

# Emulating nuclei deformation in the coupled channel formalism with the eigenvector continuation

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**Seminar on the Oct. 24**

Ref: K. Hagino. et. al., PhysRevC.112.024618  
Z. Liao. et. al., in preparation

## **Sub-barrier fusion reaction and Coupled channel model:**

**What is Low-energy sub-barrier fusion reaction?**

**How to explain the phenomenon?**

**What is the Coupled channel model?**

## **Nuclear Reaction and nuclear structure:**

**The inter section between the relativistic and low-energy heavy ion collision?**

**How to determine the nuclei shape by low-energy sub-barrier fusion reaction?**

## **Eignvector Continuation:**

**What is the  $E_c$ ?**

**What can we do with  $E_c$ ?**

## **Emulator to determine the nuclei shape:**

**How is the error performance of emulator ?**

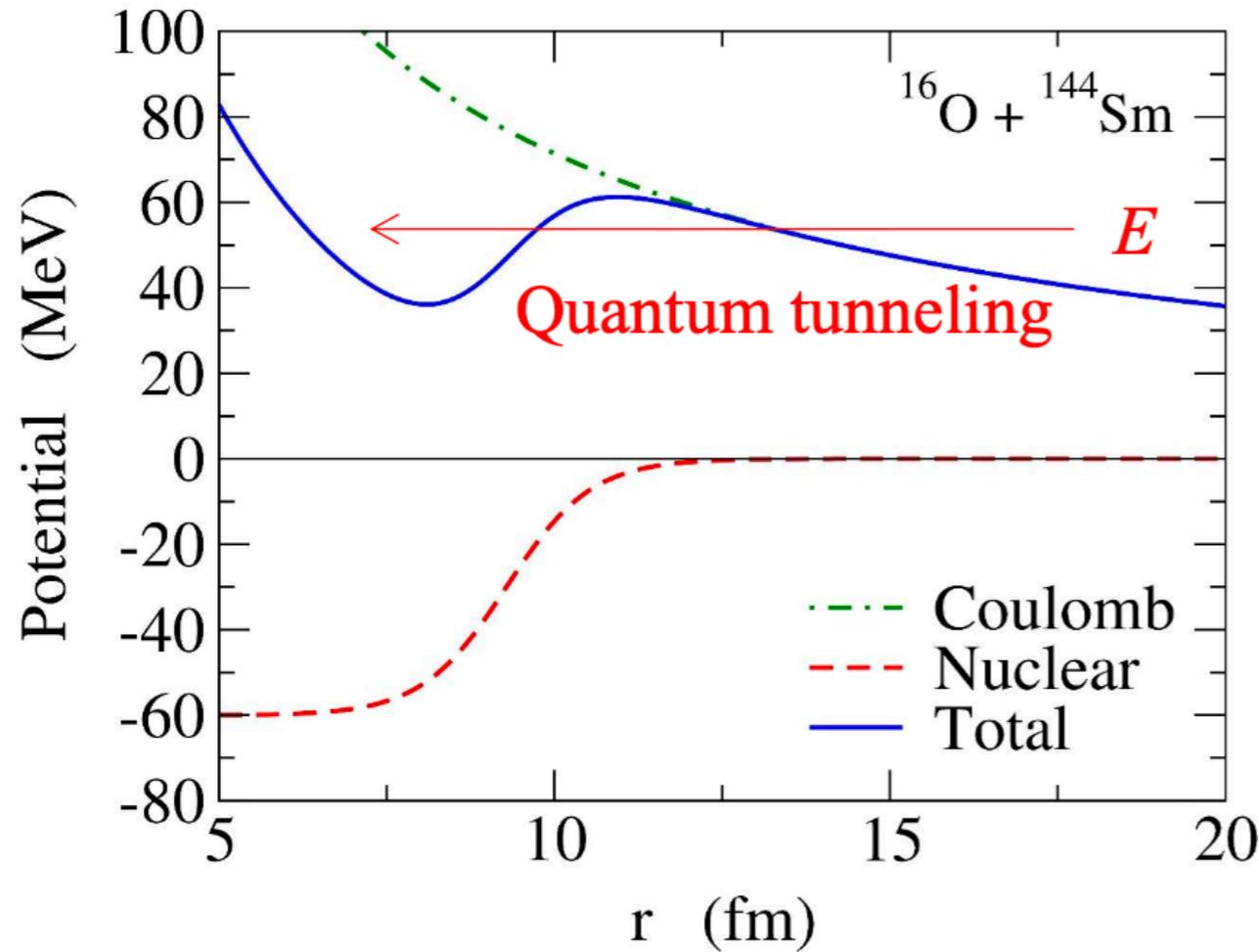
**How is the speed performance of emulator?**

**Is it feasible to built an emulator to represent CCFULL model?**

## **Summary**

# What is Low-energy sub-barrier fusion reaction?

A tunnel phenomena across the Coulomb barrier



1. **Coulomb interaction**  
long range, repulsion

2. **Nuclear interaction**  
short range, attraction



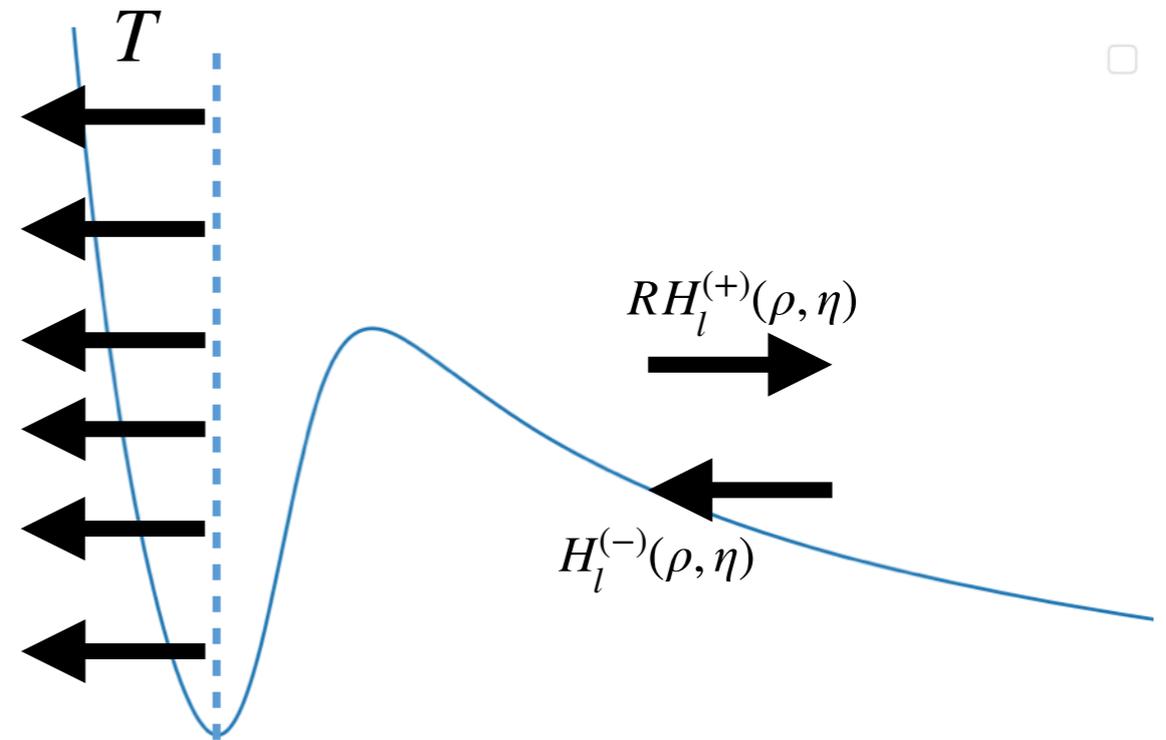
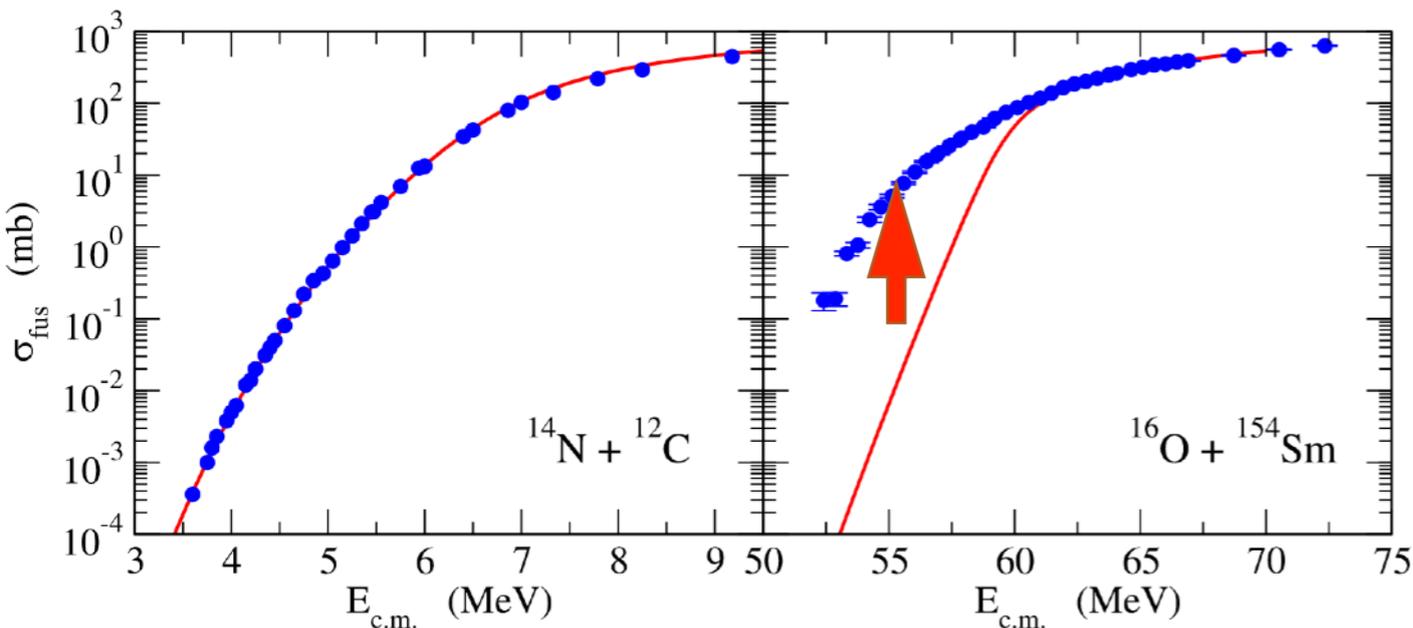
Potential barrier (**Coulomb barrier**)

**Fusion: takes place by overcoming the barrier**

the barrier height  $\rightarrow$  defines the energy scale of a system

**Fusion reactions at energies around the Coulomb barrier**

# What is Low-energy sub-barrier fusion reaction? :



$$\left[ -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{J(J+1)\hbar^2}{2\mu r^2} + V_N^{(0)}(r) + \frac{Z_P Z_T e^2}{r} - E \right] \psi_n(r) = 0,$$

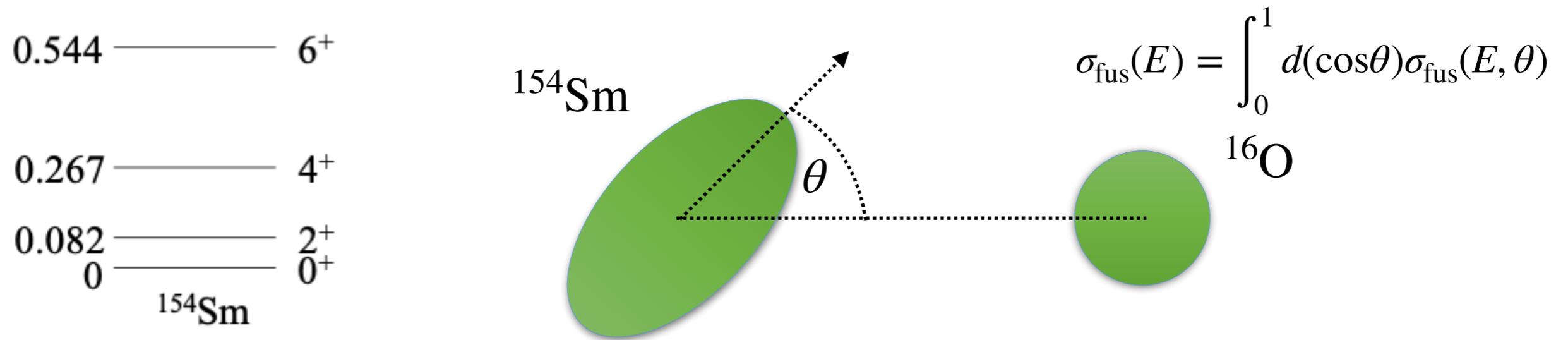
**Penetration Probability:**  $T_l = 1 - |R|^2$

**Fusion cross section:**  $\sigma_{\text{fus}}(E) = \frac{2\pi}{k^2} \sum_l (2l+1) T(E, l)$

- Works well for relatively light systems
- Underpredicts  $\sigma_{\text{fus}}$  for heavy systems at low energies

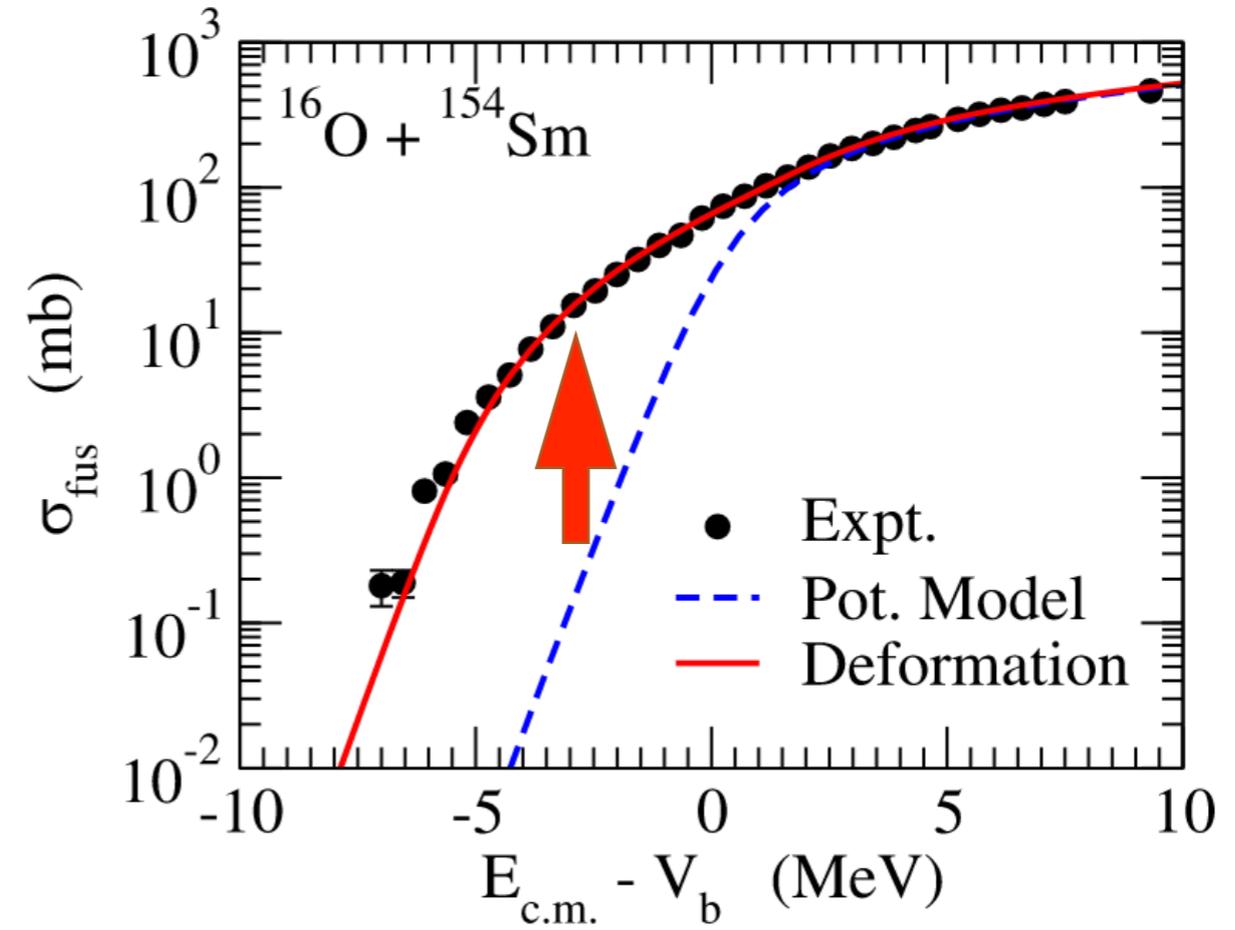
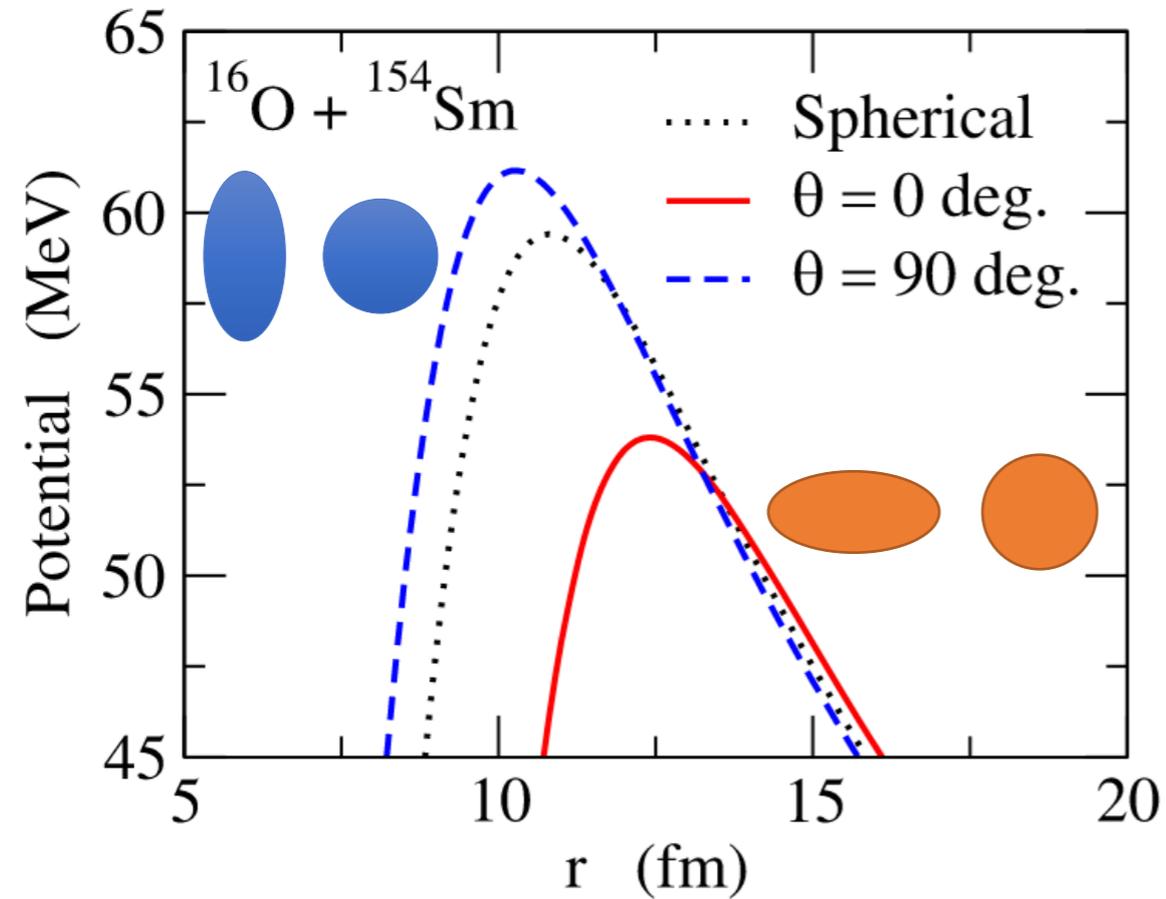
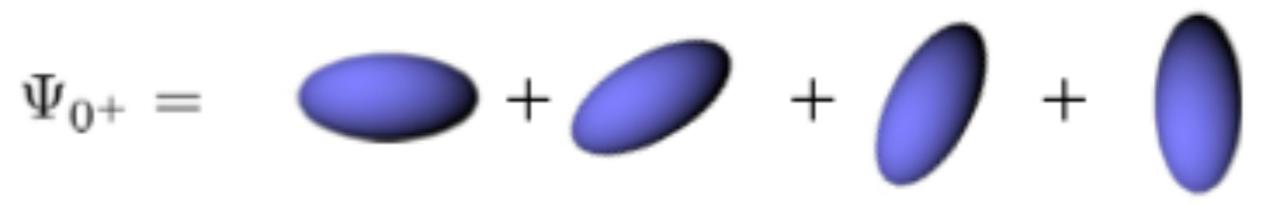


