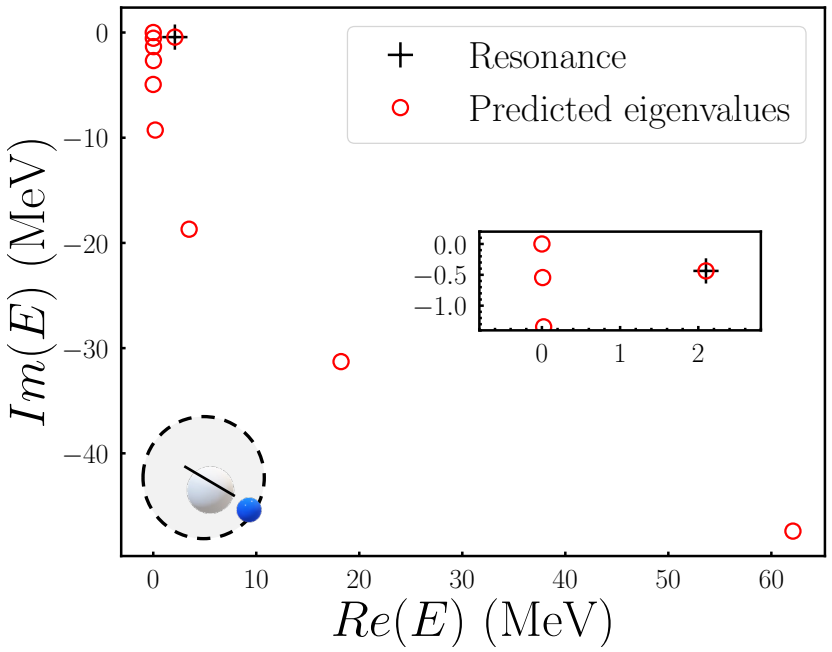


- Training basis $\boldsymbol{X}_{\mathbf{train}}$: at different parameters such as potential strength $\boldsymbol{c}$ or the complex energy $\boldsymbol{E}$
- Projecting basis $\boldsymbol{Y}_{\mathbf{proj}}$: smoothly changed subspace, such as high-momentum free-particle wave

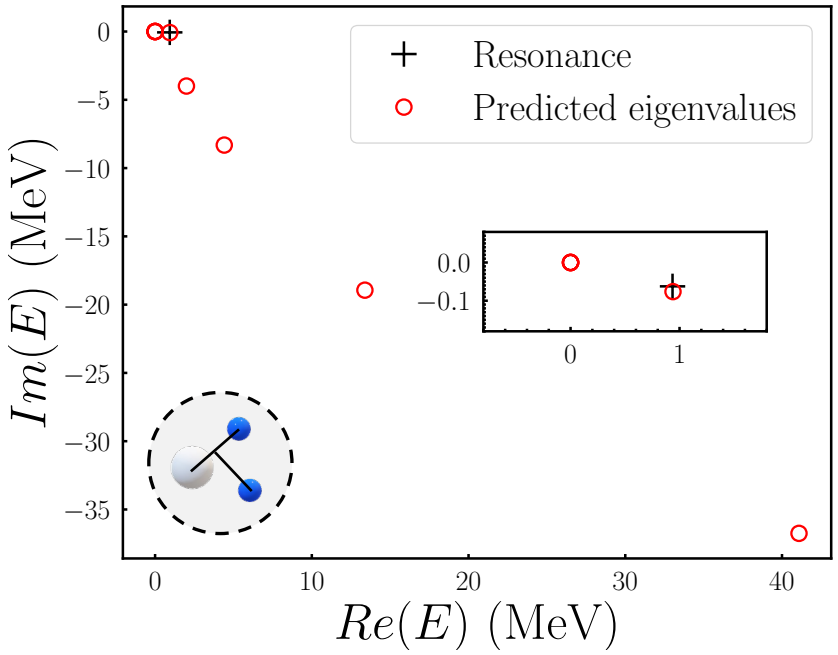
Internal region of a nucleus

RBM for resonances

Two-body system



Three-body system

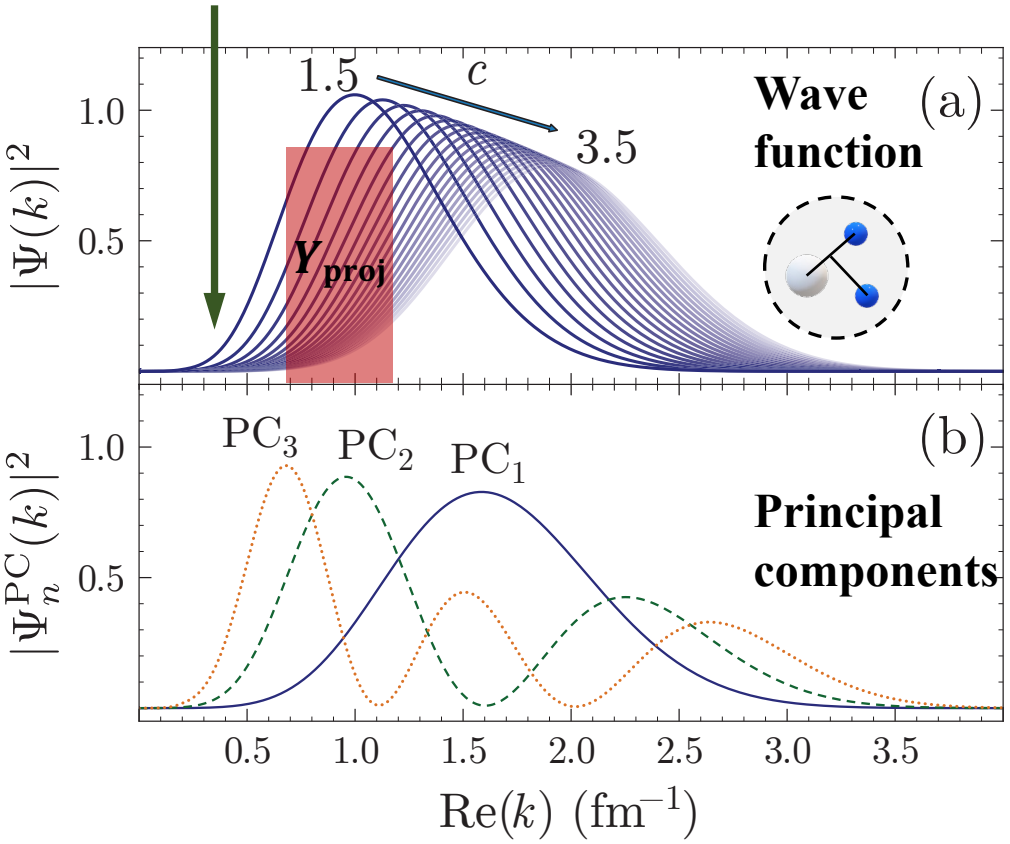


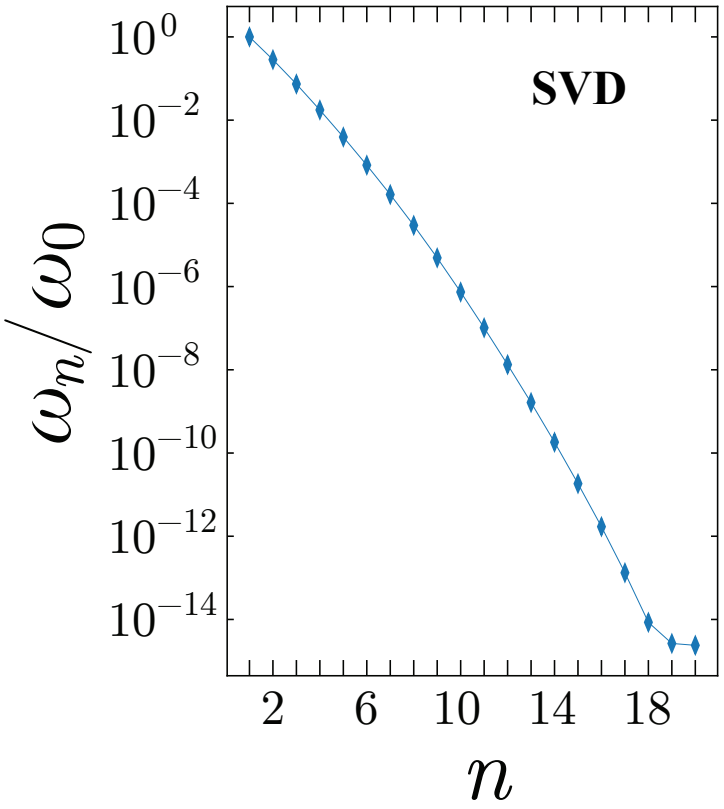
- Training basis $\boldsymbol{X}_{\mathbf{train}}$: at different parameters such as potential strength $\boldsymbol{c}$ or the complex energy $\boldsymbol{E}$
- Projecting basis $\boldsymbol{Y}_{\mathbf{proj}}$: smoothly changed subspace, such as high-momentum free-particle wave

