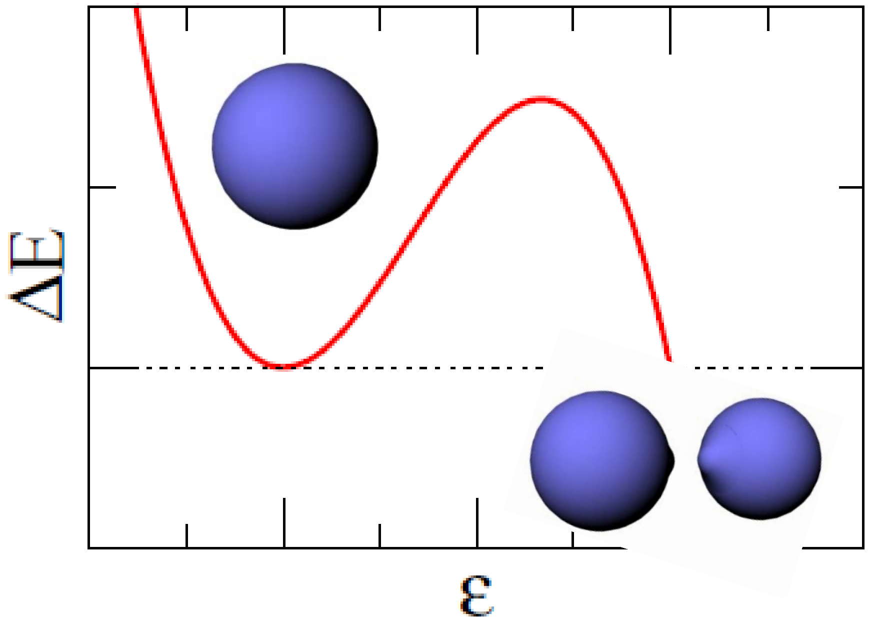
Modeling **low-energy induced fission** in a discrete-basis formalism with density functional theory

Kouichi Hagino
Kyoto University

George F. Bertsch (Seattle)
Kotaro Uzawa (Kyoto)



How well can one describe nuclear fission microscopically?

G.F. Bertsch and K.H., Phys. Rev. C107, 044615 (2023).
K. Uzawa and K.H., Phys. Rev. C110, 014321 (2024).

5th Gogny conference, Paris, Dec. 10-13, 2024.

Modeling **low-energy induced fission** in a discrete-basis formalism with density functional theory

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1. Microscopic understanding of nuclear fission
2. GCM + CI approach to induced fission
3. Calculations with the Skyrme functional
4. Discussions: applications of the Gogny interaction?

G.F. Bertsch and K.H., Phys. Rev. C107, 044615 (2023).
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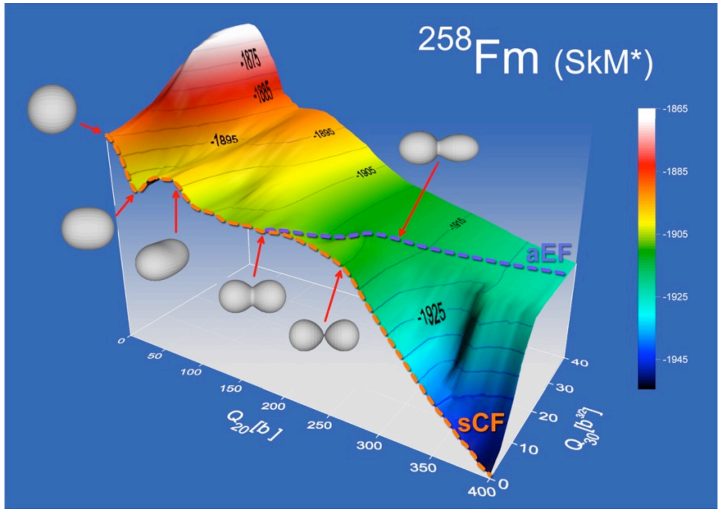
Microscopic approaches to fission
: mean-field wave functions constrained by shape degrees of freedom

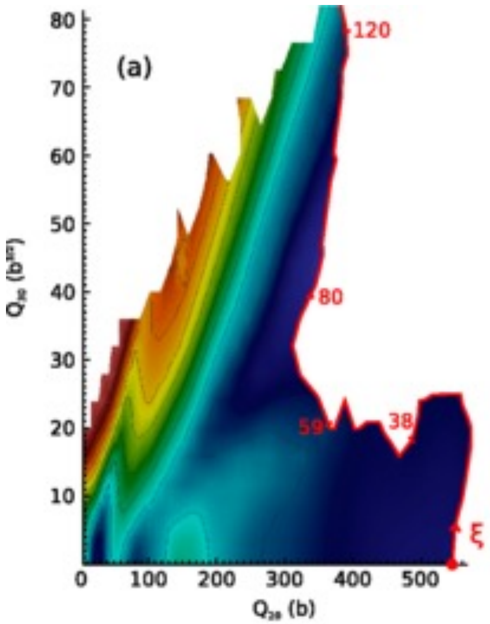
$$\delta\langle\Phi|H-\lambda Q_{20}|\Phi\rangle = 0 \quad \to \Phi(Q_{20}),\;\; E(Q_{20})$$



- WKB approximation for spontaneous fission

$$P = \exp\left[-2\int dq\sqrt{\frac{2B(q)}{\hbar^2}(V(q)-E)}\right]$$

A. Staszczak et al., PRC80 ('09) 014309



- Time-dependent GCM

$$|\Psi(t)\rangle = \int dq f(q,t)|\Phi_q\rangle \qquad \to H_{\rm coll}(q,\partial/\partial q)$$

D. Regnier et al., PRC93 ('16) 054611

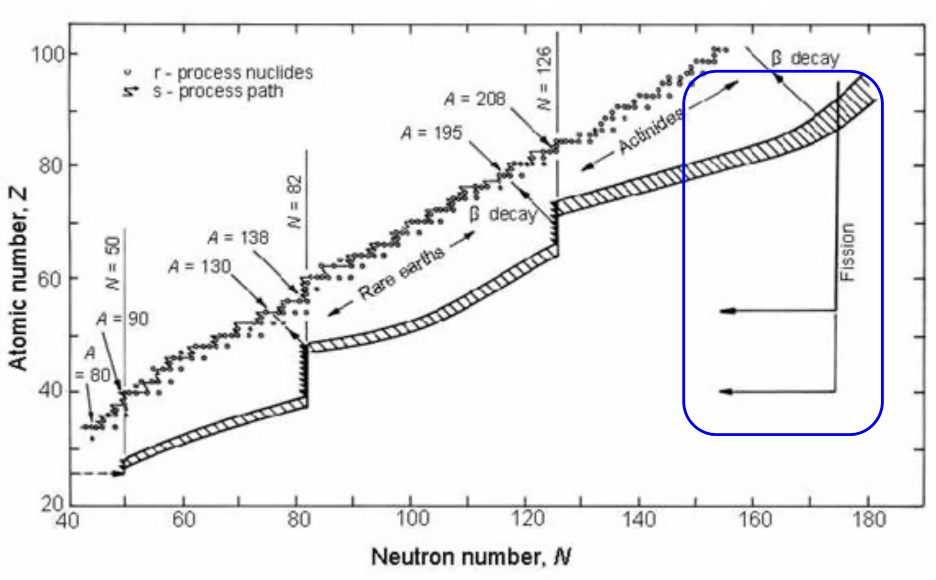
- Our approach

in the same philosophy, but with a Green's fcn

G.F. Bertsch and K.H., Phys. Rev. C107, 044615 (2023).

Why is a microscopic theory for fission important?