# How to explain the phenomenon in classical picture:



$$\sigma_{\text{fus}}(E) = \int_0^1 d(\cos\theta) \sigma_{\text{fus}}(E, \theta)$$

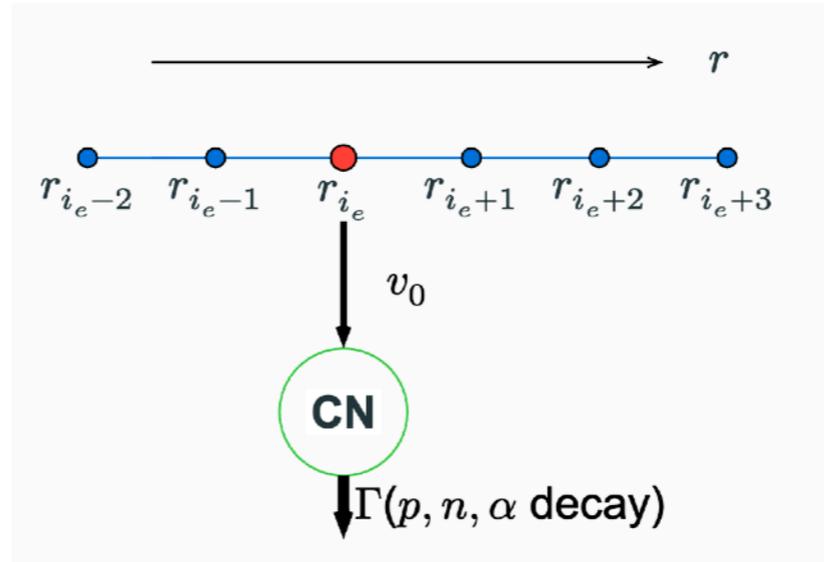
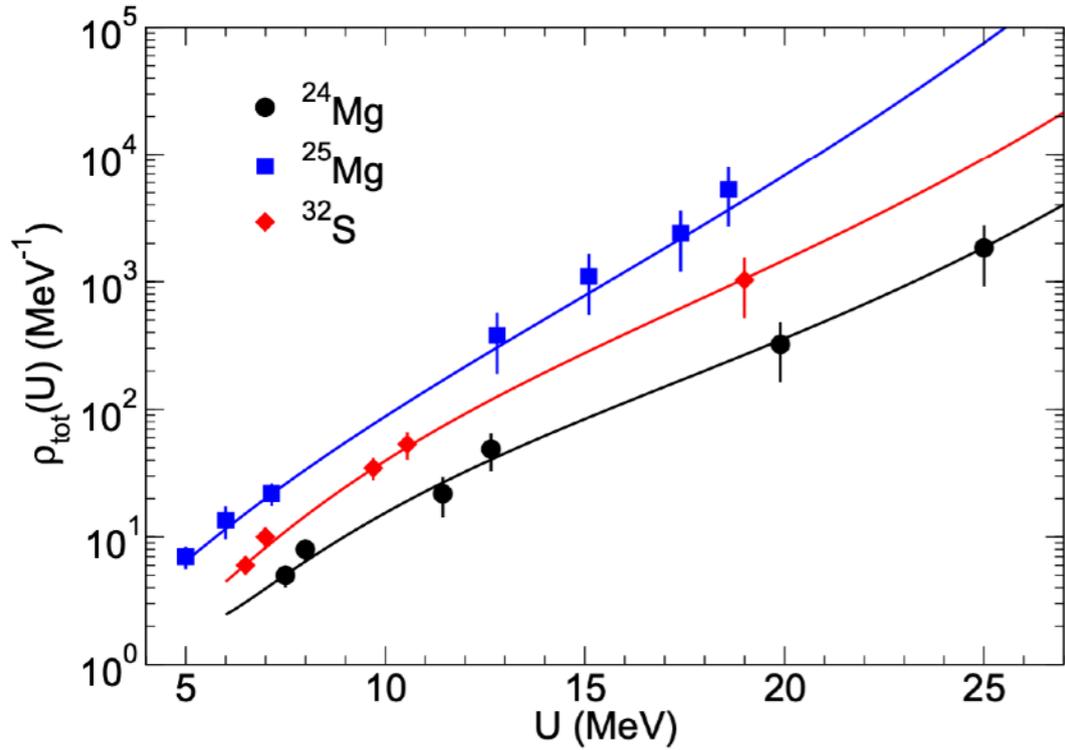
$E_{\text{rot}} \approx 0.082 \text{ MeV}$      $\tau_{\text{rot}} \approx 8 \times 10^{-21} \text{ s}$   
 $E_{\text{tunnel}} \approx 3.5 \text{ MeV}$      $\tau_{\text{tunnel}} \approx 1.9 \times 10^{-22} \text{ s}$



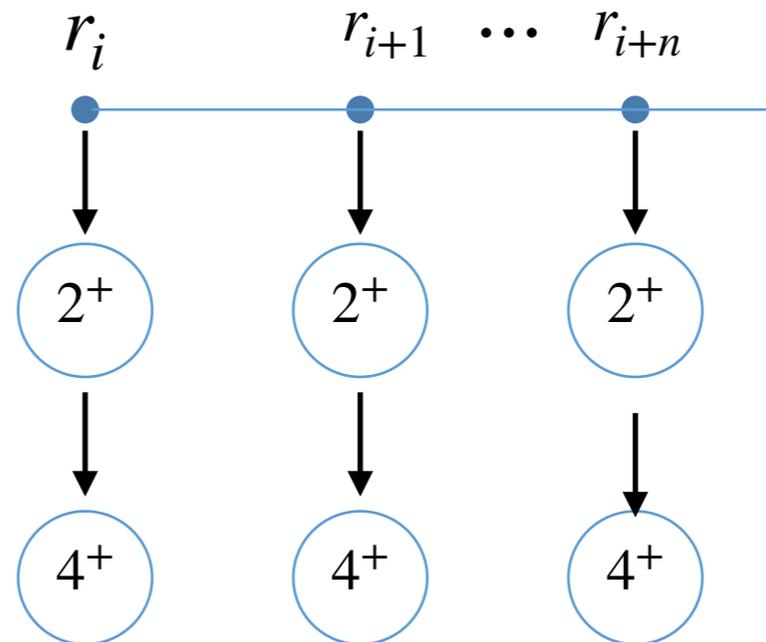
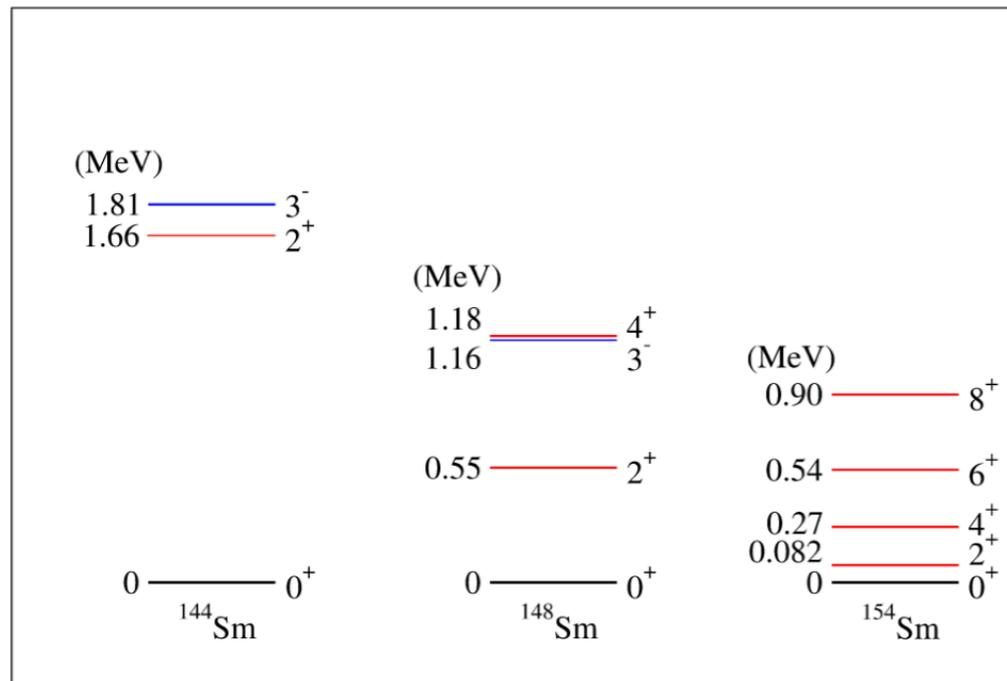
# How to explain the phenomenon in Quantum picture:

## The coupled-channel model:

Kosei Nagao's talk



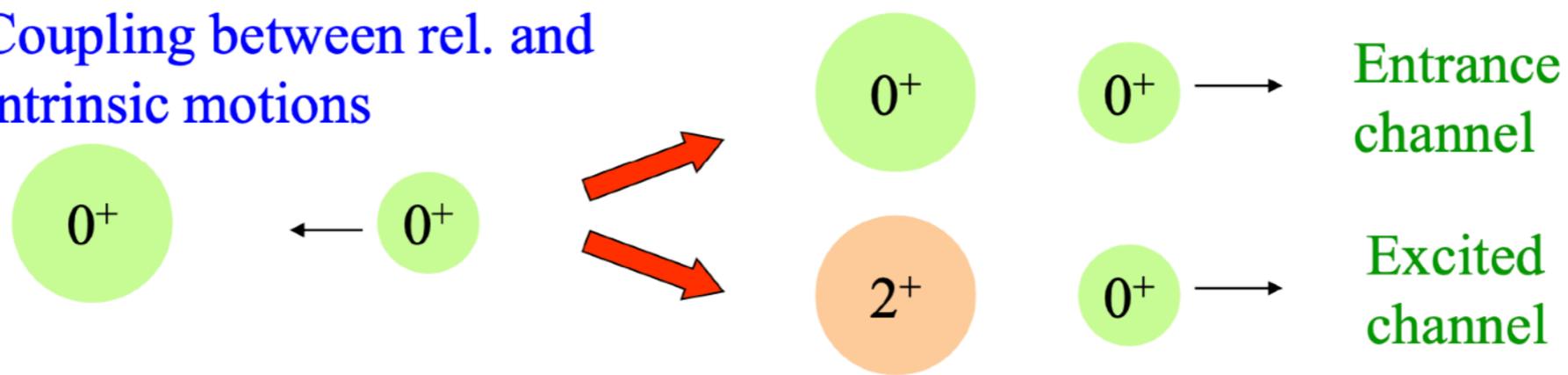
$$H = \begin{pmatrix} H_{C+C} & V \\ V^T & H_{\text{CN}} \end{pmatrix}.$$



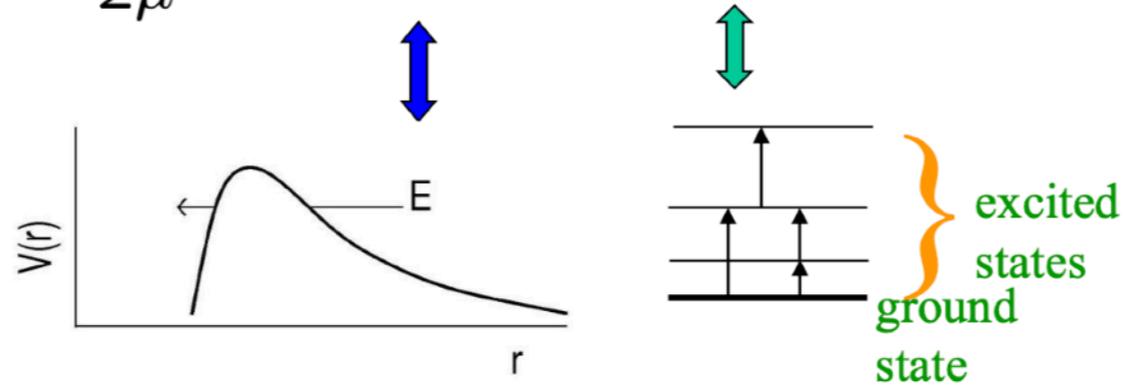
$$H = \begin{pmatrix} H_0 & V \\ V^T & H_{2^+} \end{pmatrix}$$

two-channels Hamiltonian matrix **7**

Coupling between rel. and intrinsic motions



$$H = -\frac{\hbar^2}{2\mu} \nabla^2 + V_0(r) + H_0(\xi) + V_{\text{coup}}(r, \xi)$$



$$H_0(\xi) \phi_k(\xi) = \epsilon_k \phi_k(\xi)$$

The total, three-channels Hamiltonian matrix

$$H = \begin{pmatrix} 2t + V(r_0) & -t & 0 & \dots \\ -t & 2t + V(r_0) & -t & \dots \\ 0 & -t & 2t + V(r_0) & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & \dots \\ 0 & E(2^+) & 0 & \dots \\ 0 & 0 & E(4^+) & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} + \begin{pmatrix} V_{00}(r_0) & V_{01}(r_0) & V_{02}(r_0) & \dots \\ V_{10}(r_0) & V_{11}(r_0) & V_{12}(r_0) & \dots \\ V_{20}(r_0) & V_{21}(r_0) & V_{22}(r_0) & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