Internal region of a nucleus

Principal-component analysis

Crucial region for continuum

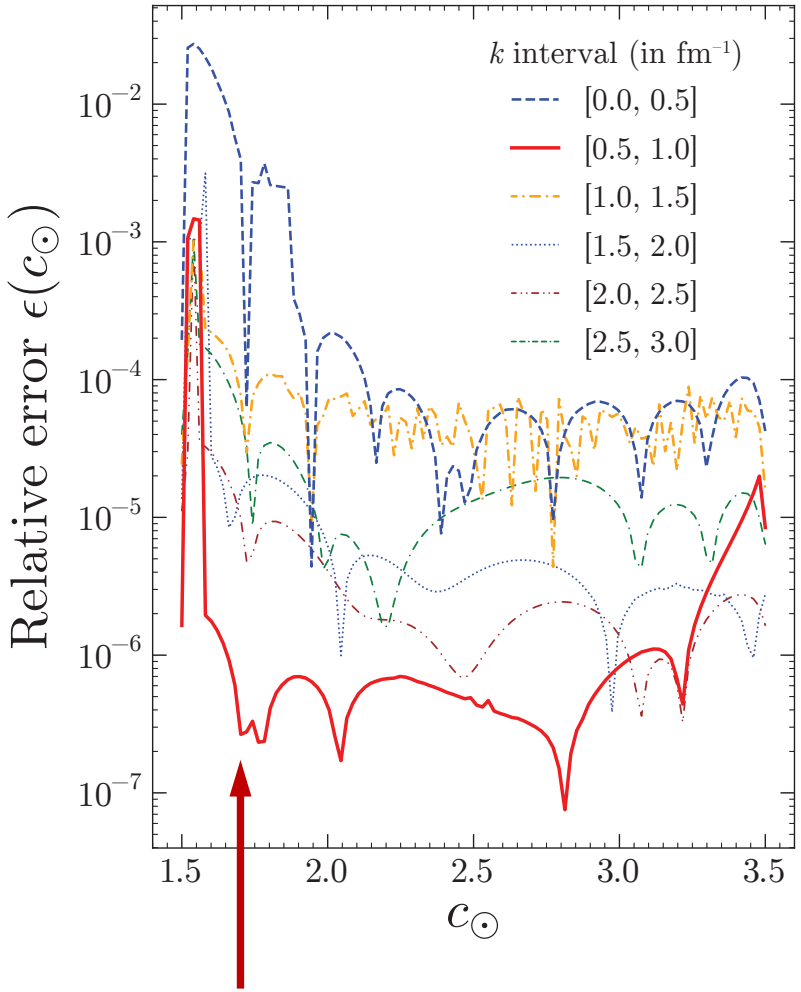


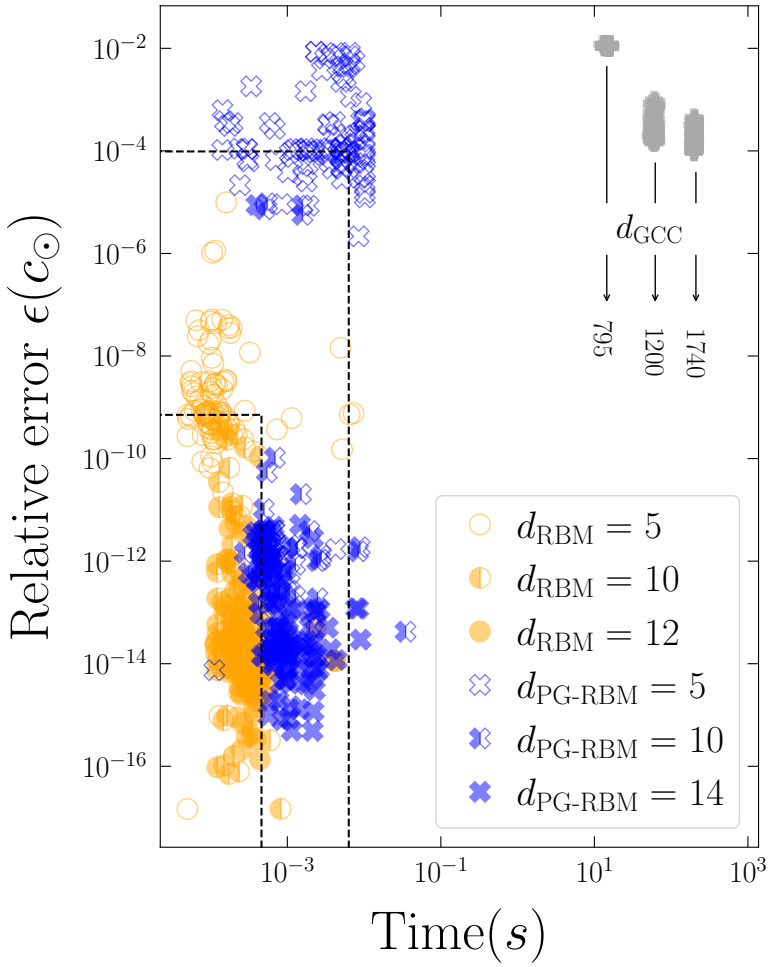


- Training wave function can be bound states

R. Y. Cheng *et al.*, Phys. Rev. C 111, 064315 (2025)

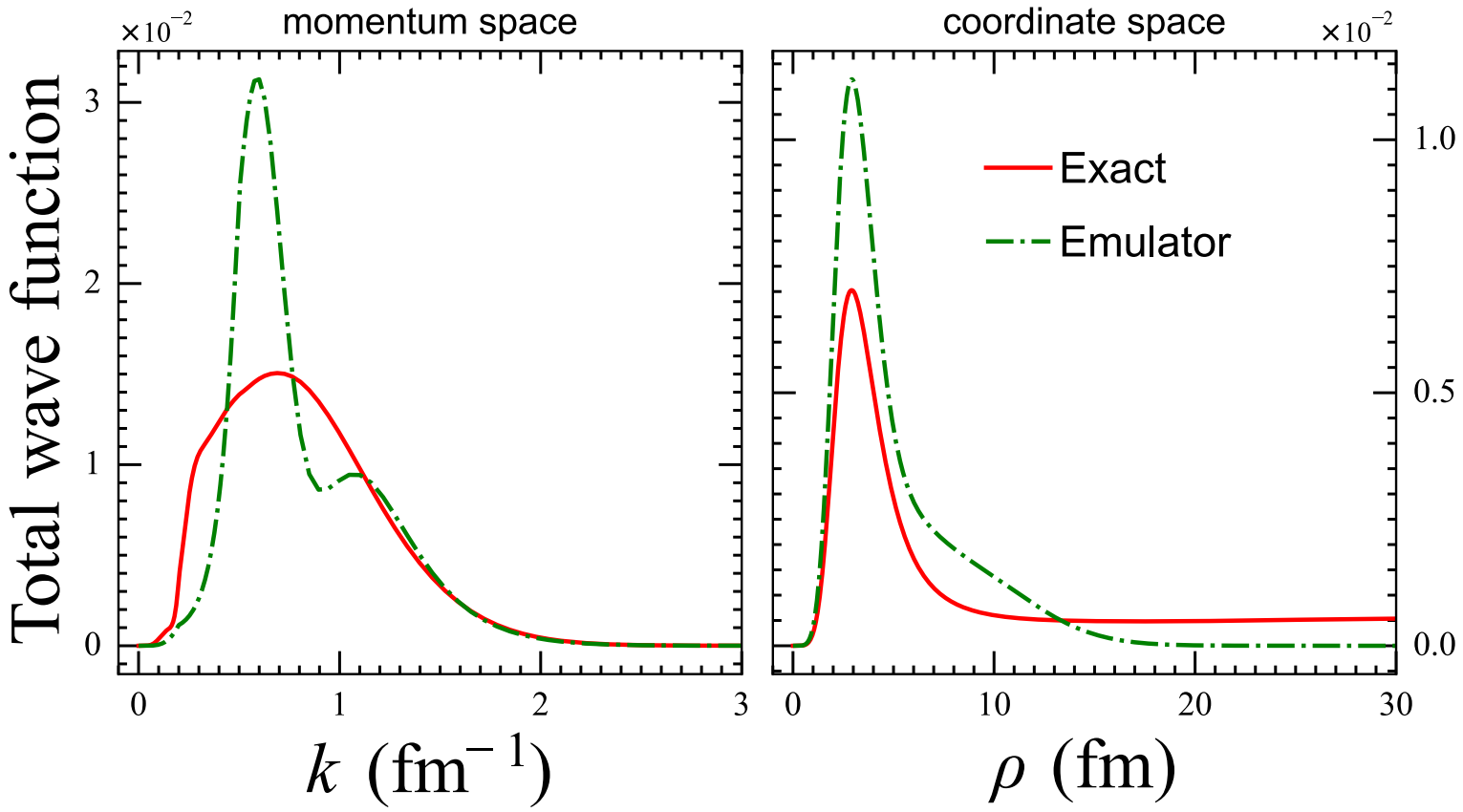
Accuracy & efficiency





$k \in [0.5, 1.0]$ corresponds to the inner-nucleus region strongly impacted by the structure

But at what cost?



- Wavefunction matches inside the nucleus (mid- & high-momenta), but fails asymptotically for both emulators
- Asymptotic-observable predictions might be challenging

Wavefunction correction

Problem: the emulated wavefunction has ignored the asymptotic behavior

$$|\Psi_{\odot}^{(\mathrm{emu})}\rangle = \sum_n a_n |\Psi_n^{\mathrm{RB}}\rangle$$ localized

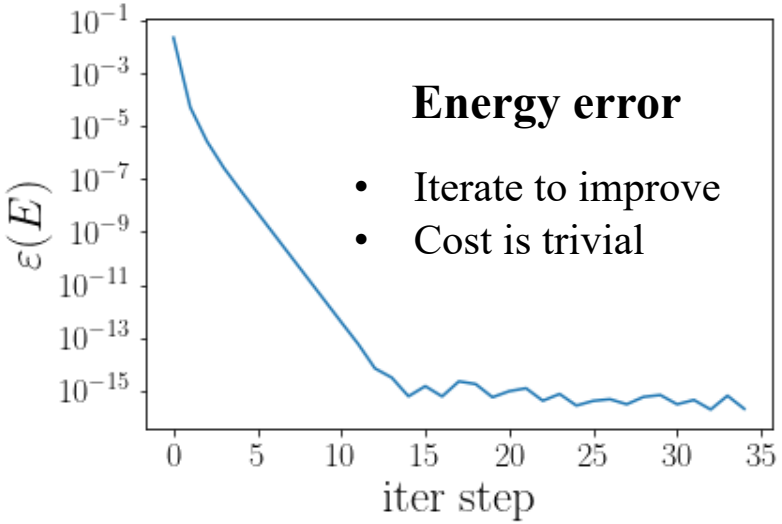
Lippmann-Schwinger equation

$$H_0|\Psi_{\odot}\rangle + \boxed{V_{\odot}|\Psi_{\odot}^{(\mathrm{emu})}\rangle} = E_{\odot}|\Psi_{\odot}\rangle \quad \Rightarrow \quad |\Psi_{\odot}\rangle = \frac{V_{\odot}}{E_{\odot} - H_0}|\Psi_{\odot}^{(\mathrm{emu})}\rangle$$

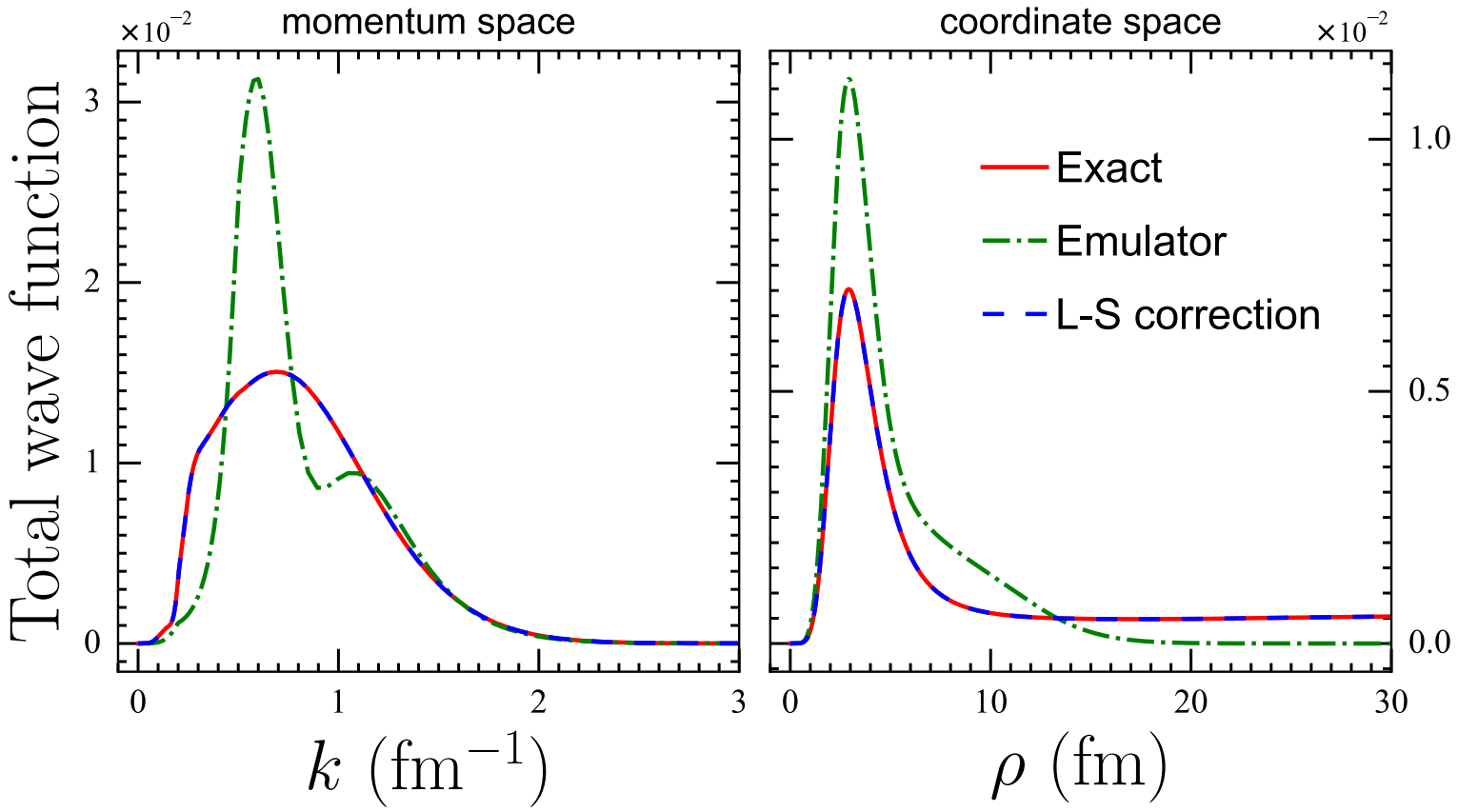
Consider the numerical stability:

$$|\Psi_{\odot}^{(i)}\rangle = (1-\omega)|\Psi_{\odot}^{(i-1)}\rangle + \omega \frac{V_{\odot}}{E_{\odot}^{(i-1)} - H_0}|\Psi_{\odot}^{(\mathrm{i\text{-}1})}\rangle$$

- Maintain the localized component as a reference



Wavefunction correction



- L-S correction improves the overall wave function
- Require additional steps

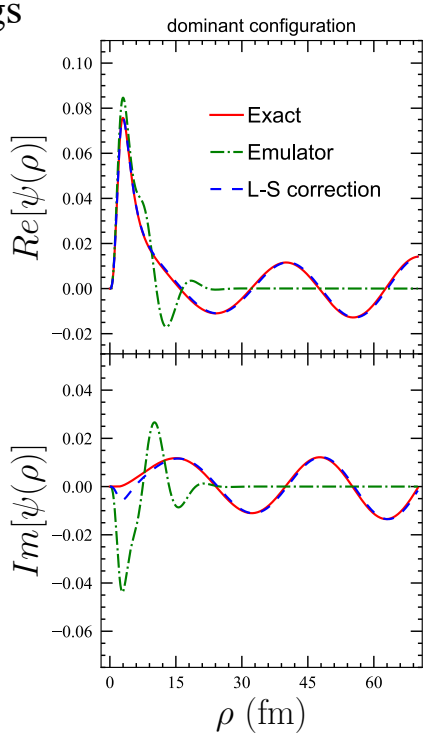
Emulator for asymptotic observables

Challenges: handle structure and asymptotic observables on the same footings

Potential solutions:

1. **RBM for resonances/response function**
   a) Good for structure & energy
   b) Require additional process for asymptotic wave function

2. **PMM for open quantum systems (ongoing project)**
   a) Maintains quantum mechanical interpretability
   b) Train energy and observable simultaneously



Underlying equations

$$\begin{cases} H(c) = H_0 + cH_1 \\ H(c)\,|\psi(c)\rangle = E(c)\,|\psi(c)\rangle \\ \langle\psi(c)|O|\psi(c)\rangle = f(c) \end{cases}$$

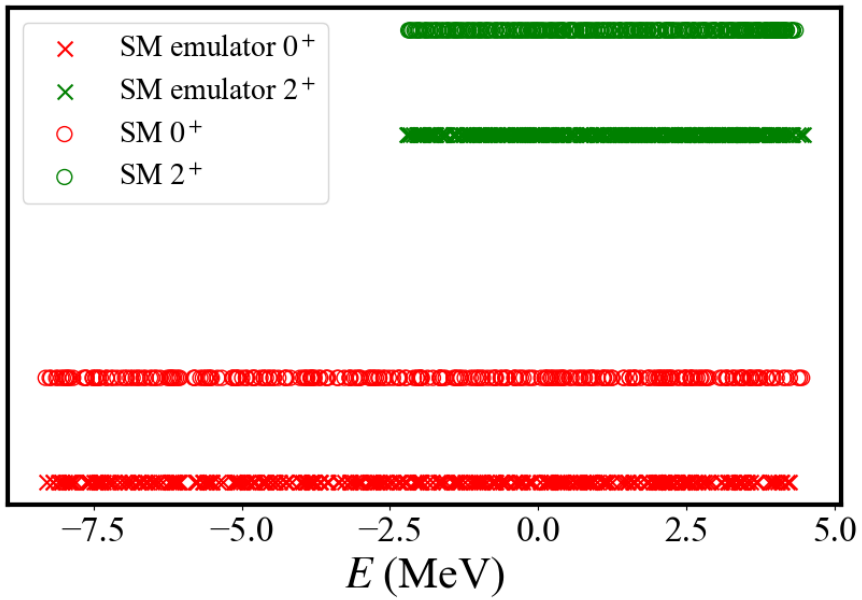
PMM

$$\begin{cases} M(c) = \underline{M_0} + c\underline{M_1} \\ M(c)\,\big|\tilde{\psi}(c)\big\rangle = \tilde{E}(c)\,\big|\tilde{\psi}(c)\big\rangle \\ \big\langle\tilde{\psi}(c)\big|\underline{X}\big|\tilde{\psi}(c)\big\rangle = \tilde{f}(c) \end{cases}$$

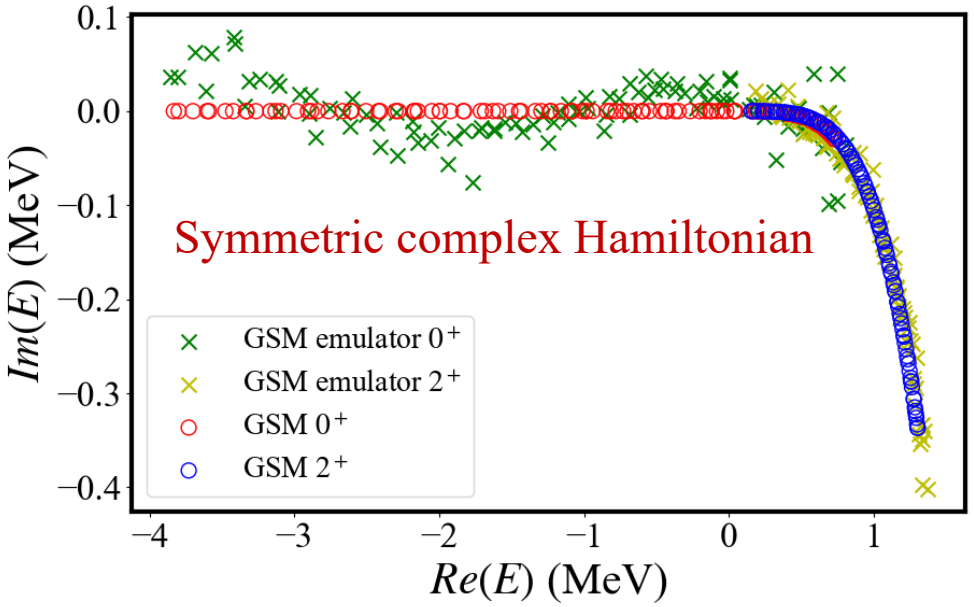
Adopted from D. Jammooa's presentation

PMM first attempt

PMM for closed systems



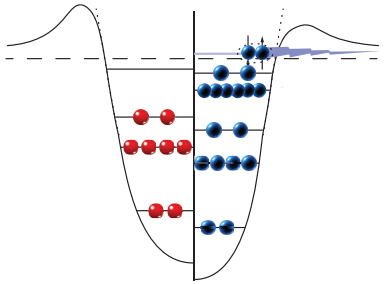
PMM for open systems

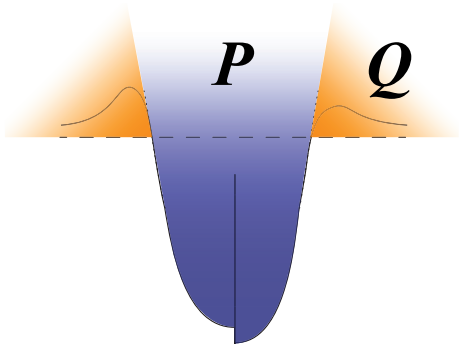


- PMM works very well for closed quantum systems (CQSs)
- Extend to rigged Hilbert space for open quantum systems (OQSs)
- Fails to reproduce the eigen values directly

Emulator for asymptotic observables

Open quantum system





Closed quantum physics

$$\begin{pmatrix} H_{\mathcal{PP}} & H_{\mathcal{PQ}} \\ H_{\mathcal{QP}} & H_{\mathcal{QQ}} \end{pmatrix} \begin{pmatrix} \mathcal{P}\Psi \\ \mathcal{Q}\Psi \end{pmatrix} = E \begin{pmatrix} \mathcal{P}\Psi \\ \mathcal{Q}\Psi \end{pmatrix}$$

Continuum physics

Continuum coupling

Prepare training data (E, O) for close and open systems

Train CQSs

$$M_{\mathcal{PP}}(c) = M^a_{\mathcal{PP}} + c\, M^b_{\mathcal{PP}}$$

$$M_{\mathcal{PP}}(c)|\Psi_{\mathcal{P}}\rangle = E_{\mathcal{P}}(c)|\Psi_{\mathcal{P}}\rangle$$

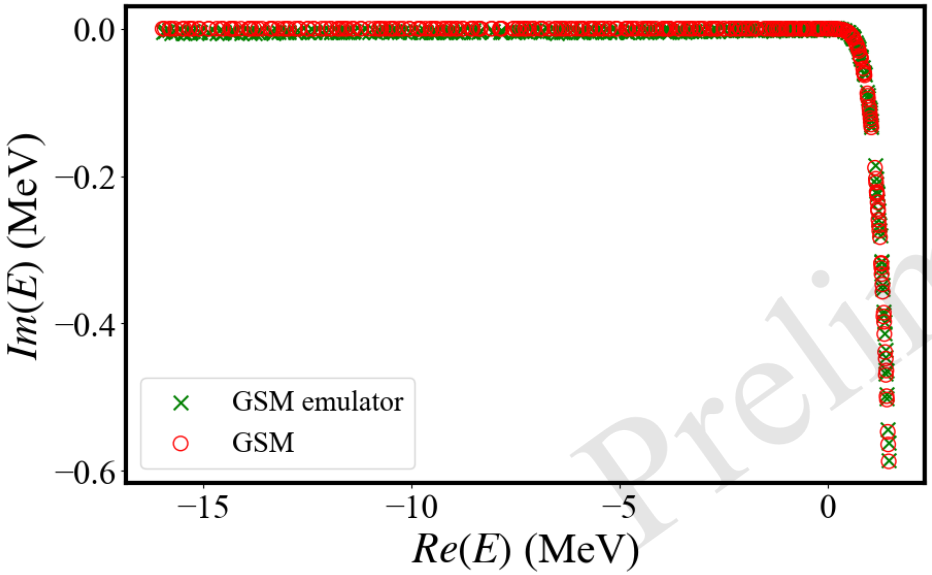
$$M = \begin{pmatrix} M_{\mathcal{PP}} & M_{\mathcal{PQ}} \\ M_{\mathcal{QP}} & M_{\mathcal{QQ}} \end{pmatrix}$$

