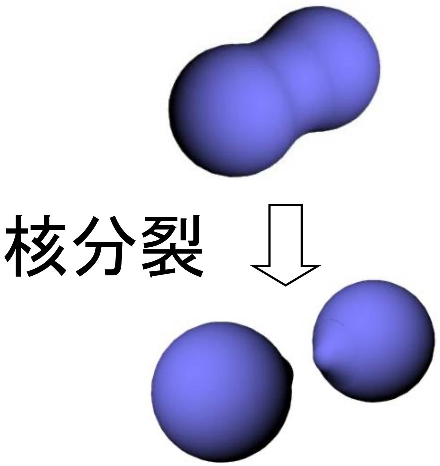
Towards a microscopic description for low-energy induced fission



Kouichi Hagino（萩野浩一）
Kyoto University　京都大学

G.F. Bertsch (Seattle)
Kotaro Uzawa（鵜沢浩太朗）(Kyoto)

1. Introduction: nuclear fission
2. Shell Model for induced fission
3. Application to low-energy fission of ^{236}U
4. A comment on the Dynamical GCM
5. Summary

G.F. Bertsch and K.H., Phys. Rev. C107, 044615 (2023).
K. Uzawa, K.H., and G.F. Bertsch, arXiv:2403.04255.

A seminar at Tongji University, 2024.4.24

Introduction: particle emission decays of unstable nuclei

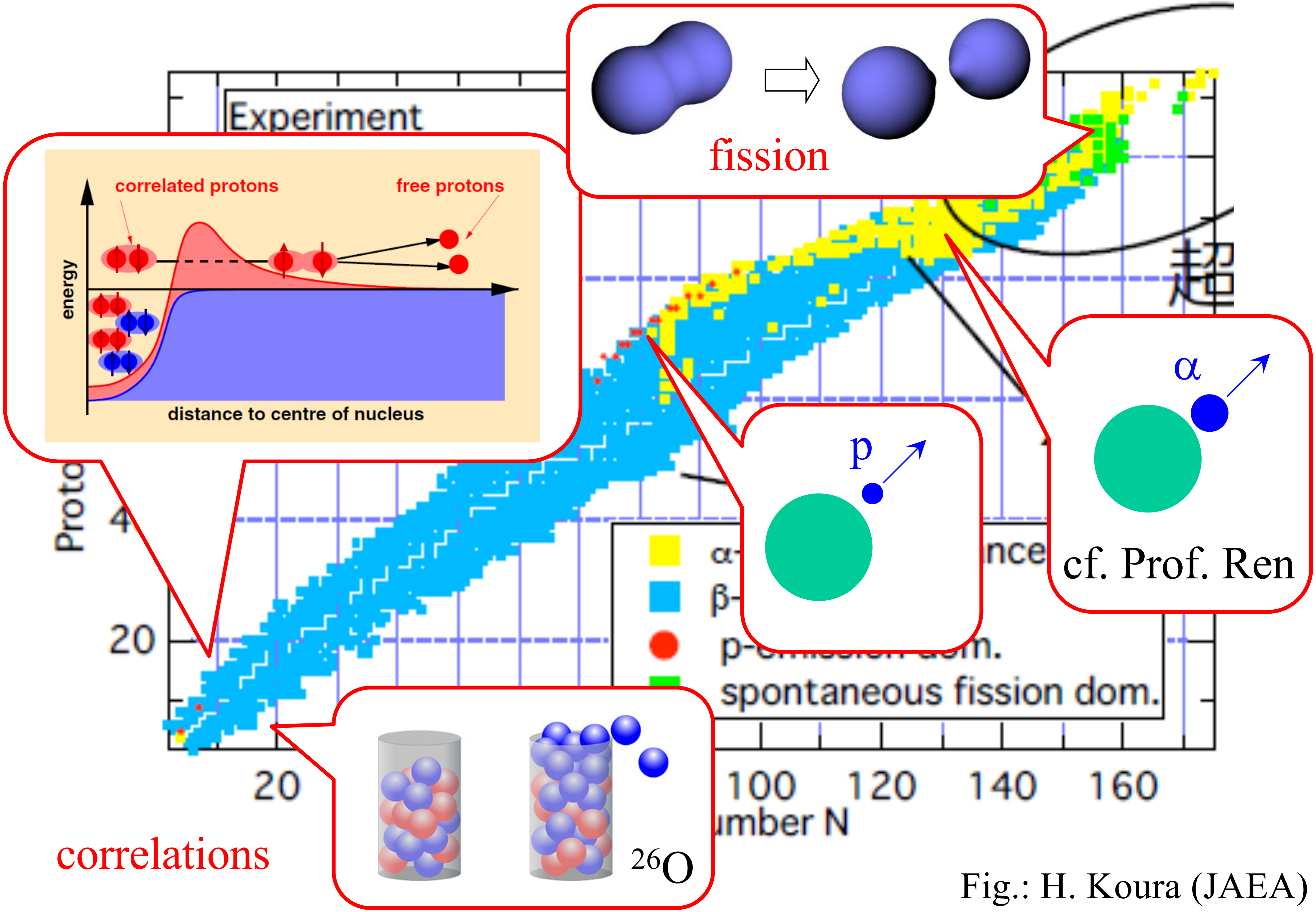
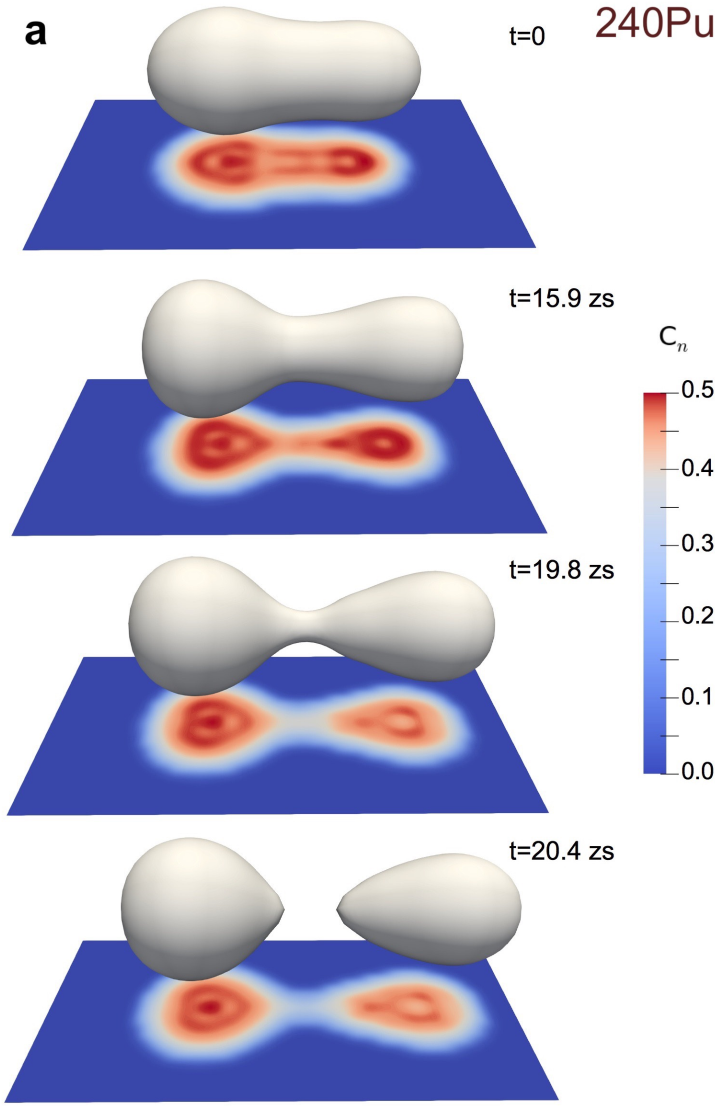


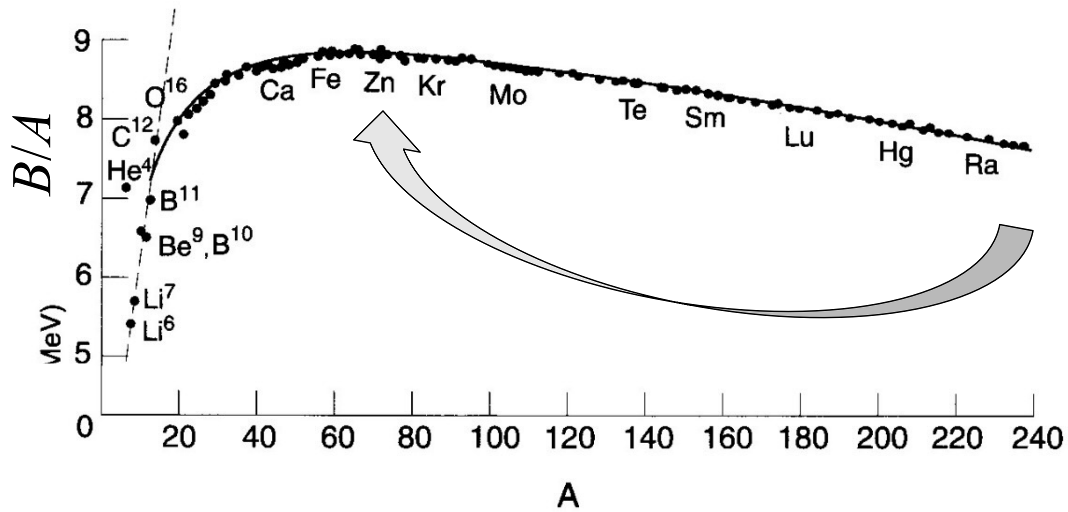
Fig.: H. Koura (JAEA)