For convenient, I just show the element where  $r = r_0$

$$V_{nm}(r_0) = V_{nm}^{(C)} + V_{nm}^{(N)}(r_0)$$

$$V_{nm}(r_0) = V_{nm}^{(C)} + V_{nm}^{(N)}(r_0)$$

The nuclear coupling Hamiltonian is thus given by:

$$V_N(r, \hat{O}) = - \frac{V_0}{1 + \exp(r - R_0 - \hat{O})/a}$$

**Dynamical operator:**  $R_0 \rightarrow R_0 + \hat{O} = R_0 + \beta_2 R_T Y_{20} + \beta_4 R_T Y_{40}$

**For the matrix element of the operator  $\hat{O}$ , here we take one example:**

**Here, we know**  $\langle \alpha' | \beta_2 R_T Y_{20} | \alpha \rangle = \int Y_{j_1 m_1}^* \beta_2 R_T Y_{20} Y_{j_1 m_1} d\theta d\varphi$

$$\int Y_{j_1 m_1}(\theta, \varphi) Y_{j_2 m_2}(\theta, \varphi) Y_{j_3 m_3}(\theta, \varphi) d\Omega = \sqrt{\frac{(2j_1 + 1)(2j_2 + 1)(2j_3 + 1)}{4\pi}} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3 \\ 0 & 0 & 0 \end{pmatrix}$$

**if we only consider axi-symmetry situation,  $m_1 = 0$**

$$\hat{O}_{I'0I0} = \beta_2 R_T \sqrt{\frac{5(2I + 1)(2I' + 1)}{4\pi}} \begin{pmatrix} I & 2 & I' \\ 0 & 0 & 0 \end{pmatrix}^2 + \beta_4 R_T \sqrt{\frac{9(2I + 1)(2I' + 1)}{4\pi}} \begin{pmatrix} I & 4 & I' \\ 0 & 0 & 0 \end{pmatrix}^2$$

**The nuclear coupling matrix elements are then evaluated as**

$$\begin{aligned} V_{nm}^{(N)} &= \langle I'0 | V_N(r, \hat{O}) | I0 \rangle - V_N^0(r) \delta_{n,m} \\ &= \sum_{\alpha} \langle I'0 | \alpha \rangle \langle \alpha | I0 \rangle V_N(r, \lambda_{\alpha}) - V_N^0(r) \delta_{n,m} \end{aligned}$$

$$V_{nm}(r_0) = V_{nm}^{(C)} + V_{nm}^{(N)}(r_0)$$

**The Coulomb component of the coupling Hamiltonian is evaluated as follows.**

$$V_C(r) = \int dr' \frac{Z_P Z_T e^2}{|r - r'|} \rho_T(r') = \sum_{\lambda} \frac{3Z_P Z_T e^2}{(2\lambda + 1)R_T^3} \sum_{\mu=-\lambda}^{+\lambda} \frac{1}{r^{\lambda+1}} Y_{\lambda\mu}^*(\hat{r}) \int_0^{2\pi} \int_0^{\pi} \frac{1}{\lambda + 3} R_T^{\lambda+3}(\theta', \phi') Y_{\lambda\mu}(\theta', \phi') d\theta' d\phi'$$

$$R_0 \rightarrow R_0 + \hat{O} = R_0 + \beta_2 R_T Y_{20} + \beta_4 R_T Y_{40}$$

**for the intergal,  $\lambda = 2$  and  $\mu = 0$  only.**

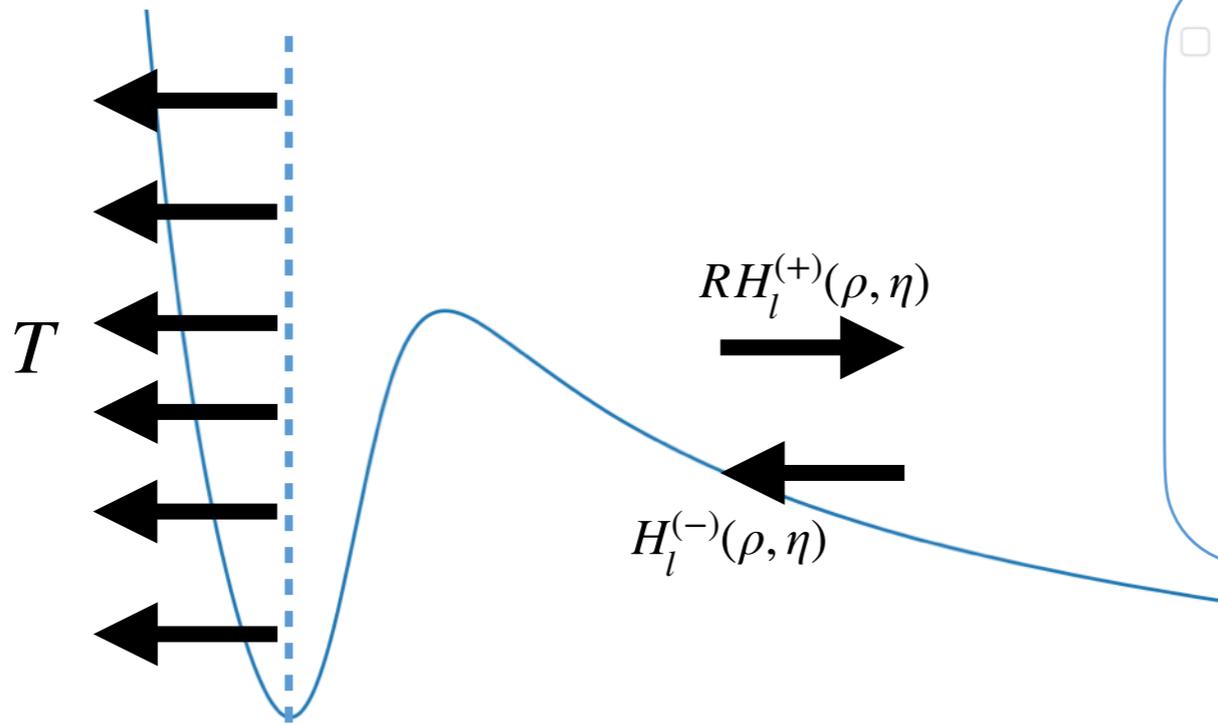
$$V_C(r) = \frac{3Z_P Z_T e^2}{5} \frac{R_T^2}{r^3} \beta_2 Y_{20}$$

**Therefore, for the matrix element  $V_{mn}(r)$**

$$\langle I'0 | V^C | I0 \rangle = \left\langle I'0 \left| \frac{3Z_P Z_T e^2}{5} \frac{R_T^2}{r^3} \beta_2 Y_{20} \right| I0 \right\rangle + \left\langle I'0 \left| \frac{3Z_P Z_T e^2}{9} \frac{R_T^4}{r^5} \beta_4 Y_{40} \right| I0 \right\rangle$$

$$V_{nm}^{(C)} = V_{I0, I'0}^{(C)} = \frac{3Z_P Z_T e^2}{5} \frac{R_T^2}{r^3} \sqrt{\frac{5(2I+1)(2I'+1)}{4\pi}} \left( \beta_2 + \frac{2}{7} \sqrt{\frac{5}{\pi}} \beta_2^2 \right) \begin{pmatrix} I2I' \\ 000 \end{pmatrix}^2$$

$$+ \frac{3Z_P Z_T e^2}{9} \frac{R_T^4}{r^5} \sqrt{\frac{9(2I+1)(2I'+1)}{4\pi}} \left( \beta_4 + \frac{9}{7} \sqrt{\frac{1}{\pi}} \beta_2^2 \right) \begin{pmatrix} I4I' \\ 000 \end{pmatrix}^2$$



□ The boundary conditions are thus expressed as

$$\rightarrow T_n \exp\left(-i \int_{r_{\min}}^r k_n(r') dr'\right), \quad r \leq r_{\min},$$

$$\rightarrow H_J^{(-)}(k_n r) \delta_{n,0} + R_n H_J^{(+)}(k_n r), \quad r > r_{\max},$$

$$\left[ -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{J(J+1)\hbar^2}{2\mu r^2} + V_N^{(0)}(r) + \frac{Z_p Z_T e^2}{r} + \epsilon_n - E \right] \psi_n(r) + \sum_m V_{nm}(r) \psi_m(r) = 0,$$

For that purpose, we extend the model space by adding  $x_N$  and  $x_{N+1}$ , and introduce the basis functions

$$\Psi \equiv \sum_s \sum_{n=0}^{N-1} b_n^{(s)} \phi_n + b_N^{(s)} \phi_{H^+} + \phi_{H^-}$$

The penetrability is then computed as,

$$\psi_n = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad \psi_{H^+} = \psi_N = \begin{bmatrix} 0 \\ \vdots \\ H_l^{(+)}(x_N) \\ H_l^{(+)}(x_{N+1}) \end{bmatrix}, \quad \psi_{H^-} = \psi_{H^+}^*$$

$$P = 1 - \sum_{s=1,2} \frac{k_s}{k_1} |b_{s0}|^2 = \sum_{s=1,2} \frac{k_s}{k_1} |b_{sN}|^2.$$

$$\sigma_{\text{fus}} = \frac{2\pi}{k^2} \sum_l (2l+1) P_l$$

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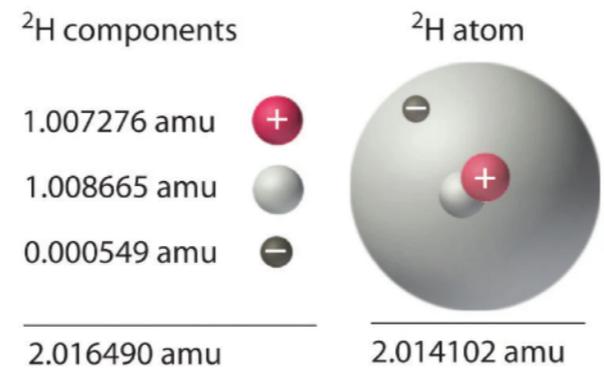
**How is the error performance of emulator ?**

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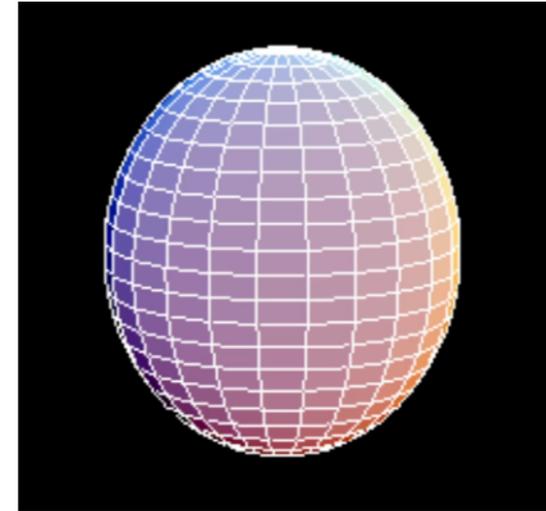
**Is it feasible to built an emulator to represent CCFULL model?**

## **Summary**

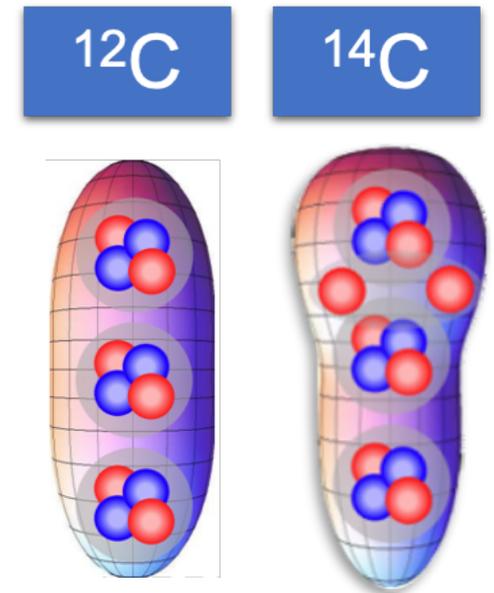
Rich properties:



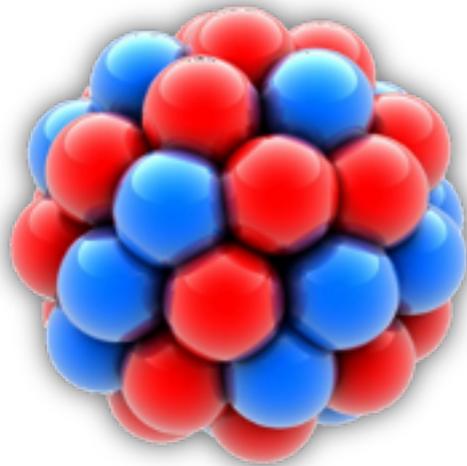
Mass



Collective mode

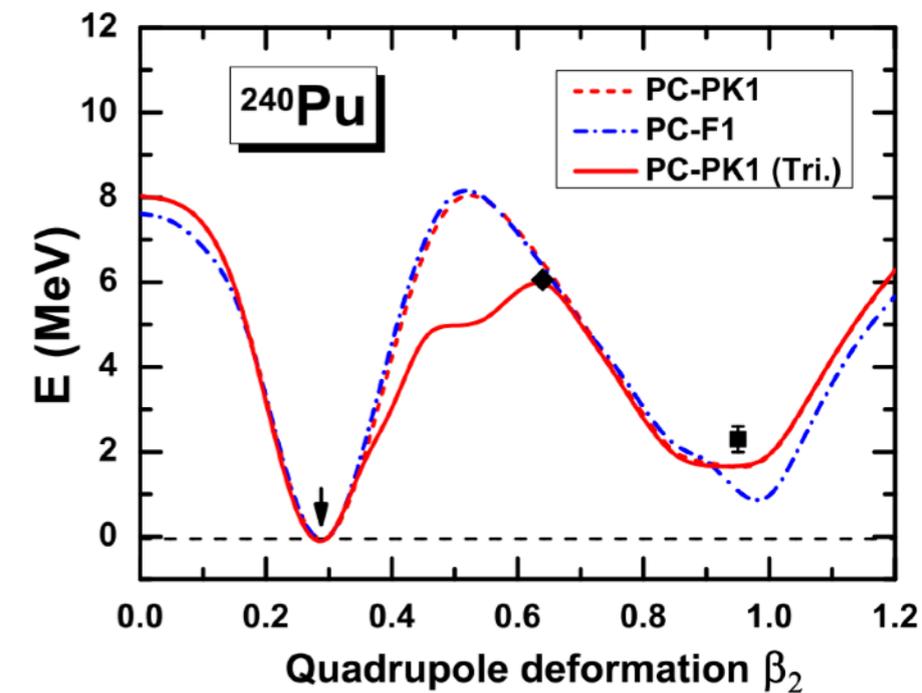
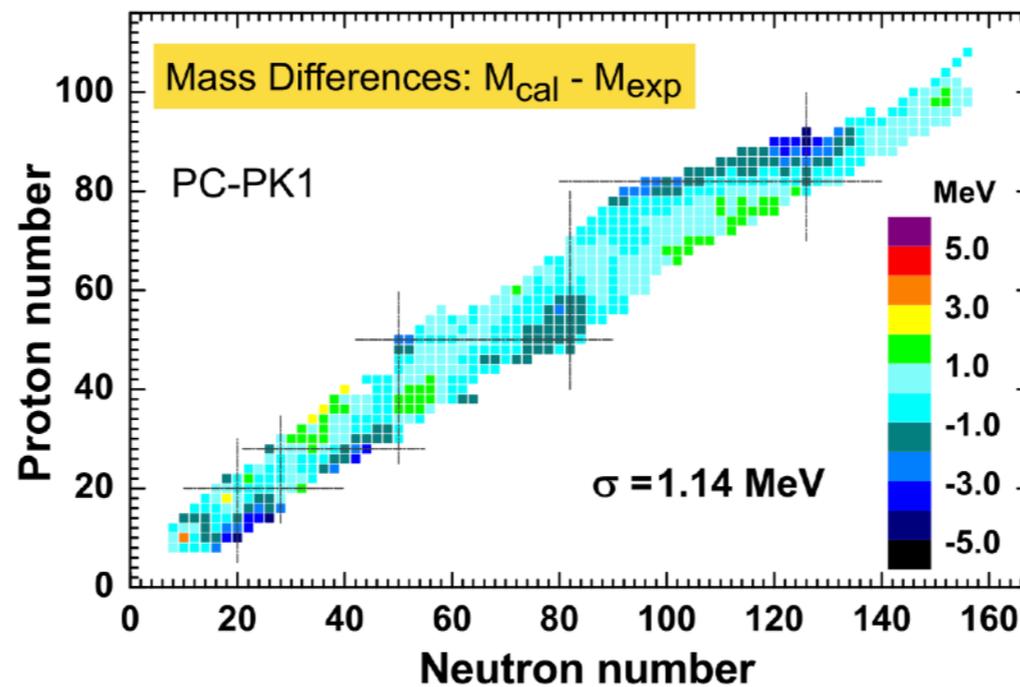