Train OQSs similarly

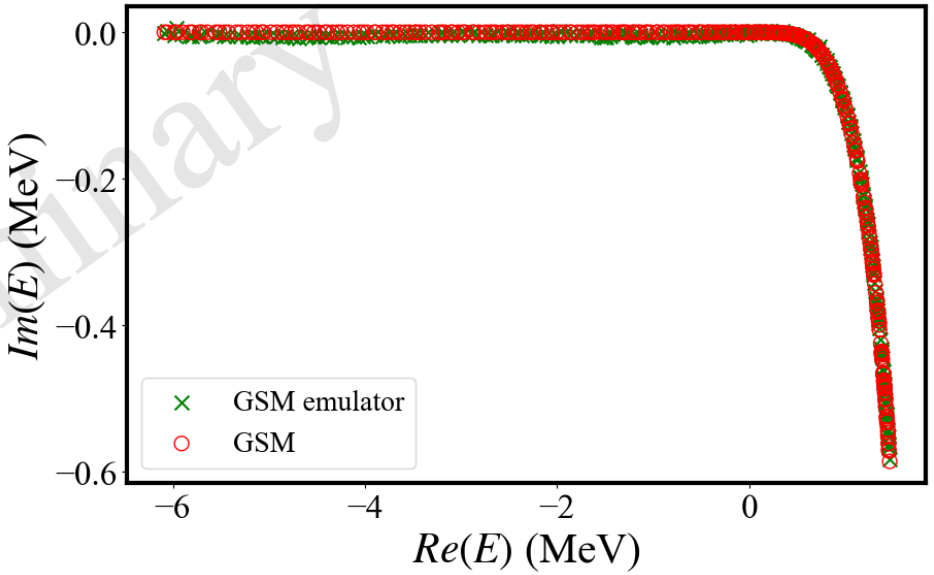
Find E through $\langle\Psi|\Psi_{\mathcal{P}}\rangle$

Emulator for asymptotic observables

^{6}He Ground state



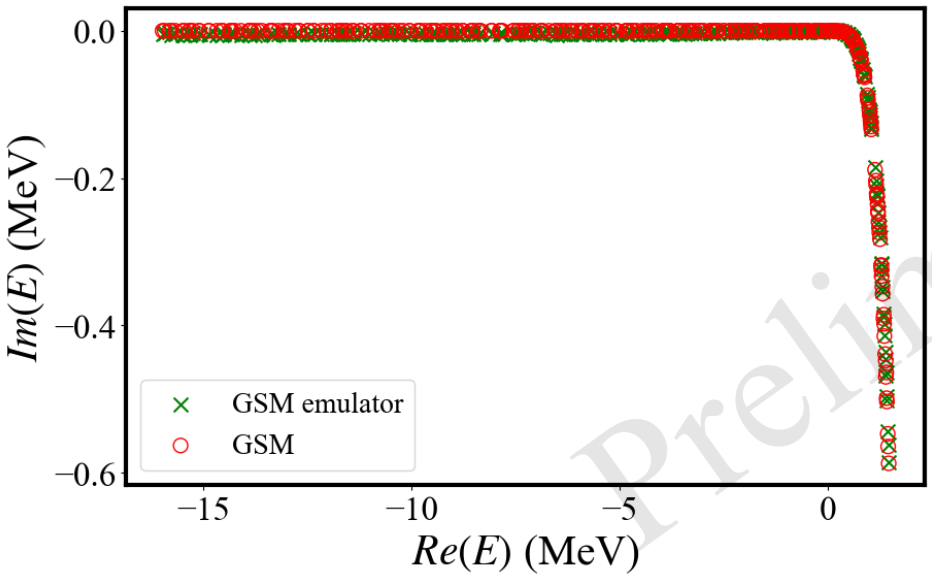
^{6}He 2^+ state



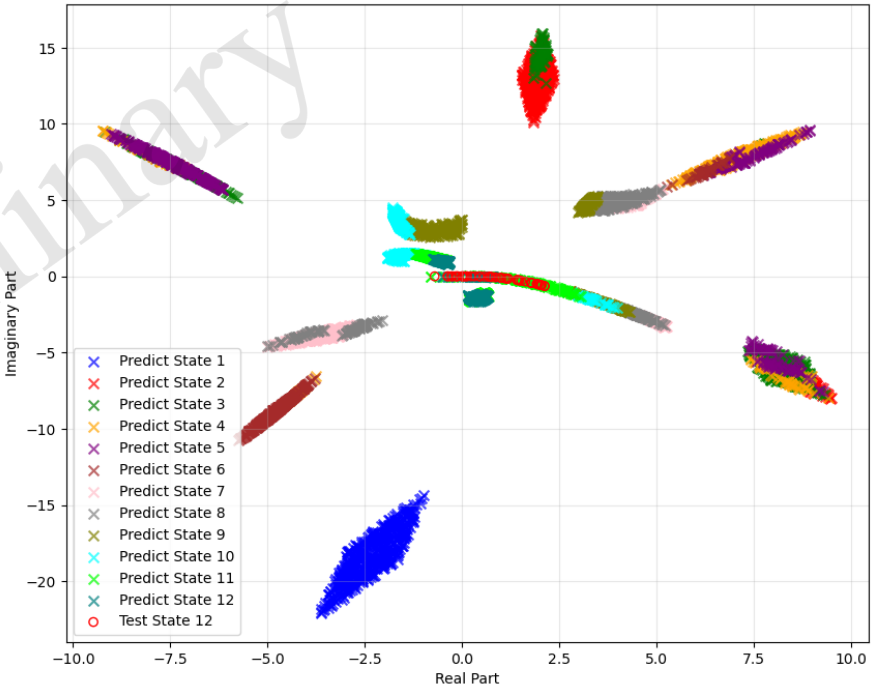
- Based on PQ method, construct GSM emulator
- Use SM emulator to obtain eigenstates, guide the selection of corresponding states
- GSM emulator reproduce the high-fidelity results very well

Emulator for asymptotic observables

^{6}He Ground state

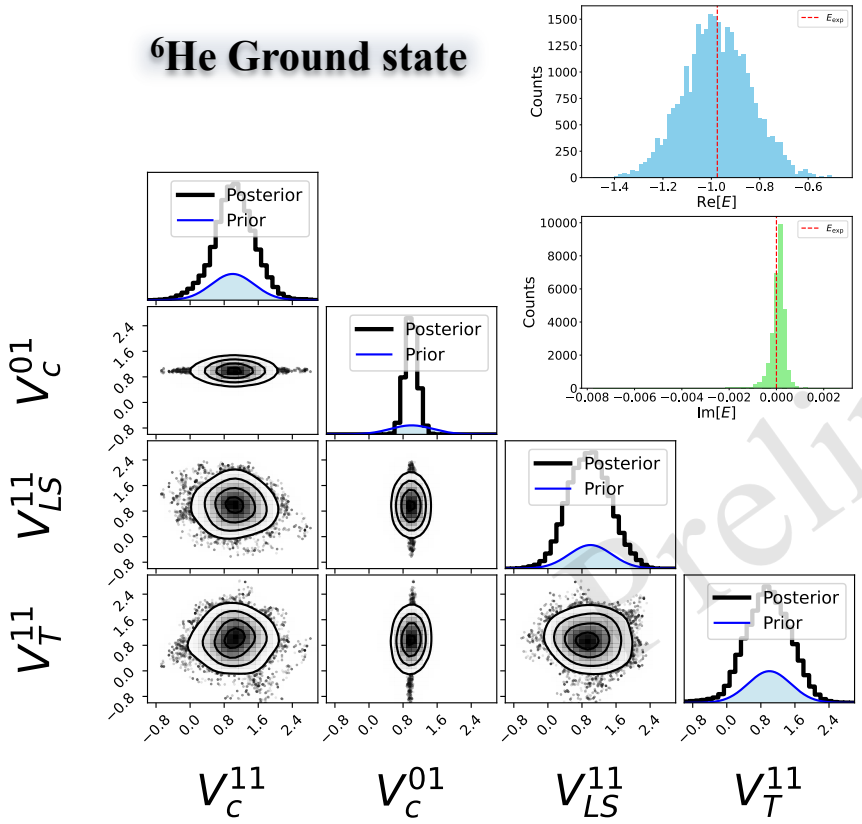


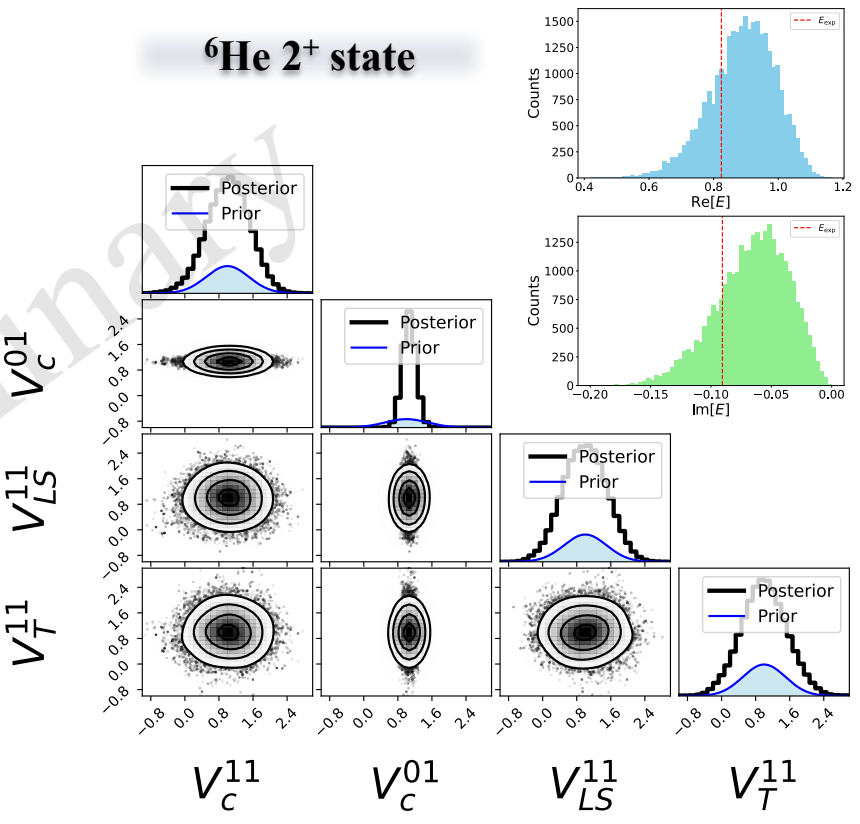
Eigenvalue distribution



- Based on PQ method, construct GSM emulator
- Use SM emulator to obtain eigenstates, guide the selection of corresponding states
- GSM emulator reproduce the high-fidelity results very well

Perspectives





- Try to study the continuum coupling
- $V_T{}^{11}$ shows weakest constraint with widest posterior distribution
- Parameter correlations reveal compensation effects in nuclear force components

Thank you for your attention!