- r-process nucleosynthesis



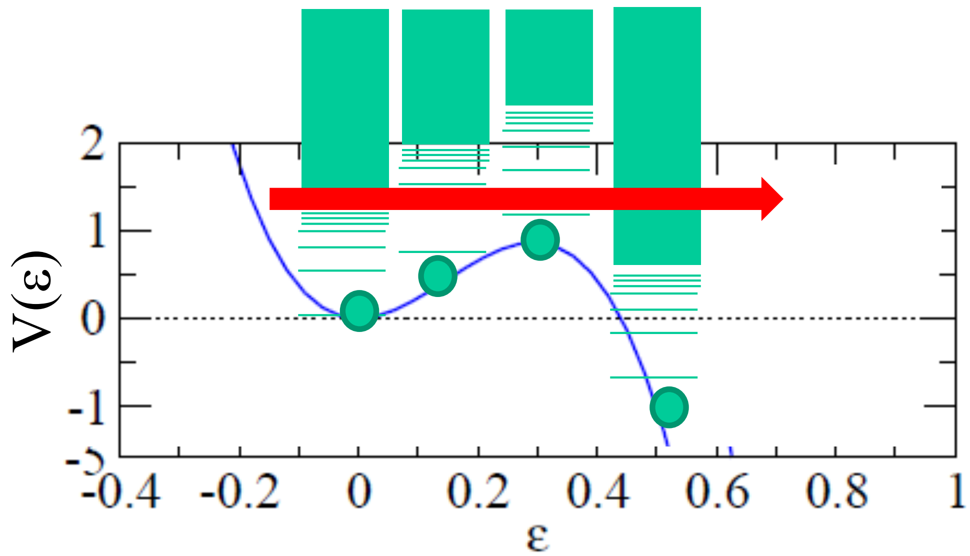
(neutron induced) fission of neutron-rich nuclei

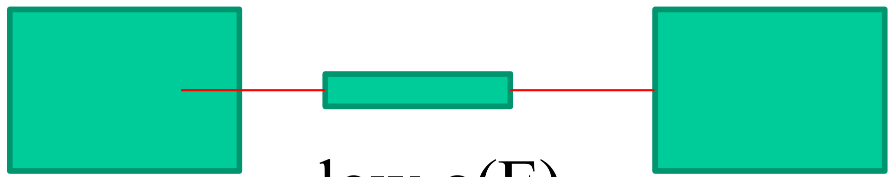
→ low E^* and low $\rho(E^*)$

✓ Validity of statistical models?

✓ Validity of the Langevin approach?

- barrier-top fission





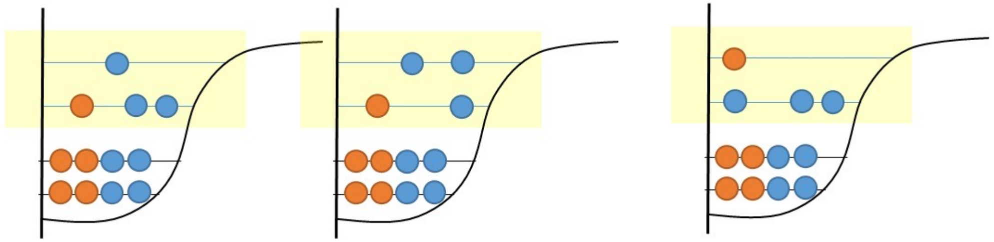
↓

discrete levels

How to connect to a many-body Hamiltonian?

Shell model approach?

Shell model



$$|\Psi\rangle = \quad v_1|m_1\rangle \quad + \quad v_2|m_2\rangle \quad + \quad v_3|m_3\rangle \quad + \cdots$$

Figure: Noritaka Shimizu (Tsukuba)

many-particle many-hole configurations
in a mean-field potential
→mixing by residual interactions

Shell model based on DFT

$$H = \sum_i \epsilon_i a_i^\dagger a_i - GP^\dagger P$$

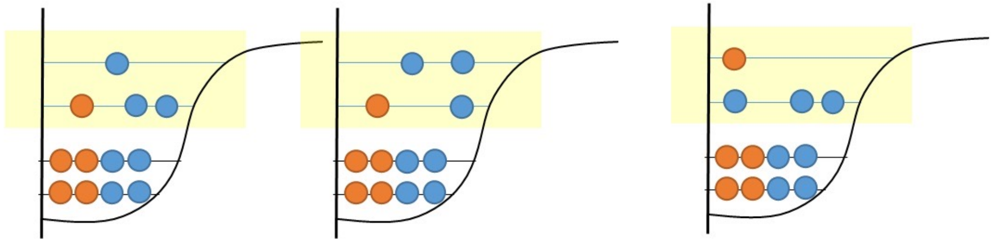
$\varepsilon_i \leftarrow$ DFT

Y.P. Wang et al., PRL132, 232501 (2024)
J. Liu et al., arXiv: 2411.05370 (2024).

Shell model approach?

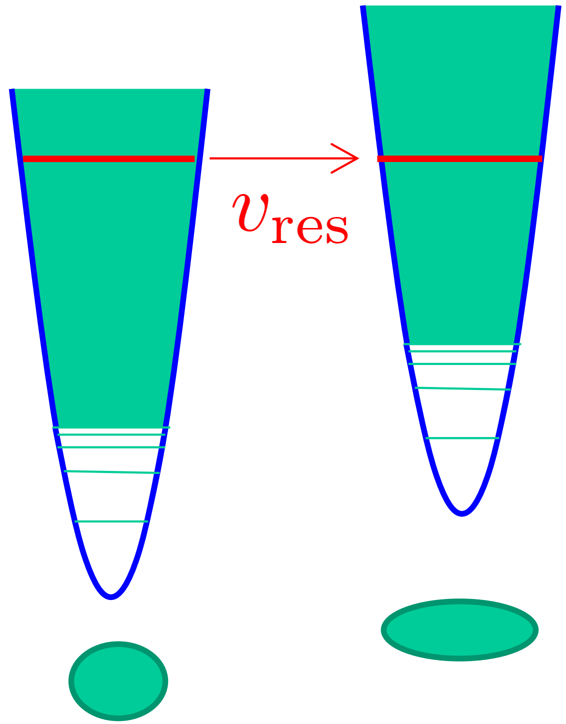
A similar approach for nuclear fission?

Shell model



$$|\Psi\rangle = v_1|m_1\rangle + v_2|m_2\rangle + v_3|m_3\rangle + \cdots$$

Figure: Noritaka Shimizu (Tsukuba)



many-particle many-hole configurations in a mean-field potential

→mixing by residual interactions

- Many-body configurations in a MF pot. for each shape
- hopping due to res. int.

→ shape evolution

a good connection to nuclear reaction theory

Shell model based on DFT

$$H = \sum_i \epsilon_i a_i^\dagger a_i - GP^\dagger P$$

ε_i ← DFT

Y.P. Wang et al., PRL132, 232501 (2024)

J. Liu et al., arXiv: 2411.05370 (2024).

Calculations for ^{235}U(n,f) based on Skyrme HF method

G.F. Bertsch and K.H., Phys. Rev. C107, 044615 (2023).

fission: along $Q = Q_{20} \longrightarrow$ discretized along the fission path

the criterion: $\langle \Psi_\mu(Q) | \Psi_\mu(Q') \rangle \sim e^{-1}$

14b	18b	22b	26b	29b	33b	37b	40b

- ✓ Dynamics of the first barrier: axial symmetry
- ✓ a scaled fission barrier with $B_f = 4$ MeV : $E_{gs}(Q) \longrightarrow f\, E_{gs}(Q)$

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fission: along $Q = Q_{20} \rightarrow$ discretized along the fission path

the criterion: $\langle \Psi_\mu(Q) | \Psi_\mu(Q') \rangle \sim e^{-1}$

714x714 Hamiltonian matrix

dim. =100	42	97	153	125	65	32	100
GOE	18b	22b	26b	29b	33b	37b	GOE

✓ Dynamics of the first barrier: axial symmetry

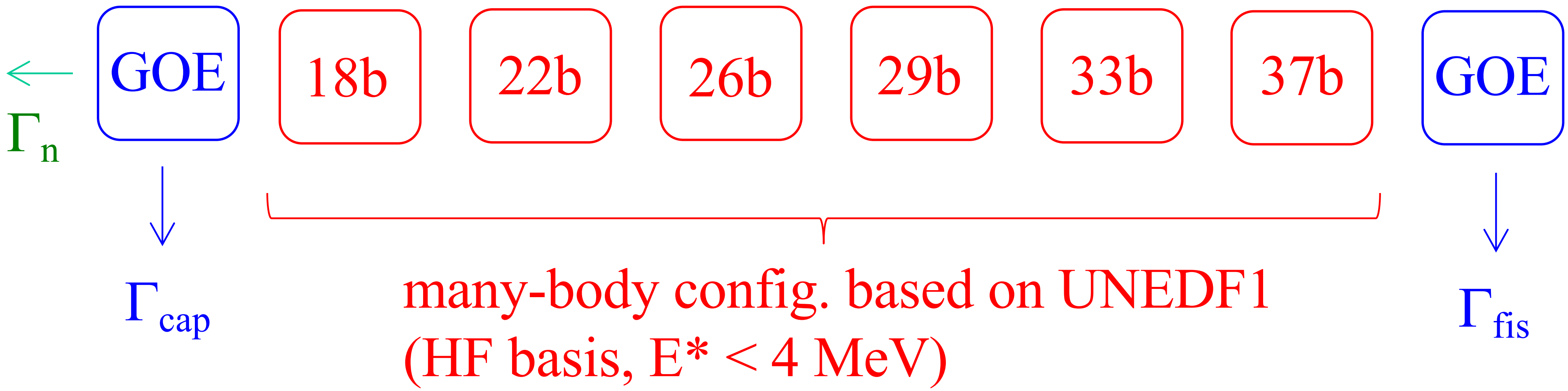
✓ a scaled fission barrier with $B_f = 4$ MeV : $E_{gs}(Q) \rightarrow f\, E_{gs}(Q)$

construct excited configurations at each Q with Skyrme UNEDF1

- neutron seniority zero configurations only
- truncation at $E^* = 4$ MeV
- GOE for the CN and the pre-scission blocks

Calculations for ^{235}U(n,f) based on Skyrme HF method

G.F. Bertsch and K.H., Phys. Rev. C107, 044615 (2023).