Exotic structure

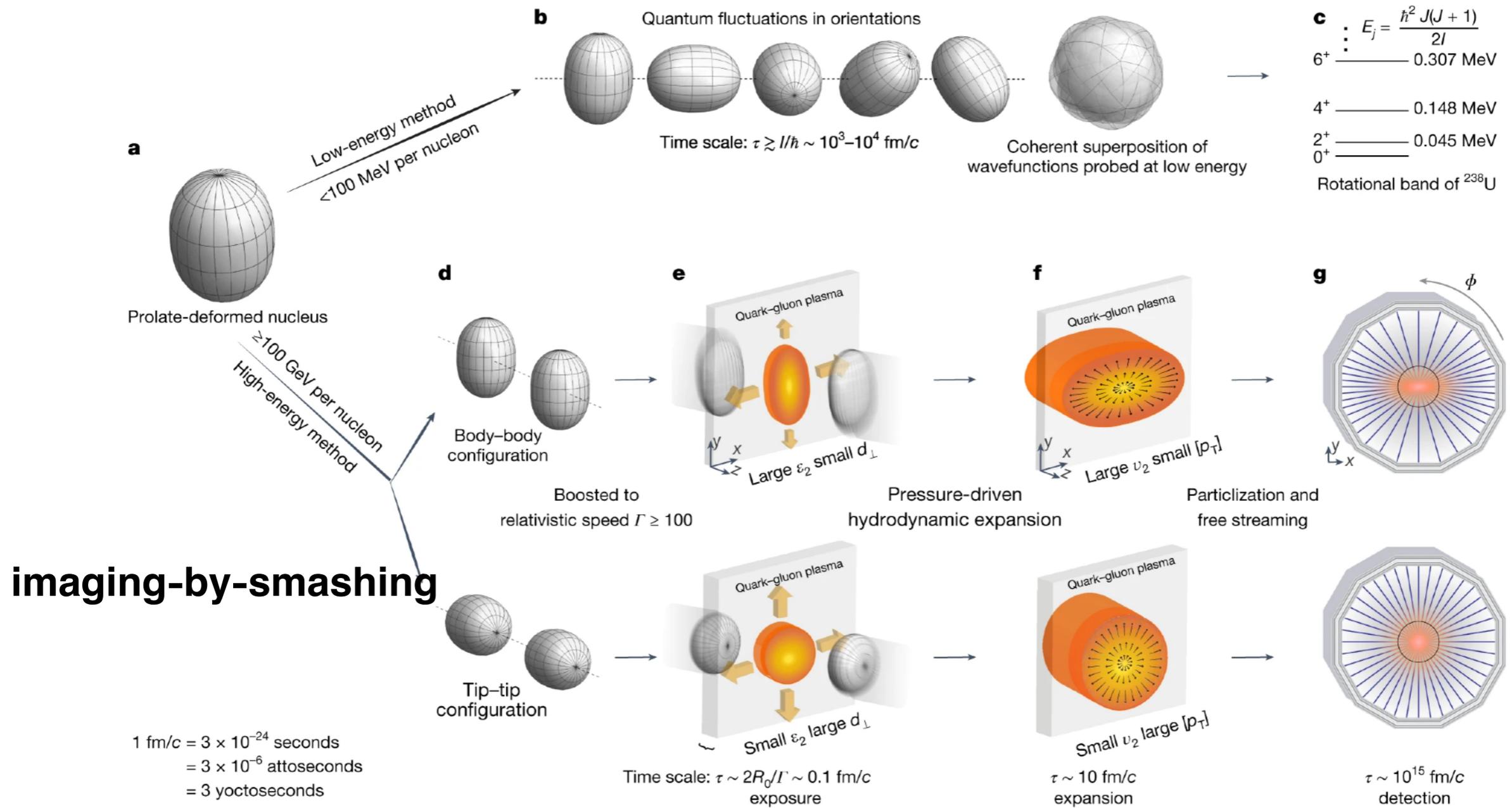


Quantum many-body systems

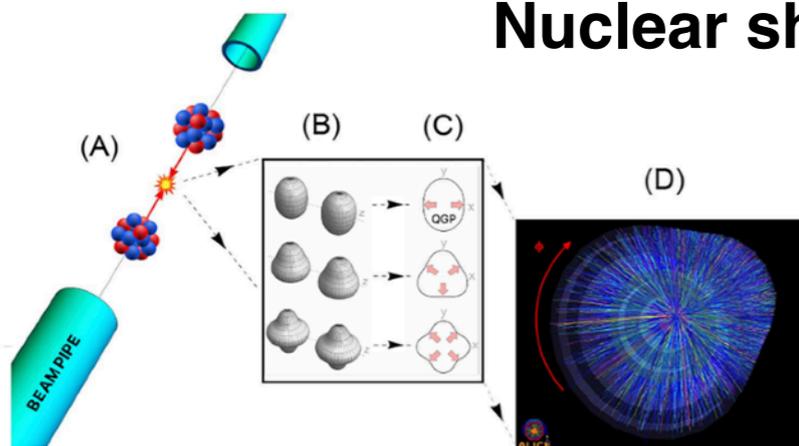
DFT determines these properties:



# Probing nuclear shapes in Relativistic H.I. collisions



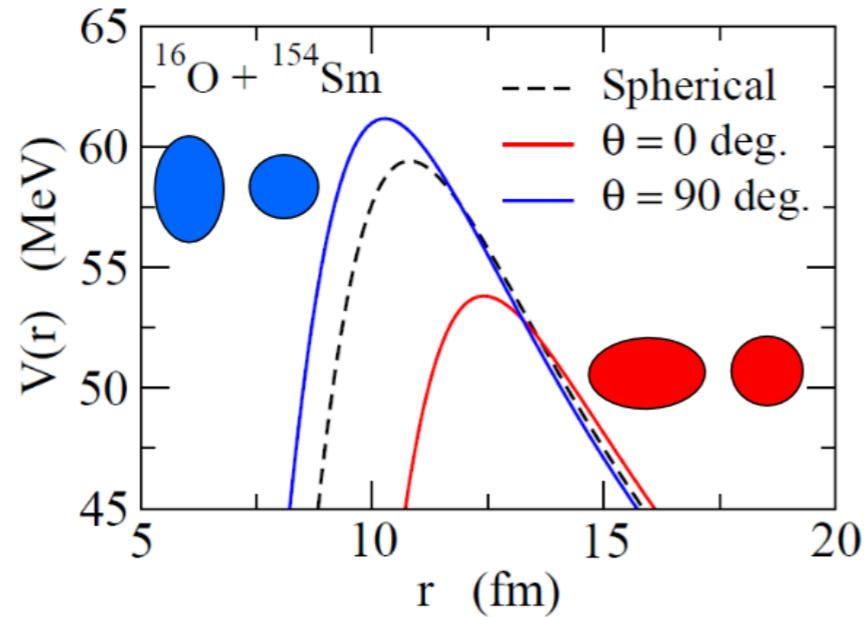
## Nuclear shapes are encoded during quark-gluon plasma formation and evolution



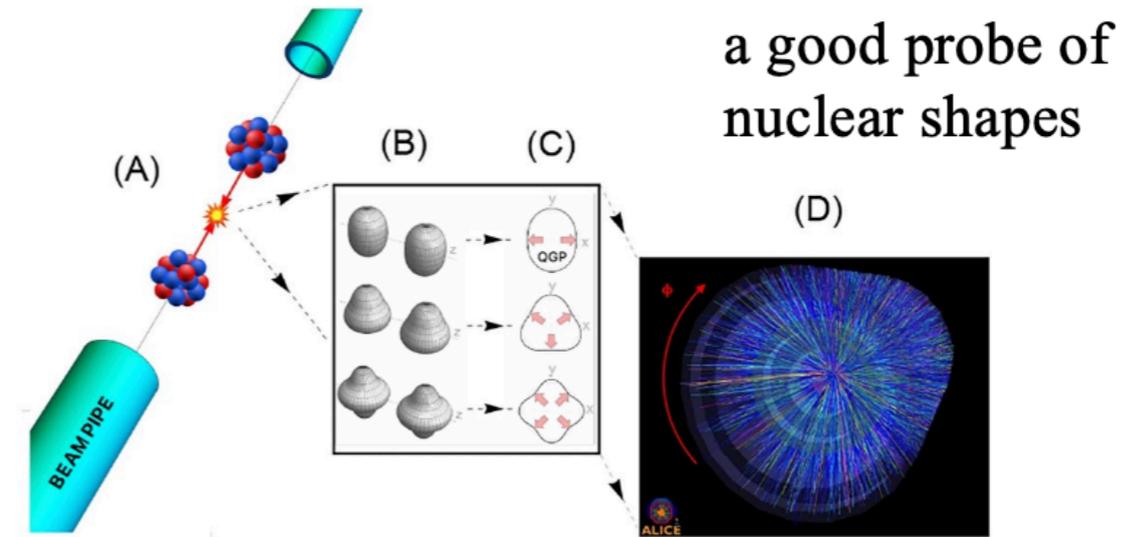
M.I. Abdulhamid et al. (STAR collaboration) Nature 635, 67 (2024)

J. Jia et al., Nucl. Sci. Tech. 35, 220 (2024)

**low-energy H.I. fusion reactions of a deformed nucleus**



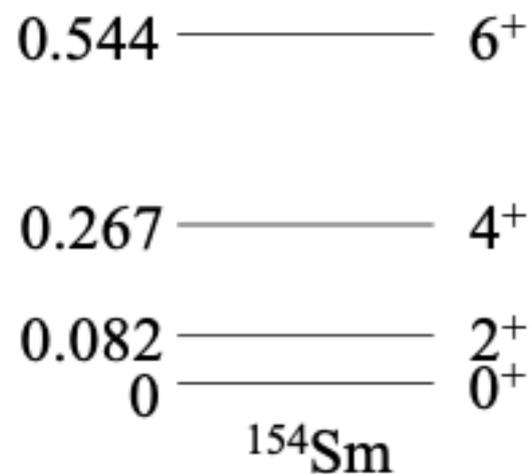
**relativistic H.I. collisions with a deformed nucleus**



J. Jia et al.,  
Nucl. Sci. Tech. 35, 220 (2024)

increasing interests in recent years

Large similarities → intersection of **High E** and **Low E** HI collisions

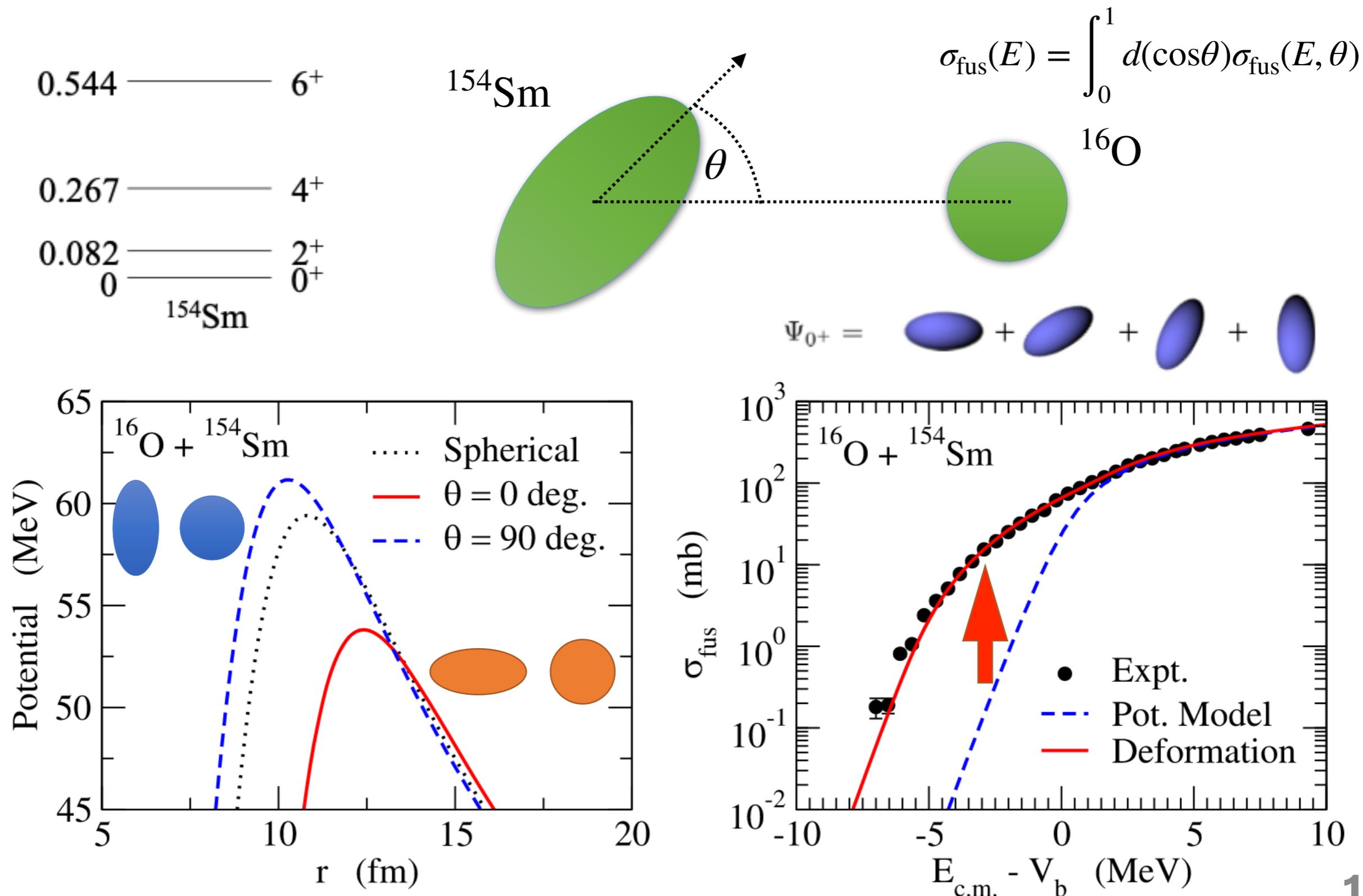


$$E_{\text{rot}} \approx 0.082 \text{ MeV} \quad \tau_{\text{rot}} \approx 8 \times 10^{-21} \text{ s}$$

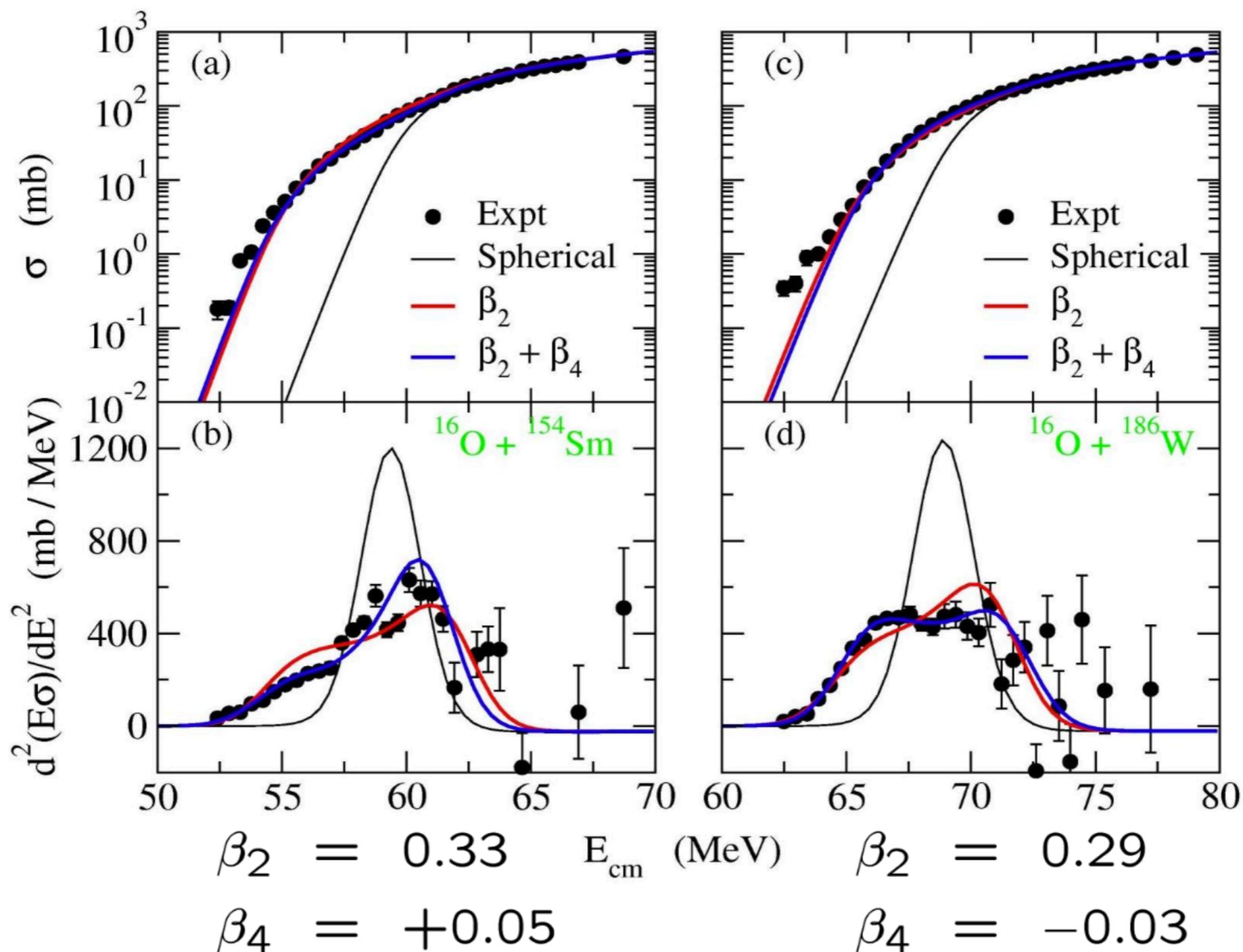
$$E_{\text{tunnel}} \approx 3.5 \text{ MeV} \quad \tau_{\text{tunnel}} \approx 1.9 \times 10^{-22} \text{ s}$$

