INPC-2025, 5/2025, Daejeon

A Complex Scaling Method for Efficient and Accurate Scattering Emulation in Nuclear Reactions

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Comput. Phys. Commun. 311 (2025) 109568

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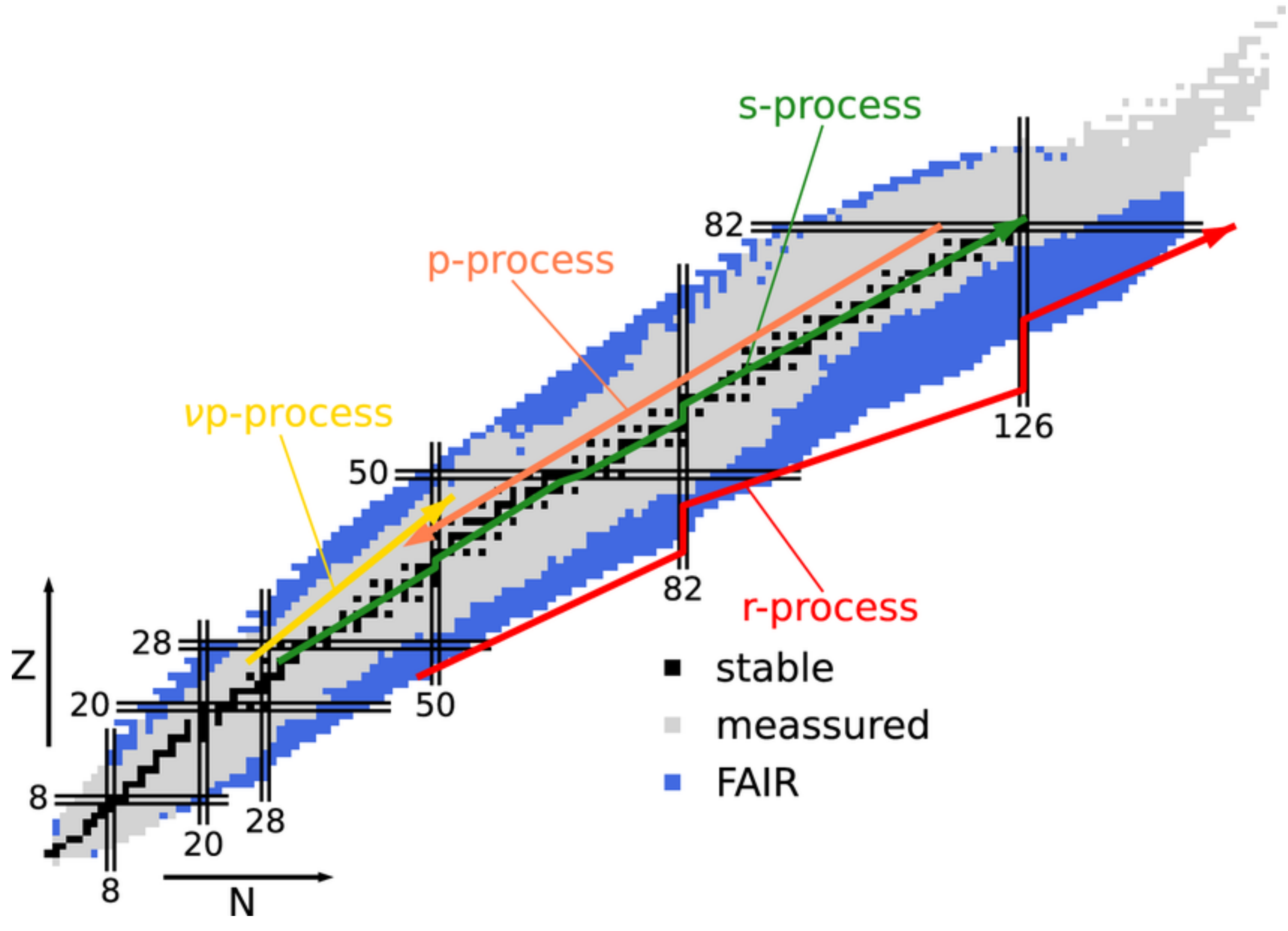
Uncertainty quantification



Arcones et al., Astron. Astrophys. Rev. 31,1 2022

Nucleosynthesis
Element abundance

Requires nuclear reaction cross sections as input

Reaction calculation relies on the phenomenological optical model potential(OMP)

Error propagates to astrophysical results

Uncertainty quantification is crucial

Bayesian statistics provides a powerful and practical framework

Errors in experiment or truncation → **Errors in predictions**

$$p(\boldsymbol{\alpha} \mid D, I) = \frac{p(D \mid \boldsymbol{\alpha}, I)p(\boldsymbol{\alpha} \mid I)}{p(D \mid I)}$$

- D : exp. Data
- α : model parameter
- I : prior information

Need for Emulator

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Optical Model Potentials $U_N(r;\boldsymbol{\omega}) = V_C(r;R_c) + V_0 f\left(r;R_R,a_R\right) + iW_0 f\left(r;R_W,a_W\right) + iW_S\frac{\mathrm{d}}{\mathrm{d}r}f\left(r;R_{ws},a_{ws}\right)$

Parameter set $\boldsymbol{\omega} = \{V_0, R_R, a_R, W_0, R_W, a_W, W_S, R_{ws}, a_{ws}, R_c\}$ **10 dimensions!**

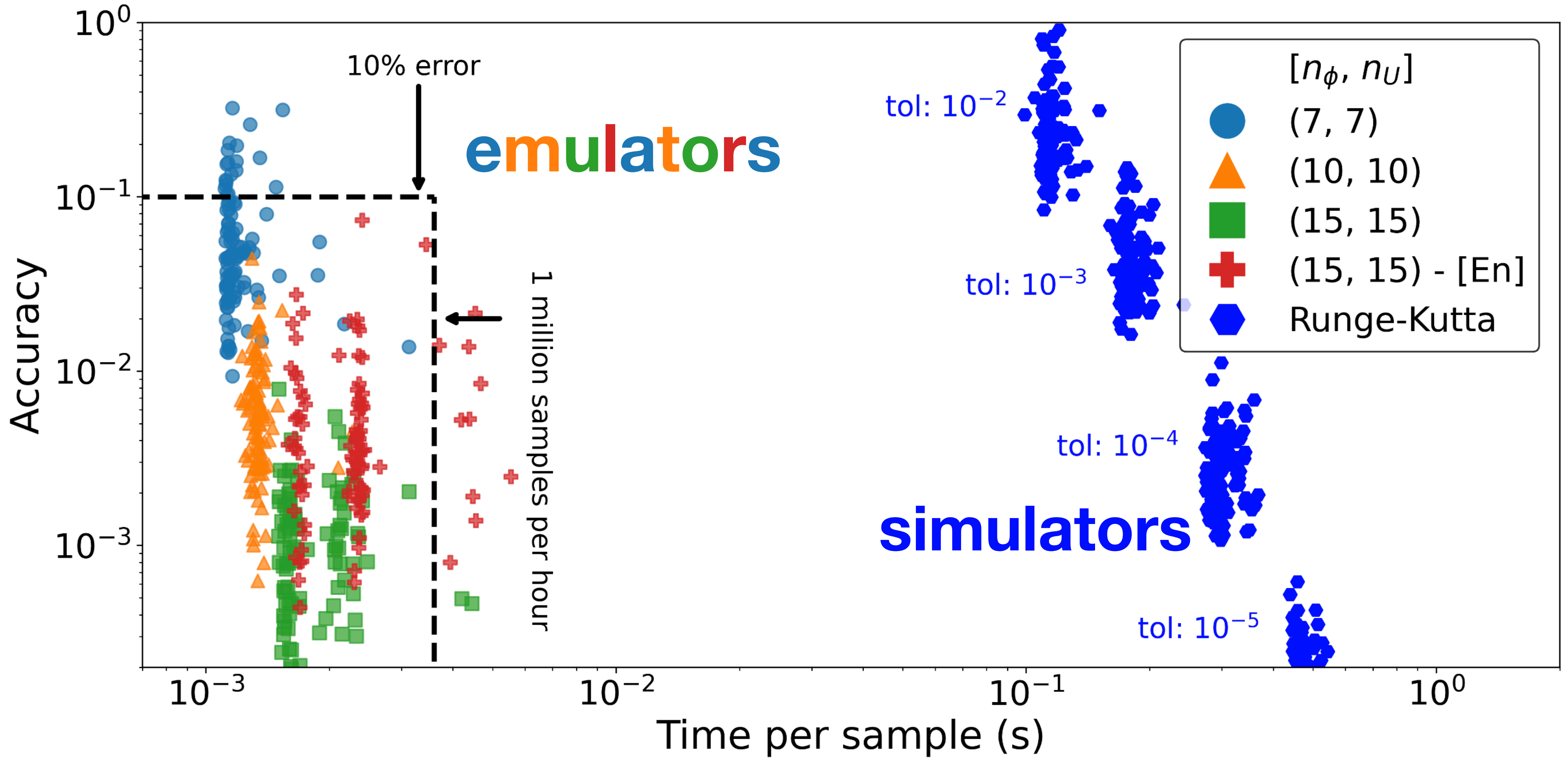
Markov chain Monte Carlo (MCMC) to sample posterior:

- Reduced model
- Approximated
- Fast

Emulator ⟷ **Simulator**

- High-fidelity
- Accurate
- Slow

Fig. Taken from: Odell et al,. PRC **109**, 044612



e.g. 50000 samples

- **Emulator: 50000*0.001s = 50s**
- **Simulator: 50000*0.1s = 5000s**

100x acceleration!