Summary

1. **Open quantum systems:** complex physics, asymptotic behavior, decaying property
2. **Emulators**
   a) EC for response function
   b) RBM for resonance energy/width
   c) PMM for continuum coupling
3. **Perspectives**
   a) Uncertainty quantifications
   b) Time evolution
   c) Other observables: *nn* correlations

Acknowledgements

FRIB · Universitas Varsoviensis · Washington University in St. Louis · Florida State University · Peking University · UMass Lowell · IMP · GSI · GANIL (laboratoire commun CEA/DRF – CNRS/IN2P3) · Spiral2 · …

Collaborators

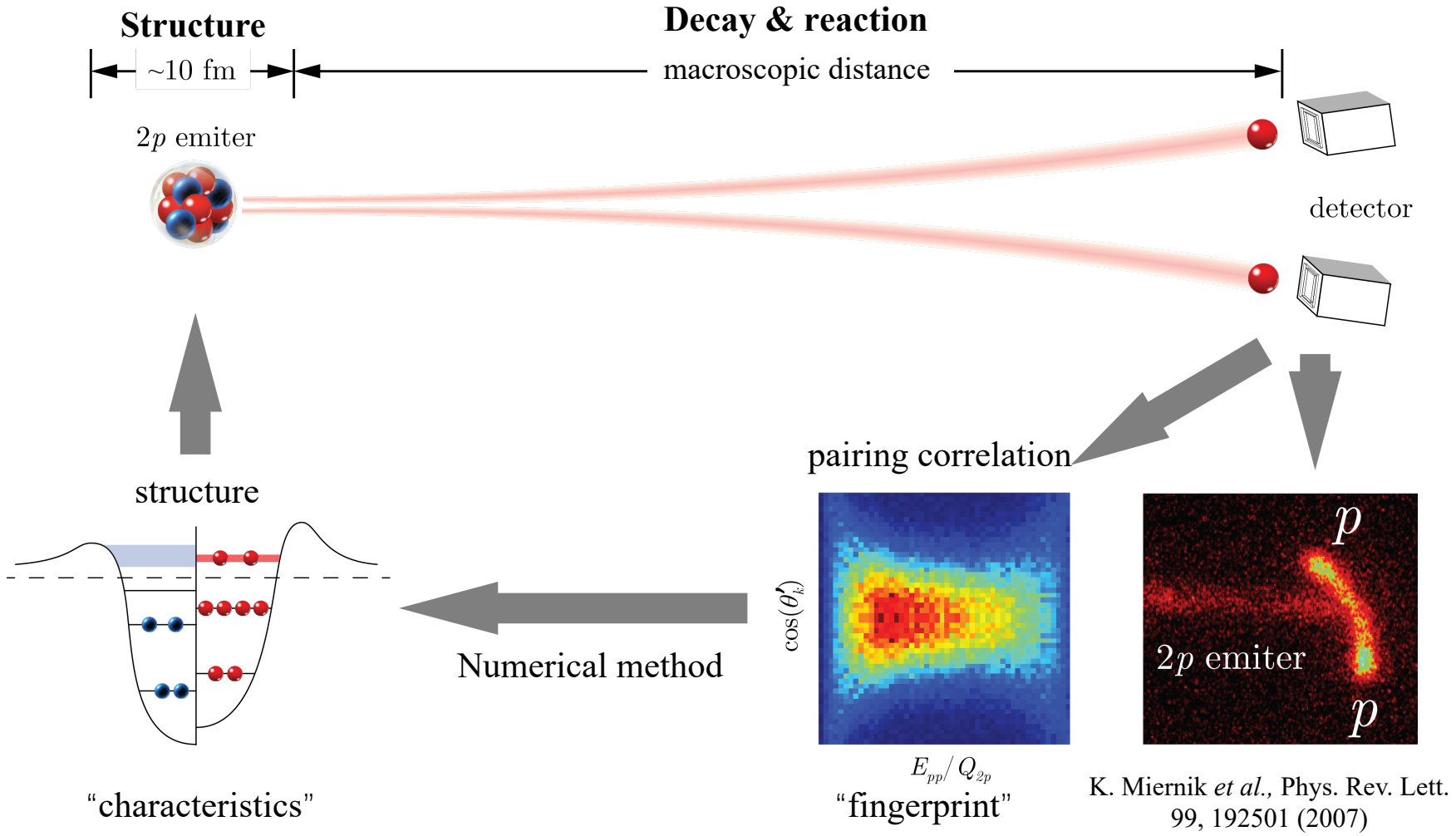
- R. Y. Cheng
- K. Godbey
- W. Nazarewicz
- A. Volya
- Z. C. Xu
- X. L. Zhang
- Y. G. Ma
- …

Questions

1. How to handle both internal and external wave function properly?
2. How to connect the asymptotic observables with structure information?
3. How to improve the prediction power of an emulator?
4. If there are some uncertainties/errors in the training data, can the emulator handle it?
5. A data driven PMM?

Backup

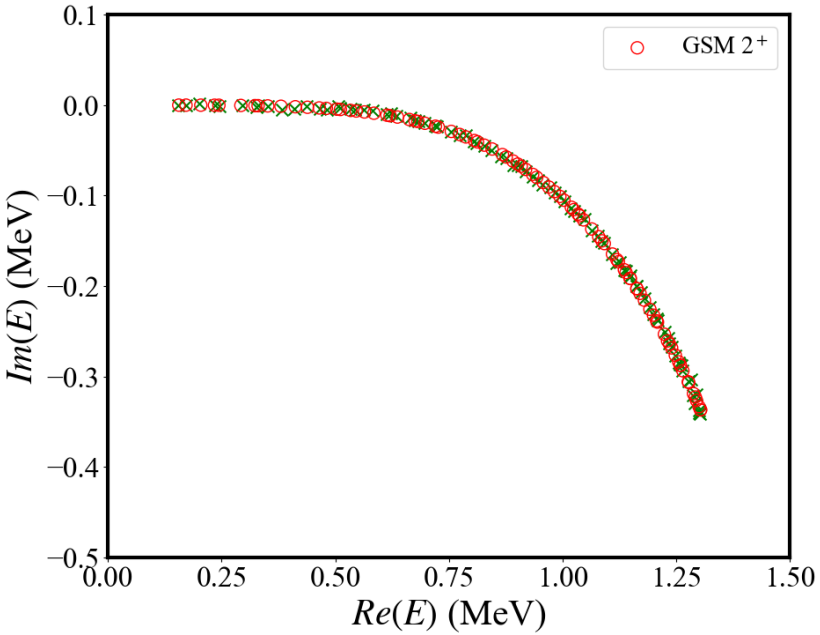
Structure ⟷ Asymptotic observables



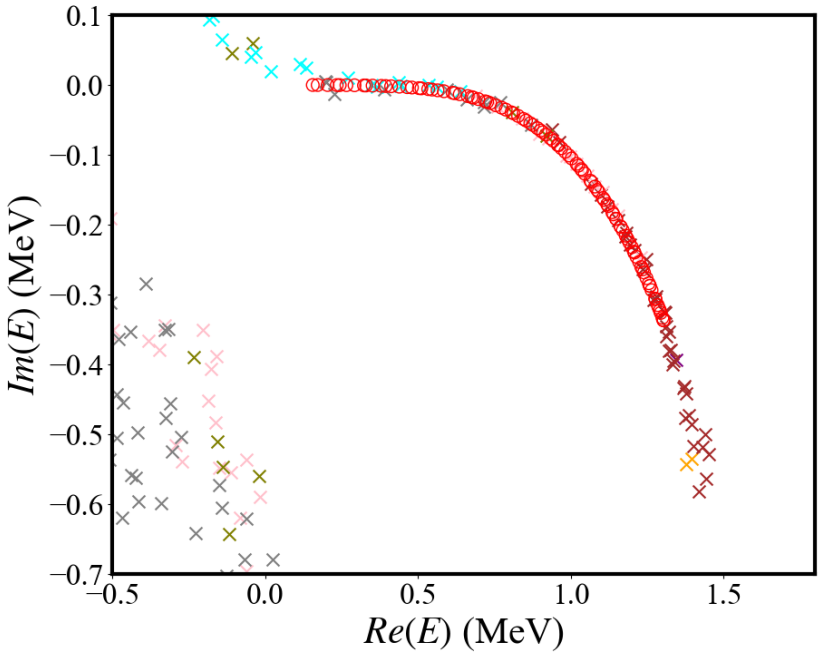
K. Miernik *et al.*, Phys. Rev. Lett. 99, 192501 (2007)

GSM emulator extrapolation

We change the way to train the emulator, in which we find the closest value to train. The results is better, but not good enough.



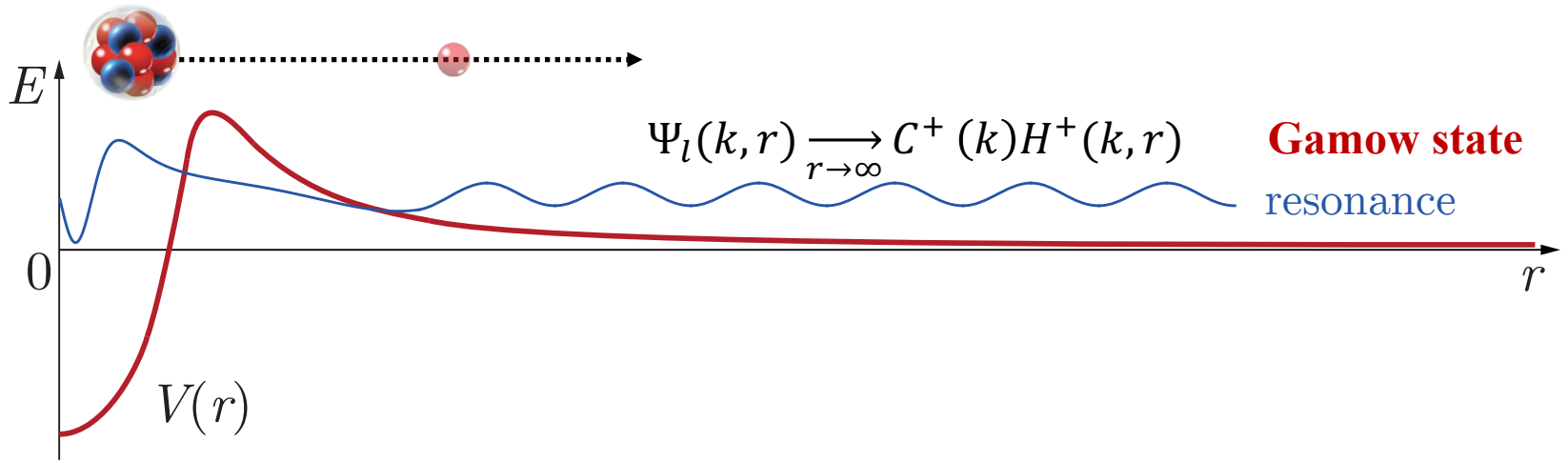
train data



extrapolation

- The eigenvalues of the matrices are widely dispersed.
- The extrapolation capability appears to be bad.
- The eigenvalues on the extrapolation line do not originate from the same energy level series.