- introduce the decay widths for the configurations at Q=14 and 40 b
  - ✓ Γ_{cap}: exp. data (scaled according to N_{GOE}), Γ_{fis}: insensitivity

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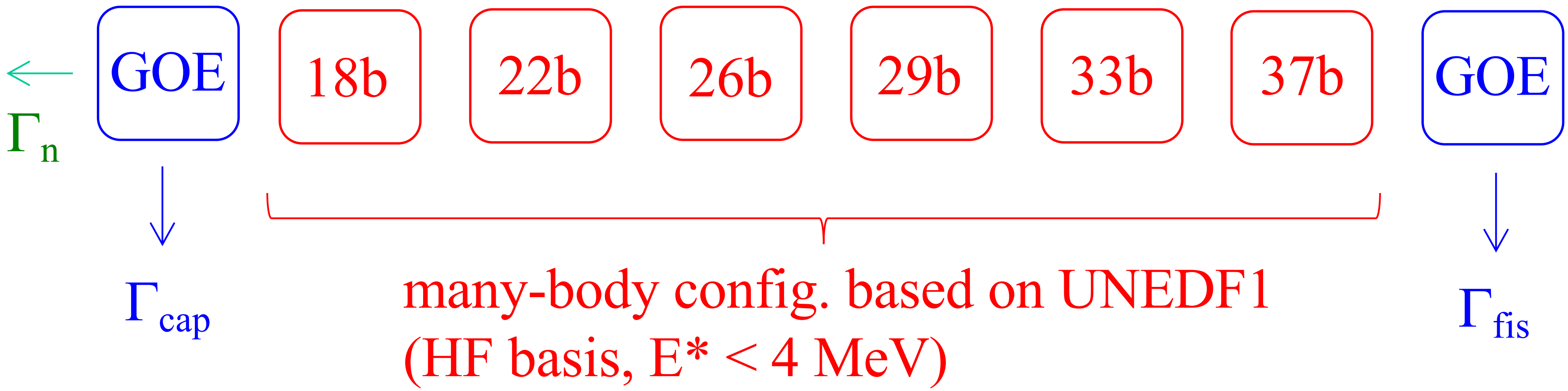


- introduce the decay widths for the configurations at Q=14 and 40 b
  - ✓ Γ_{cap}: exp. data (scaled according to N_{GOE}), Γ_{fis}: insensitivity

Reaction theory (absorption probability):

$$T_{\text{fis}} = Tr[\Gamma_n G(E) \Gamma_{\text{fis}} G^\dagger(E)]$$

$$T_{\text{cap}} = Tr[\Gamma_n G(E) \Gamma_\gamma G^\dagger(E)]$$

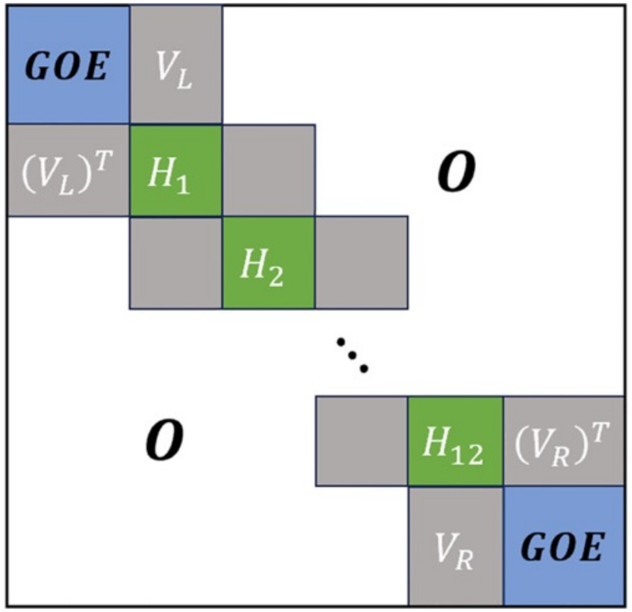
"Datta formula"

$$G(E) = [H - i\Gamma/2 - EO]^{-1}$$

Calculations for ^{235}U(n,f) based on Skyrme HF method

G.F. Bertsch and K.H., Phys. Rev. C107, 044615 (2023).

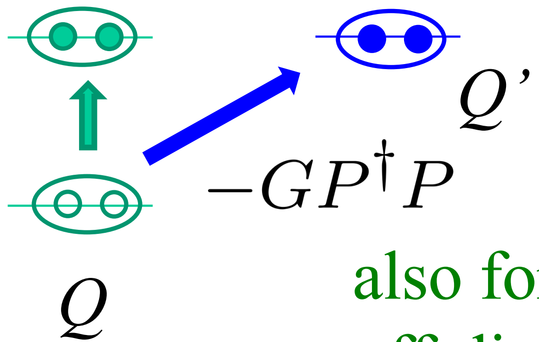
$$H \sim H_0 + V_{\rm pair} + V_{\rm diabatic} = H_0 - GP^\dagger P + V_{\rm diabatic}$$



$$H_k = \sum_i \epsilon_i(Q_k) a_i^\dagger(Q_k) a_i(Q_k) - GP^\dagger P$$

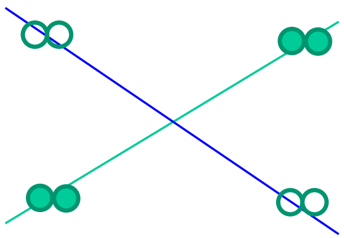
$$P^\dagger = \sum_i a_i^\dagger(Q_k) a_{\bar{i}}^\dagger(Q_k)$$

from DFT



also for off-diagonals

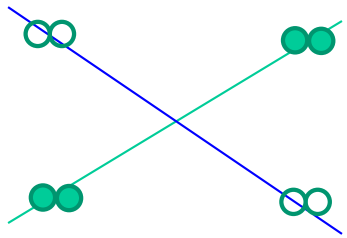
diabatic couplings



Gaussian Overlap Approximation (GOA)

$$\frac{\langle \Psi_\mu(Q)|H|\Psi_\mu(Q')\rangle}{\langle \Psi_\mu(Q)|\Psi_\mu(Q')\rangle} \sim E_\mu(\bar{Q}) - h_2(\Delta\zeta)^2$$