Nuclear Fission



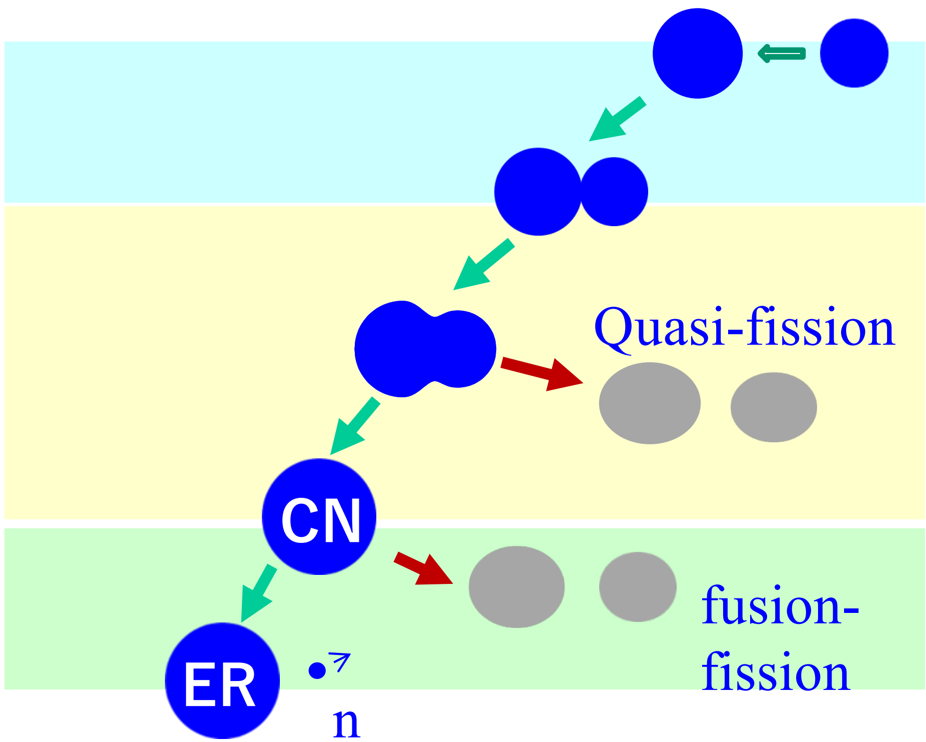
G. Scamps and C. Simenel, Nature 564 (2018) 382

- discovered about 80 years ago (in 1938) by Hahn and Strassmann
- a primary decay mode of heavy nuclei

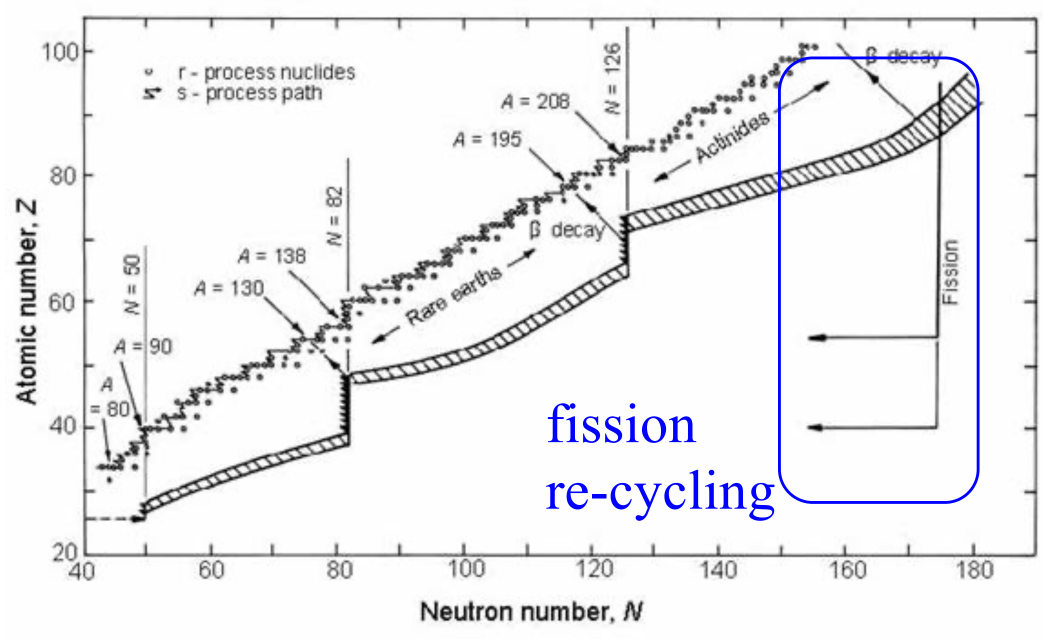


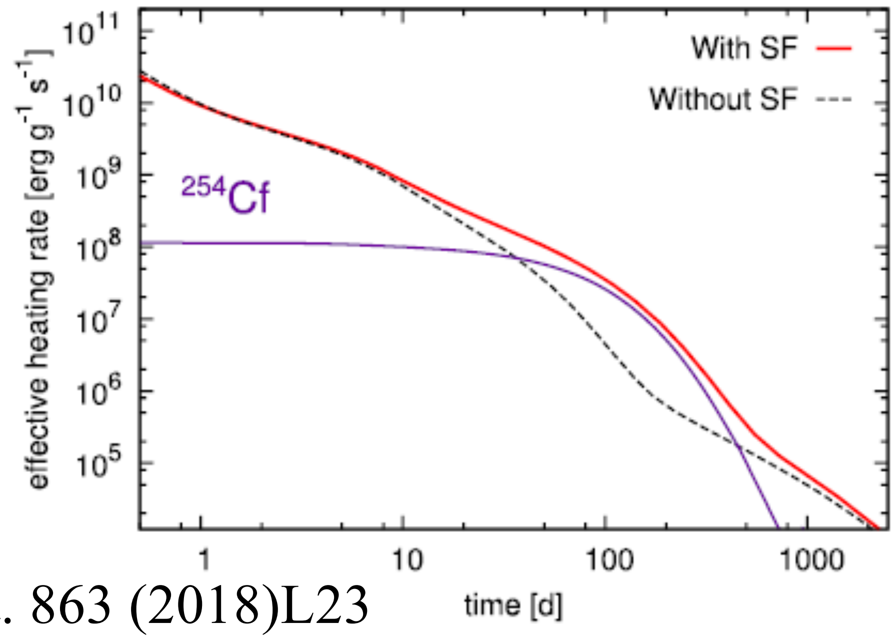
- important role in:
  - energy production
  - superheavy elements
  - r-process nucleosynthesis
  - production of neutron-rich nuclei

Superheavy elements



fission in r-process nucleosynthesis





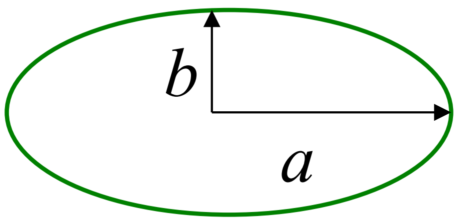
Y. Zhu et al.,
Astrophys. J. Lett. 863 (2018)L23

a macroscopic understanding of fission

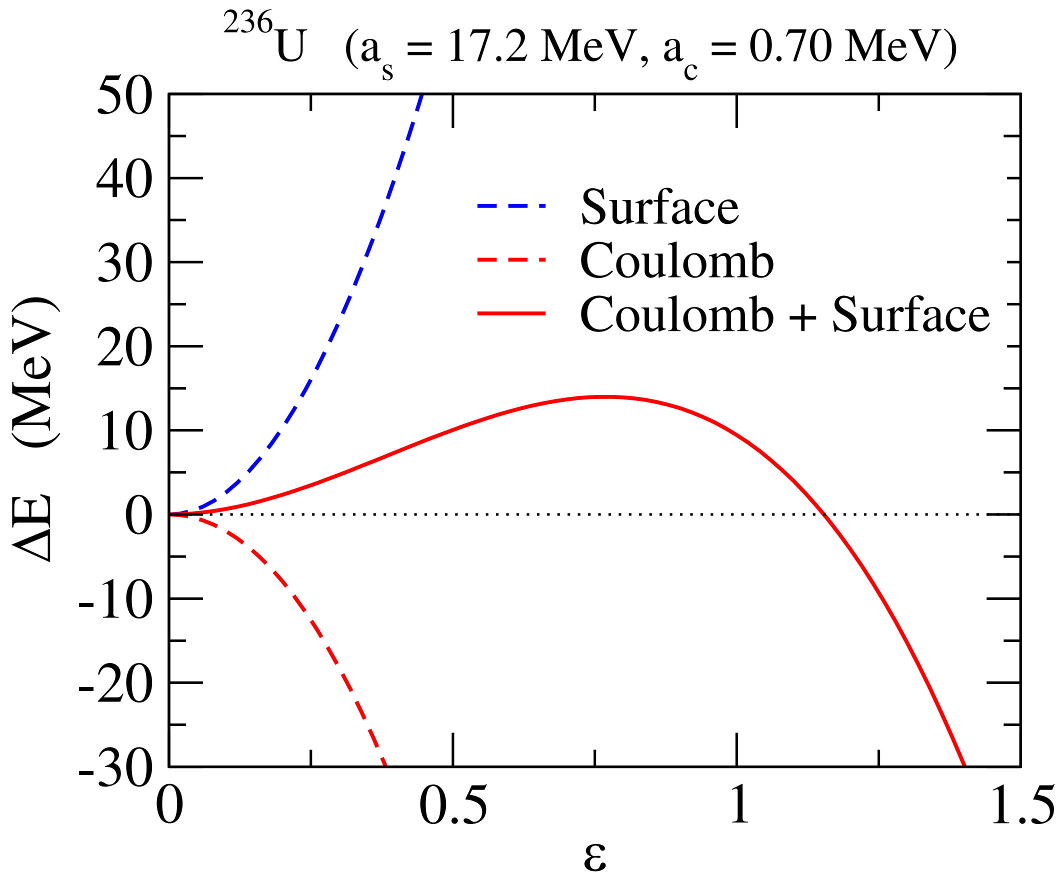
competition between the surface and the Coulomb energies