Quantum picture of decay



Real-energy expansion

$$|\Psi\rangle \propto \oint_L \frac{1}{E-\tilde{E}}|E\rangle \mathrm{d}E$$

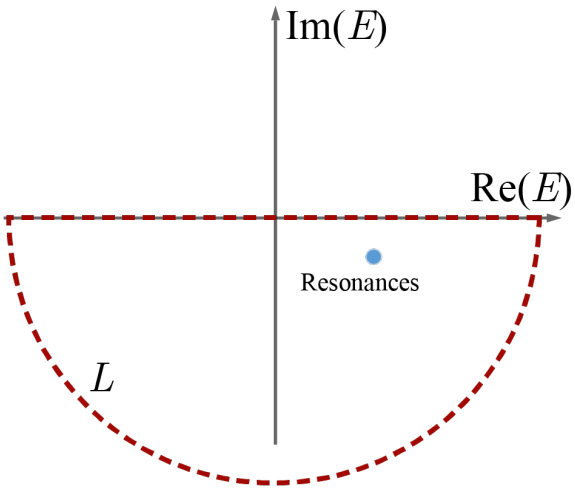
Survival probability

$$\mathcal{S}(t) = |\langle \Psi(t) \mid \Psi(0)\rangle|^2$$

$$\propto \left| \oint_L \frac{\langle E \mid E\rangle}{|E-\tilde{E}|^2} e^{-i\frac{E}{\hbar}t}\, \mathrm{d}E \right|^2$$

Spectral function

Complex energy plane



Gamow coupled-channel (GCC) method

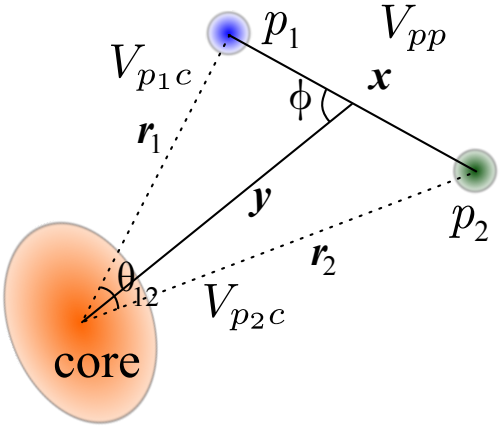
- The 3-body **Hamiltonian** can be written as:

$$\hat{H} = \sum_{i=1}^{3} \frac{\hat{\vec{p}}_i^2}{2m_i} + \sum_{i=1}^{2} V_{p_i c} + V_{pp} + \hat{H}_{\rm core} - \hat{T}_{\rm c.m.}$$

- **Total wave-function** $\Psi^{J\pi} = \sum_{J_p \pi_p j_c \pi_c} \left[\Phi^{J_p \pi_p} \otimes \phi^{j_c \pi_c} \right]^{J\pi}$

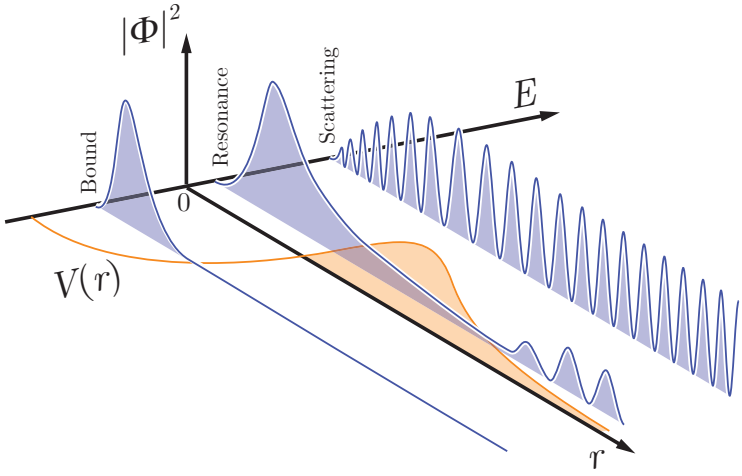
valence nucleons

deformed core



1. **Jacobi coordinates**
   a) No spurious center-of-mass motion
   b) Proper 3-body asymptotic behavior
2. **Berggren basis**
   a) Bound, scattering, and Gamow states
   b) Structure and decay information

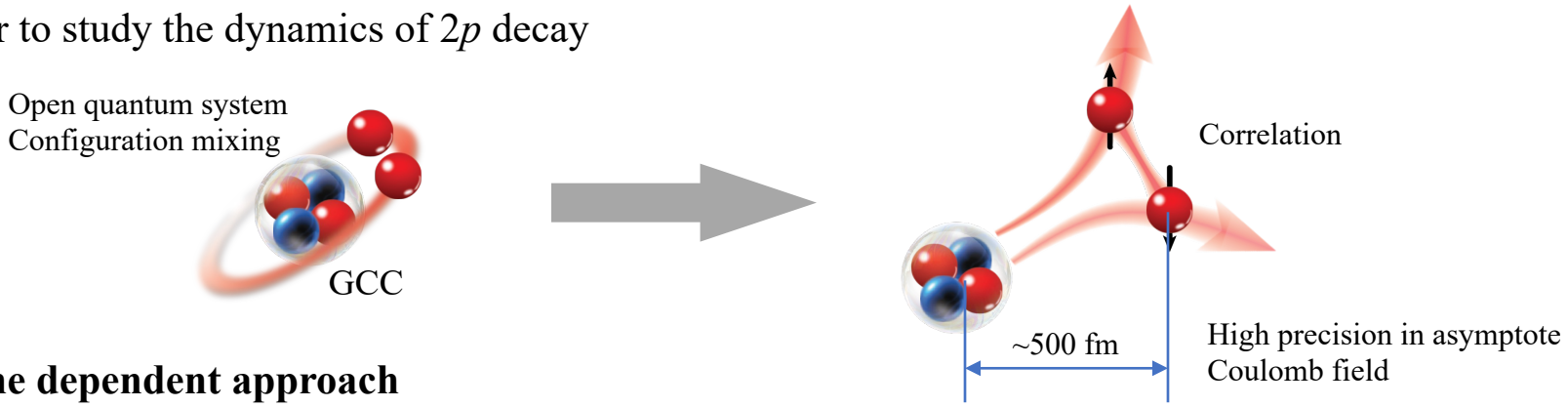
Berggren basis



SW and W. Nazarewicz, Phys. Rev. Lett. 120, 212502 (2018)

Time dependent (TD) approach

In order to study the dynamics of 2*p* decay



- **Time dependent approach**

$$e^{-i\frac{\hat{H}}{\hbar}t} = \sum_{n=0}^{\infty}(-i)^n\,(2-\delta_{n0})\,J_n(t)T_n(\hat{H}/\hbar)$$

  - Time propagator can be expanded with Chebyshev polynomials.
  - Initial wave function is obtained by GCC, which includes configuration mixing and proper asymptote.
  - Two-proton wave function has been propagated to over 500 fm.

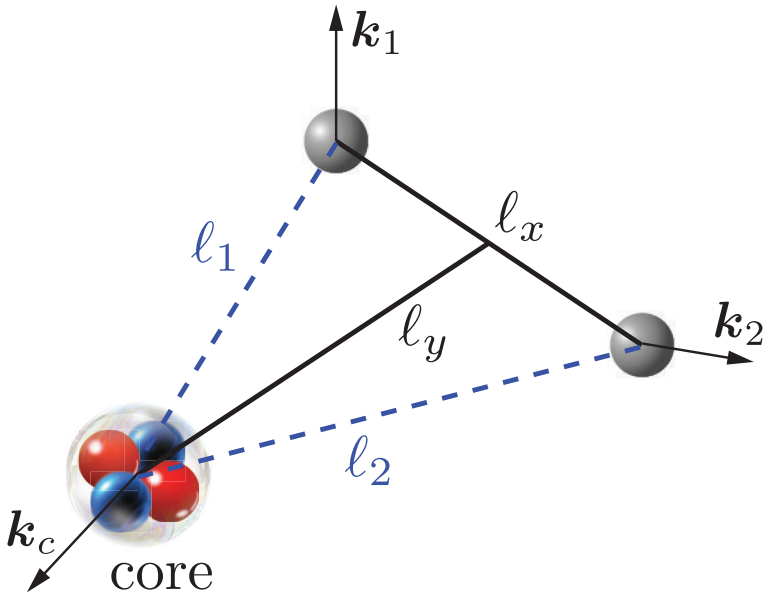
- **Green's functional method** to benchmark

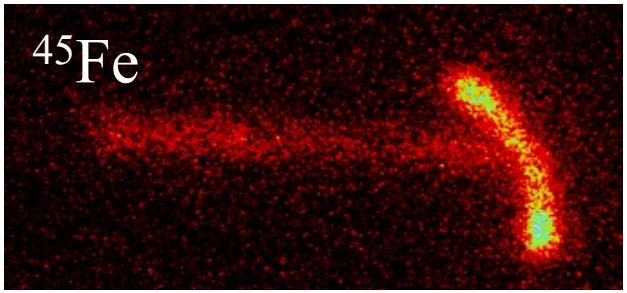
$$G(E) = \frac{1}{E-H} = -i\int_0^{\infty} dt\ \exp(iEt)\exp(-iHt)$$

  - Time propagator and Green's function can be connected by Fourier transformation.