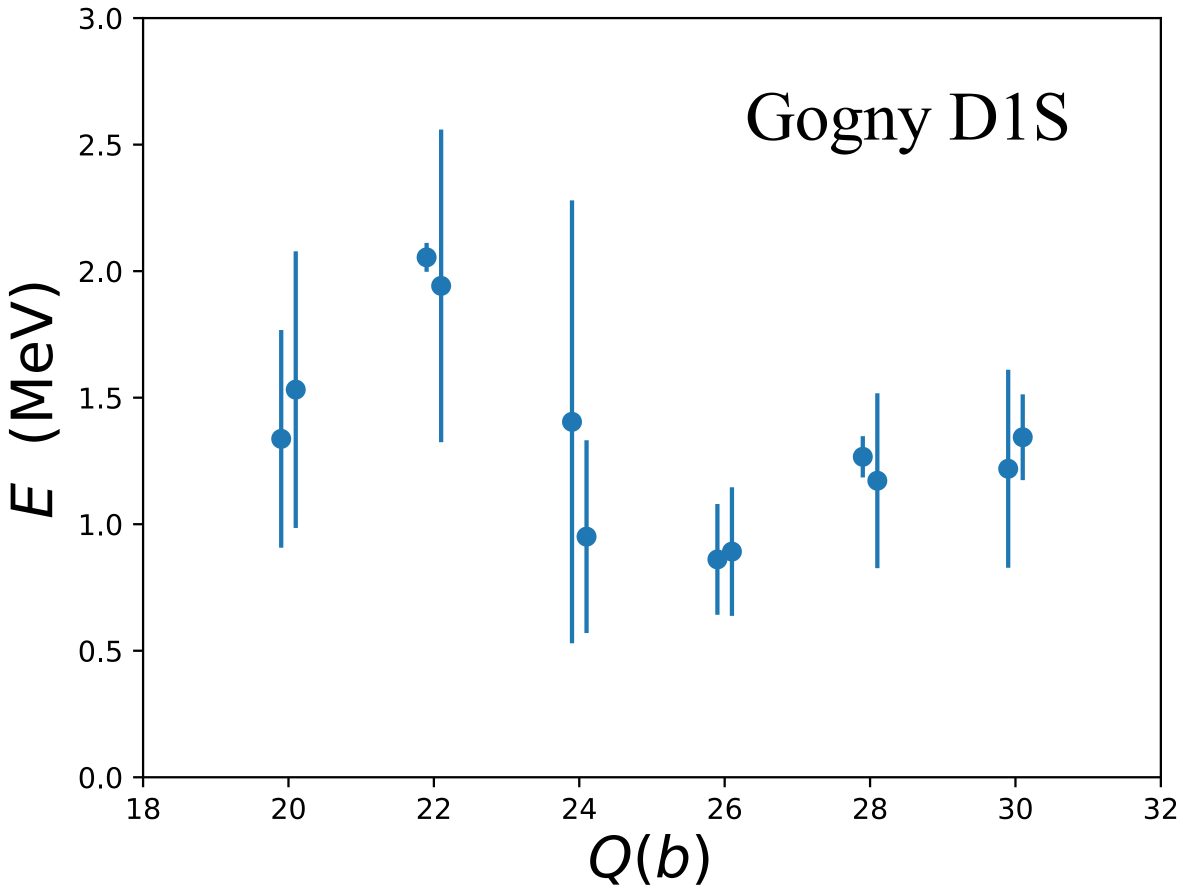
diabatic couplings



$$\frac{\langle \Psi_\mu(Q) | H | \Psi_\mu(Q') \rangle}{\langle \Psi_\mu(Q) | \Psi_\mu(Q') \rangle} \equiv \langle \Psi_\mu(Q) | V_{\text{diabatic}} | \Psi_\mu(Q') \rangle$$

$$\sim \; E_\mu(\bar{Q}) - h_2 (\Delta\zeta)^2$$

$$\langle \Psi_\mu(Q) | \Psi_\mu(Q') \rangle = e^{-(\Delta\zeta)^2}$$

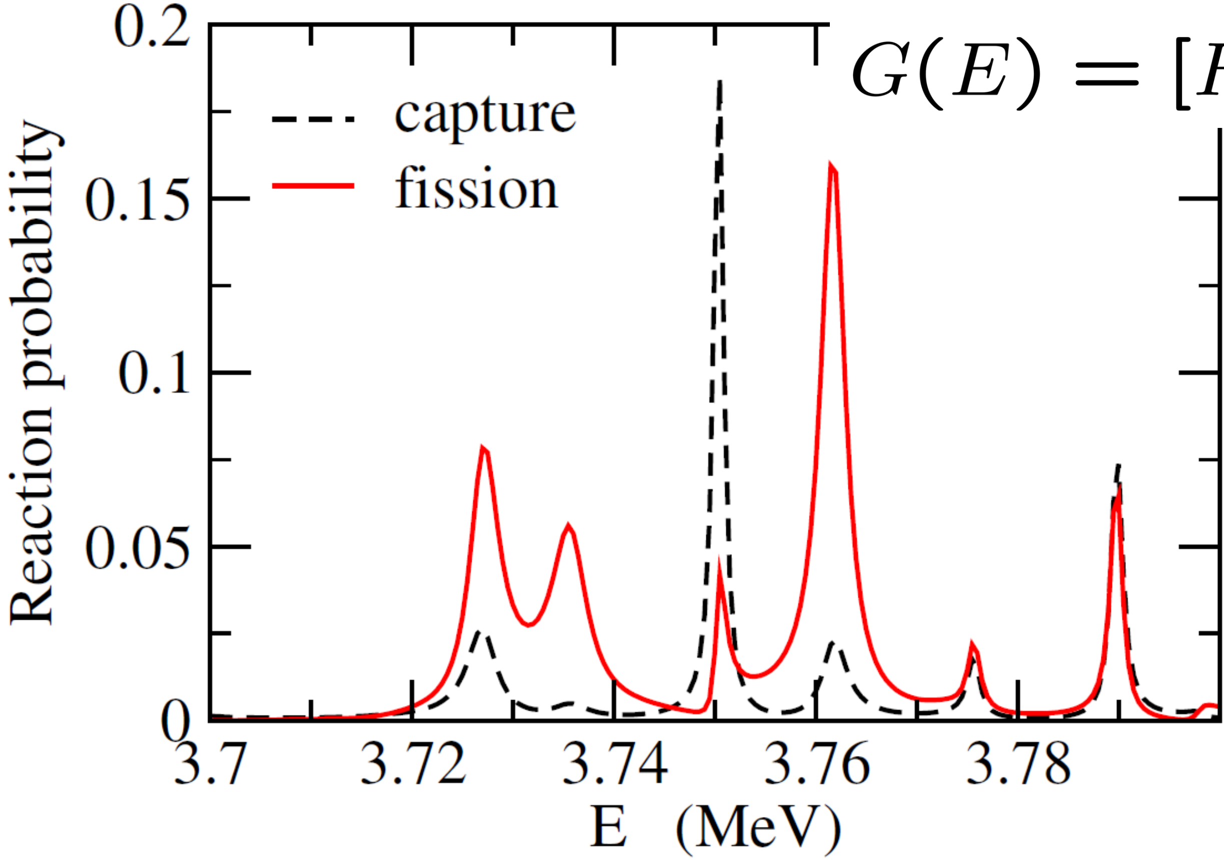


$\rightarrow h_2 \sim 1.5$ MeV

$$T_{\mathsf{fis}}(E) = Tr[\Gamma_{\mathsf{in}} G(E) \Gamma_{\mathsf{fis}} G^{\dagger}(E)]$$

$$T_{\mathsf{cap}}(E) = Tr[\Gamma_{\mathsf{in}} G(E) \Gamma_{\gamma} G^{\dagger}(E)]$$