$\rightarrow$ fission barrier

Liquid Drop Model

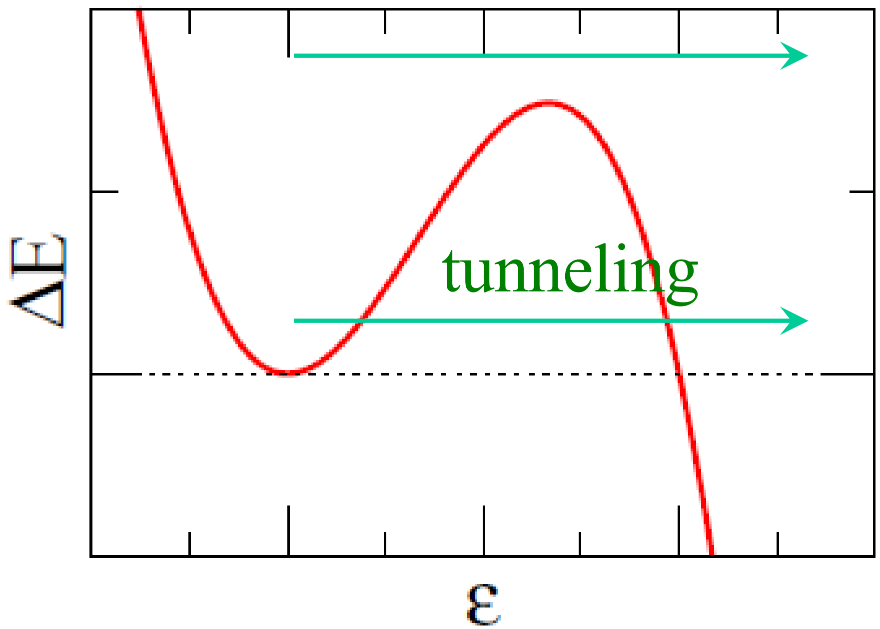


$$a = R\cdot(1+\epsilon)$$
$$b = R\cdot(1+\epsilon)^{-1/2}$$

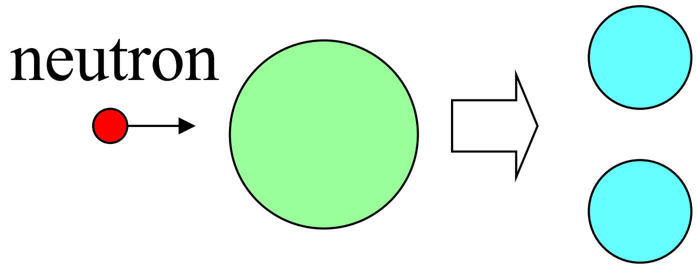


$$E_S(\epsilon) = \left(1+\frac{2}{5}\epsilon^2-\frac{4}{105}\epsilon^3+\cdots\right)$$
$$E_C(\epsilon) = E_C^{(0)}\left(1-\frac{1}{5}\epsilon^2-\frac{4}{105}\epsilon^3+\cdots\right)$$