SW and W. Nazarewicz, Phys. Rev. Lett. 126, 142501 (2021)

Two-proton ($2p$) decay





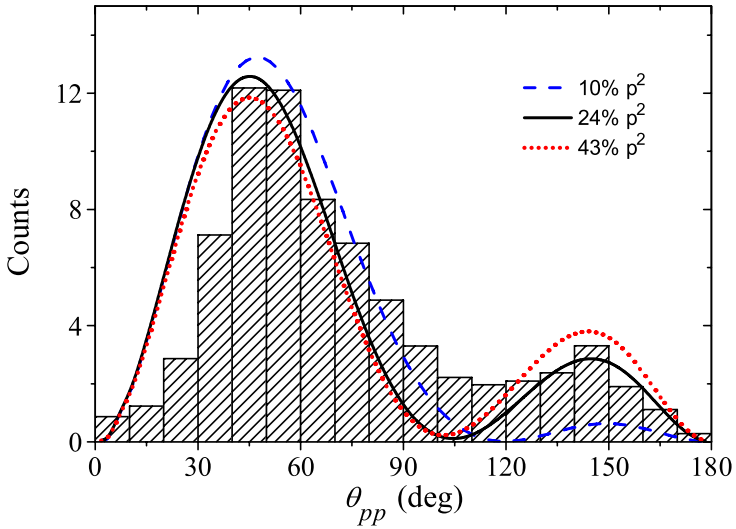
J. Giovinazzo *et al.*, Phys. Rev. Lett. 89, 102501 (2002)

Jacobi ⟷ **Single-particle**

(ℓ_x, ℓ_y) ⟷ (ℓ_1, ℓ_2)

$(0, 0)$ ⟷ (s, s), (p, p), (d, d), (f, f)

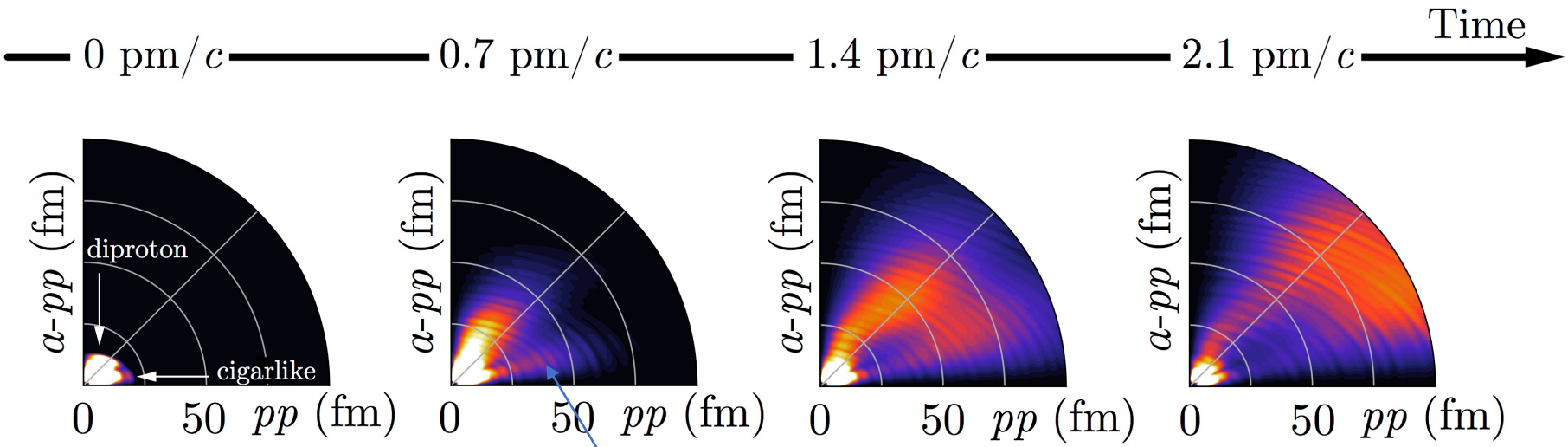
clustering

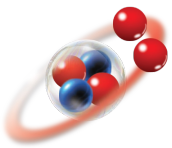


K. Miernik *et al.*, Phys. Rev. Lett. 99, 192501 (2007)

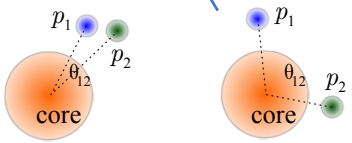
- Diproton structure will introduce configuration mixing.

2*p* decay in ^{6}Be

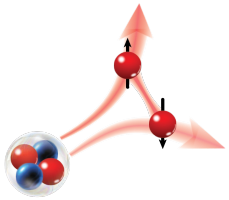




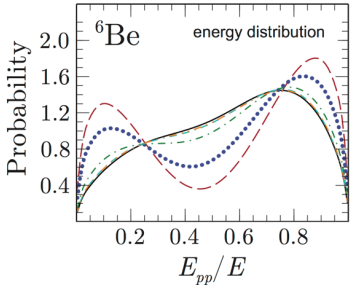
Protons inside nucleus



Two types of tunneling:
1. diproton (primarily)
2. cigarlike



Diproton branch bends due to Coulomb repulsion



Asymptotic correlation begin to converge

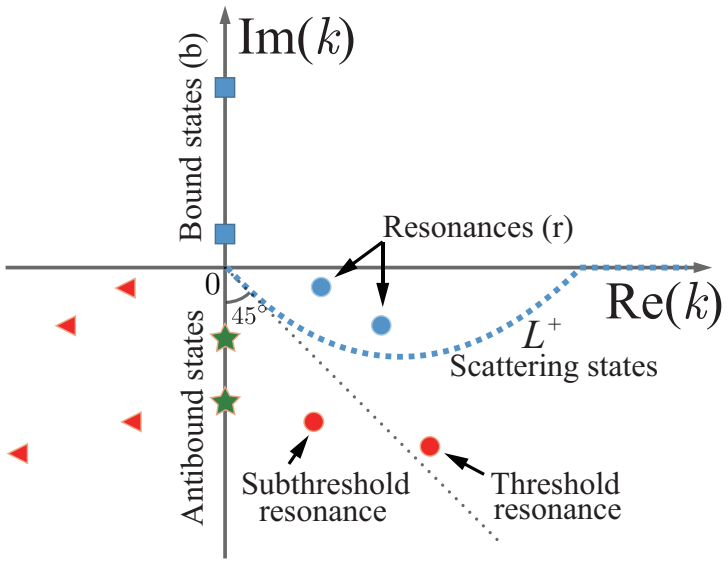
SW and W. Nazarewicz, Phys. Rev. Lett. 126, 142501 (2021)

Complex-plane framework

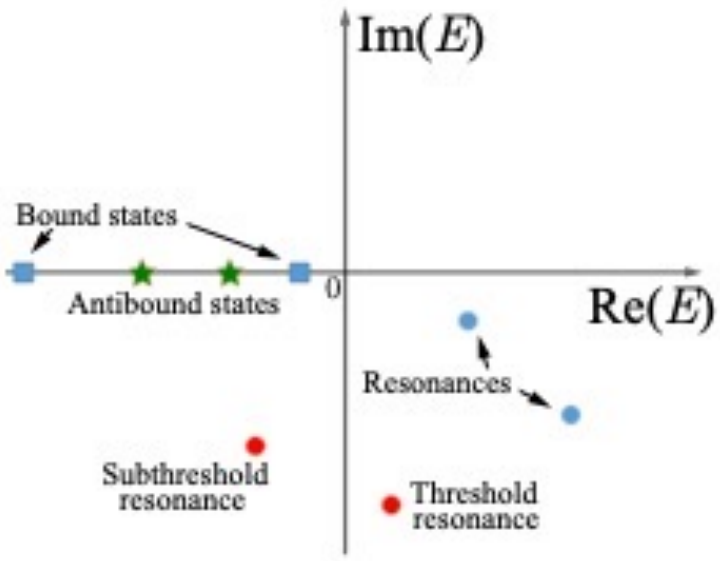
- **Decay width/Lifetime**
  - Complex symmetric Schrödinger equation

$$\hat{H}\Psi = \tilde{E}\Psi, \text{ where } \tilde{E} = E - i\frac{\Gamma}{2}$$