$$G(E) = [H - i\Gamma/2 - EO]^{-1}$$



$\Gamma_{in} = 0.01$ MeV

$\Gamma_{cap} = 0.00125$ MeV

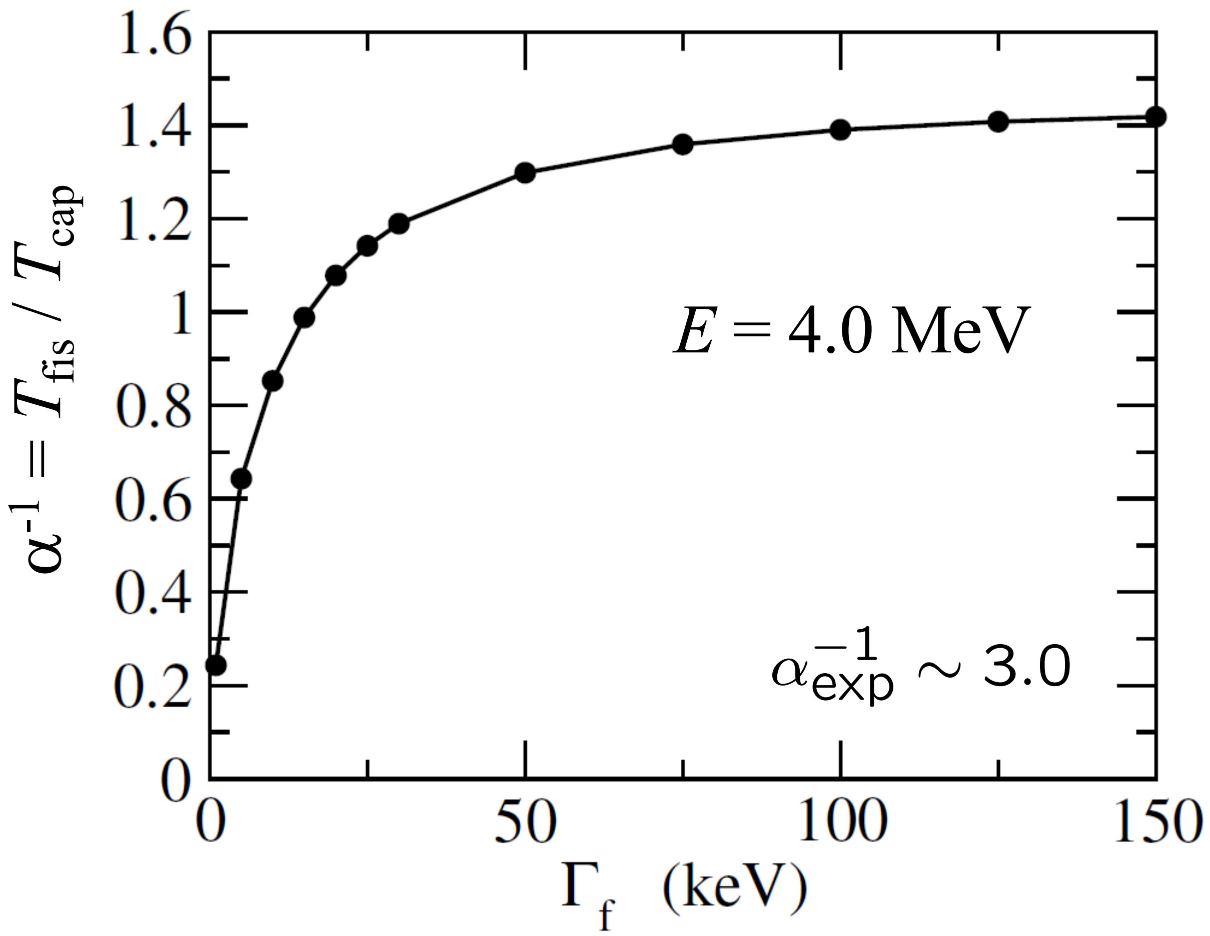
$\Gamma_{fis} = 0.015$ MeV

energy average

$$\alpha^{-1} = \frac{\int_{\Delta E} T_{\mathsf{fis}}(E')dE'}{\int_{\Delta E} T_{\mathsf{cap}}(E')dE'}$$

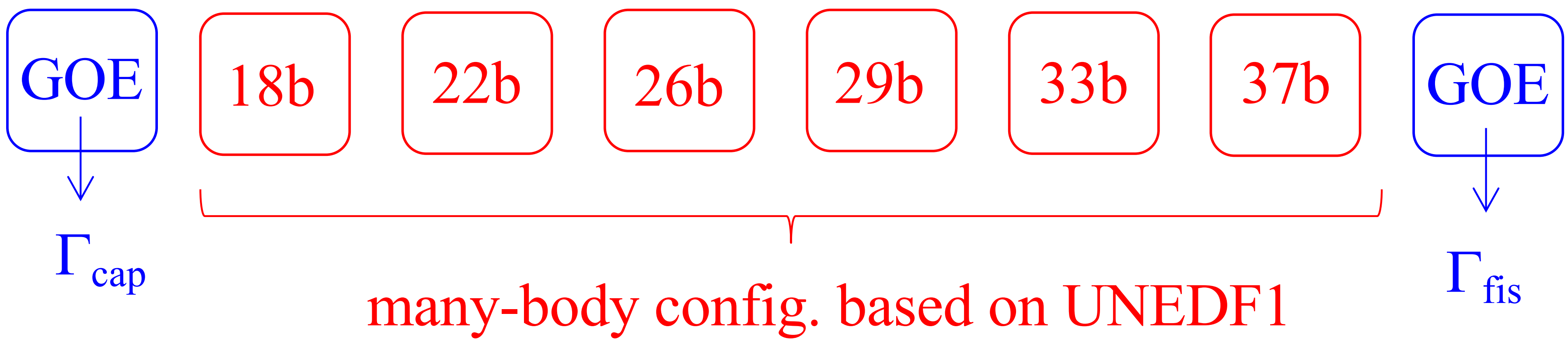
$\Delta E = 0.5$ MeV

insensitivity property

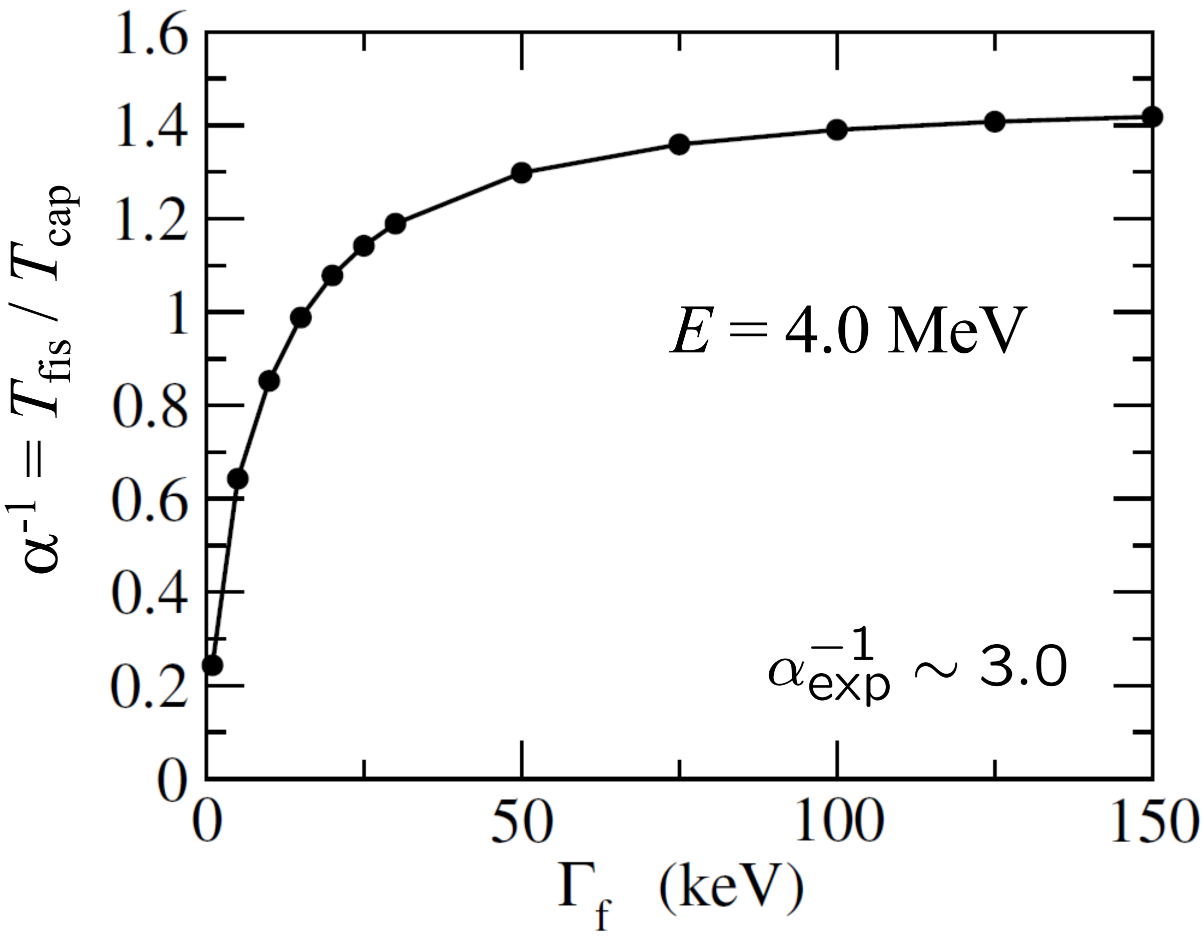


insensitive to Γ_f
(post-barrier dynamics)
→the main assumption
of TST

cf. Analytic discussion
with a 2GOE+1Q model
K.H. and G.F. Bertsch,
JPSJ93, 064003 (2024)