Eigenvector Continuation

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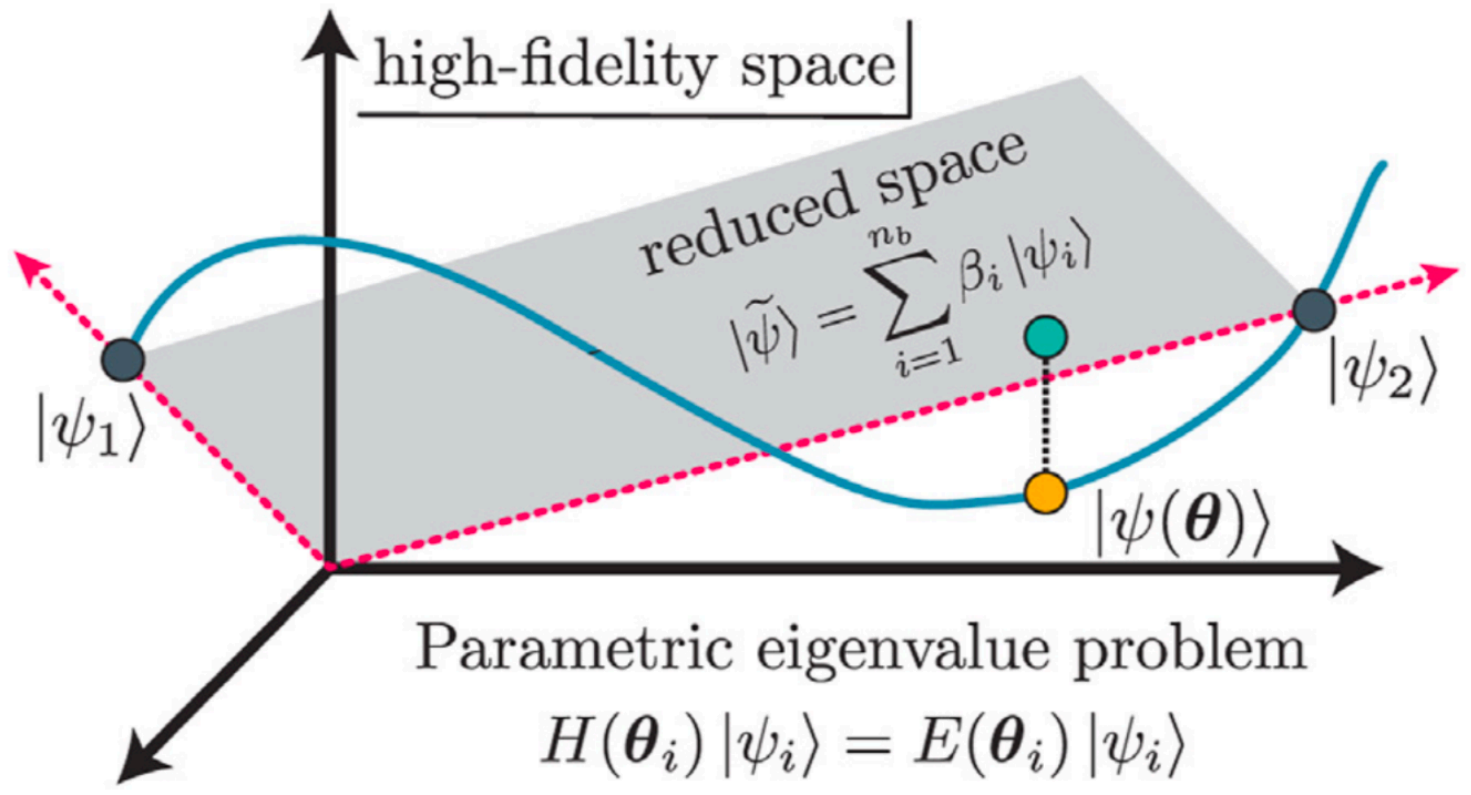
Basic procedure of Eigenvector Continuation Frame et al., PRL 121 032501 (2018)

- Calculate $|\psi(\Omega_i)\rangle, i = 1, \ldots, N_{\mathrm{EC}}$ on different training parameter points, Ω_is are randomly sampled from the whole parameter space
- Use this set of solutions $|\psi(\Omega_i)\rangle, i = 1, \ldots, N_{\mathrm{EC}}$ as the new unorthogonal variational basis to solve the eigenvalue problem/linear equation on the target point



Drischler et al., Front. Phys. 10 1092931 (2022)

"…The key insight is that while an eigenvector resides in a linear space with enormous dimensions, the eigenvector trajectory generated by smooth changes of the Hamiltonian matrix is well approximated by a very low-dimensional manifold.…"

Frame et al., PRL 121 032501 (2018)

Many extensions:

- NCSM: König et al,. PLB 810 135814 (2020)
- CC : Ekström et al,. PRL 123 252501 (2019)
- Pairing Hamiltonian: Companys et al,. PRC 109, 024311 (2024)
- Resonance: Yapa et al., PRC 107, 064316 (2023)

…….

Scattering Emulator

Kohn variational principle (KVP)

Furnstahl et al., PLB 809 135719 (2020)

- The functional $\beta[|\psi_{\rm trial}\rangle] \equiv \tau_{\rm trial} - 2\mu\langle\psi_{\rm trial}|H(\boldsymbol{\theta}) - E|\psi_{\rm trial}\rangle$ should be stationary for $|\psi_{\rm trial}\rangle$

General complex KVP

Drischler et al., PLB 821 13677 (2021)

- Consider multiple boundary conditions to mitigate the Kohn anomalies, at the cost of extending matrix size

Kohn anomaly singularity:

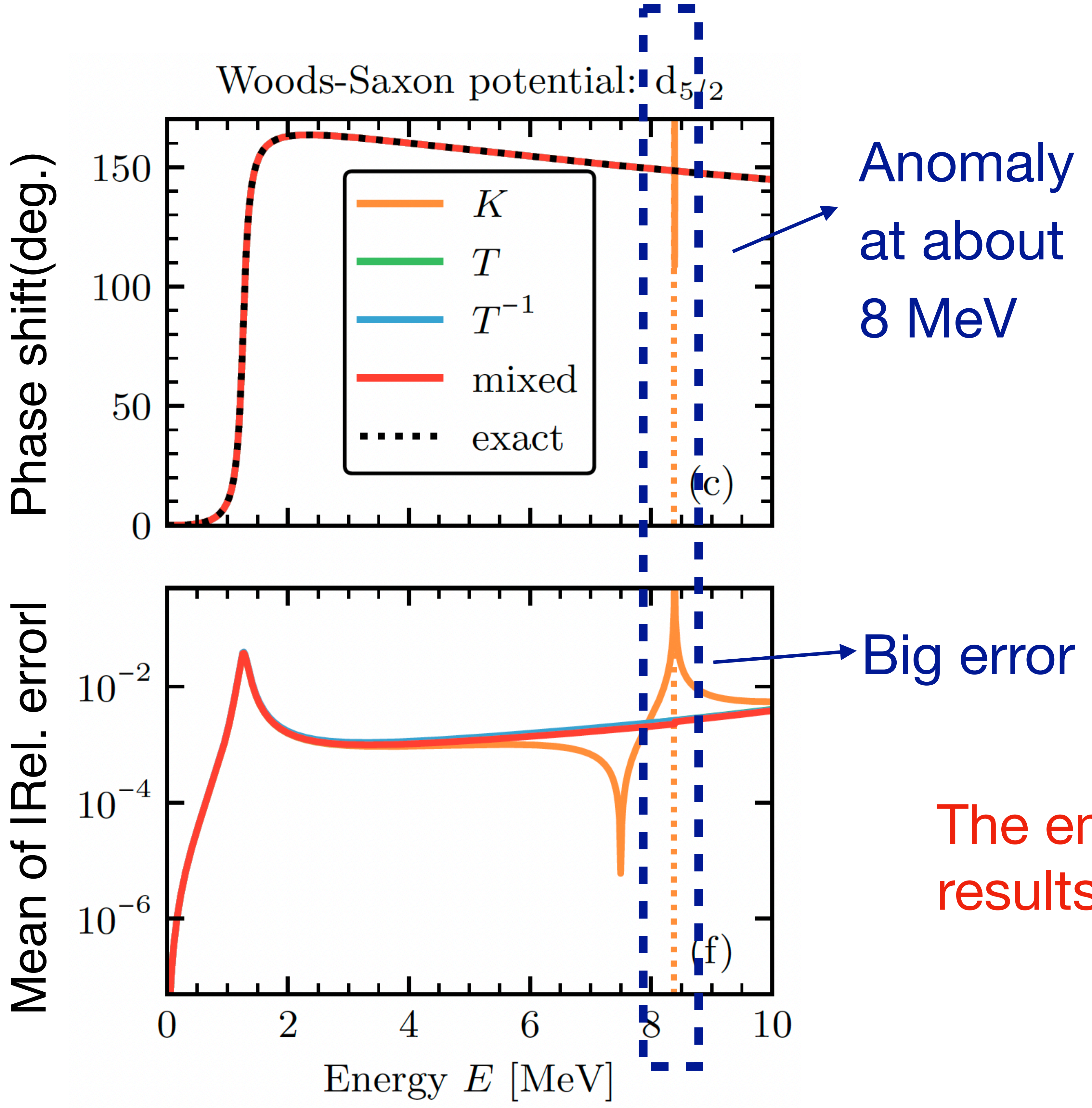
A numerical problem encountered in KVP

- At some specific energy point
- When the basis size is big

The result will suffer from sudden change and explode

e.g. $n + {}^{10}\mathrm{Be}\quad \mathrm{d}_{5/2}$ state

Resonance at about 1.274 MeV



The emulated results are unstable

Fig. taken from Drischler et al., PLB 821 13677 (2021)

Scattering Emulator

Kohn variational principle (KVP) Furnstahl et al., PLB 809 135719 (2020)

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General complex KVP Drischler et al., PLB 821 13677 (2021)

- Consider multiple boundary conditions to mitigate the Kohn anomalies, at the cost of extending matrix size

$R-$**matrix formalism:** division of the configuration space Bai et al., PRC 103 014612 (2021)

Runge-Kutta+RBM "ROSE" Odell et al,. PRC 109, 044612

Limitation: different reduced basis are needed for different partial waves !

Different Basis sets → Different Matrix elements + Big amount Of storage

Different Hamiltonian matrix elements should be calculated for different angular momentum

Scattering Emulator

Kohn variational principle (KVP)

Furnstahl et al., PLB 809 135719 (2020)

- The functional $\beta[|\psi_{\rm trial}\rangle] \equiv \tau_{\rm trial} - 2\mu\langle\psi_{\rm trial}|H(\boldsymbol{\theta}) - E|\psi_{\rm trial}\rangle$ should be stationary for $|\psi_{\rm trial}\rangle$

General complex KVP

Drischler et al., PLB 821 13677 (2021)

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Runge-Kutta+RBM "ROSE"

Odell et al,. PRC 109, 044612

Limitation: different reduced basis are needed for different partial waves !