- various fission processes

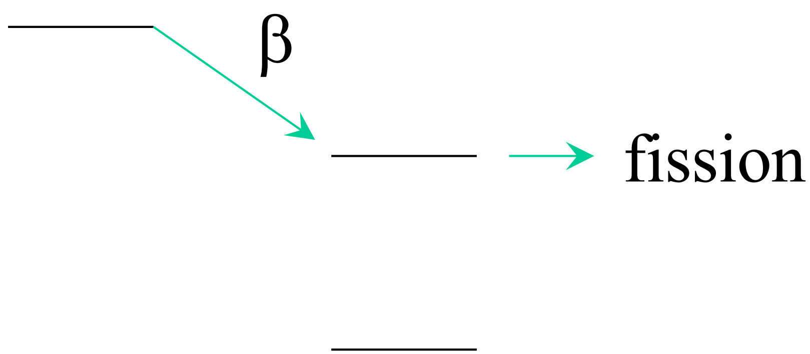


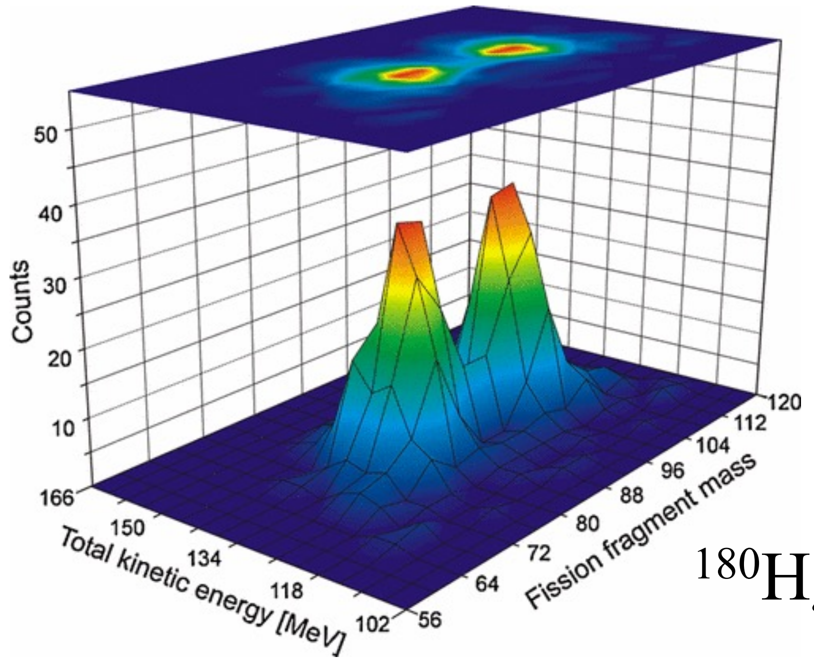
induced fission



spontaneous fission

beta-delayed fission





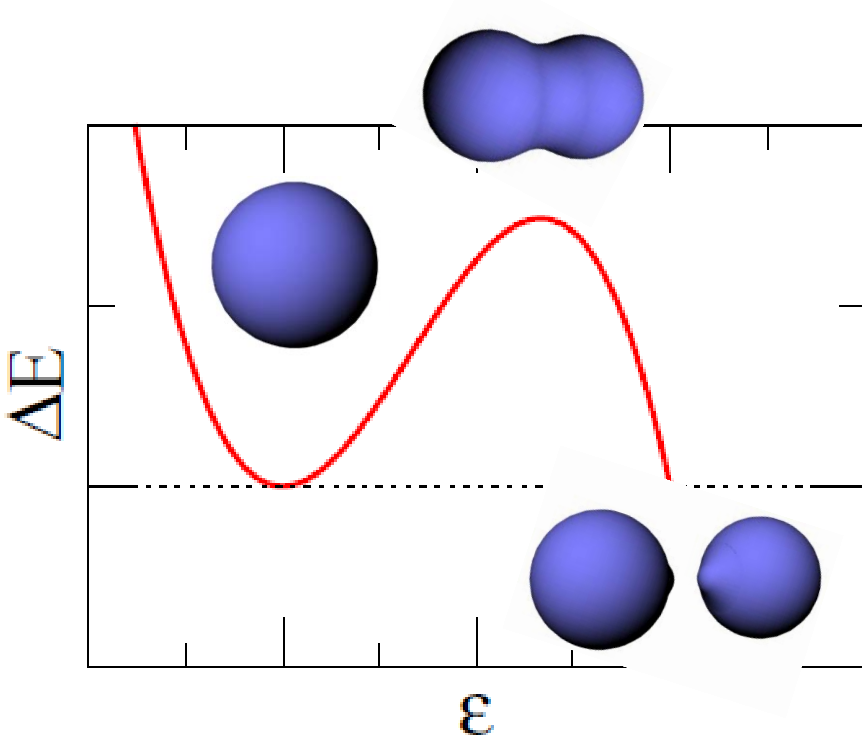
^{180}Hg

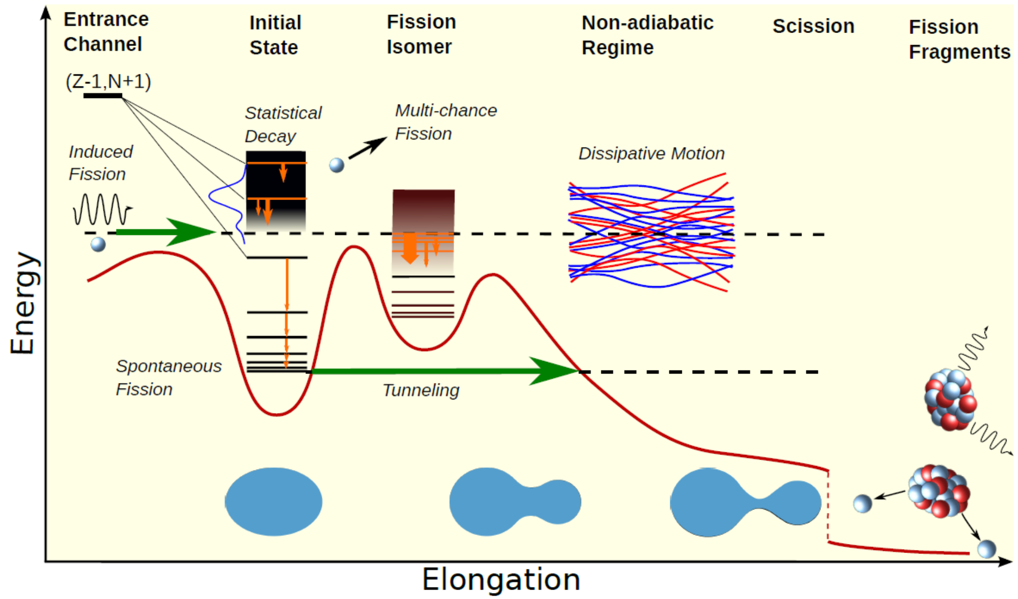
A.N. Andreyev et al., PRL105(‘10)252502

➢ macroscopic understanding:

competition between the surface and the Coulomb energies

→ fission barrier





"Future of fission theory"
M. Bender et al., J. of Phys. G47, 113002 (2020)

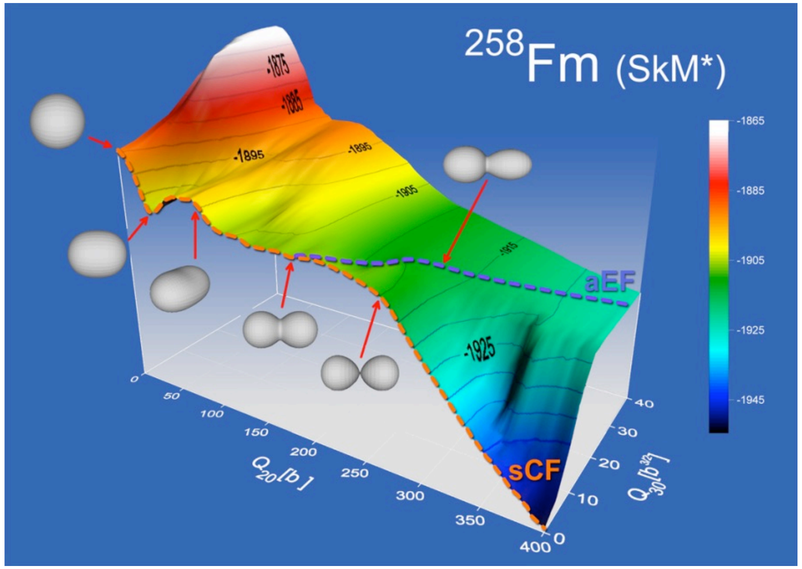
➢ a microscopic understanding:

large change of nuclear shape

→ microscopic description : far from complete

an ultimate goal of nuclear physics

➤ spontaneous fission



A. Staszczak, A. Baran, J. Dobaczewski, and W. Nazarewicz, PRC80 ('09) 014309

constrained Hartree-Fock (+B) method:

$$\delta\langle\Phi|H-\lambda Q_{20}|\Phi\rangle=0$$

$$\rightarrow \Phi(Q_{20}),\ \ E(Q_{20})$$

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

➤ induced fission

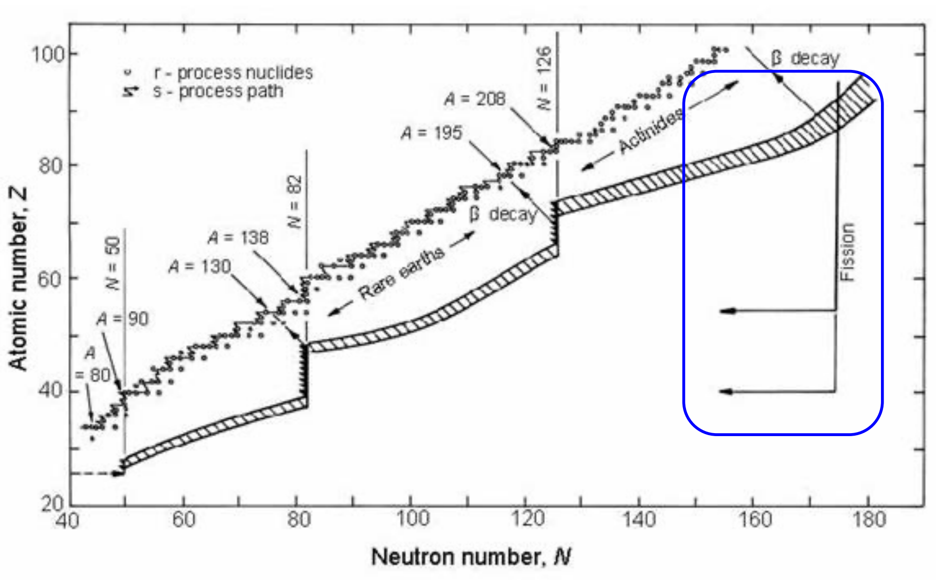
almost nothing has been developed for a microscopic theory

↓

the topic of this talk

Why do we need a microscopic approach?

- r-process nucleosynthesis

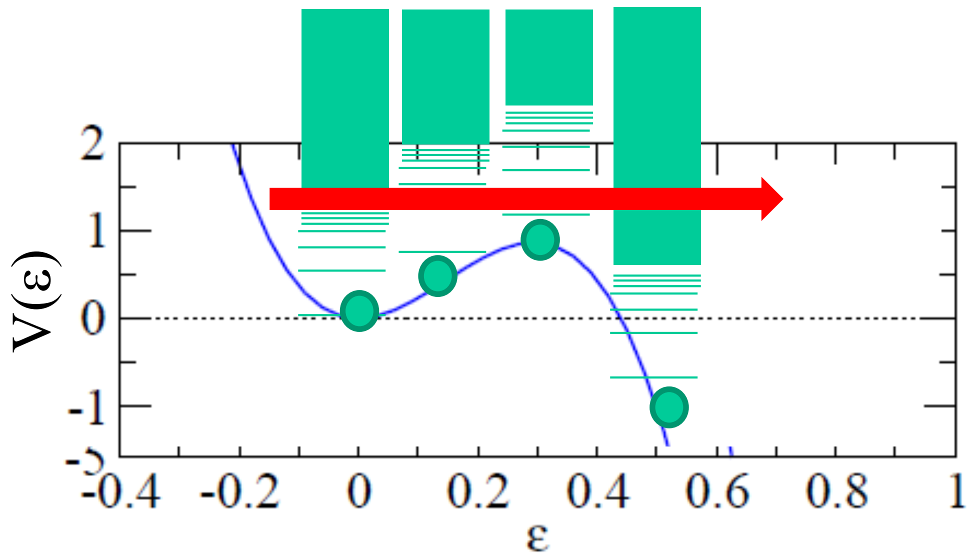


(neutron induced) fission of neutron-rich nuclei

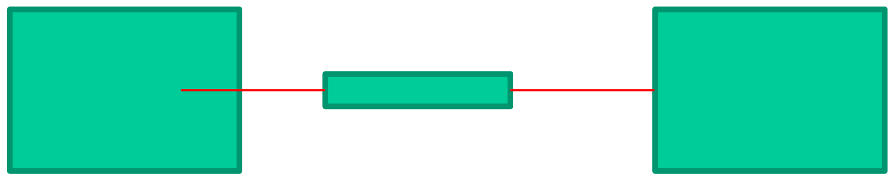
→ low E^* and low $\rho(E^*)$

- ✓ Validity of statistical models?
- ✓ Validity of the Langevin approach?