# Probing nuclear shapes in Low-energy H.I. collisions

A good example of the interplay between structure and reaction



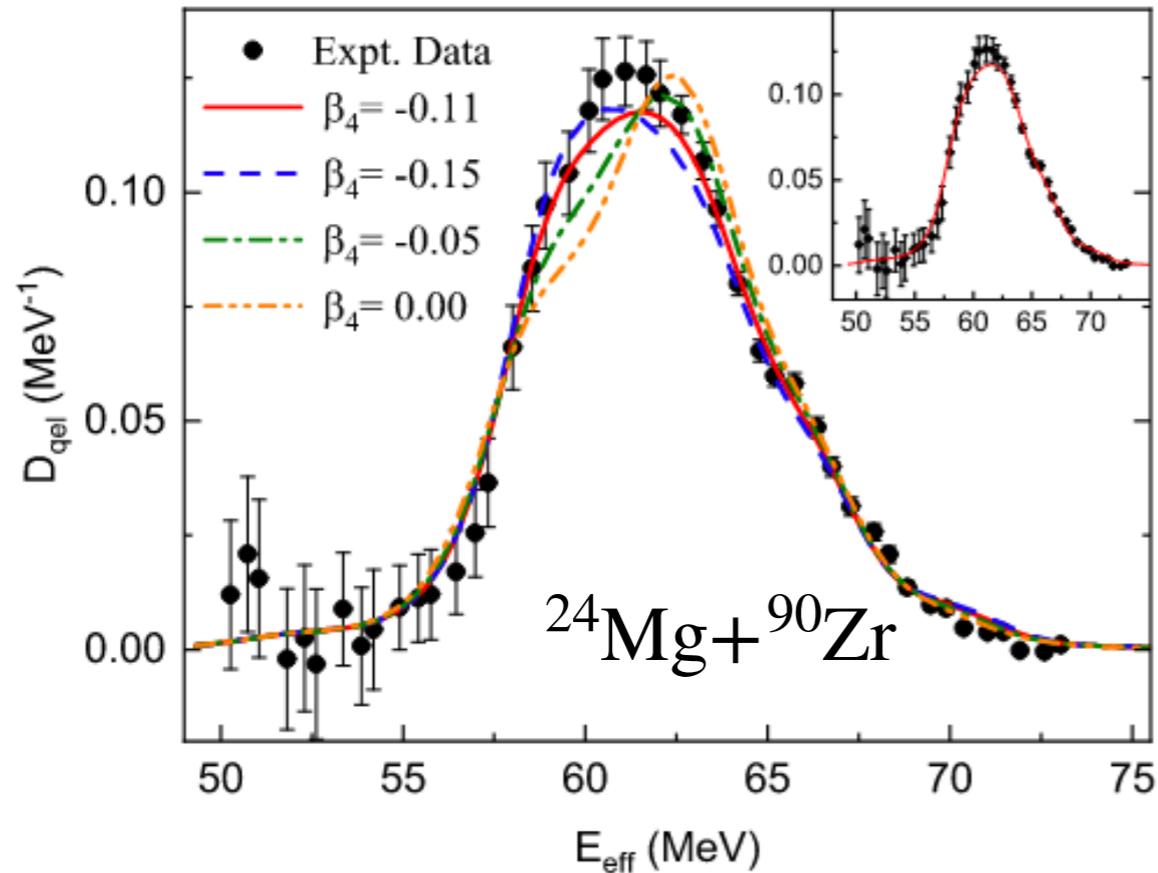
# Fusion reaction could be a probe to nuclei deformation.



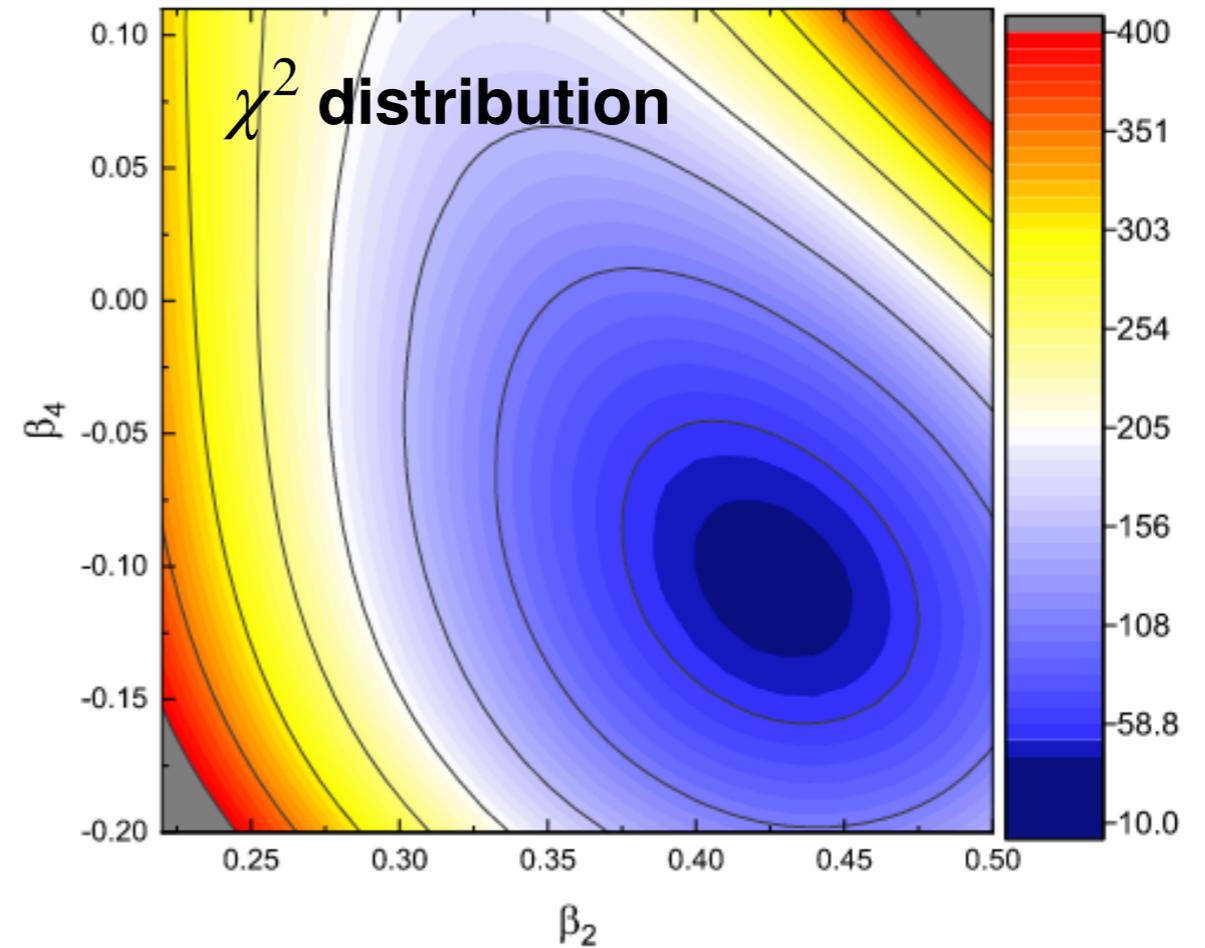
K. Hagino' talk in INPC 2025

J.R. Leigh et al., PRC52 ('95) 3151

# Determination of hexadecapole deformation of the light-mass nucleus $^{24}\text{Mg}$ using quasi-elastic scattering measurements



$$\beta_2 = 0.43, \quad \beta_4 = -0.11$$



cf. (p,p'):  $\beta_2 = 0.47, \quad \beta_4 = -0.05 \pm 0.08$

R. De Swiniarski et al., PRL23, 317 (1969)

$$\chi^2(\beta_2, \beta_4) = \sum_{i=1}^N \frac{[Y_i - f(\beta_2, \beta_4)]^2}{\sigma_i^2}$$

$Y_i$  : the experimental value at the  $i^{\text{th}}$  energy point,  
 $\sigma_i$  : the uncertainty in the data,  
 $f(\beta_2, \beta_4)$  : CCFULL calculation for a particular  $(\beta_2, \beta_4)$ .

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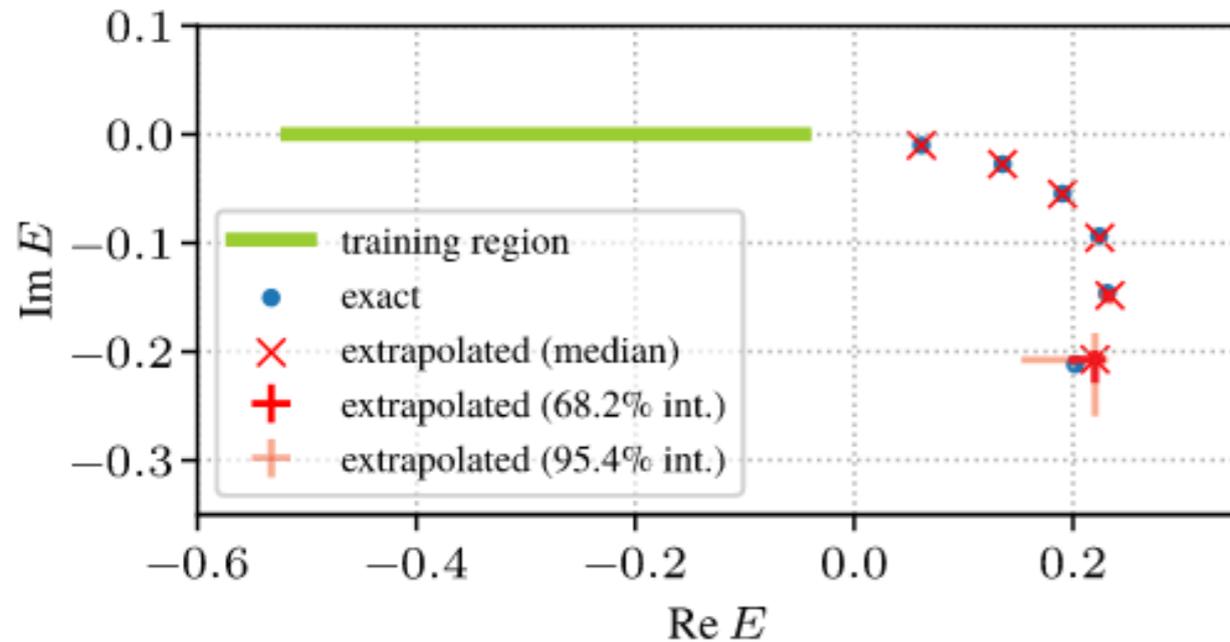
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## **Summary**

# Eigenvector Continuation:

EC is highly effective for **extrapolation**

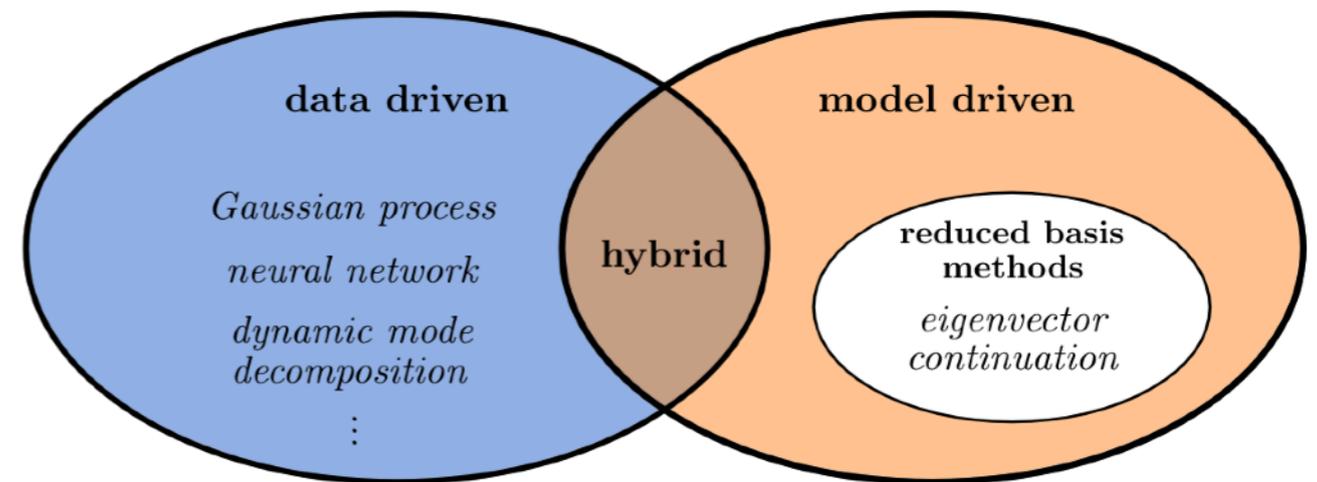
Shoujirou Mizutori san 's tall



**It can extend the applicability of existing computational methods to regions where the parameter values are beyond the methods original calculation thresholds.**

EC functions as a powerful emulator

**reduced order models**



## Data-driven methods:

typically interpolate the outputs of high-fidelity models without requiring an understanding of the underlying model structure

## Model-driven methods

solve reduced-order equations derived from the full equations, so they are physics based and respect the underlying structure

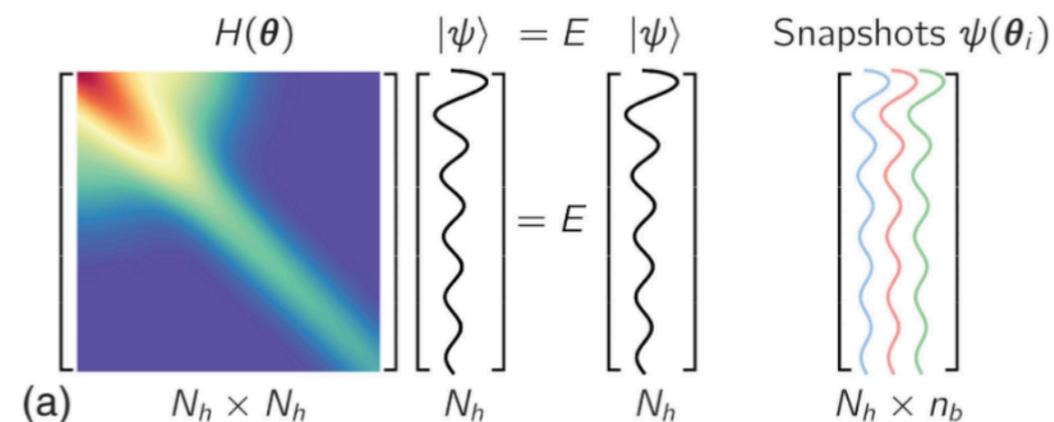
Yapa, N., and S. Konig, 2022, Phys. Rev. C 106, 014309.

Yapa, N., K. Fosse, and S. Konig, 2023, Phys. Rev. C 107, 064316.