Complex momentum plane

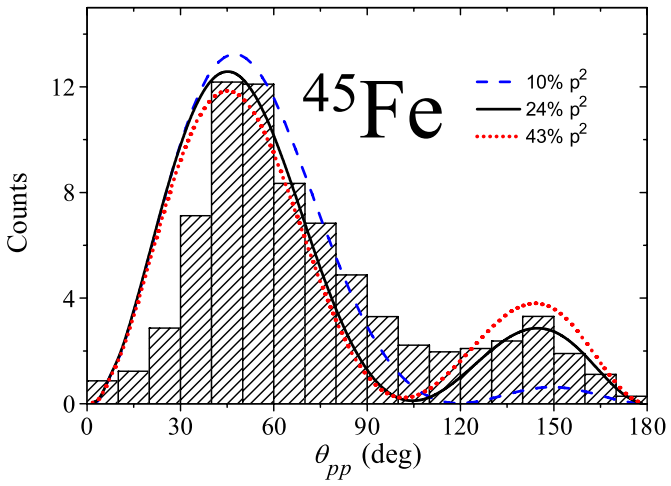


Complex energy plane

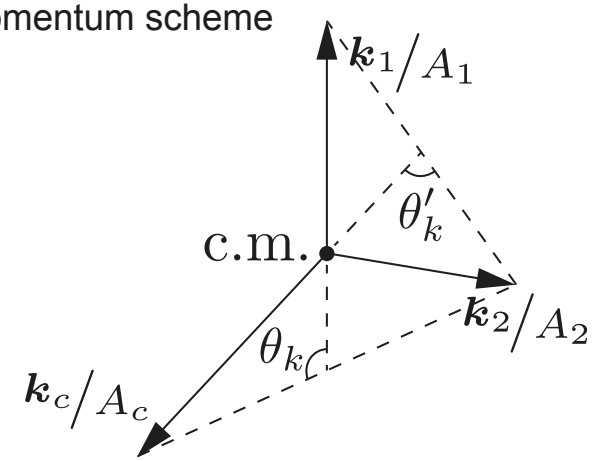


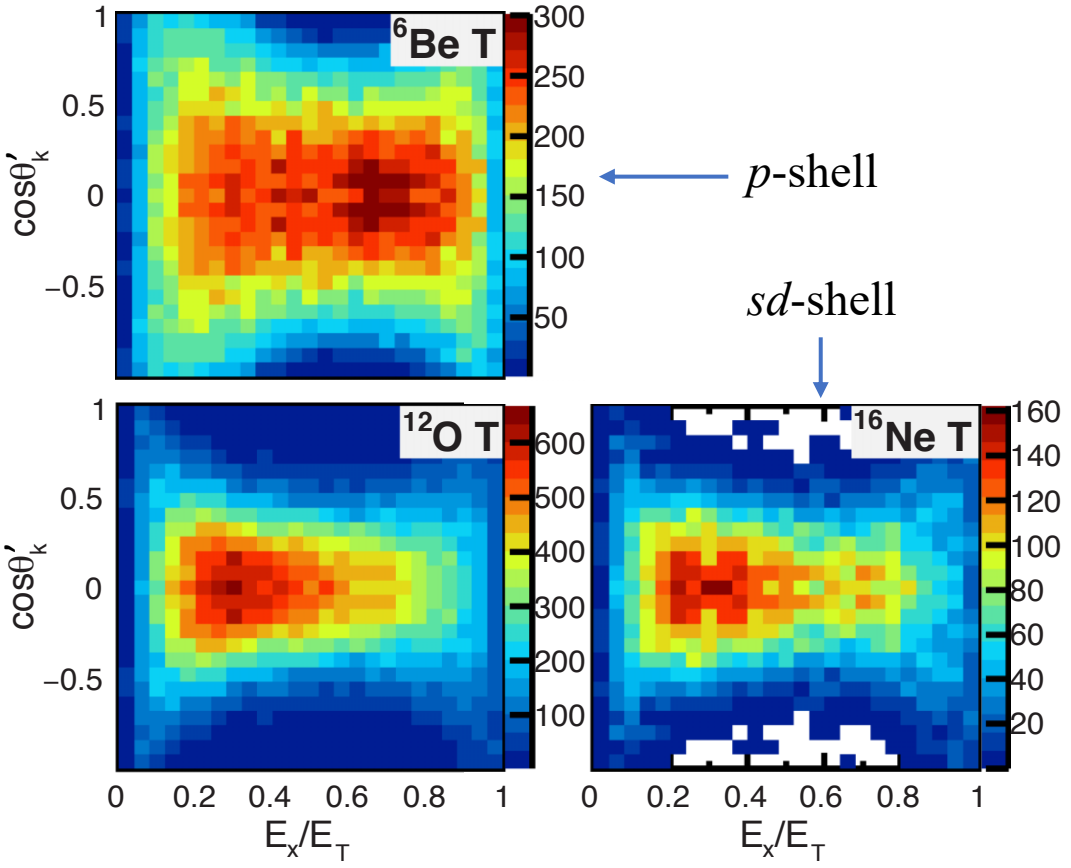
Asymptotic nucleon-nucleon correlation

K. Miernik *et al.* PRL 99, 192501 (2007)



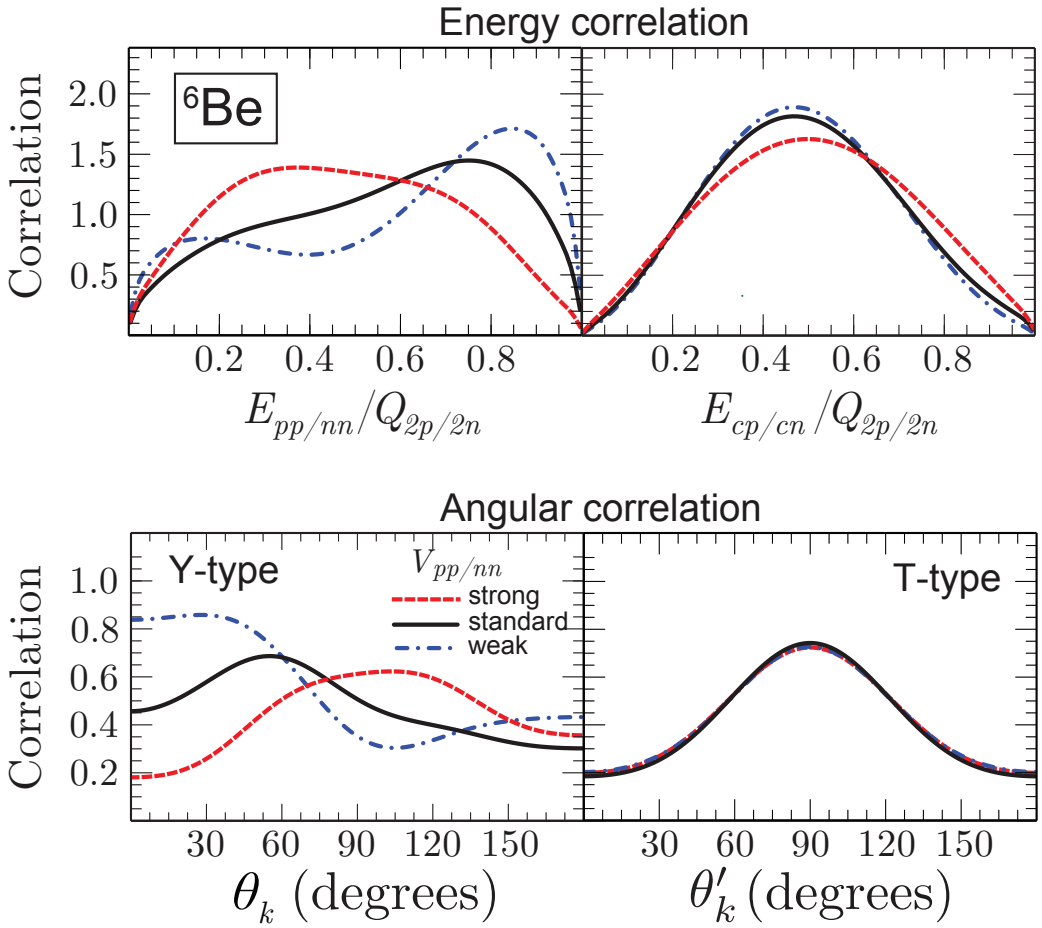
Momentum scheme

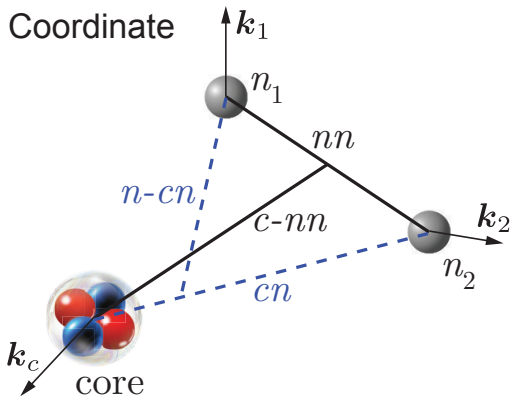


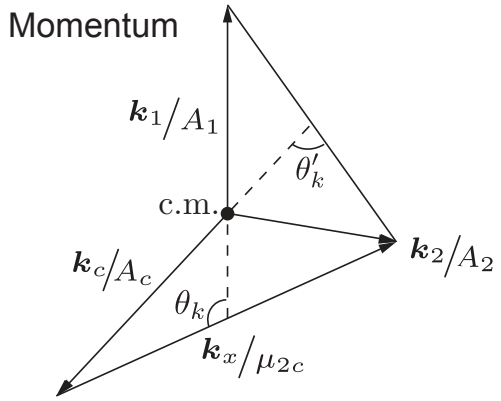


T.B. Webb *et al.* Phys. Rev. C 100, 024306 (2019)

Asymptotic correlations

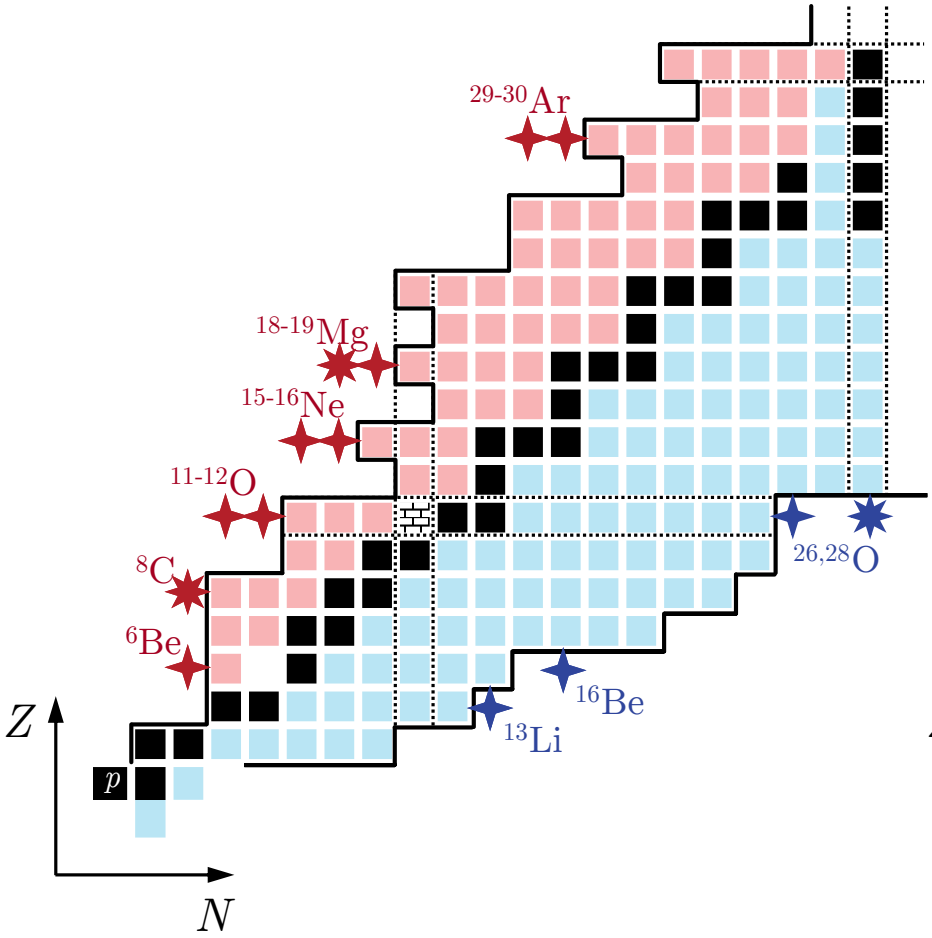


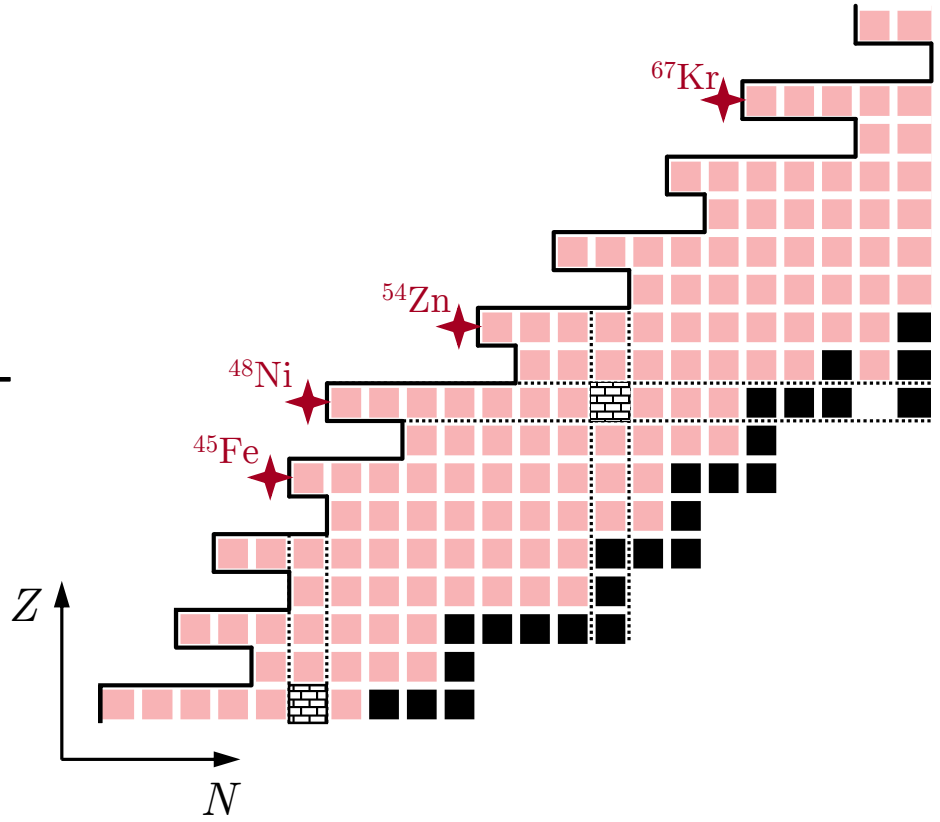




- E_{pp} and Y-type angular correlations are strongly impacted by nucleon-nucleon interaction.

Observed 2*p* emitters





Correlations of light-mass nuclei