- barrier-top fission



CN | barrier-top | post barrier



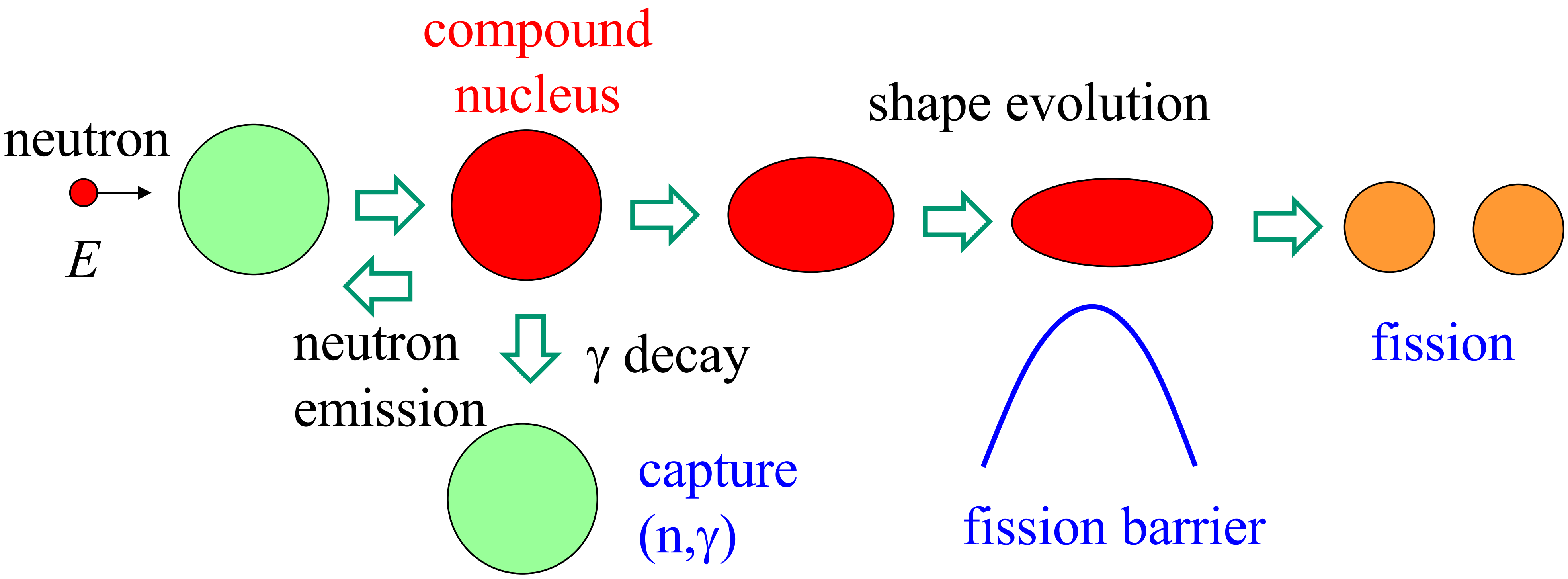
high ρ(E) | low ρ(E) | high ρ(E)

↓

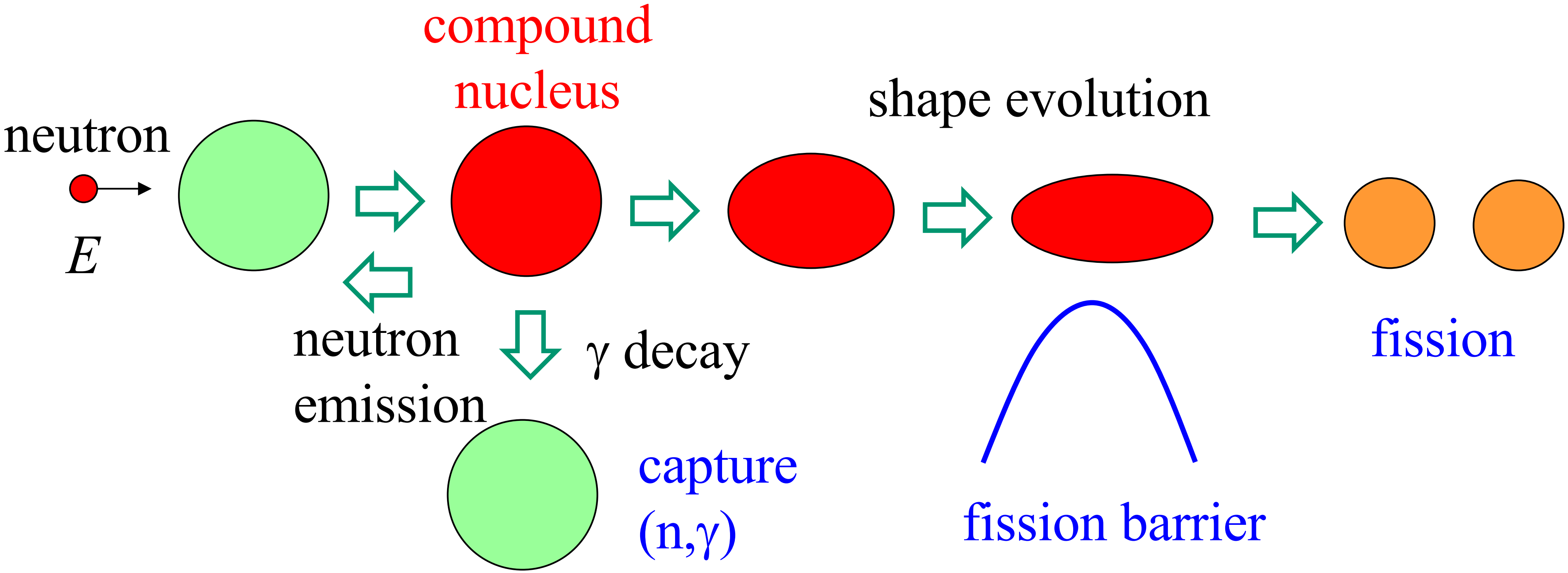
discrete levels

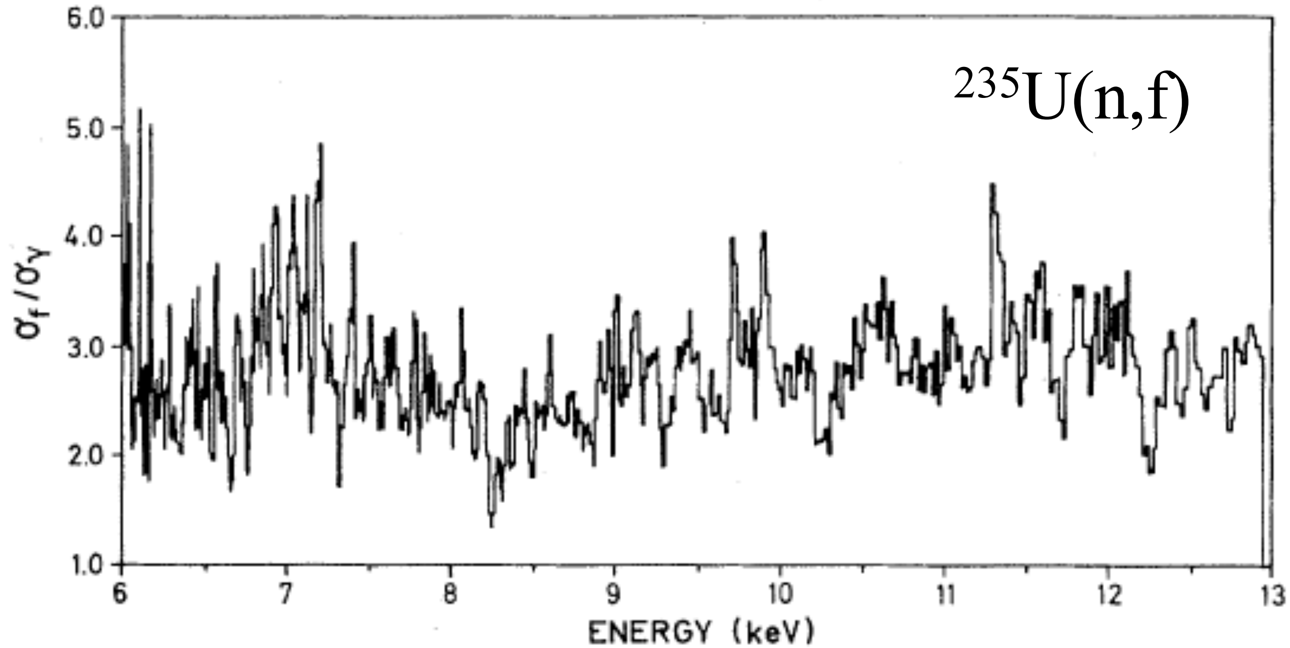
How to connect to a many-body Hamiltonian?

a process which we would like to dicscuss



a process which we would like to dicscuss



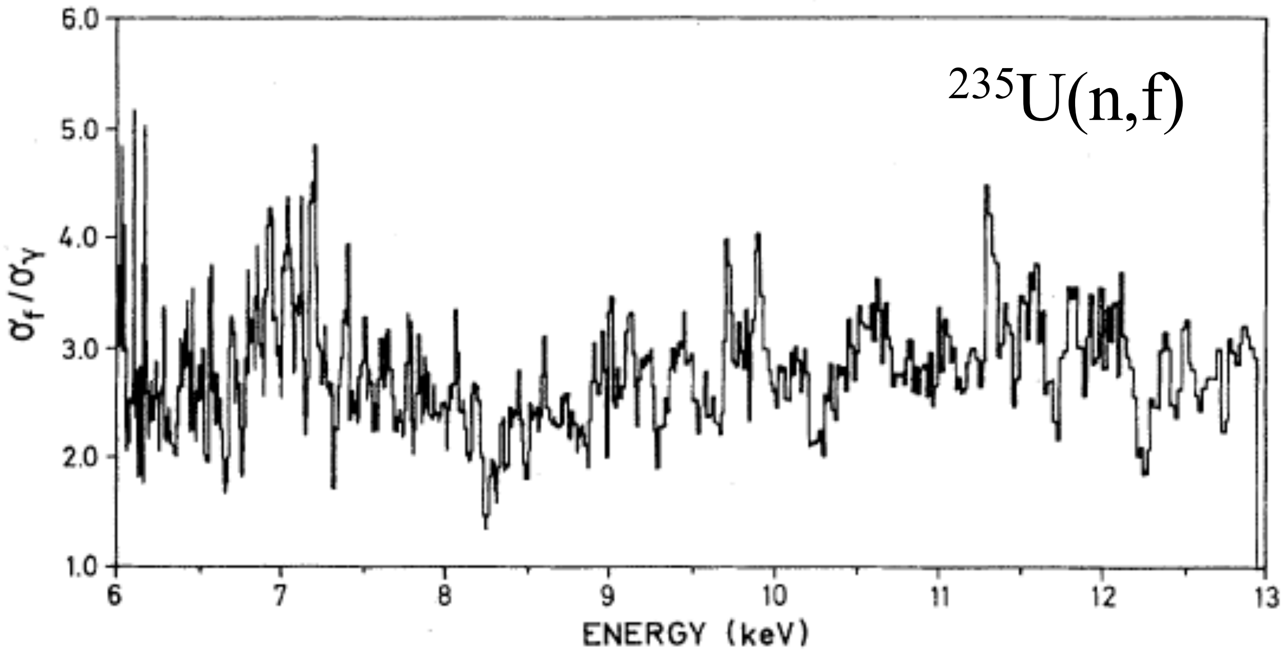


branching ratio

$$\alpha^{-1} = \frac{\sigma_f}{\sigma_\gamma}$$

sensitive to intermediate structure

M.S. Moore et al., PRC30 ('84) 214



branching ratio

$$\alpha^{-1} = \frac{\sigma_f}{\sigma_\gamma}$$

Important questions for r-process nucleosynthesis

- How will a fission barrier be modified for neutron-rich nuclei?
- What is an influence of pairing for (n,f) reactions?
- How does the branching ratio evolve towards n-rich nuclei?