Motivation: Can all the partial waves share a single set of reduced basis?

ℓ is a parameter in the Hamiltonian

$$H_l(r) = \frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2} + U_N(r,\omega)$$

ℓ specifies the boundary condition

$$u_l(r) \to \frac{i}{2}e^{i\sigma_l}\left[H_l^{(-)}(r) - S_l H_l^{(+)}(r)\right]$$

Basis trained on ℓ can not be easily extrapolated to ℓ'

Because it cannot reproduce the different boundary condition

Eliminate the difference of boundary condition!

Complex Scaling method

Complex scaling method is first introduced to handle resonance

Rotate the coordinate $r \to re^{i\theta}$, $\hat{S}(\theta)F(r) = e^{i\theta/2}F(re^{i\theta})$

For a historical review of complex scaling method, see Lazauskas, arXiv:1904.04675

Asymptotic behavior

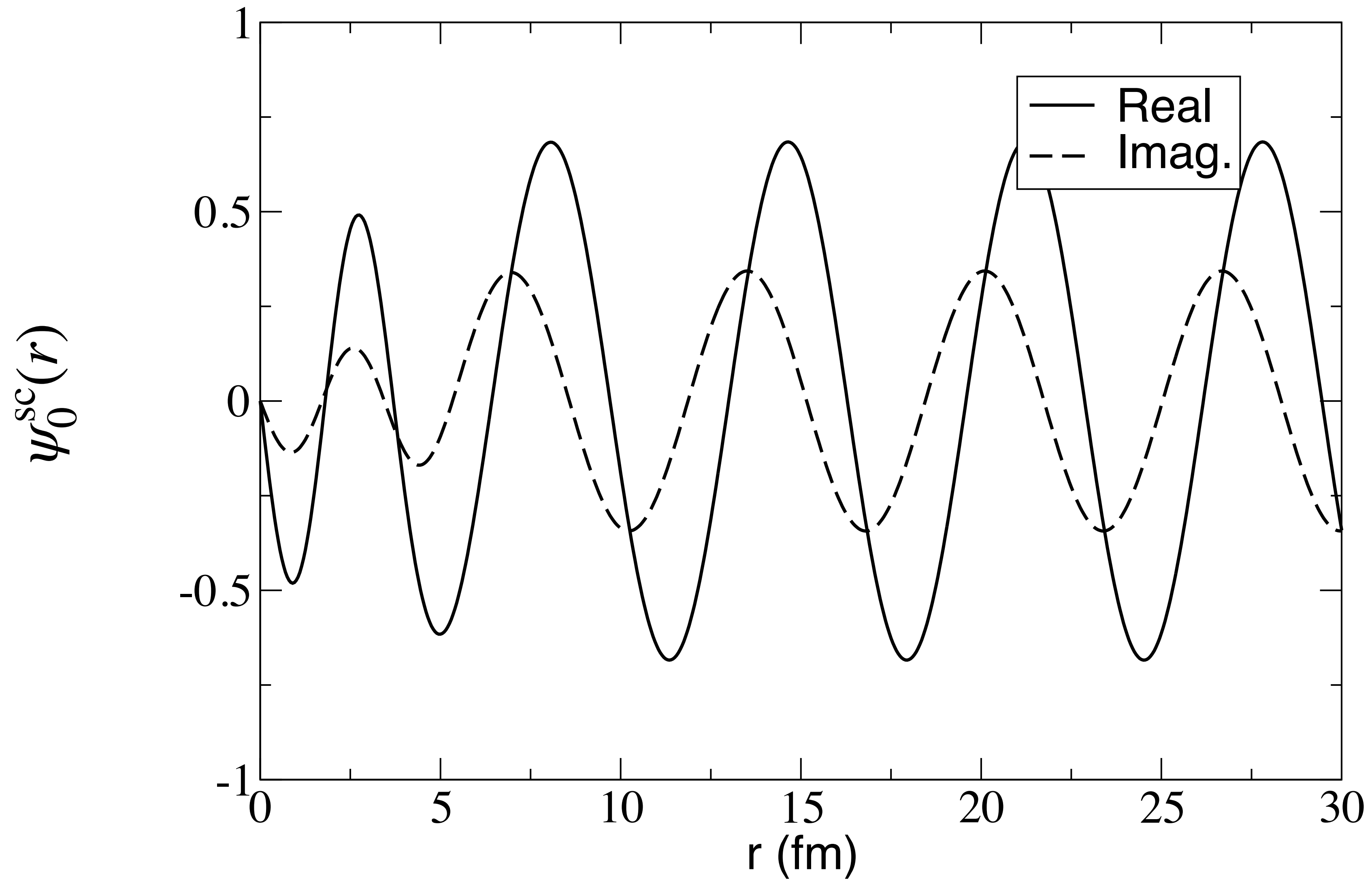
$$\psi_l(r) = F_l(\eta, kr)e^{i\sigma_l} + \boxed{\psi_l^{\rm sc}(r)},$$

Scattered part of wave function

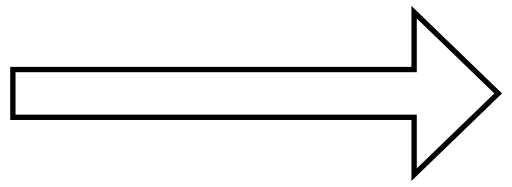
$$\psi_l^{\rm sc}(r) \propto_{r\to\infty} e^{i\left(kr - \frac{1}{2}l\pi - \eta\ln 2kr + \sigma_l\right)}$$

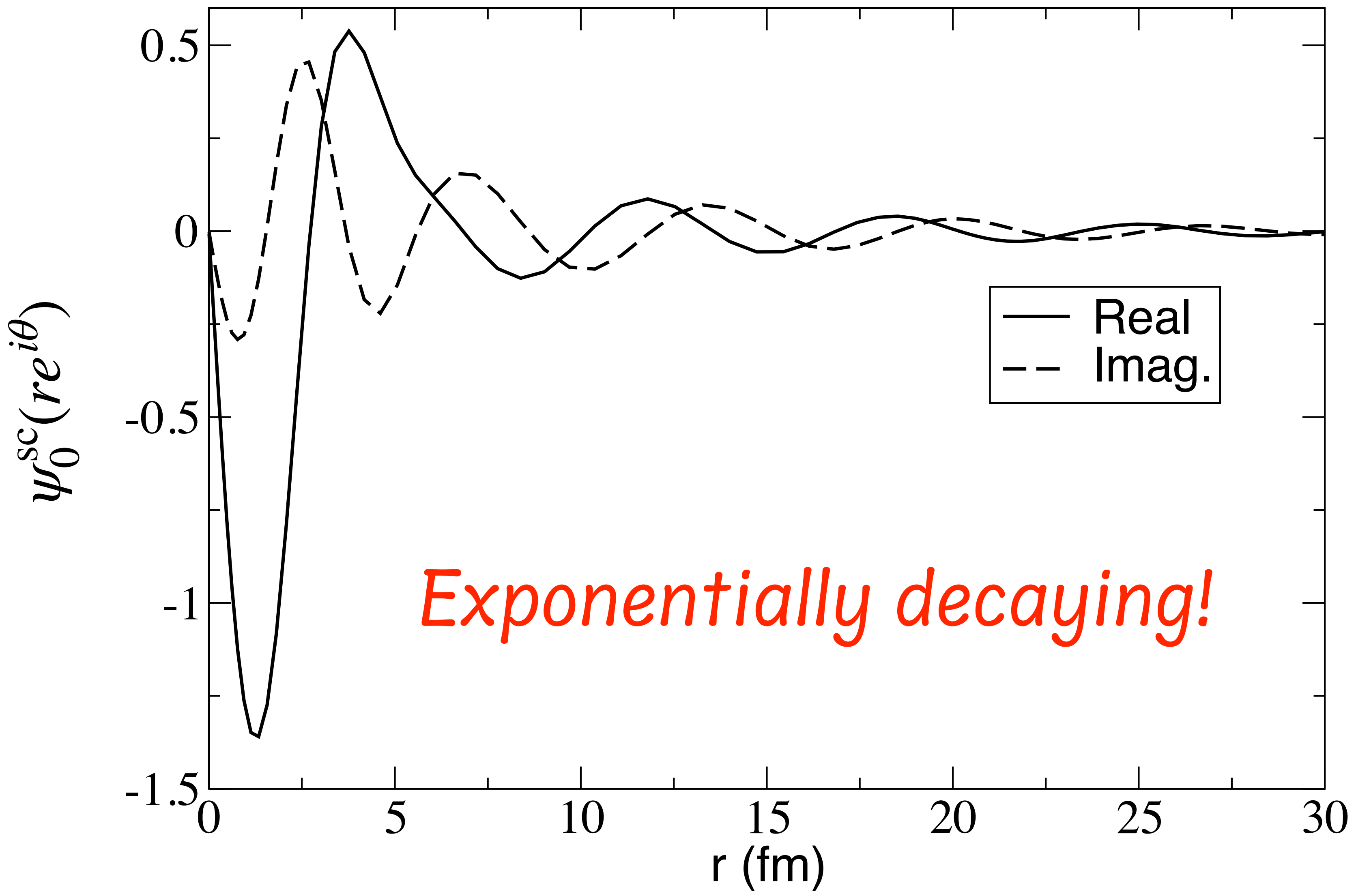
$$\psi_l^{{\rm sc},\theta}(r) = \hat{S}(\theta)\psi_l^{\rm sc}(r) = e^{i\theta/2}\psi_l(re^{i\theta})$$