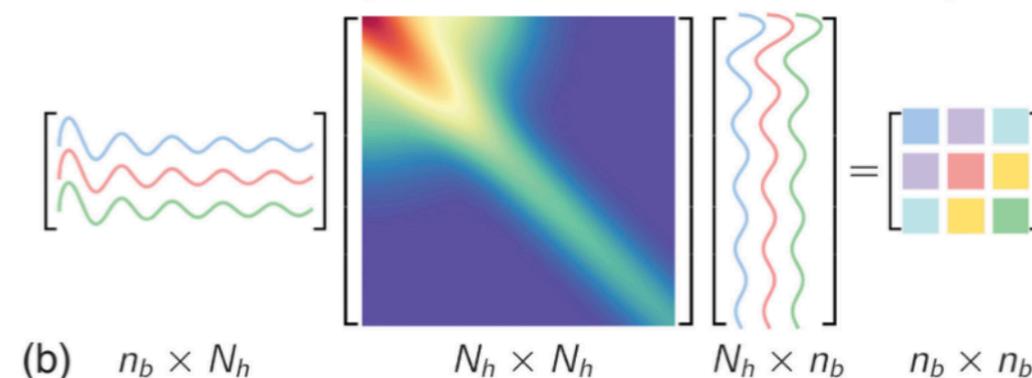
RevModPhys.96.031002

# Eigenvector Continuation:

- Select a small number of **training parameter values**  $\theta_i$ . Calculate the corresponding exact eigenvectors, or “**snapshots**,”
- The EC method uses these snapshots to span a **low-dimensional variational subspace**
- For any new parameter value  $\theta_{\text{new}}$ , the original large Hamiltonian  $H(\theta_{\text{new}})$  is projected onto the much smaller EC subspace.
- A tiny, effective projected eigenvalue problem is solved:



Projection (after orthonormalizing snapshots)



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

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

$$\begin{bmatrix} \text{grid} \end{bmatrix} \begin{bmatrix} \bullet \\ \blacklozenge \\ \blacktriangledown \end{bmatrix} = \tilde{E} \begin{bmatrix} \bullet \\ \blacklozenge \\ \blacktriangledown \end{bmatrix}$$

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

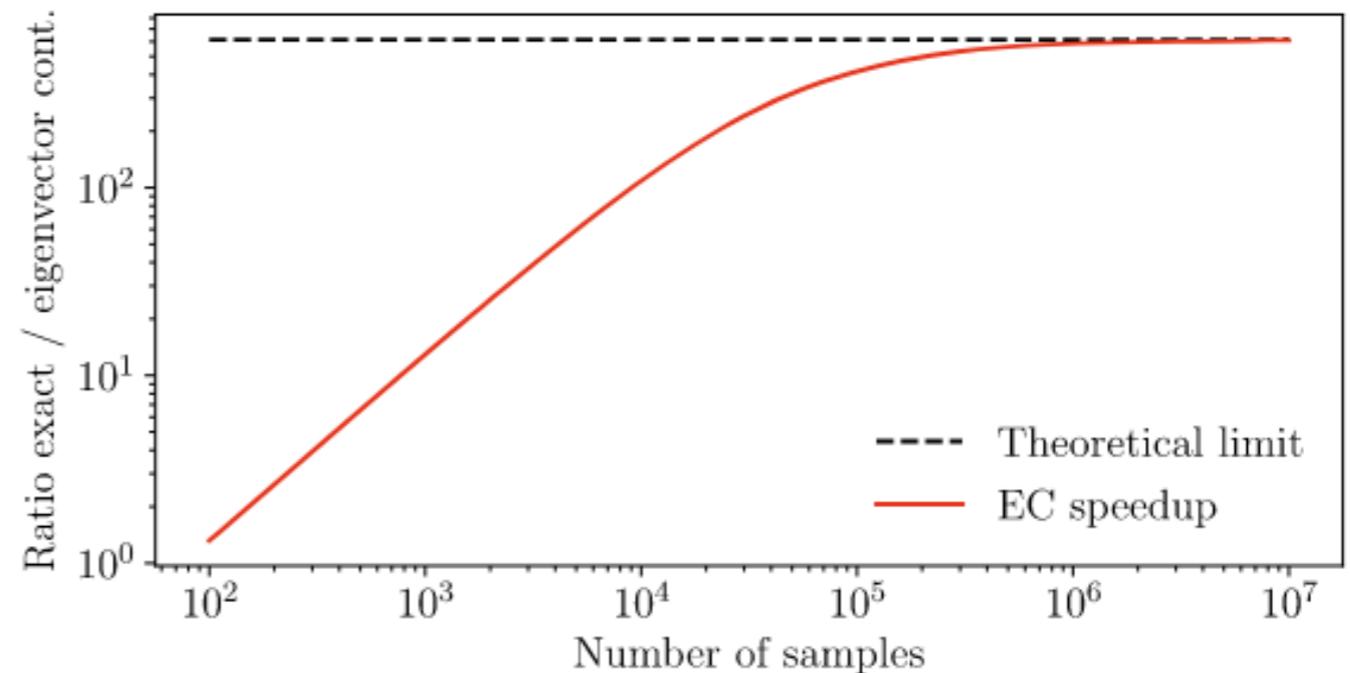
(c) All size- $n_b$  operations

# Eigenvector Continuation:

## Application to no-core shell-model calculation of ${}^4\text{He}$

The parameters  $\theta$  considered by König *et al.* (2020) are the low-energy constants of the chiral effective field theory ( $\chi\text{EFT}$ ) potential used in that work. Overall, there are  $d = 16$  individual parameters subsumed in  $\theta$  that determine two- and three-nucleon interactions in the potential. Setting up an EC emulator proceeds following the on-line–off-line scheme described in Sec. II for the generic RBM workflow.

- (i) Picking a training set  $\{\theta_i\}_{i=1}^{n_b}$  of  $n_b$  parameters, using space-filling Latin hypercube sampling (McKay, Beckman, and Conover, 1979) in the  $d$ -dimensional parameter domain (or some subset thereof).
- (ii) Performing exact calculations (for the ground states of  ${}^3\text{H}$  and  ${}^4\text{He}$ ) in the case of König *et al.* (2020) for each point in the training set.
- (iii) Constructing a pair of Hamiltonian and norm matrices as described in Sec. II for each evaluation of the emulator at a target parameter point  $\theta_*$ .



**EC emulator that can be rapidly evaluated at many different parameter points. This approach achieves significant speedup factors**

König, S., A. Ekström, K. Hebeler, D. Lee, and A. Schwenk, 2020, “Eigenvector continuation as an efficient and accurate emulator for uncertainty quantification,” *Phys. Lett. B* 810, 135814.

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## **Eignvector Continuation:**

**What is the  $E_c$ ?**

**What can we do with  $E_c$ ?**

## **Emulator to determine the nuclei shape:**

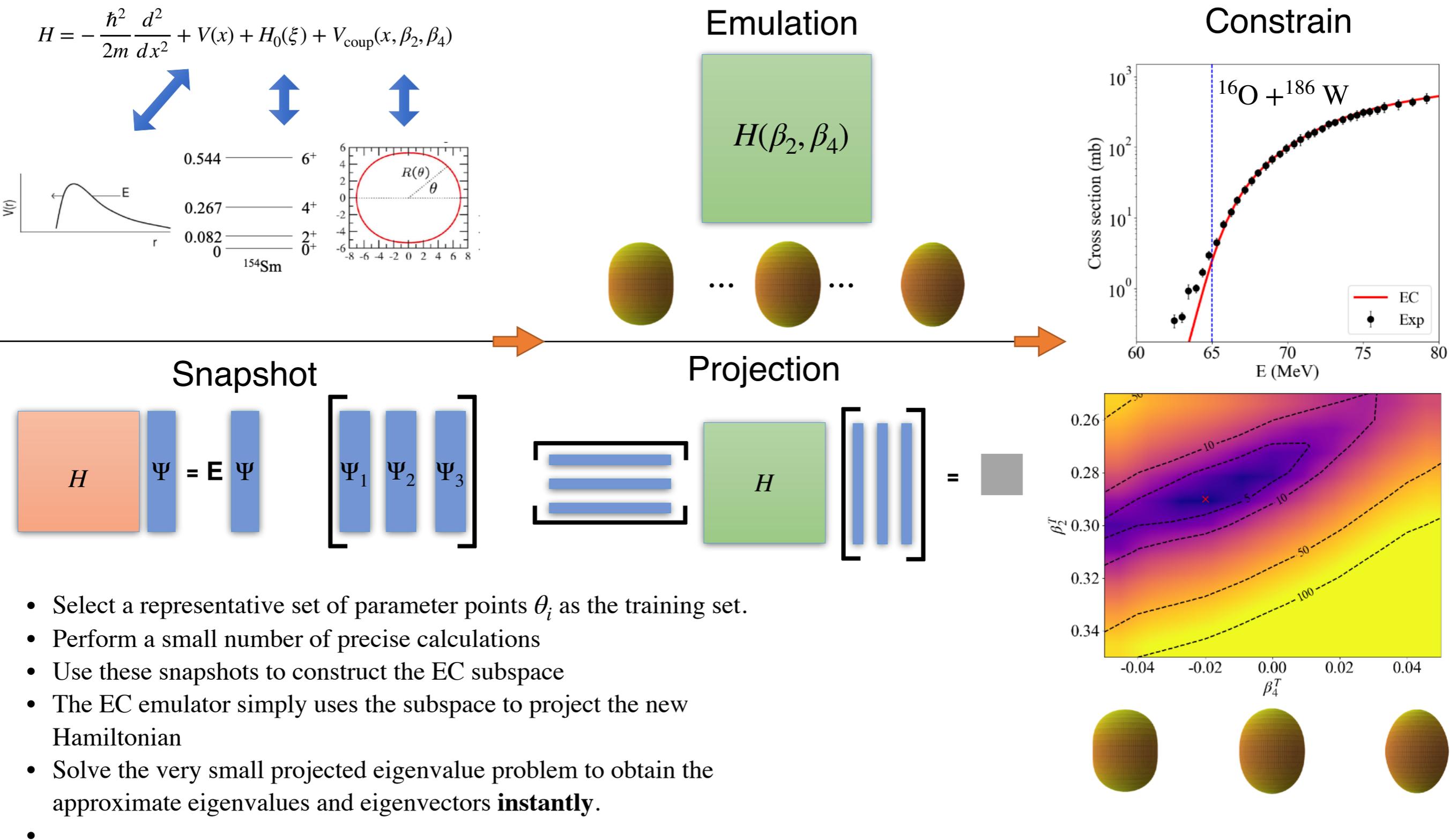
**How is the error performance of emulator ?**

**How is the speed performance of emulator?**

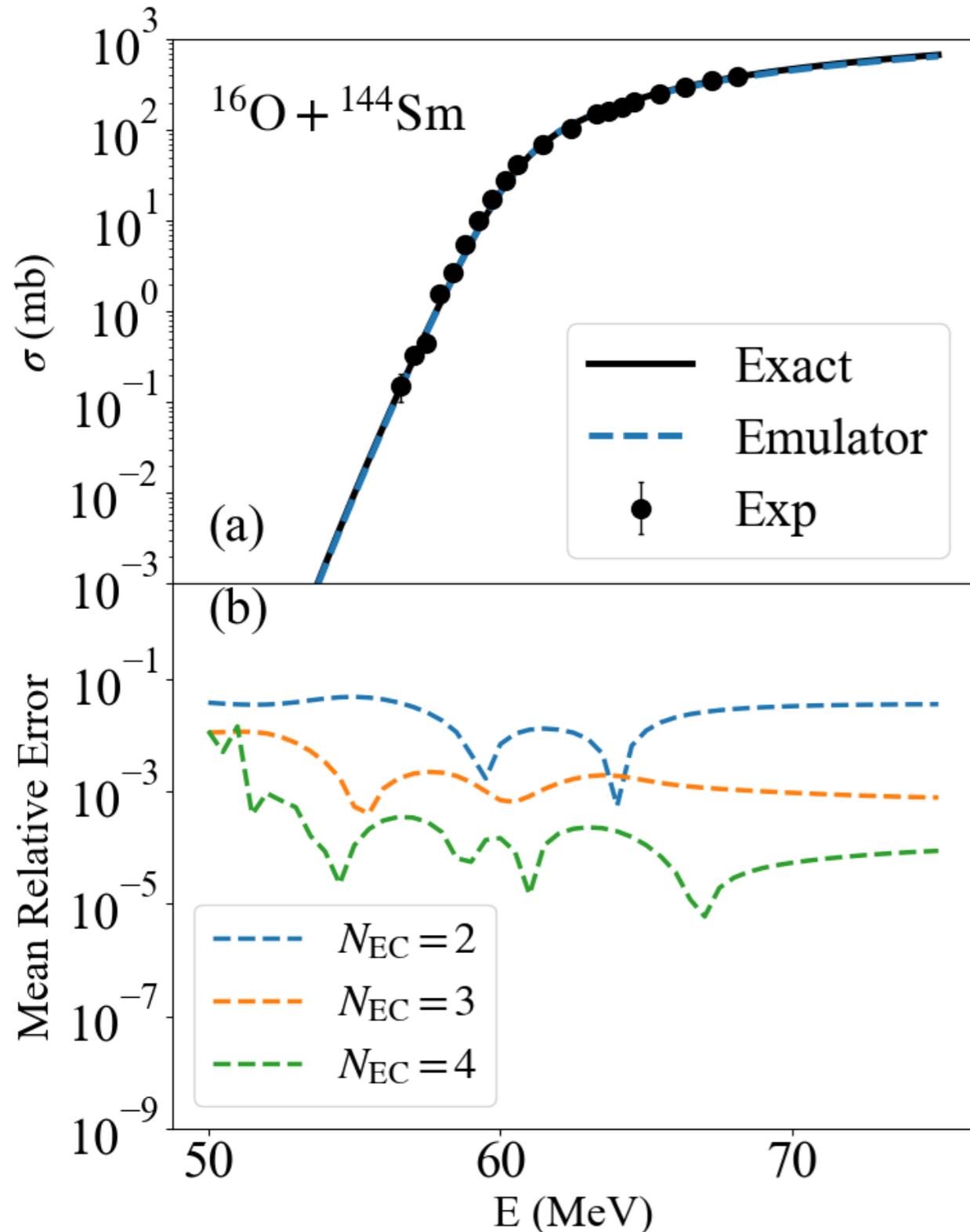
**Is it feasible to built an emulator to represent CCFULL model?**

## **Summary**

# Emulator for Coupled Channel Model



# Emulator: Accuracy performance



For the exact result into ccfull model

■ The octupole vibration deformation parameter  $\beta_3 = 0.21$

For the Ec calculation, we show the case  $N_{\text{EC}} = 2$ .

■ For the this case, we choose the basis  $(\beta_3^{(i)} = 0.23, 0.25)$  to emulate the exact case

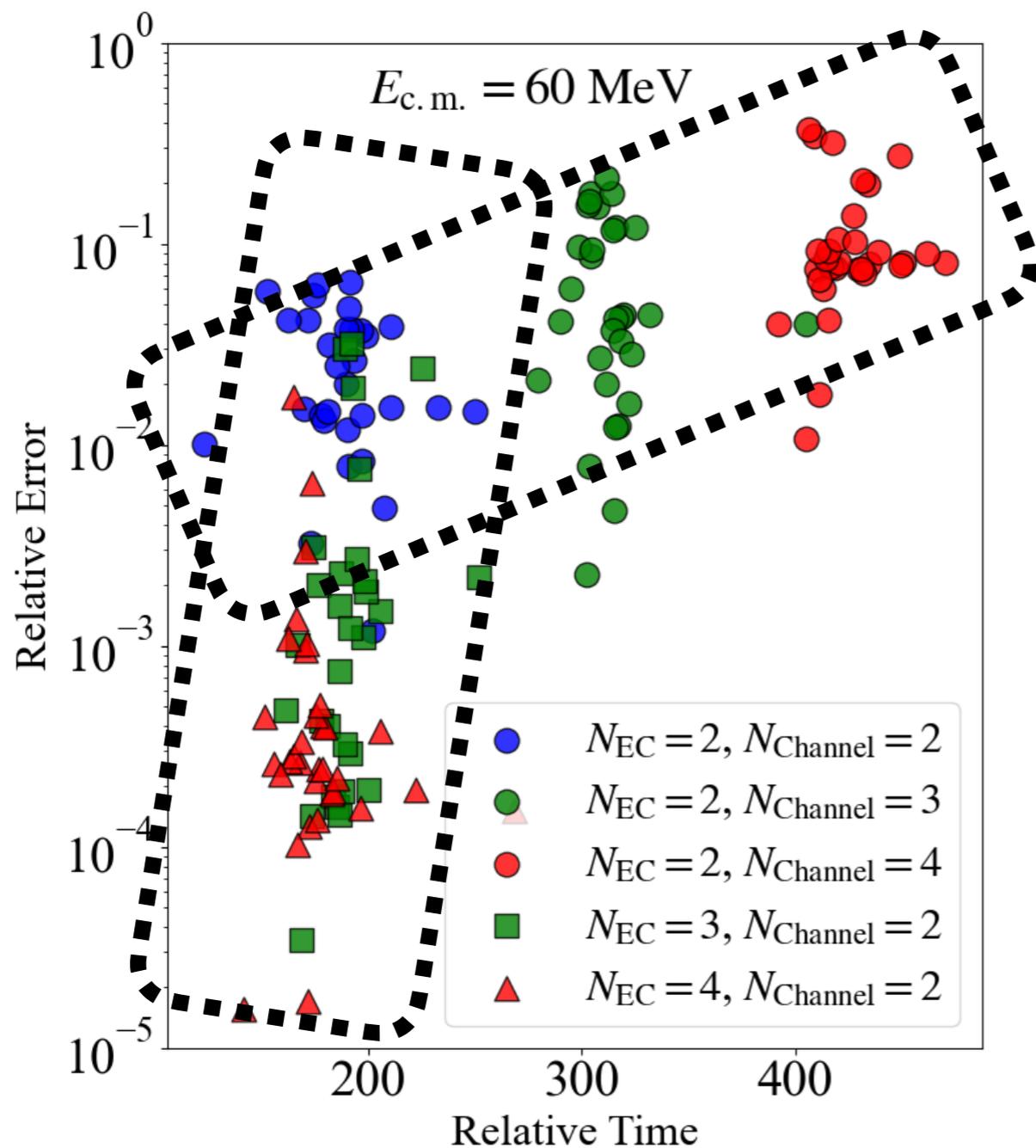
the values of  $\beta_3$  are chosen randomly in the range of (0.15, 0.25) and an ensemble average is taken for 5 different samples.