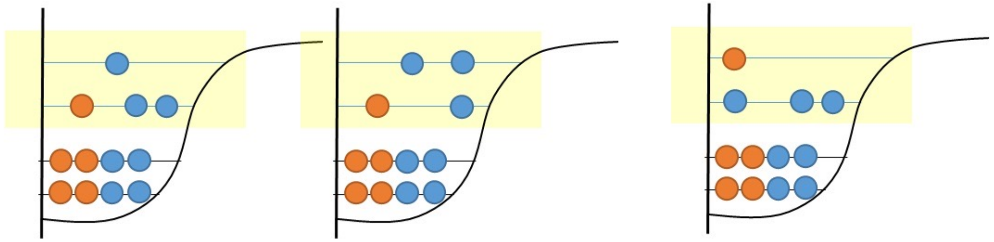
  (n,f) versus (n,γ)

- How does fission compete with alpha/cluster decays in neutron-rich heavy nuclei?

a microscopic approach may be crucial to address these questions

Shell model approach?

Shell model

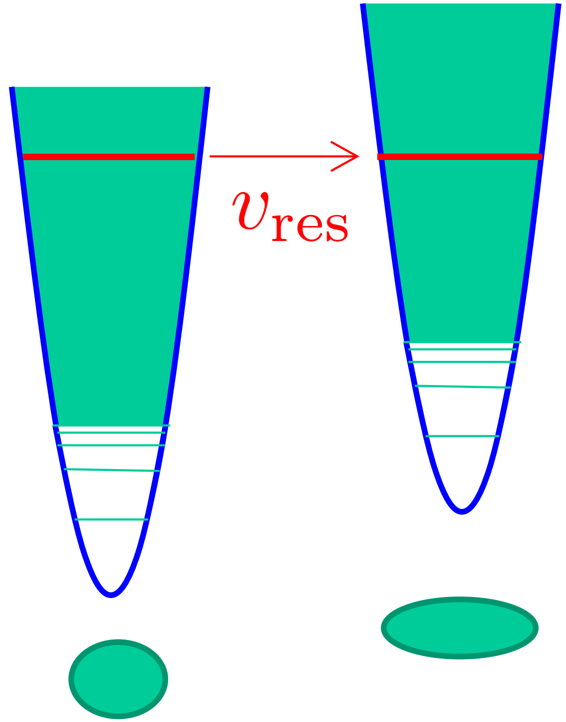


$|\Psi\rangle = v_1|m_1\rangle + v_2|m_2\rangle + v_3|m_3\rangle + \cdots$

Figure: Noritaka Shimizu (Tsukuba)

many-particle many-hole configurations in a mean-field potential
→mixing by <u>residual interactions</u>

A similar approach for nuclear fission?

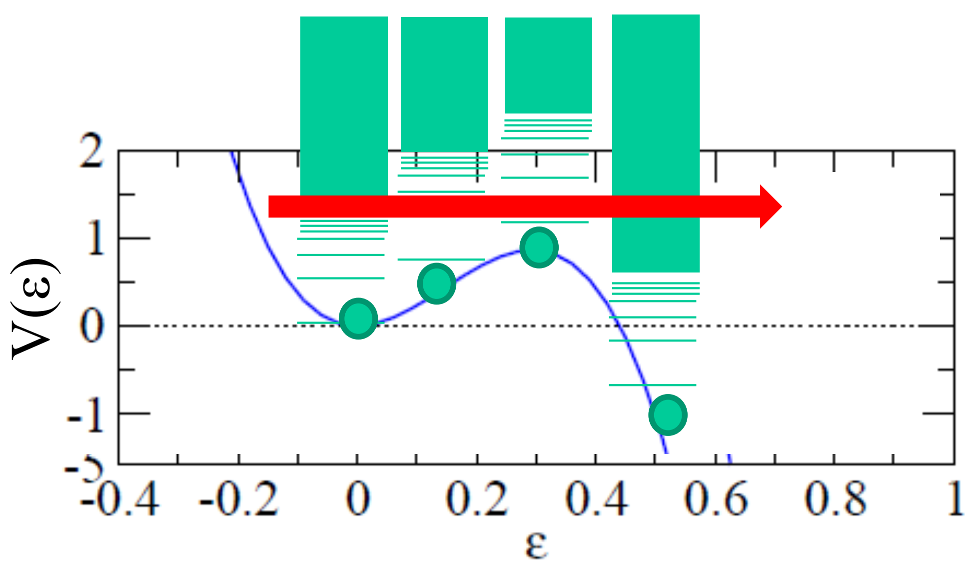


- Many-body configurations in a MF pot. for each shape
- hopping due to res. int.

→ shape evolution

a good connection to nuclear reaction theory

Shell model approach?

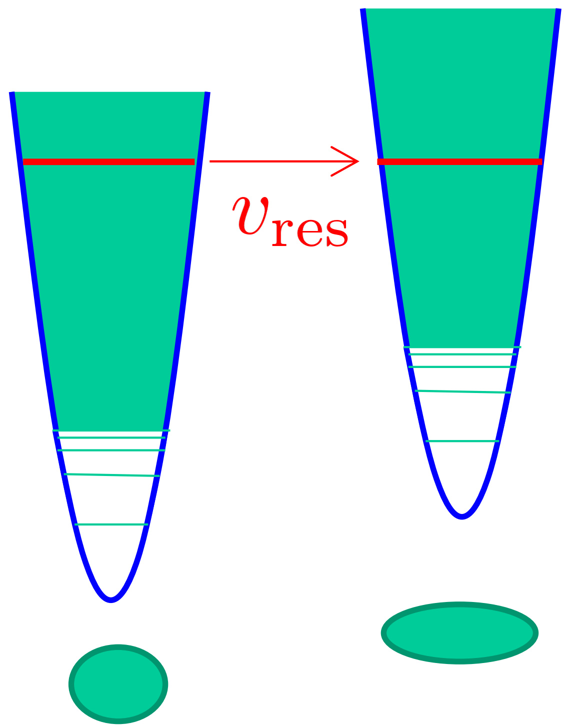


$$|\Psi\rangle = \int dQ \sum_i f_i(Q)|\Phi_Q(i)\rangle$$

GCM with excited states

cf. the usual GCM:

$$|\Psi\rangle = \int dQ\, f(Q)|\Phi_Q(g.s.)\rangle$$



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

→ shape evolution

a good connection to nuclear reaction theory

GCM methodology for transmission channels

GCM calculations for nuclear structure

1. construct $\{|\Psi_i\rangle\}$ by discretizing $Q=(q_1,q_2,\ldots,q_N)$

2. compute

$$H_{ij} = \langle\Psi_i|H|\Psi_j\rangle$$
$$N_{ij} = \langle\Psi_i|\Psi_j\rangle$$

3. solve the Hill-Wheeler equation

$$\sum_j H_{ij} f_j = E \sum_j N_{ij} f_j$$

a many-body wf is then:

$$|\Phi\rangle = \sum_i f_i |\Psi_i\rangle$$

GCM calculations for transmission

1. construct $\{|\Psi_i\rangle\}$

2. compute H_{ij} and N_{ij}

3. introduce imaginary terms

$$-i(\Gamma_i)_{kk'}/2$$

representing the decay width of the state i

4. compute the Green's function

$$\boldsymbol{G}(E) = \left(\boldsymbol{H} - i\sum_i \boldsymbol{\Gamma}_i/2 - \boldsymbol{N}E\right)^{-1}$$

5. the transmission probability from i to j is then computed as

$$T_{i\to j} = \mathrm{Tr}[\boldsymbol{\Gamma}_i \boldsymbol{G} \boldsymbol{\Gamma}_j \boldsymbol{G}^\dagger]$$

GCM methodology for transmission channels

GCM calculations for transmission

1. construct $\{|\Psi_i\rangle\}$
2. compute H_{ij} and N_{ij}
3. introduce imaginary terms

$$-i(\Gamma_i)_{kk'}/2$$

representing the decay width of the state i

←Fermi's Golden Rule

$$\Gamma_i \sim \frac{2\pi}{\hbar} \sum_k |\langle k|v|i\rangle|^2 \delta(E_k - E_i)$$