insensitivity property



$E = 4.5$ MeV

base set

$G_{pair} = 0.2$ MeV

$h_2 = 0.15$ MeV

$\rightarrow \alpha^{-1} = 0.95$

$G_{pair} \rightarrow G_{pair}/2$

$G_{pair} = 0.1$ MeV

$h_2 = 0.15$ MeV

$\rightarrow \alpha^{-1} = 0.37$

sensitive to the pairing, though less than in spontaneous fission

Fluctuations of fission width

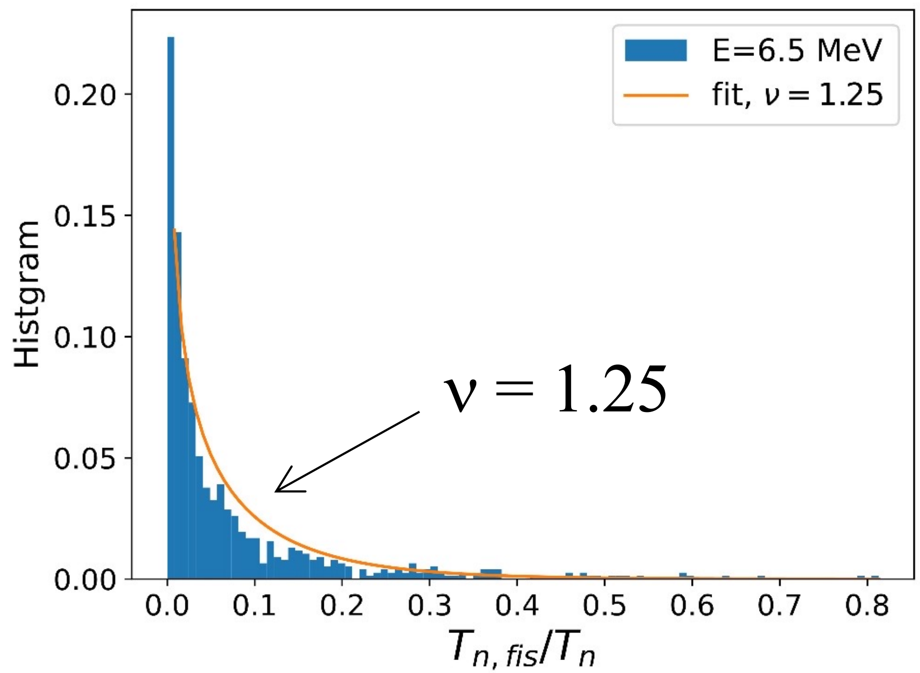
K. Uzawa and K.H., Phys. Rev. C110, 014321 (2024).

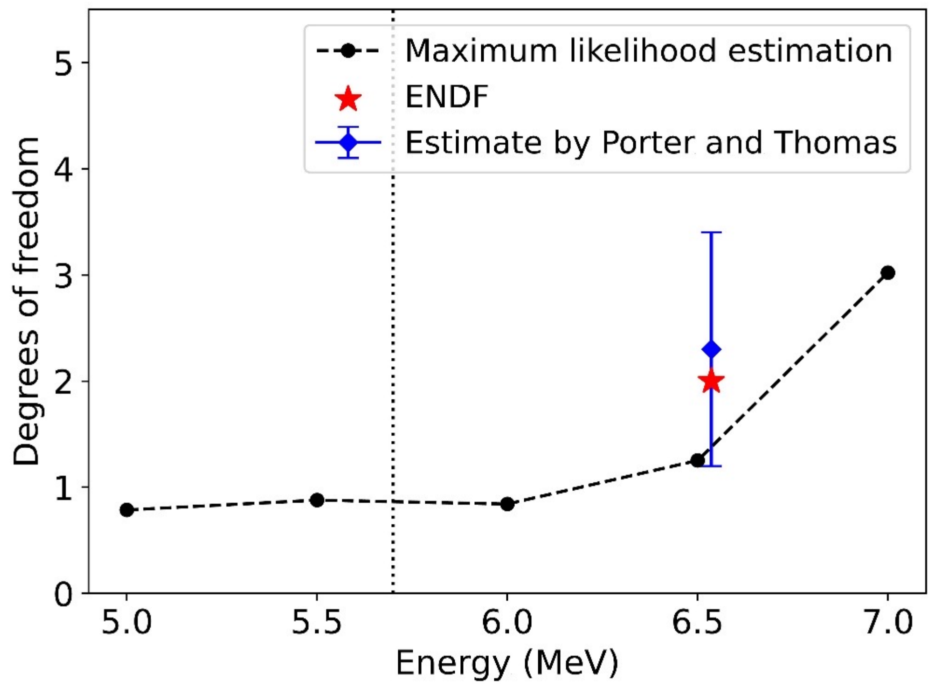
chi-square distribution:

$$P_\nu(x) = \frac{\nu}{2\Gamma(\nu/2)}\left(\frac{\nu x}{2}\right)^{\nu/2-1} e^{-\nu x/2}$$

ν: # of d.o.f.

(ν=1: the PT distribution)





a small number of d.o.f. for induced fission ← transition state theory

Fluctuations of fission width

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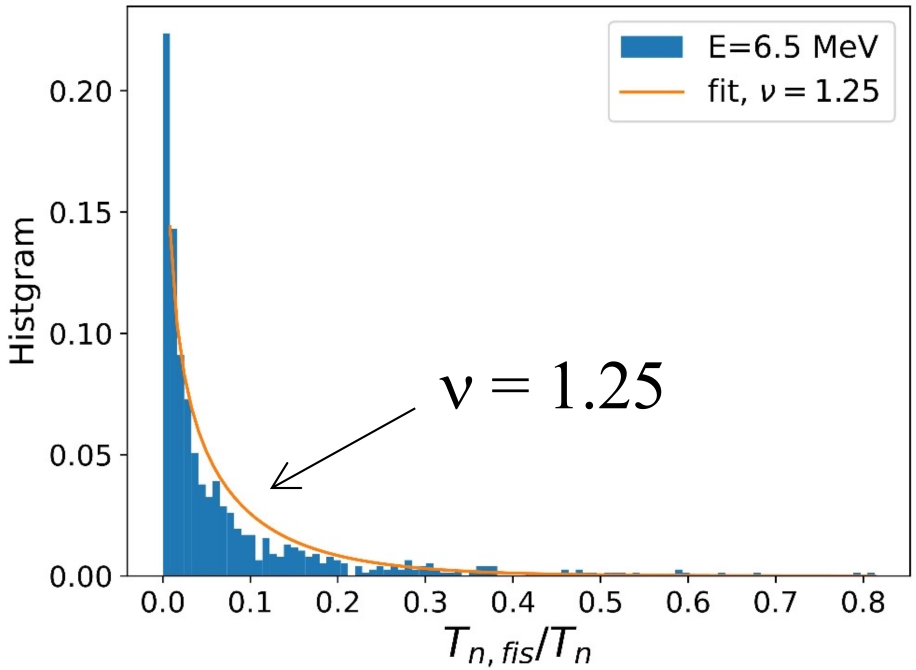
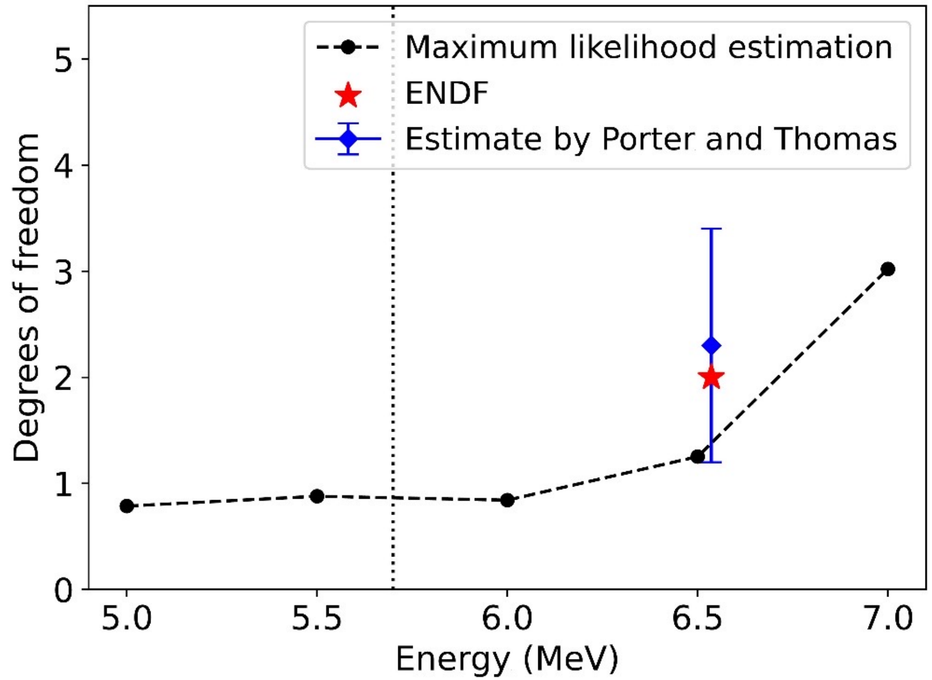




a small number of d.o.f. for induced fission ← transition state theory

$$G(E_n) = \frac{1}{H - i\Gamma/2 - E_n} = \sum_\alpha \frac{|\phi_\alpha\rangle\langle\tilde{\phi}_\alpha|}{E_\alpha - E_n}$$

only a few eigenstates with $\mathrm{Re}(E_\alpha) \sim E_n$ contribute

"transition states"

Towards a large-scale calculation

K. Uzawa and K.H., PRE110, 055302 (2024).

seniority zero config. → non-zero config.