$$\psi_l^{{\rm sc},\theta}(r) \propto_{r\to\infty} \boxed{e^{-kr\sin\theta}}$$



Complex Scaling

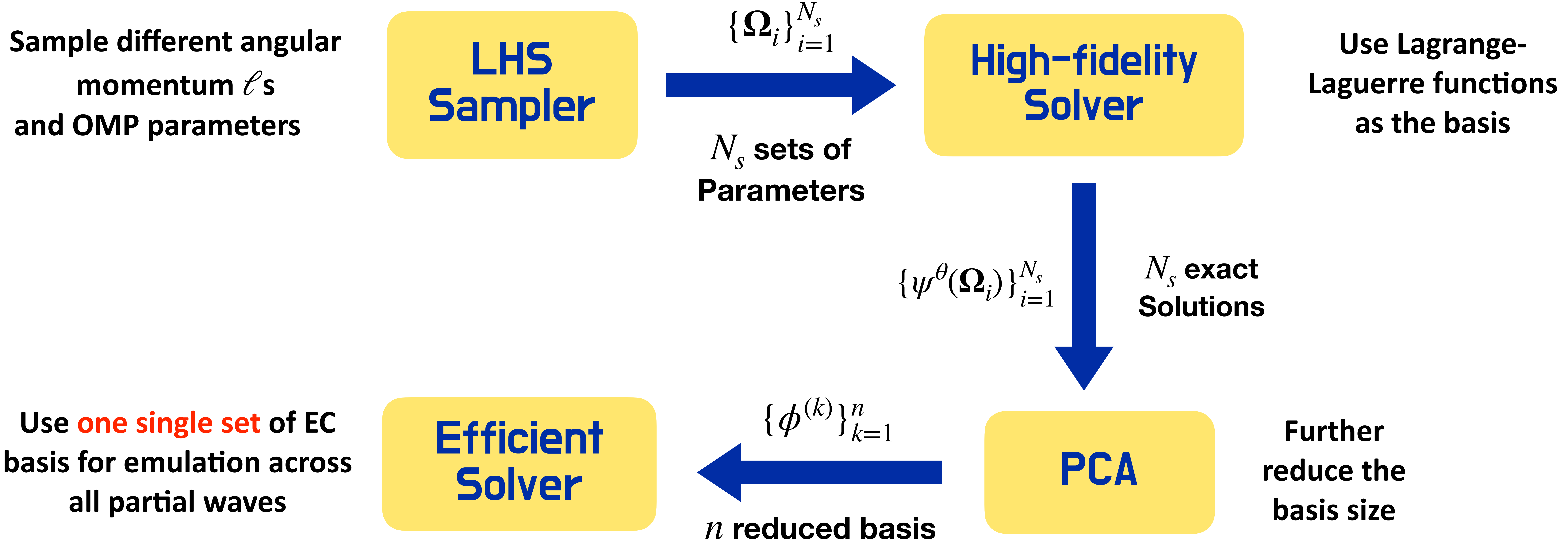




For more details and open source code, see:
Comput. Phys. Commun. 311 (2025) 109568
Computer code COLOSS: non-local, coupled-channel..

Emulate the rotated scattered part of the wave function instead of the original wave function

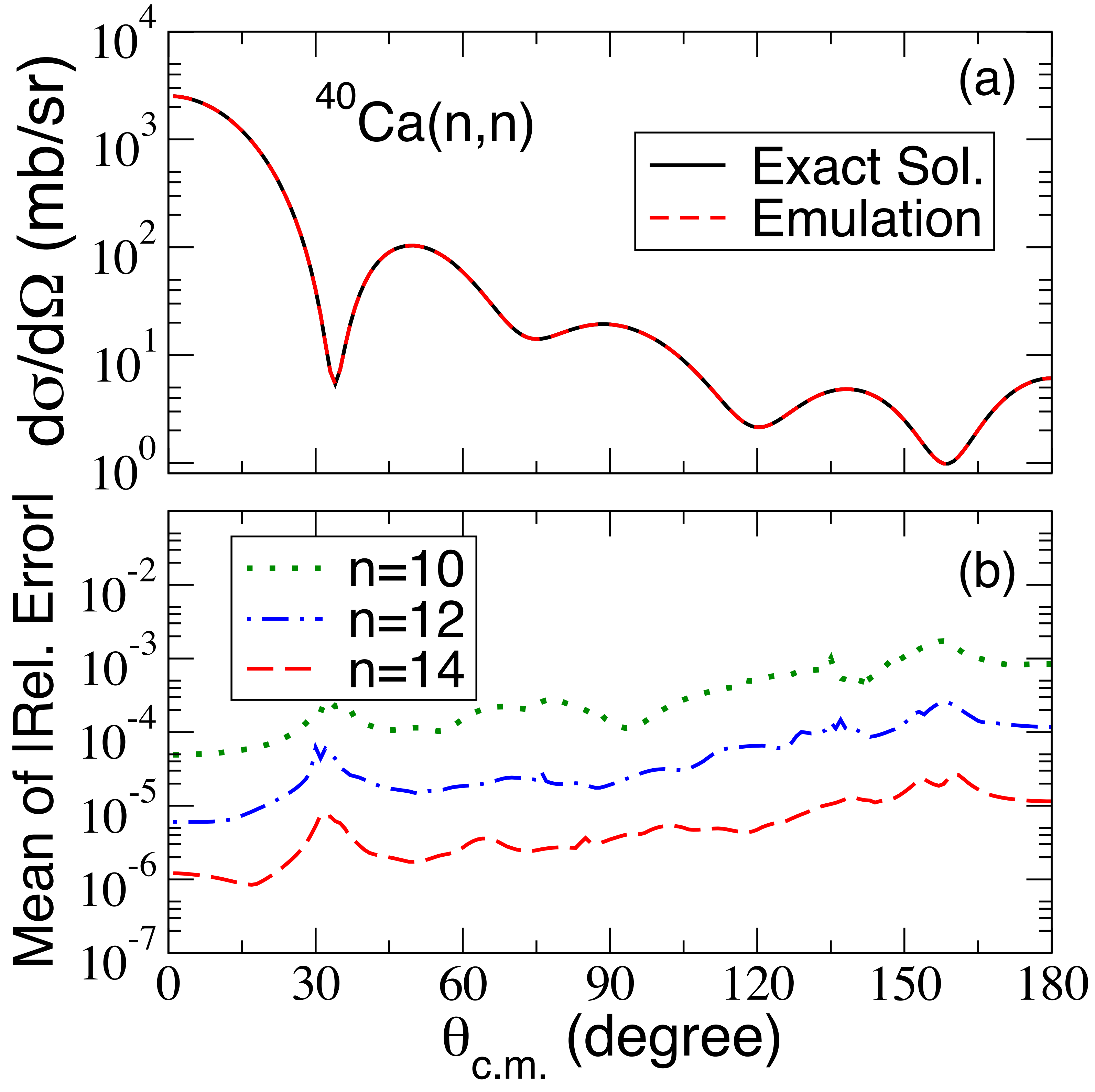
Algorithm for emulator

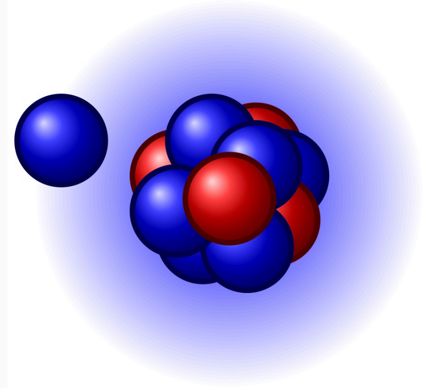


Principle component analysis (PCA):
An unsupervised machine learning technique to reduce the number of dimensions in large datasets

Results

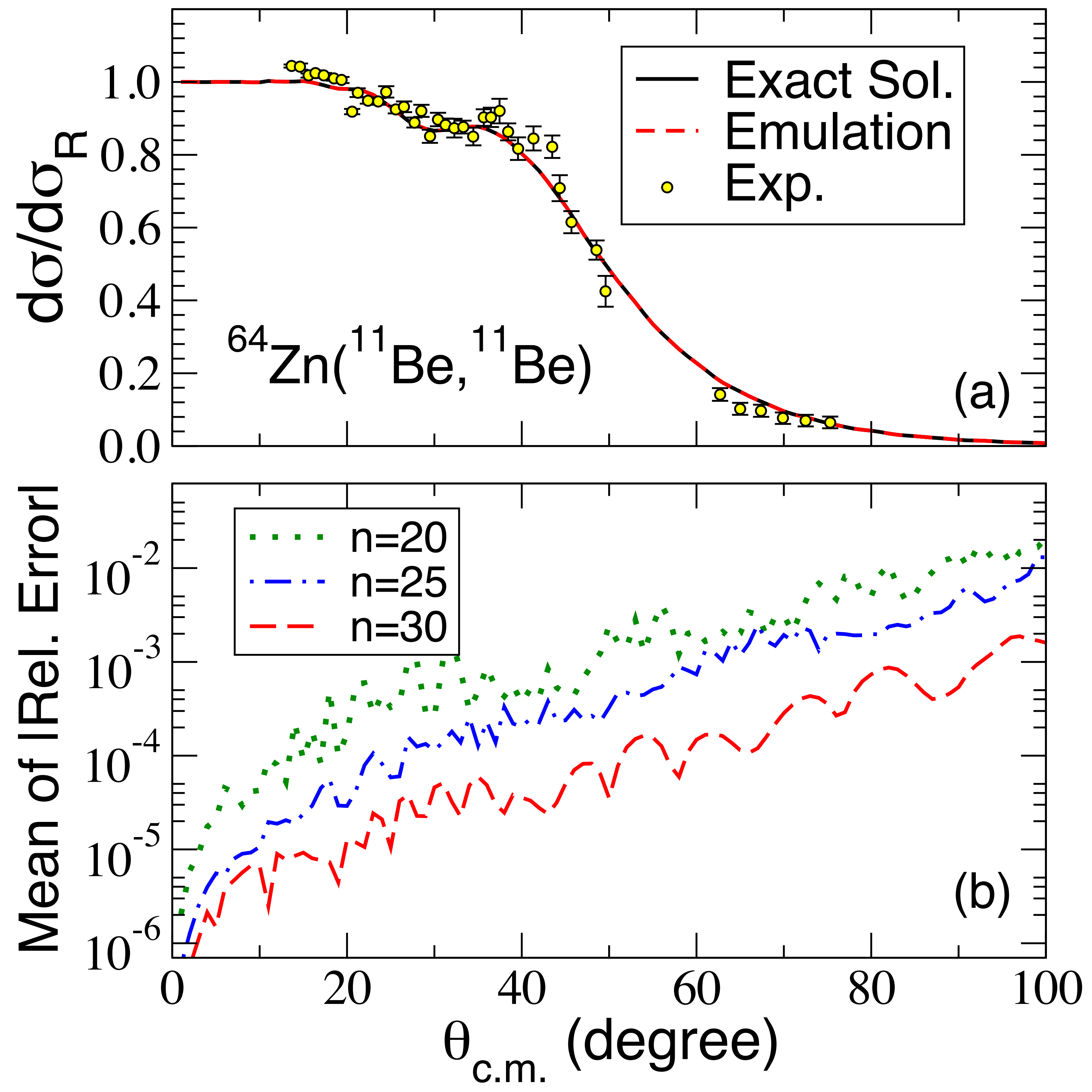
$n + {}^{40}\mathrm{Ca}$ Elastic scattering





$^{11}\mathrm{Be} + {}^{64}\mathrm{Zn}$ Elastic scattering

Need $\ell_{\max} = 60$ for convergence!