The more basis number, The less error

$$\epsilon = \frac{1}{N} \sum_i \frac{|\sigma_{\text{Ec}}^i(E) - \sigma_{\text{Exact}}(E)|}{\sigma_{\text{Exact}}(E)}$$

# Emulator: Speed performance

Comparison for the penetration probabilities at an energy of  $E = 60\text{MeV}$  across different angular momenta.



As the number of basis states  $N_{\text{EC}}$  increases, the deviation from the exact result decreases.

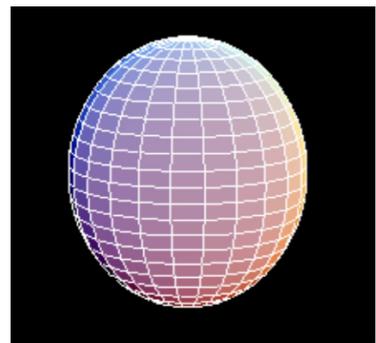
The complete space has a dimension of  
 $\sim 900$  for  $N_{\text{Channel}} = 2$  channels  
 $\sim 1300$  for  $N_{\text{Channel}} = 3$  channels.

As the number  $N_{\text{Channel}}$  increases, The accelerate ability increases

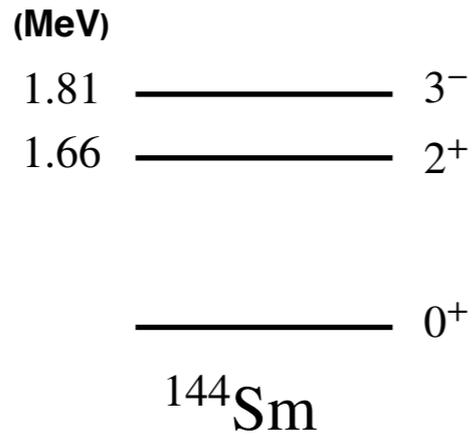
$$\text{Relative error} = |P_{\text{Ec}}(E = 60\text{MeV}, J) - P_{\text{Exact}}(E = 60\text{MeV}, J)| / P_{\text{Exact}}(E = 60\text{MeV}, J)$$

$$\text{Relative time} = \tau_{\text{Exact}}(E = 60\text{MeV}, J) / \tau_{\text{Ec}}(E = 60\text{MeV}, J)$$

# Case 1: $^{16}\text{O} + ^{144}\text{Sm}$



$^{144}\text{Sm}$

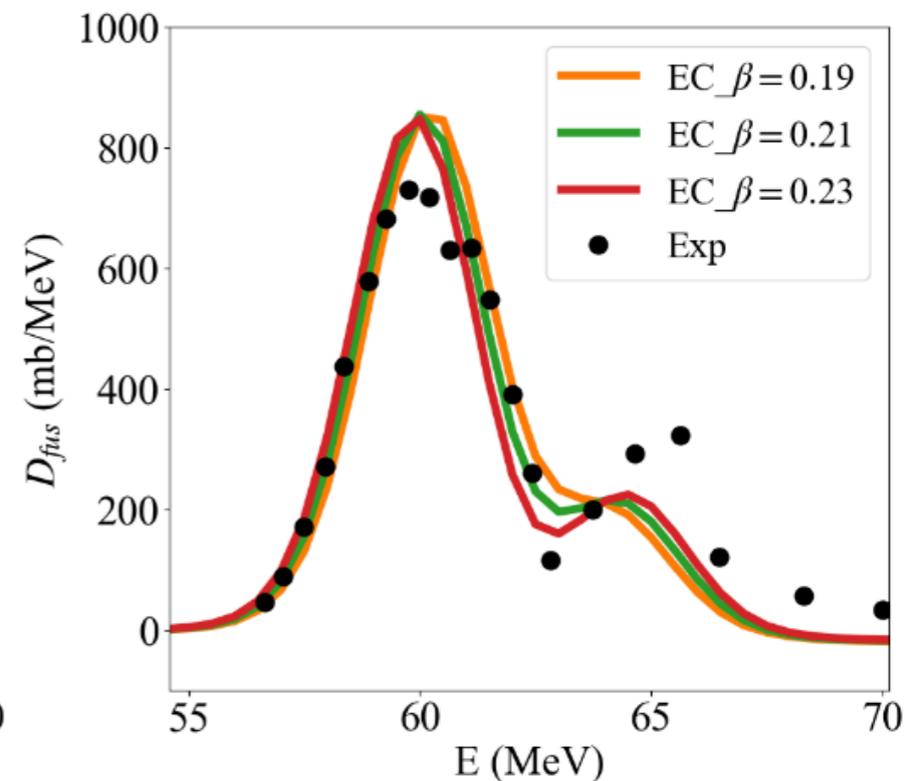
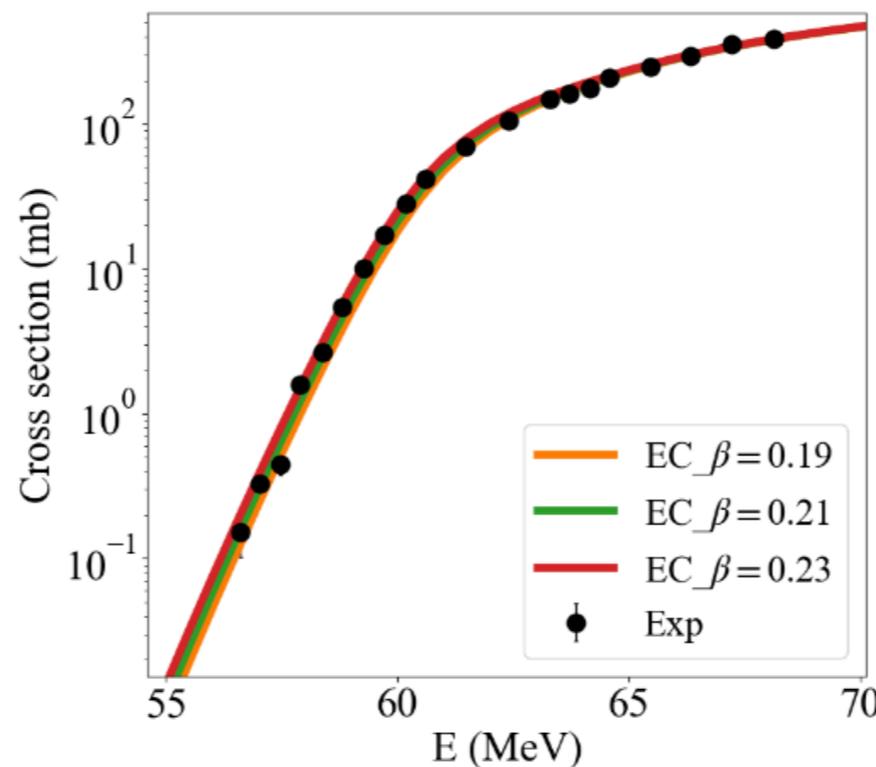
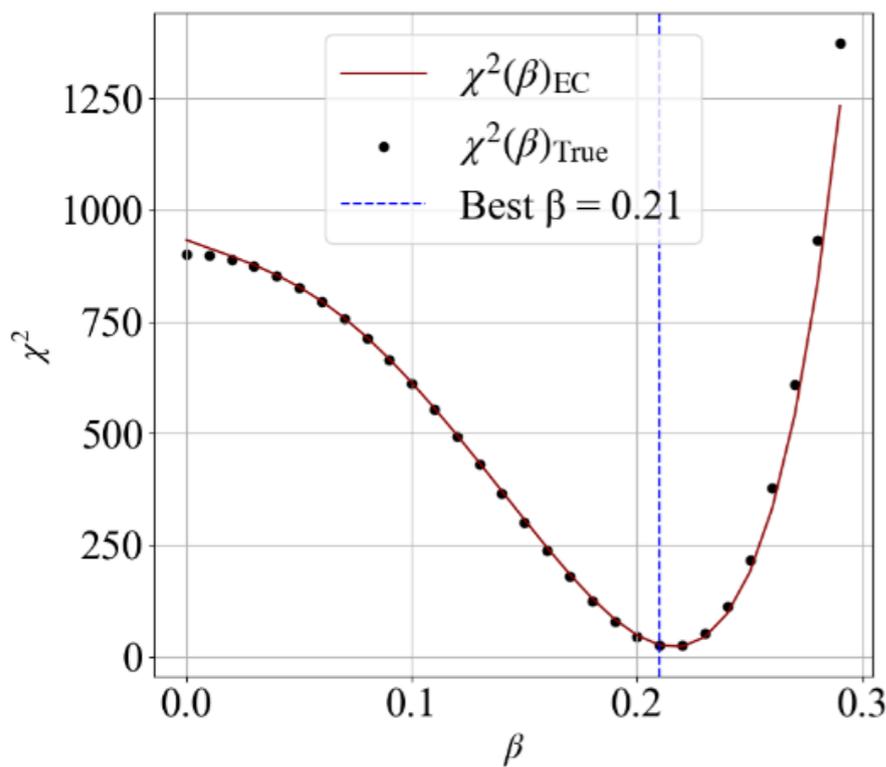


The  $\beta^\lambda$  can be obtained from measured transition probability using:

$$\beta^\lambda = \frac{4\pi}{3ZR^\lambda} \left[ \frac{B(E\lambda)}{e^2} \right]^2$$

cf. :  $\beta_3 = 0.21$ ,

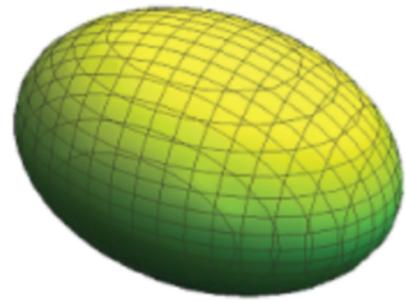
A.T. Kruppa et. al. Nucl. Phys. A560, 845 (1993)



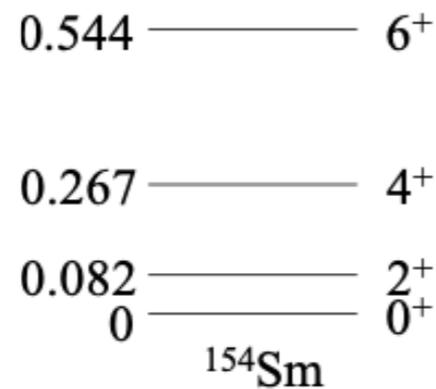
CCFULL model obtained optimal deformation strength  $\beta_3 = 0.21$

- CCFULL model can serve as a reliable theoretical tool for constraining nuclear deformation.
- It shows that the emulator can significantly reproduce this process

# Case 2: $^{16}\text{O} + ^{154}\text{Sm}$



$^{154}\text{Sm}$



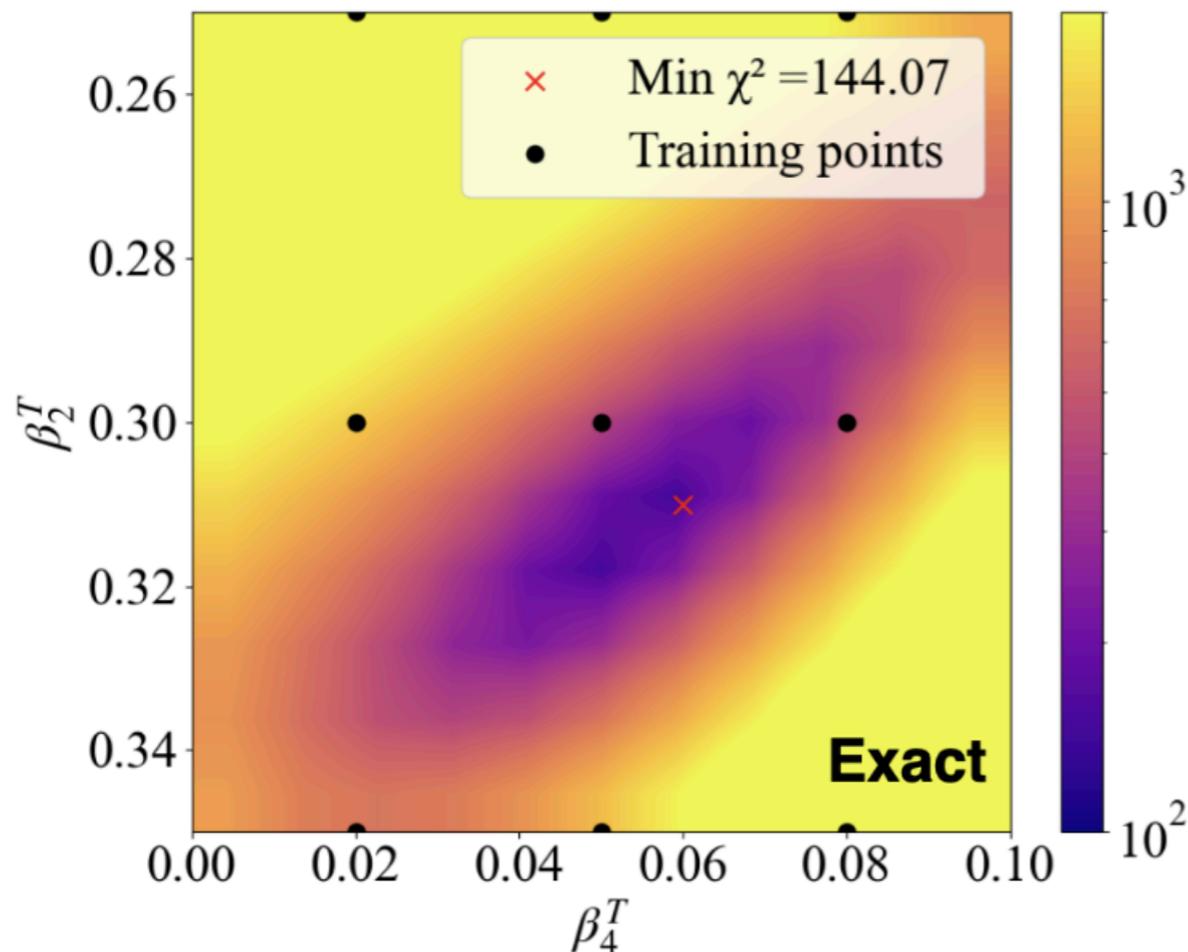
re-analysis by radius parameter  $r = 1.06$  fm

cf. ( $\alpha$  scattering) :  $\beta_2 = 0.317$  and  $\beta_4 = 0.07$

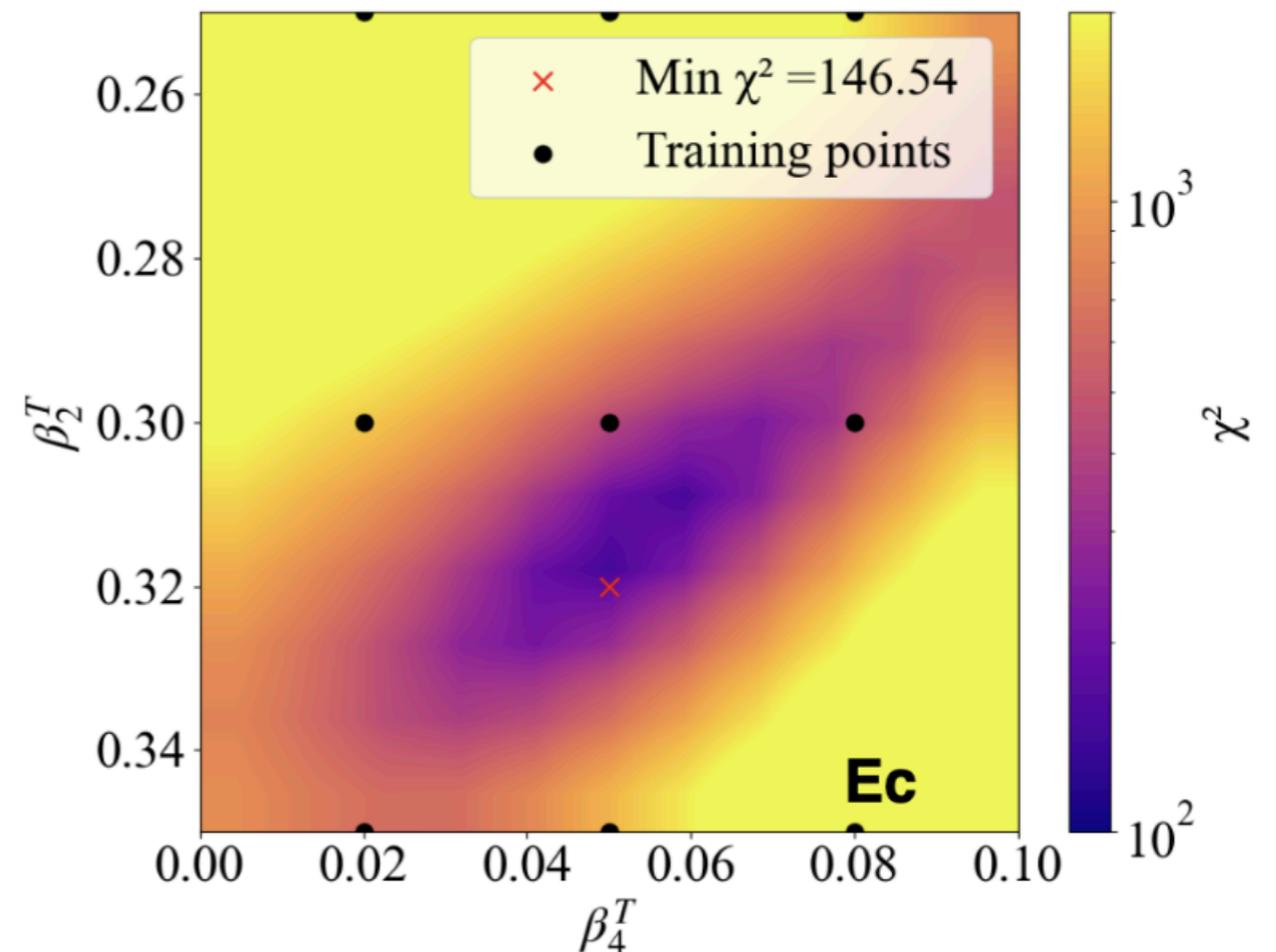
A. A. Aponik, Jr. et. al., Nucl. Phys. A159, 367 (1970).