→ a large scale calculation (~ 10^6 dim.)

Notice: large scale CI calculations → the Lanczos method
for an efficient iterative method to obtain the ground state

shift-invert Lanczos method

$$G(E_n) = \frac{1}{H - i\Gamma/2 - E_n} = \sum_\alpha \frac{|\phi_\alpha\rangle\langle\tilde{\phi}_\alpha|}{E_\alpha - E_n}$$

only a few eigenstates with $\mathrm{Re}(E_\alpha) \sim E_n$ contribute

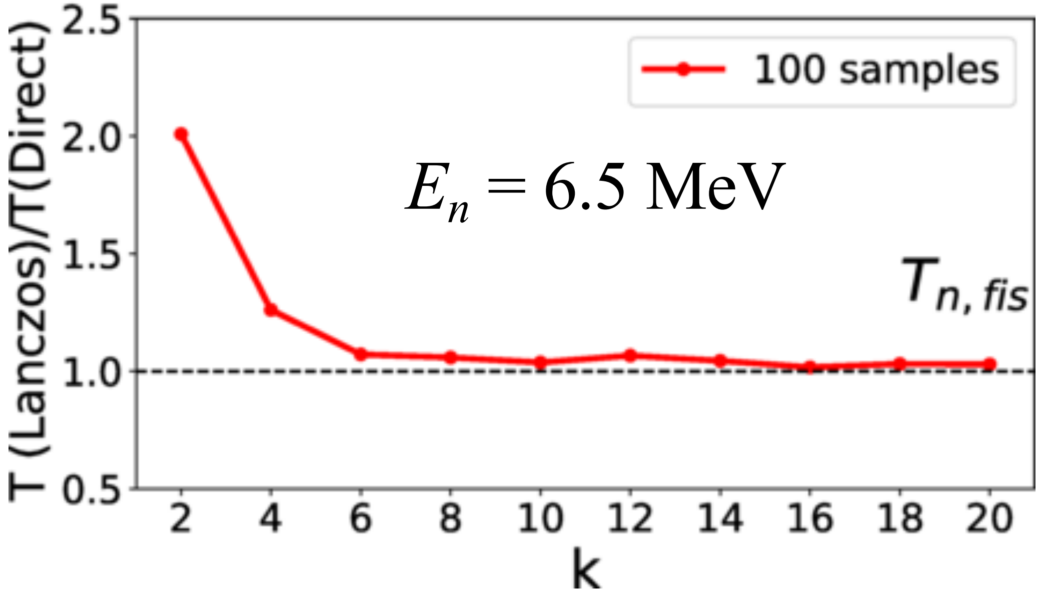
In general, the "transition states" are in the middle of the spectrum
→ the shift-invert Lanczos method

$$H\phi_\alpha = E_\alpha\phi_\alpha \to \underline{(H - E_n)^{-1}}\phi_\alpha = (E_\alpha - E_n)^{-1}\phi_\alpha$$

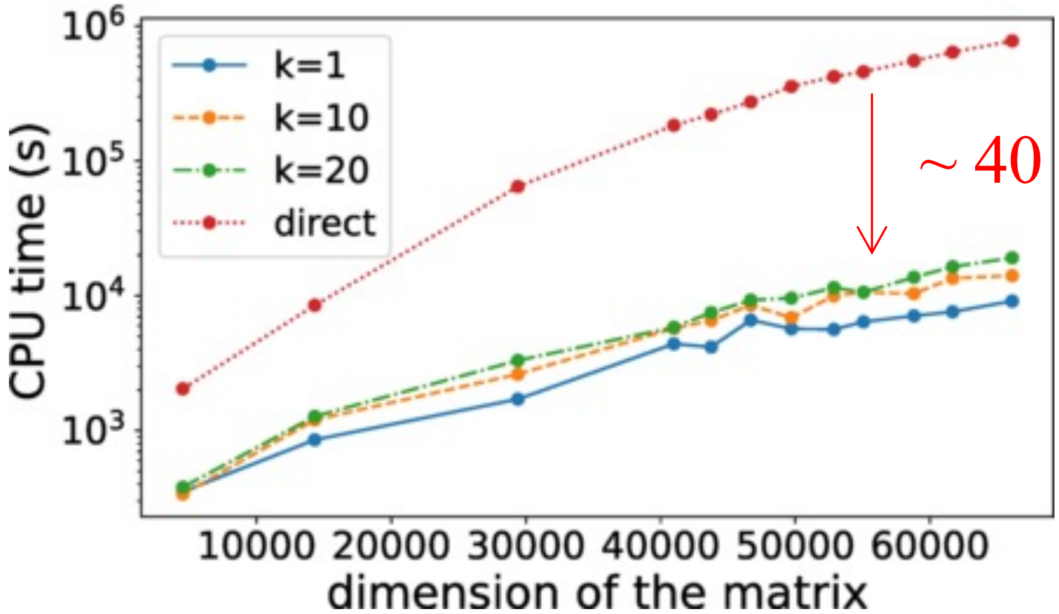
→ Lanczos

Towards a large-scale calculation

K. Uzawa and K.H., PRE110, 055302 (2024).



← # of iteration



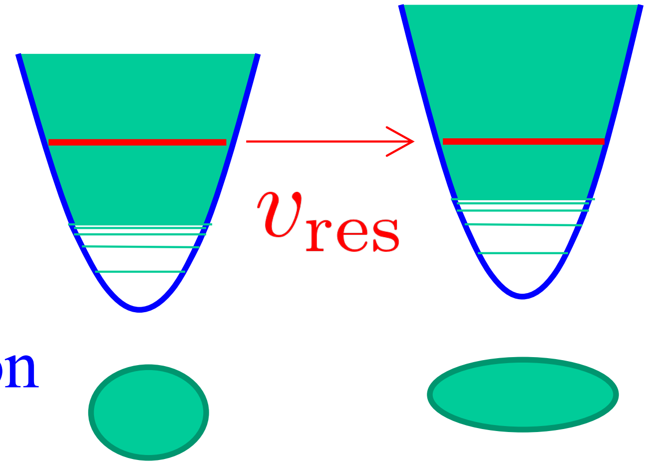
~ 40 times faster!

Summary and discussions

r-process nucleosynthesis: fission of neutron-rich nuclei

requires a microscopic approach applicable to low E^* and $\rho(E^*)$

➡ a new approach: shell model + GCM



an application to induced fission of ^{236}U based on Skyrme EDF

→ • the insensitive property
• an importance of the pairing interaction
• a small value of d.o.f.

← the transition state theory

Future perspectives: seniority non-zero config. → pn res. interaction

K. Uzawa and K. Hagino, PRC108 ('23) 024319

a large scale calculation (~ 10^6 dim.)