- Emulated results are accurate
- Reduced basis size is small
- The results converged rapidly

Exp. Data taken from Di Pietro et al. PRL 105, 022701

Define the mean of absolute relative error: $$\epsilon = \sum_i \frac{|\sigma_{E,i} - \sigma_{0,i}|}{\sigma_{0,i}}$$

No detection of anomaly

$n + ^{10}\mathrm{Be}$ $\mathrm{d}_{5/2}$ Resonance at 1.274 MeV

A Woods-Saxon + spin-orbit coupling term $V(r) = -V_0 f(r;R,a) + \vec{\ell}\cdot\vec{s}\,\frac{V_{\mathrm{LS}}}{r}\frac{\mathrm{d}}{\mathrm{d}r}f(r;R,a)$

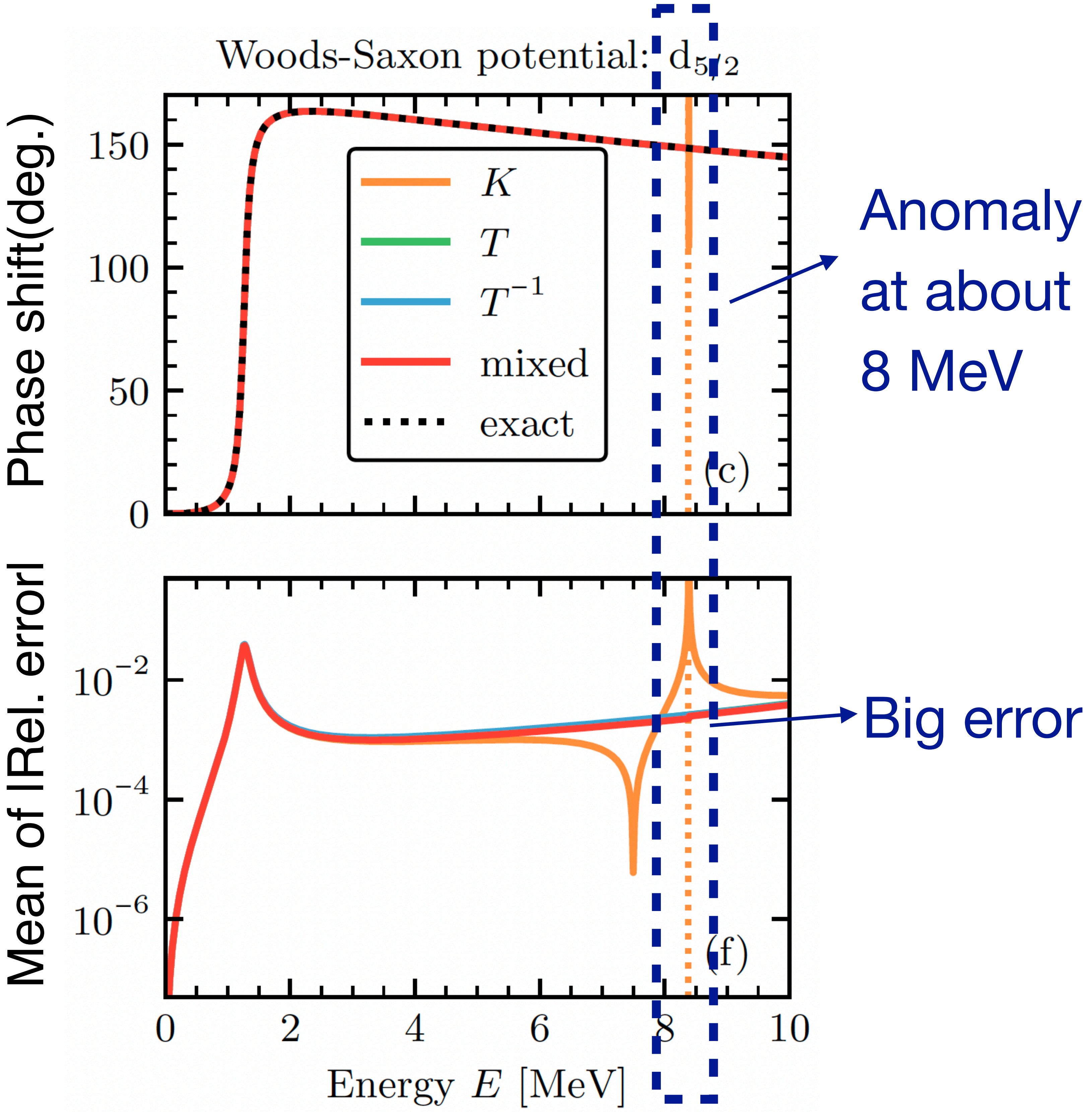
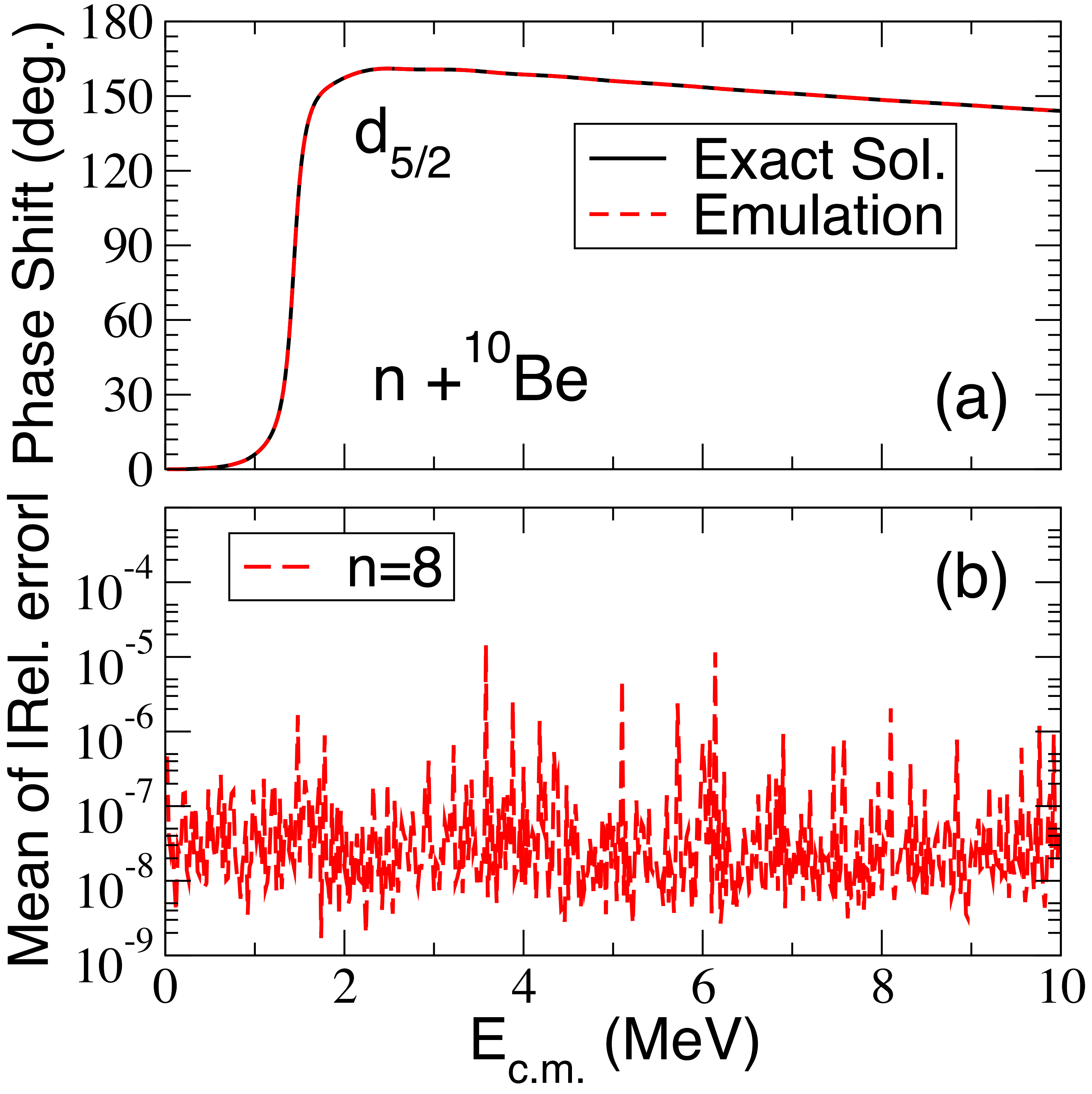


Fig. taken from Drischler et al., PLB 821 13677 (2021)

Test on a very Fine grid of c.m. kinetic energy:

$\Delta E_{\mathrm{c.m.}} = 0.02$ MeV

No anomaly in phase shift!



Stable rel. error

Summary

Conclusions：

1. Complex scaling based emulators have great accuracy and performance.
2. Different channels can share one set of reduced basis for emulation.
3. No anomaly is detected, this method shows great stability and robustness.

Outlooks：

- Building emulators for continuum discretized coupled channel(CDCC) calculation
- Next generation of optical model potentials, errors from experiment can be handled better


[261]
Db
[262]
Sg
[266]
lanthanum
57
La
cerium
58
Ce
140.12
praseodymium
59
Pr
140.91
neodymium
60
Nd
144.24
promethium
61
Pm
[145]
Bh
Hs
Mt
Ds
Sm
Eu
thorium
Th
protactinium
91
uranium
92
U
neptunium
93
Np
94
Pu
Am

Thank you!