T. Rumin, K. Hagino, N. Takigawa. Phys. Rev. C, 61, 014605

The emulator Consist 9 basis ( $\beta_2 = \{0.25, 0.30, 0.35\}$ ,  $\beta_4 = \{0.02, 0.05, 0.08\}$ ).

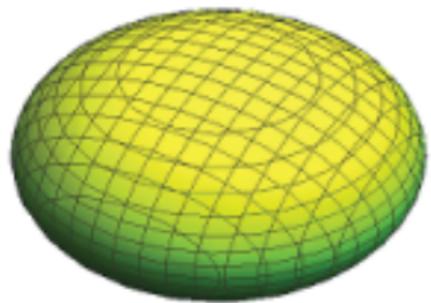


$\chi^2 = 144.07$  at  $\text{Beta}2T = 0.31$ ,  $\text{Beta}4T = 0.06$



$\chi^2 = 146.54$  at  $\text{Beta}2T = 0.32$ ,  $\text{Beta}4T = 0.05$

# Case 3: $^{16}\text{O} + ^{186}\text{W}$



$^{186}\text{W}$

re-analysis by radius parameter  $r = 1.06$  fm

cf. (Mass calculation) :  $\beta_2 = 0.25$  and  $\beta_4 = -0.117$

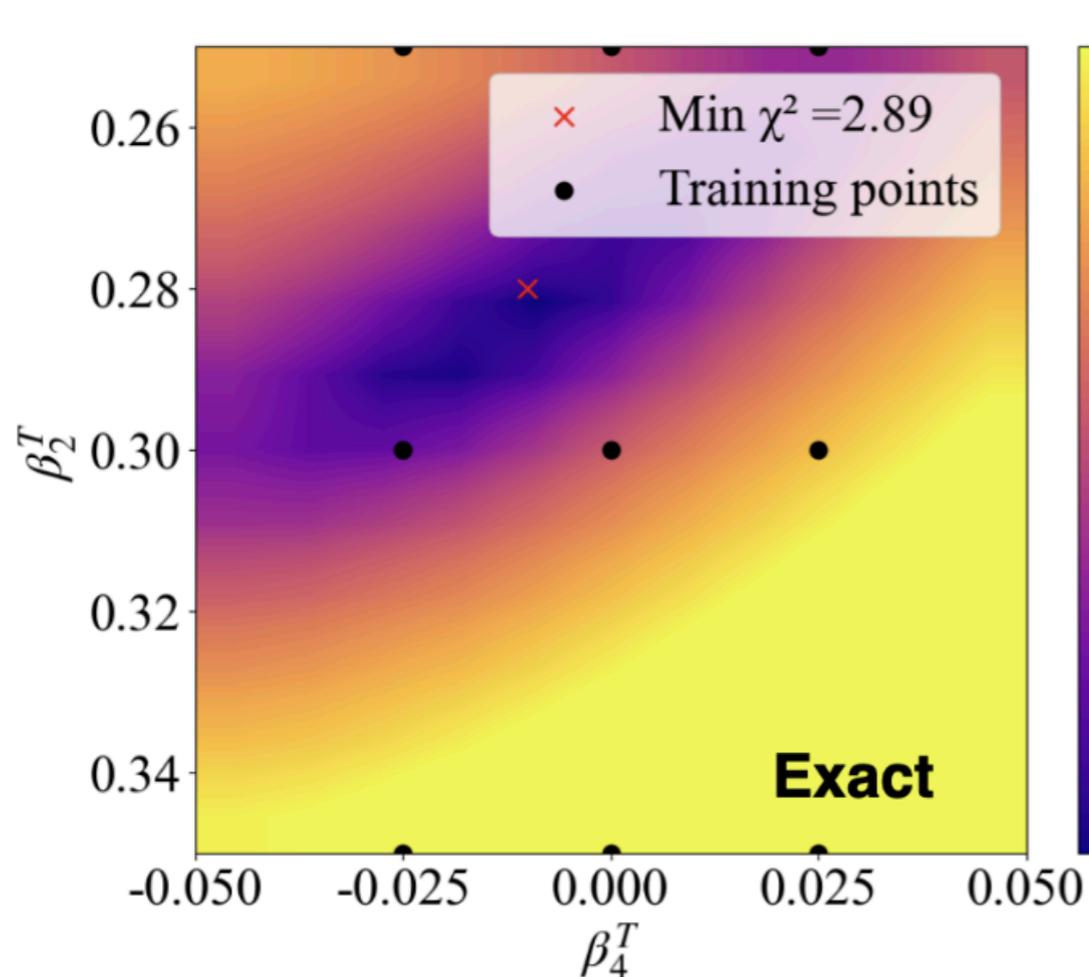
cf. (Neutron scattering):  $\beta_2 = 0.203$  and  $\beta_4 = -0.057$

P. Moller. et. al, At. Data Nucl. Data Tables 59, 185 (1995).

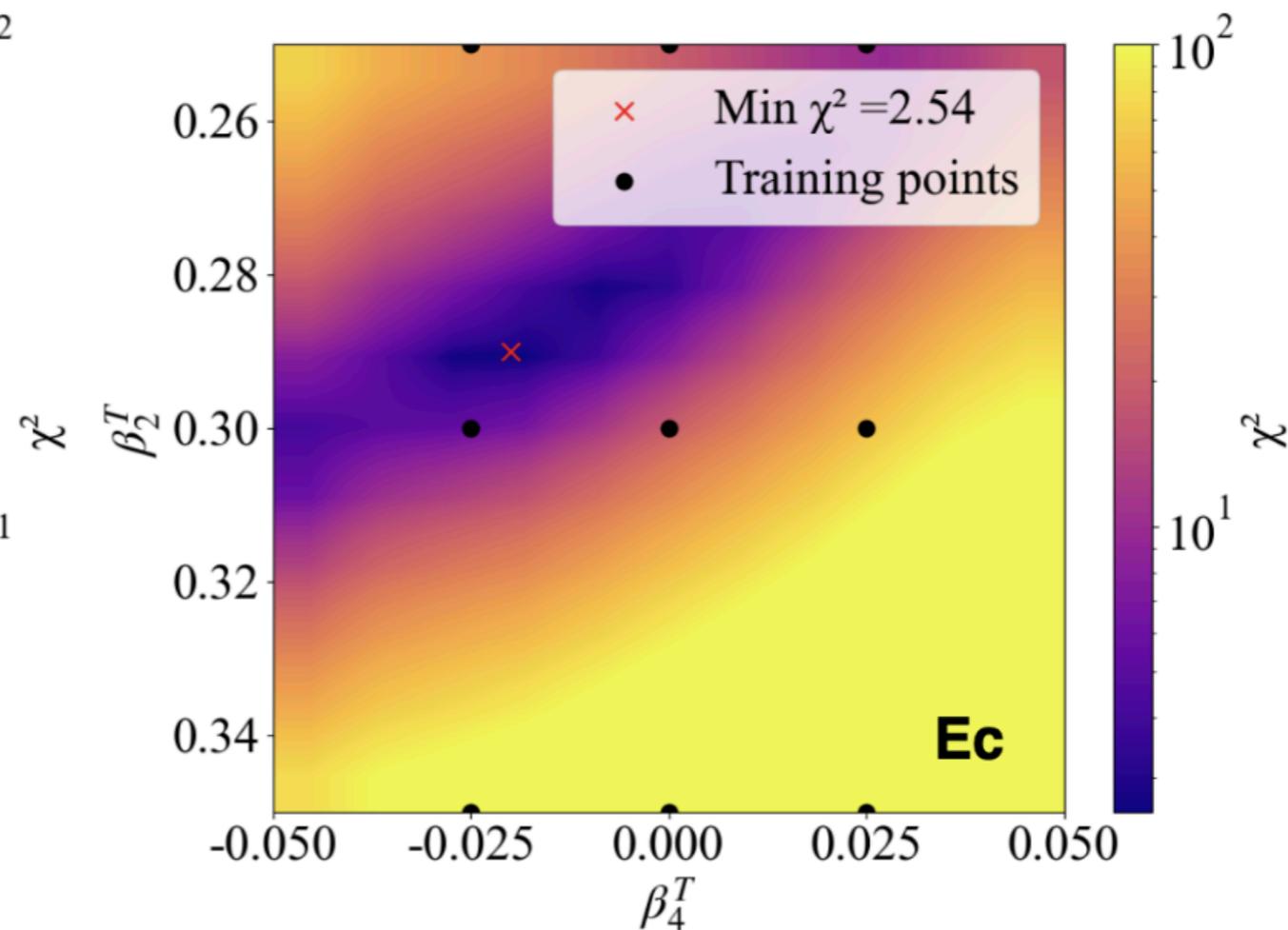
J. P. Delaroche, Phys. Rev. C 26, 1899 (1982).

T. Rumin, K. Hagino, N. Takigawa. Phys. Rev. C, 61, 014605

The emulator Consist 9 basis ( $\beta_2 = \{0.25, 0.30, 0.35\}$ ,  $\beta_4 = \{-0.025, 0.0, 0.025\}$ ).



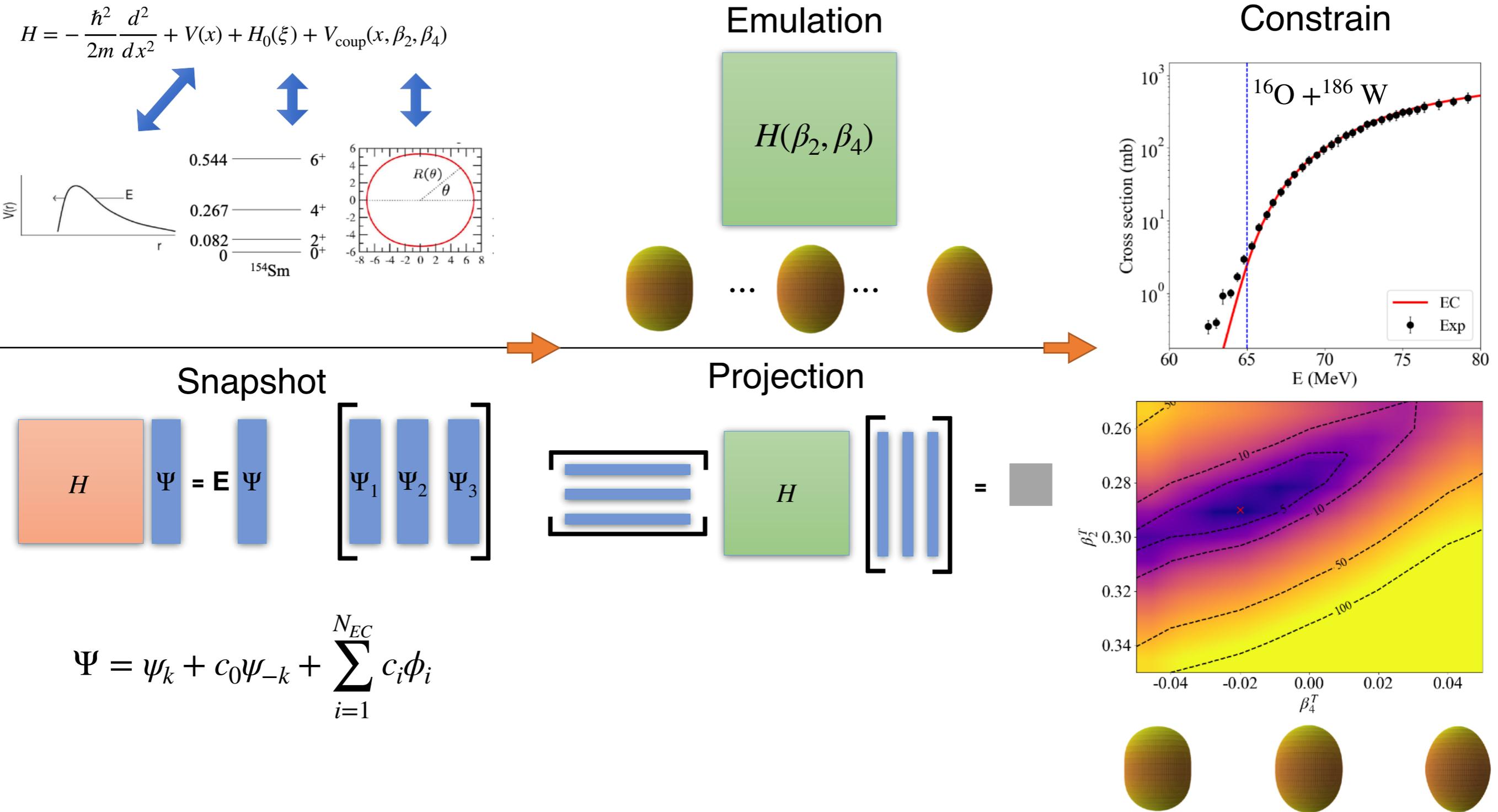
$\chi^2 = 2.89$  at Beta2T = 0.28, Beta4T = -0.01



$\chi^2 = 2.54$  at Beta2T = 0.29, Beta4T = -0.02

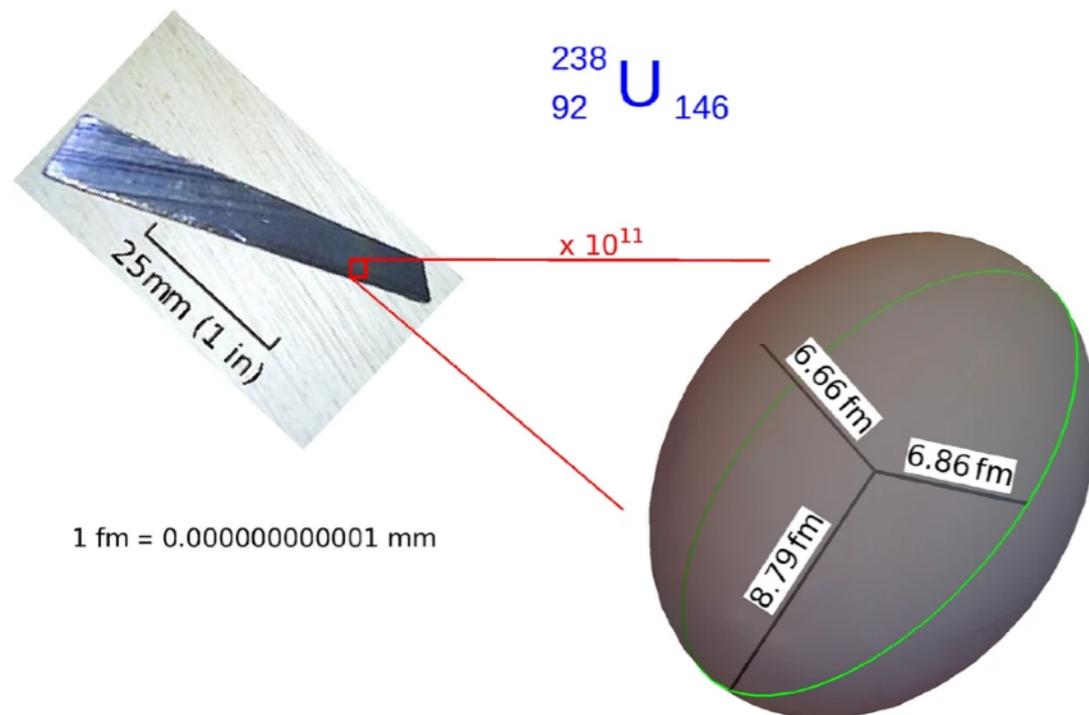
# Summary

- CCFULL model can serve as a reliable theoretical tool for constraining nuclear deformation.
- We construct an emulator to accelerate this process with Eigenvector continuation



quadrupole, hexadecapole

# Future Work



- **Uranium-238** is a typical Triaxial nuclei
- Triaxial deformation should be considered in CCFULL model

$$R(\theta, \phi) = R_0 [1 + \beta_2 (Y_2^0(\theta) \cos \gamma + Y_2^2(\theta, \phi) \sin \gamma)]$$