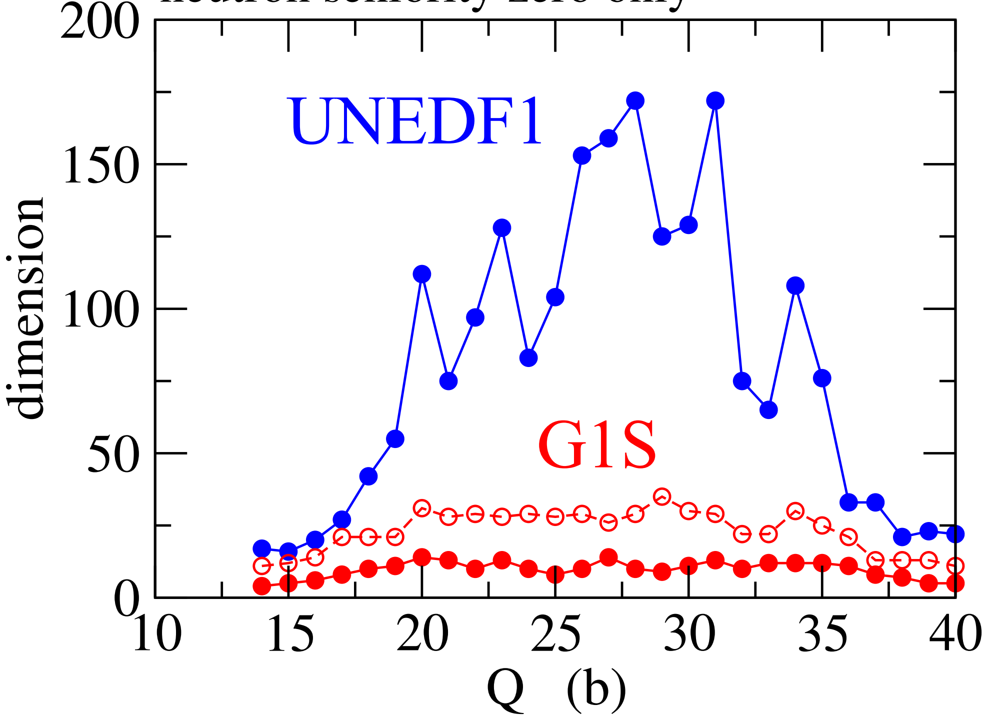
→ the shift-invert Lanczos method

K. Uzawa and K.H., PRE110, 055302 (2024)

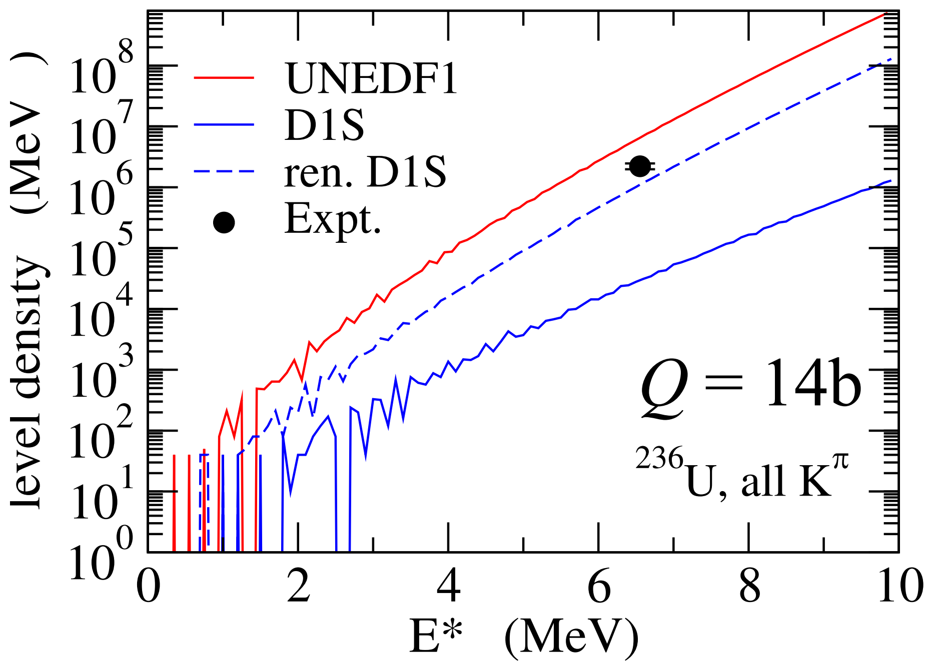
Summary and discussions

Applications with the Gogny interaction?

In principle, any EDF can be used for the calculations, but….



m^* = 1.01 (UNEDF1)
0.697 (D1S)



the # of configurations are too small with D1S

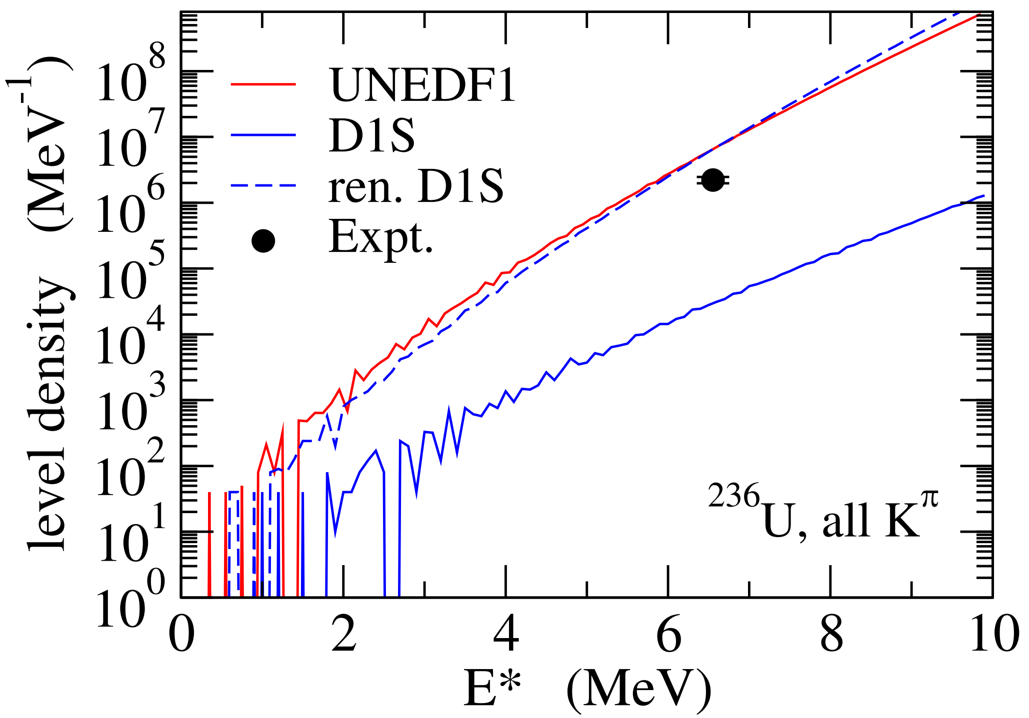
$\rho(E)$ is too small

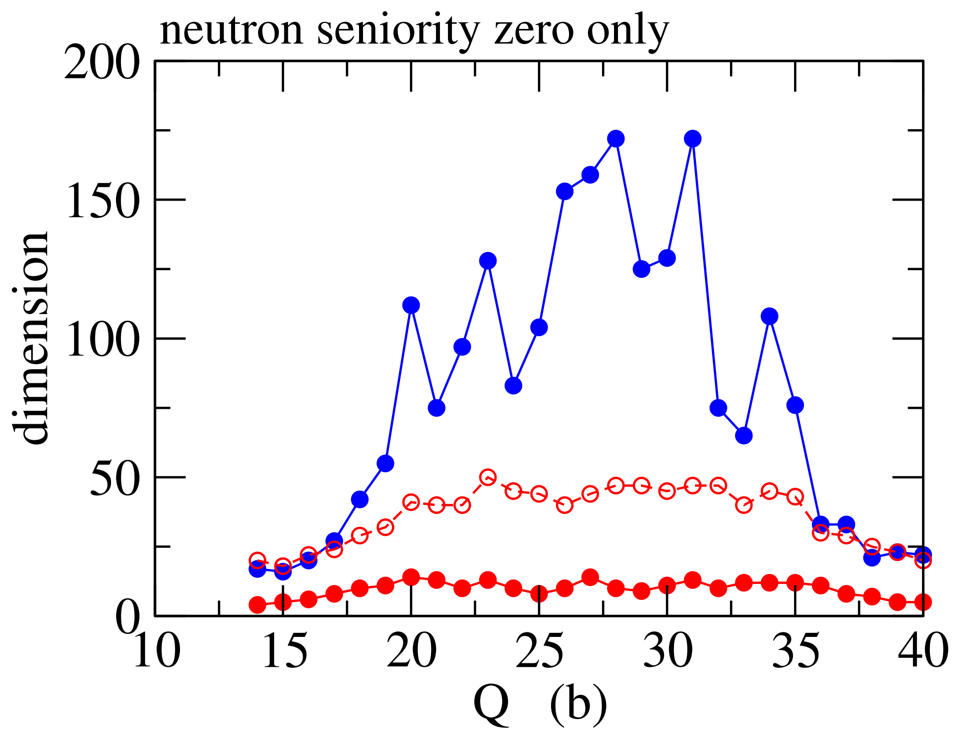
renormalization of $e_i \rightarrow (m^*/m)\ e_i$

Discussions

Applications with the Gogny interaction?

To find a renormalization factor
to match with ρ(*E*) of UNEDF1 at Q = 14b





a *Q*-dep. renormalization factor

A new Gogny parameter set with $m^* \sim 1$?