Backup slides

Details on CS method

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Schrödinger equation: $$\left[-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2}+U_N(r;\boldsymbol{\omega})\right]\psi_\ell(r)=E\psi_\ell(r)$$

Make a seperation: $$\psi_\ell(r)=e^{i\sigma_\ell}F_\ell(\eta,kr)+\psi_\ell^{\mathrm{sc}}(r)$$

Carry out CS: $$\left[E-H^\theta(r;\boldsymbol{\Omega})\right]\psi_\ell^{\mathrm{sc},\theta}(r)=e^{i\theta/2}e^{i\sigma_\ell}\tilde{U}_N(re^{i\theta};\boldsymbol{\Omega})F_\ell(\eta,kre^{i\theta})$$

Expand the wave function: $$\psi_\ell^{\mathrm{sc},\theta}(r)=\sum_j^{N_r}c_jg_j(r)$$

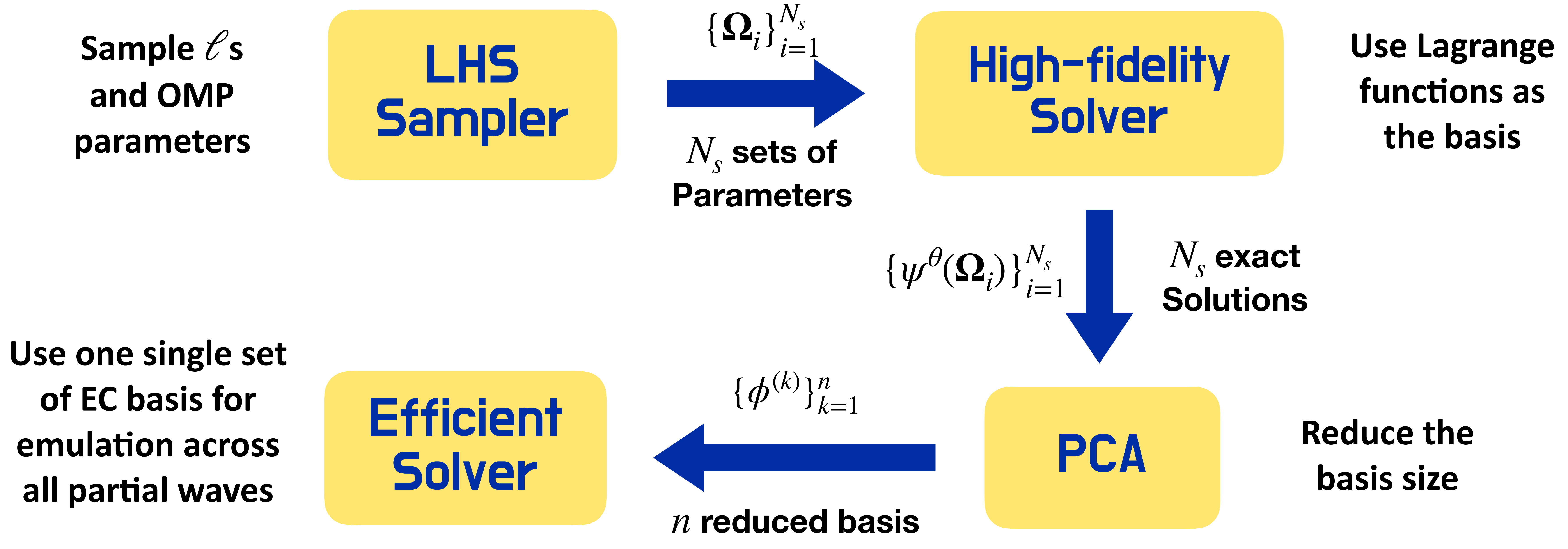
Get linear equation: $$\sum_j\left[E\mathbf{N}_{ij}-\mathbf{H}_{ij}^\theta(\boldsymbol{\Omega})\right]c_j(\boldsymbol{\Omega})=b_i^\theta(\boldsymbol{\Omega})$$

Algorithm for emulator

- Use Latin Hypercube method to randomly sample N_s training points $\{\mathbf{\Omega}_i\}_{i=1}^{N_s}$
- Perform high-fidelity calculation on these parameters and N_s solutions $\psi^{\theta}(\mathbf{\Omega}_i)$
- Carry out the principal component analysis (PCA) to extract n reduced basis:

$$\{\phi^{(k)}\}_{k=1}^{n} = \text{PCA}\left[\{\psi^{\theta}(\mathbf{\Omega}_i)\}_{i=1}^{N_s}\right]$$

- Calculate the matrix for the target Hamiltonian regarding the new basis and solve the corresponding linear equation