4. compute the Green's function

$$\boldsymbol{G}(E) = \left(\boldsymbol{H} - i\sum_i \boldsymbol{\Gamma}_i/2 - \boldsymbol{N}E\right)^{-1}$$

← "Non-equilibrium Green's function (NEGF)"

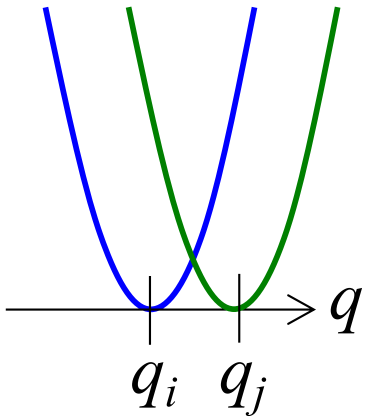
5. the transmission probability from i to j is then computed as

$$T_{i\to j} = \mathrm{Tr}[\boldsymbol{\Gamma}_i \boldsymbol{G} \boldsymbol{\Gamma}_j \boldsymbol{G}^\dagger]$$

← "Datta formula"

A test with a simple model

G.F. Bertsch and K. Hagino, PRC105, 034618 (2022)



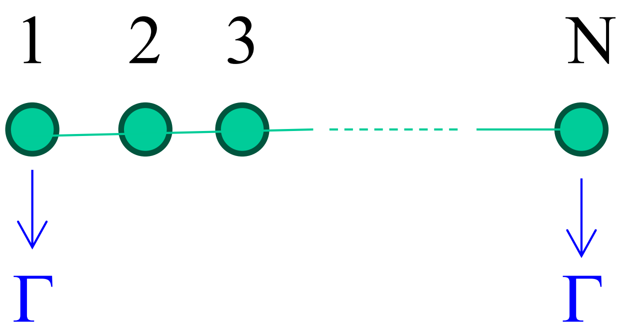
CM in HO $\Psi_{q_i}(q) = (\pi s^2)^{-1/4} e^{-(q-q_i)^2/4s^2}$

$(q_1, q_2, \ldots, q_N)$ with Δq

$$\langle \Psi_{q_i} | \Psi_{q_j} \rangle = \exp\left(-(q_i - q_j)^2/4s^2\right)$$

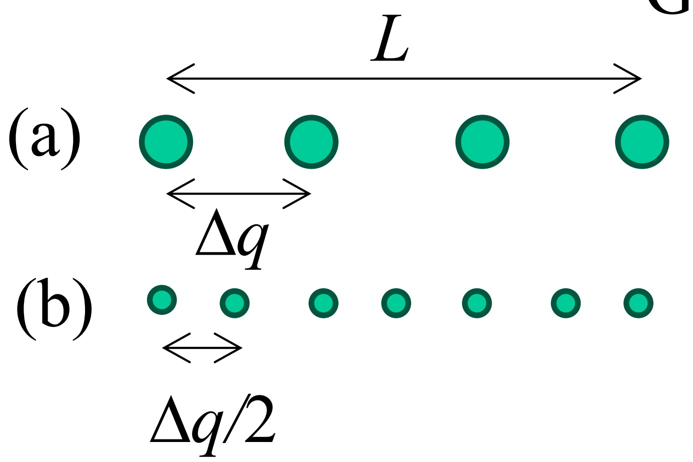
$$\left\langle \Psi_{q_i} \left| -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial q^2} \right| \Psi_{q_j} \right\rangle = E_K \left(1 - \frac{(q_i - q_j)^2}{2s^2}\right) N_{ij}$$

$$E_K = \frac{\hbar^2}{2Ms^2}$$



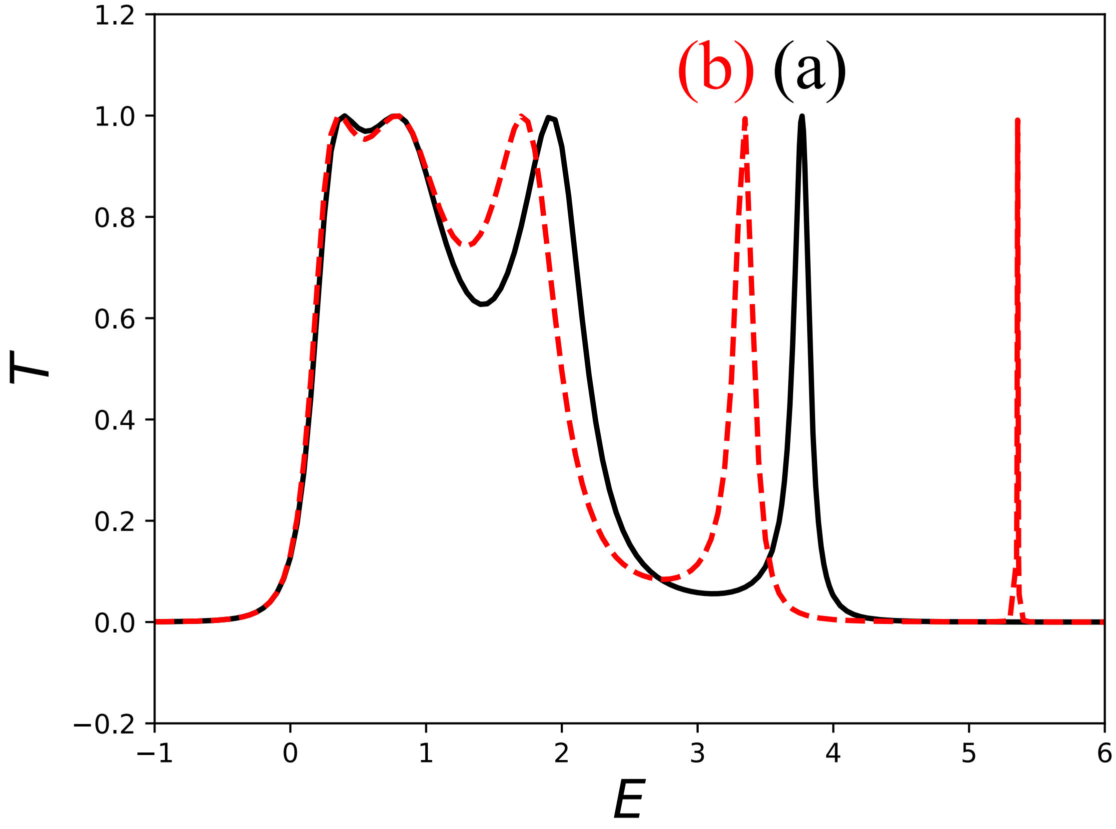
$$(\mathbf{\Gamma}_1)_{ij} = \gamma N_{i1} N_{j1}$$
$$(\mathbf{\Gamma}_N)_{ij} = \gamma N_{iN} N_{jN}$$
$$\mathbf{\Gamma}_k = 0 \quad (k \neq 1, N)$$

G.F. Bertsch and K.H., PRC105, 034618 (2022)



4 configurations with $L = 3\Delta q$

7 configurations with $L = 6\,(\Delta q/2)$



$$s = 1/\sqrt{5},\ \Delta q = 1,$$
$$E_K = 5/4$$
$$\gamma = 1$$

A low E behavior is similar.

→ one can take a large mesh.

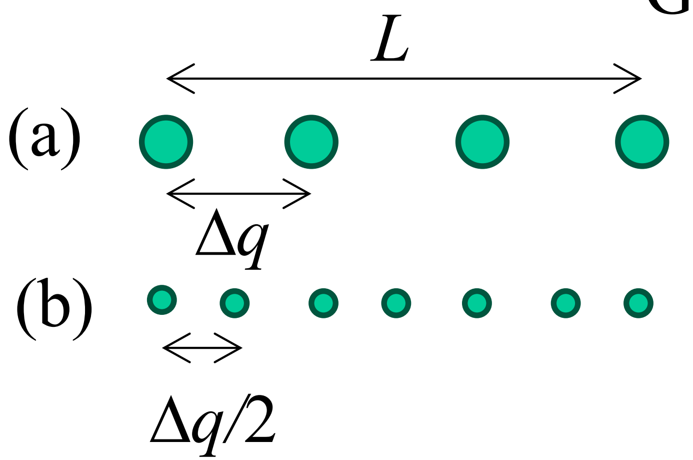
$$I \equiv \int_{-\infty}^{\infty} dE\, T(E)$$

$= 1.69\ E_K$ for (a)

$1.65\ E_K$ for (b)