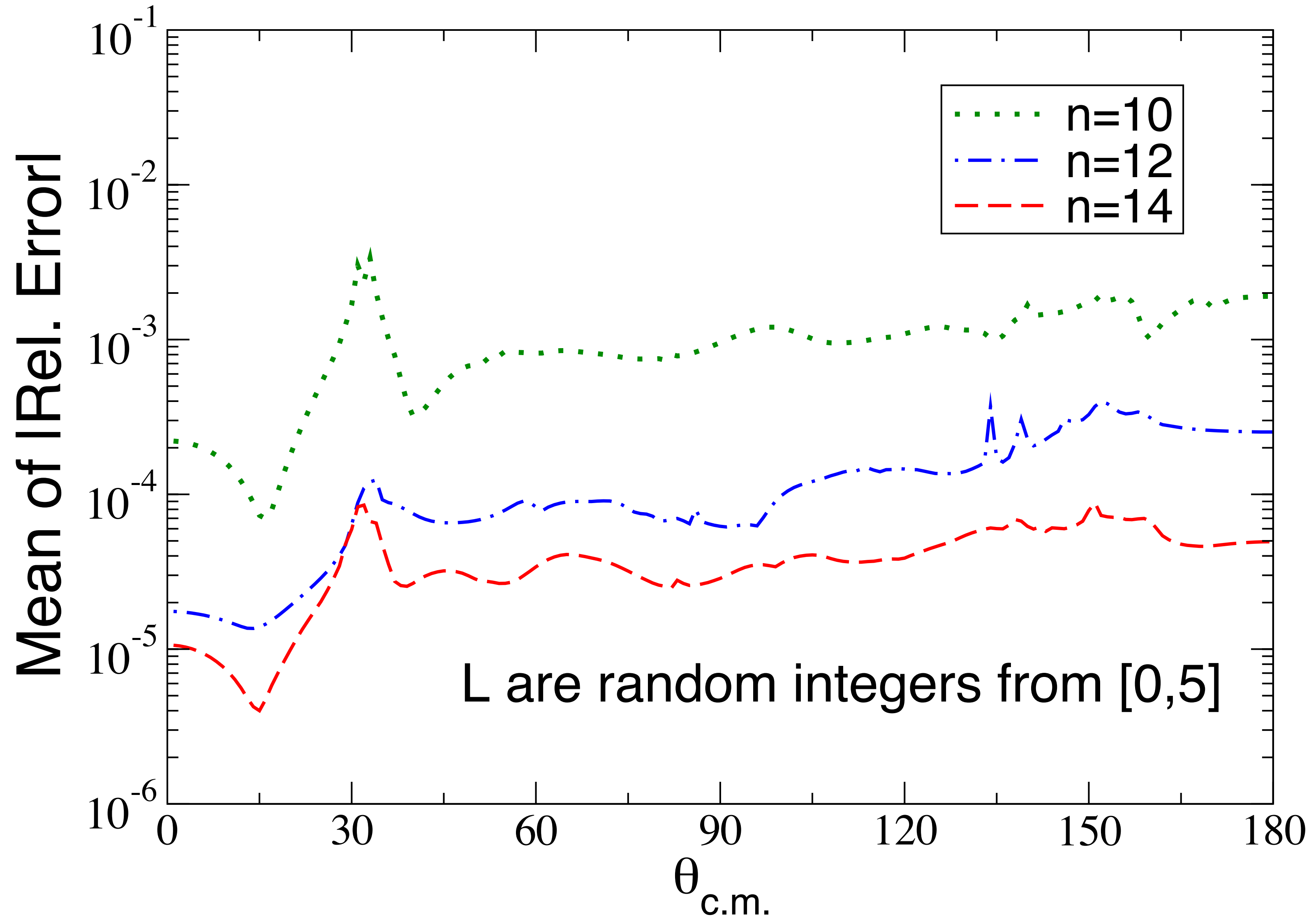


Selection for ℓs in training set

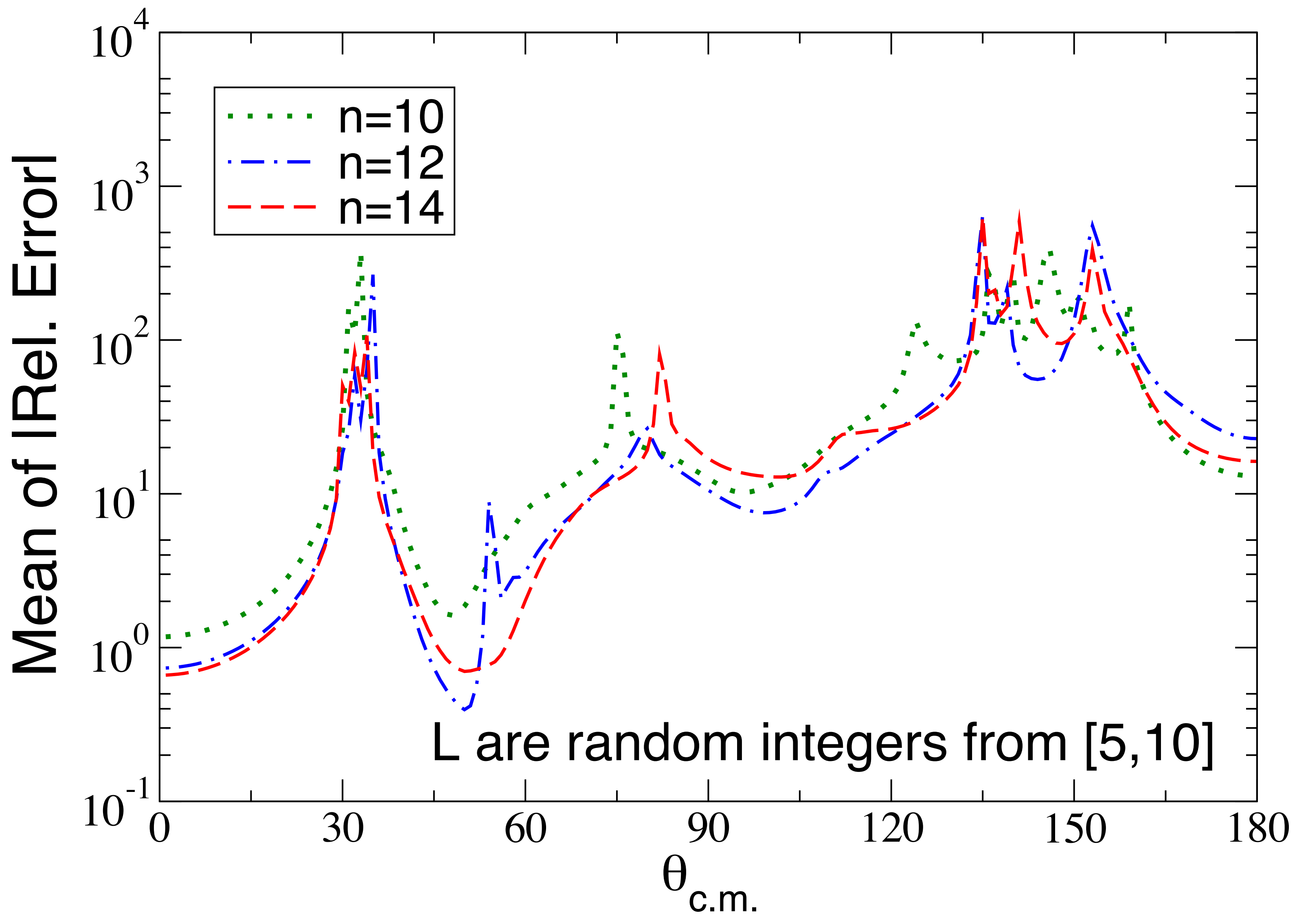
Our strategy: randomly generate integers in $[0,\ell_{\max}]$

Training point with small ℓs are crucial, while big ℓs are useless to some extent

[0, 5]



[5, 10]



Centrifugal barrier term will dominate over the OMP terms, which makes it hard to capture the analytical structure of OMPs.

Results

$n + ^{40}\mathrm{Ca}$ Elastic scattering

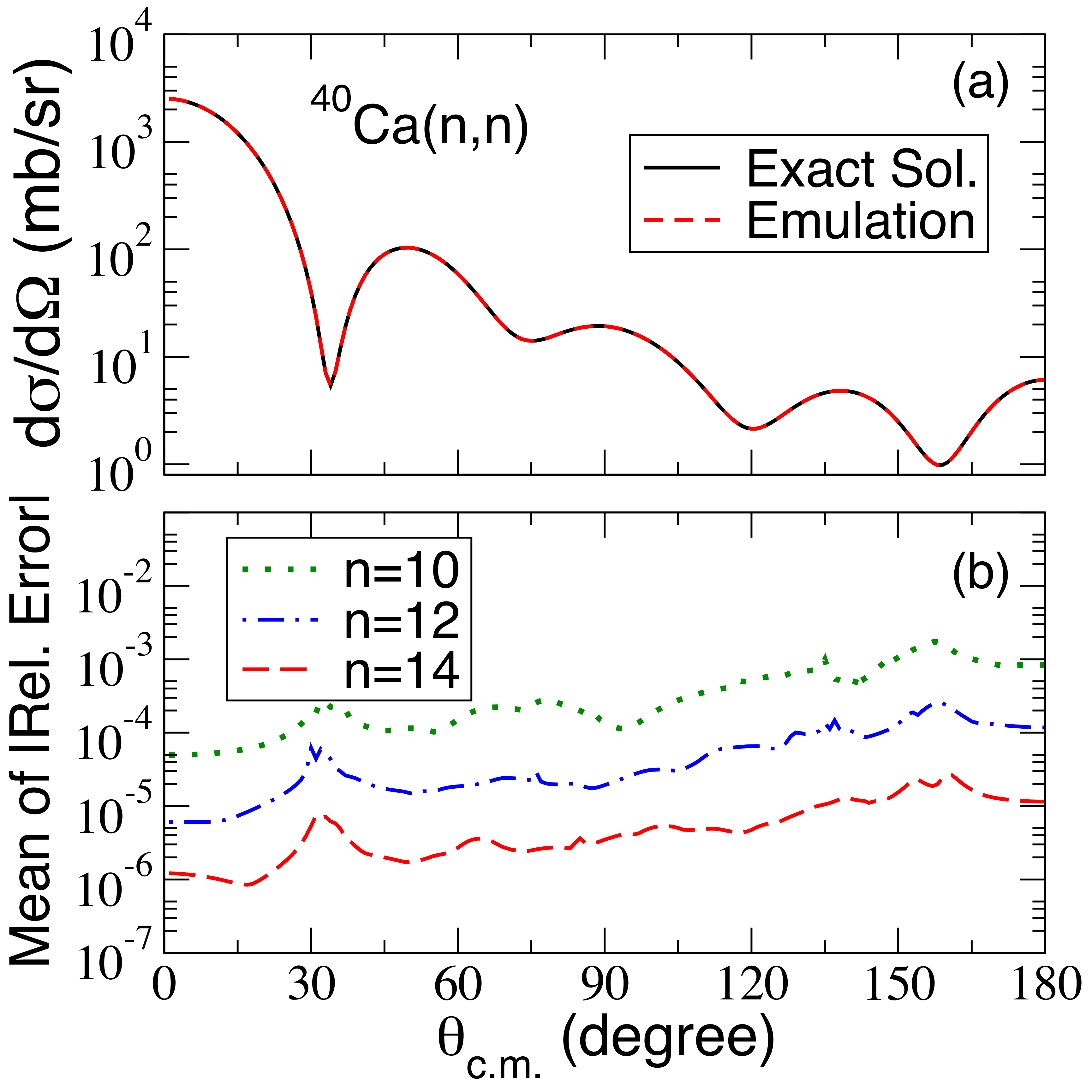
Need $\ell_{\max} = 10$ for convergence

- Randomly sample 100 training points within a ±20% range centered in the optimal values in Koning-Delaroche (KD) parameterization
- Select 10, 12, 14 principle components as the EC basis

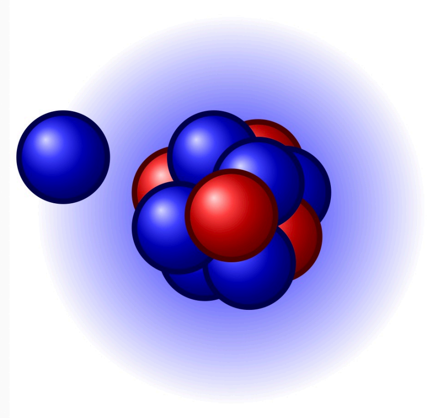
100 sets of target parameters are also randomly generated, calculate the mean of absolute relative error:

$$\epsilon = \sum_{i}^{100} \frac{|\sigma_{E,i} - \sigma_{0,i}|}{\sigma_{0,i}}$$

Optimal OMP parameter taken from:
Koning et al,. NPA 713 231310



Results



^{11}Be $+^{64}$ Zn Elastic scattering

Di Pietro et al. PRL 105, 022701

Reaction involving halo nucleus has some exotic mechanism

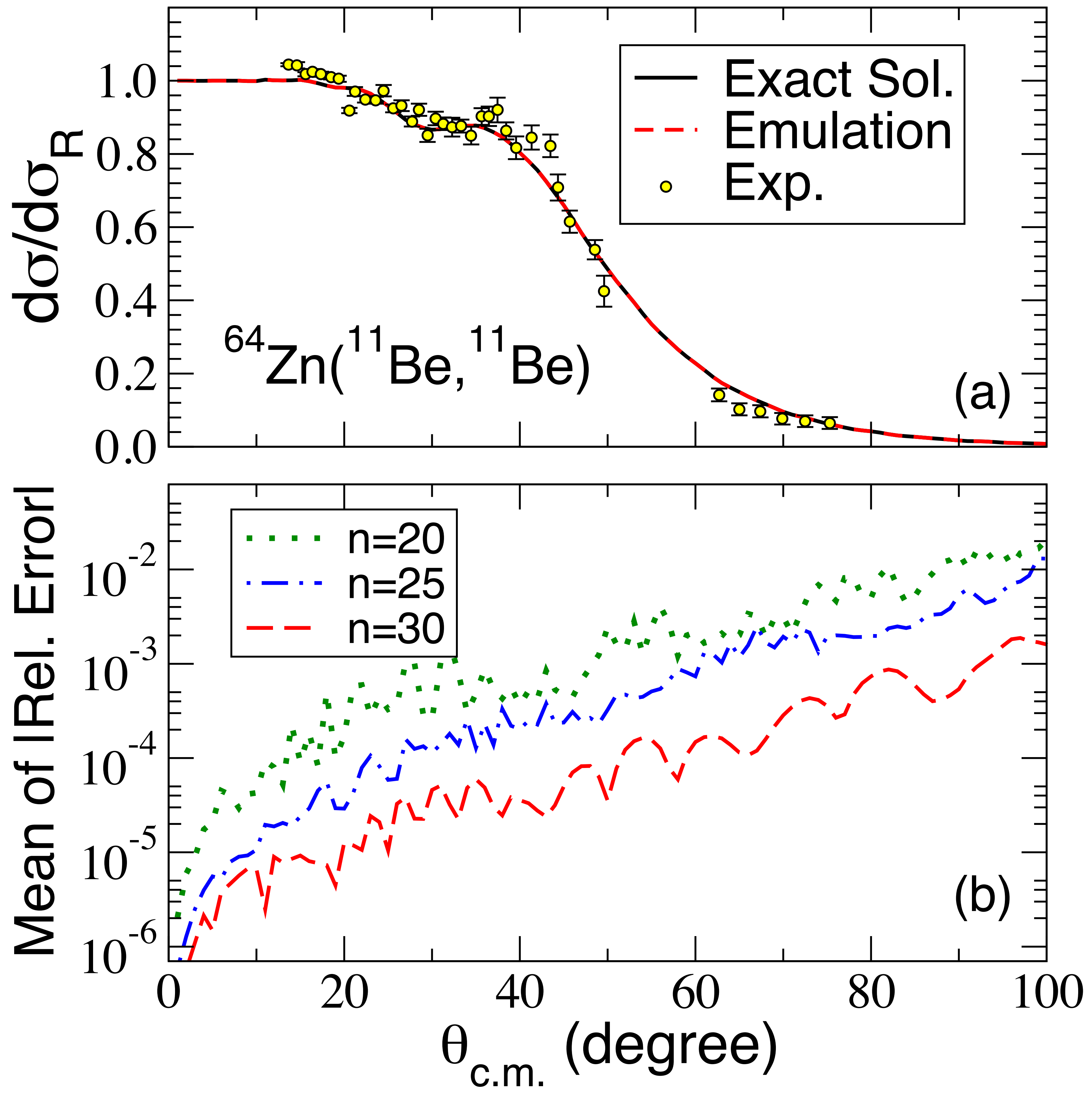
Need $\ell_{max} = 60$ for convergence

Need to prepare 61 sets of EC basis

Matrix elements computed 61 times

- Randomly sample 200 training points within a ±20% range centered in the values given by A. Di Pietro et al. PRL 105, 022701
- Select 20, 25, 30 principle components as the EC basis

100 sets of target parameters are also randomly generated for accuracy test



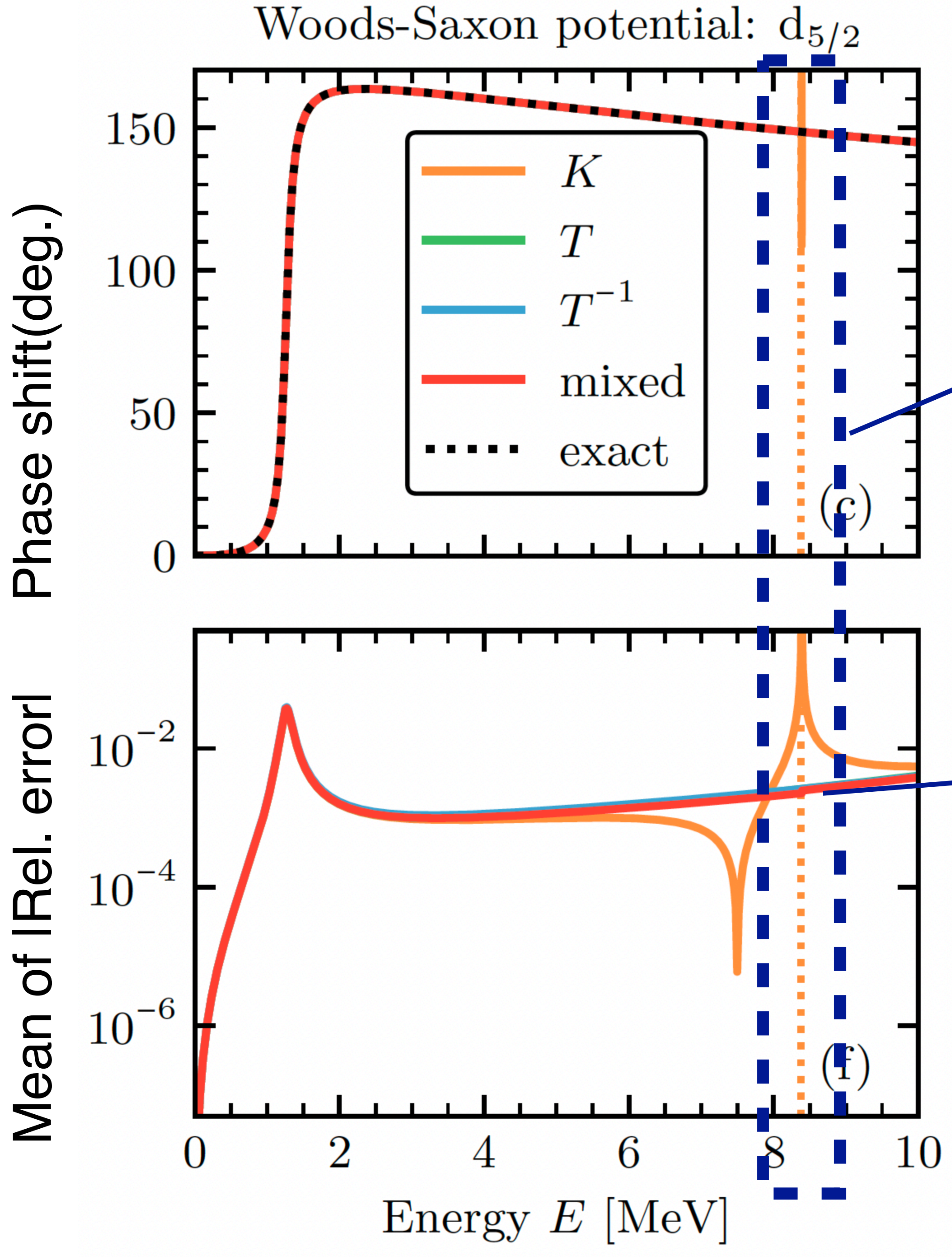
Exp. Data taken from Di Pietro et al. PRL 105, 022701

No detection of anomaly

Kohn anomaly: numerical problem in KVP

$n + ^{10}\mathrm{Be}$ $\mathrm{d}_{5/2}$ Resonance at 1.274 MeV

$$V(r) = -V_0 f(r; R, a) + \vec{\ell} \cdot \vec{s}\, \frac{V_{\mathrm{LS}}}{r} \frac{\mathrm{d}}{\mathrm{d}r} f(r; R, a)$$

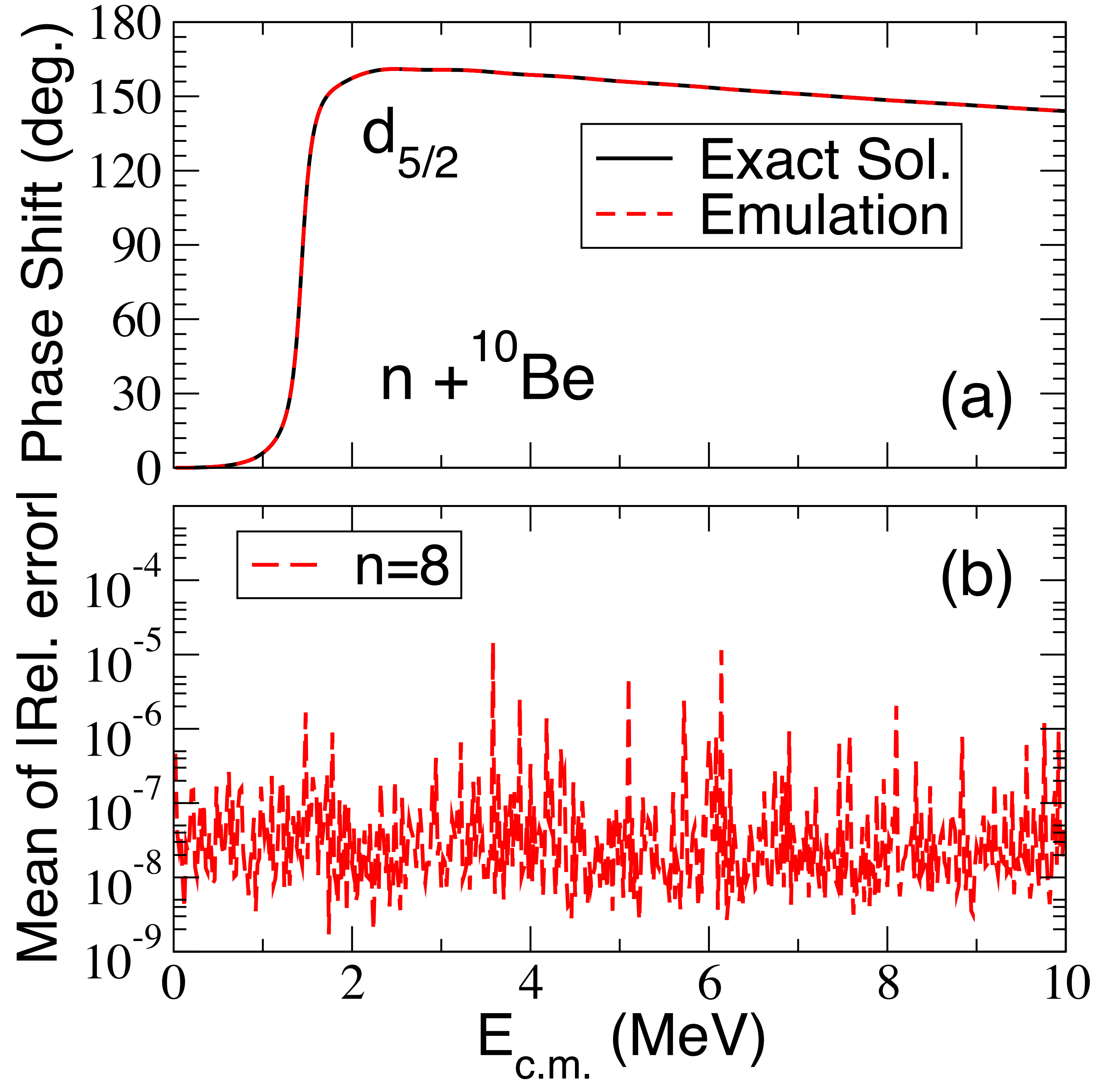


Anomaly at about 8 MeV

Big error

Fig. taken from Drischler et al., PLB 821 13677 (2021)

- Randomly sample 15 training points within a ±20% range centered in the values given by Capel et al. PRC 70 064605
- Select 8 principle components as the EC basis
- Emulate 20 times at each energy point



$\Delta E_{\mathrm{c.m.}} = 0.02$ MeV