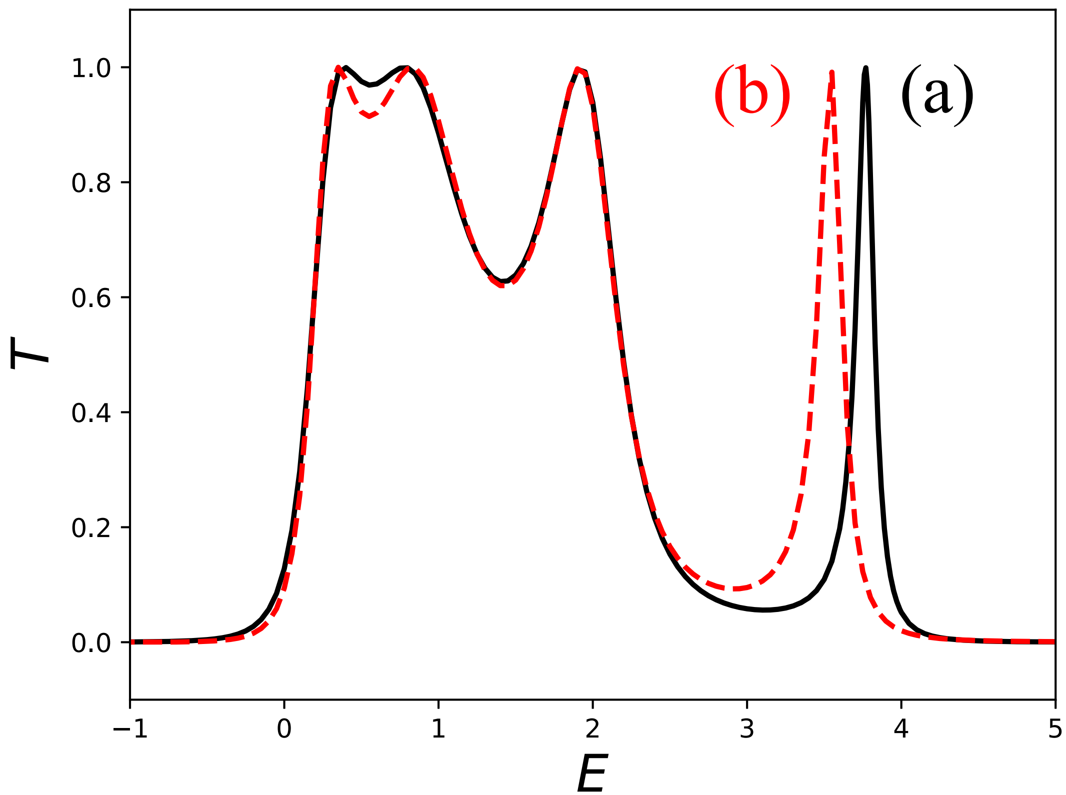
* qualitatively similar even with a barrier

G.F. Bertsch and K.H., PRC105, 034618 (2022)



4 configurations with $L = 3\Delta q$

7 configurations with $L = 6(\Delta q/2)$



Eigenvalues of N_{ij}

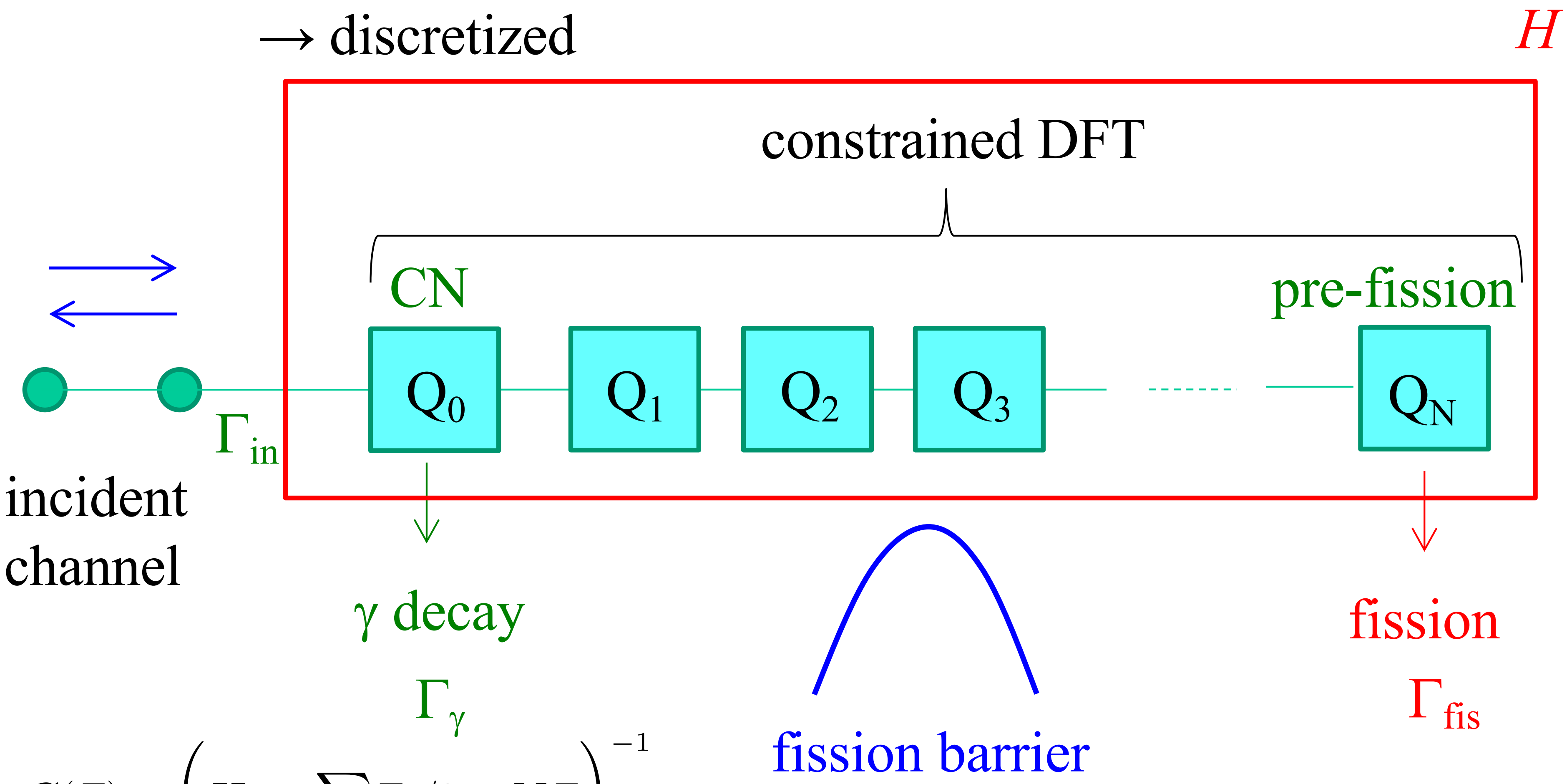
model (a)	model (b)
1. 1.47	1. 2.85
2. 1.17	2. 2.07
3. 0.82	3. 1.22
4. 0.54	4. 0.57
	5. 0.22
	6. 0.062
	7. 0.012

red: model (b), but including only 4 eigenstates of N

Application to low-energy fission of ^{236}U

G.F. Bertsch and K.H., Phys. Rev. C107, 044615 (2023).
K. Uzawa, K.H., and G.F. Bertsch, arXiv:2403.04255.

Assumption: fission occurs along Q_{20} as a collective coordinate
$\longrightarrow$ discretized



$$\boldsymbol{G}(E) = \left(\boldsymbol{H} - i\sum_i \boldsymbol{\Gamma}_i/2 - \boldsymbol{N}E\right)^{-1}$$

Application to low-energy fission of ^{236}U

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

✓ Constrained Skyrme Hartree-Fock with the UNEDF1 parameter set
✓ Hartree-Fock basis (the pairing interaction: external)
✓ Axial and Time-reversal symmetries
✓ HF Solver: SkyAx ← 2D coordinate space

P.-G. Reinhard et al., CPC258, 107603 (2021).

Simplifications:

✓ ^{236}U : only neutron configurations, up to 4 MeV
✓ Dynamics of the first barrier: axial symmetry
✓ seniority-zero config. only: occupation of (K, -K)
✓ the end configurations: replaced by GOE
✓ a scaled fission barrier with $B_f = 4$ MeV

Application to low-energy fission of ^{236}U

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

Simplifications:

- ✓ ^{236}U : only neutron configurations, up to 4 MeV
- ✓ Dynamics of the first barrier: axial symmetry
- ✓ seniority-zero config. only: occupation of (K, -K)
- ✓ discretization:

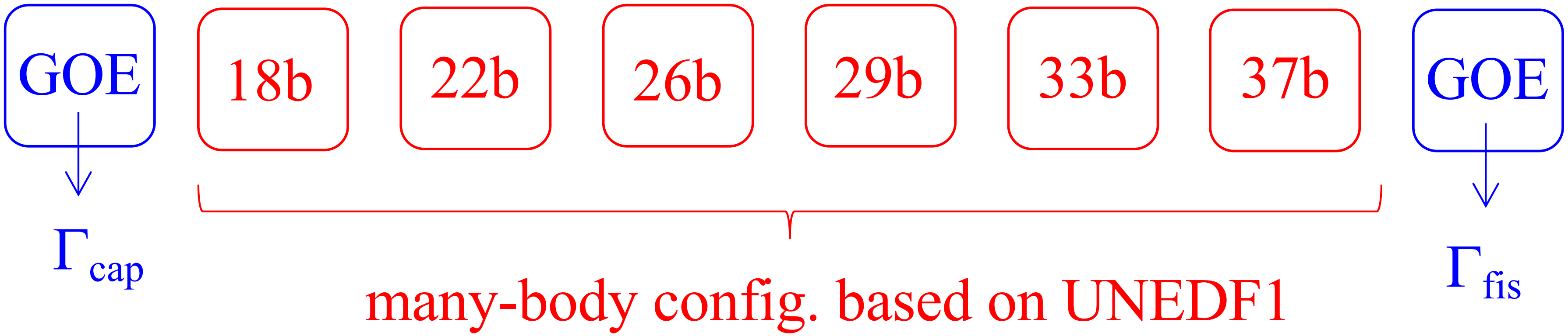
$$\langle \Psi_\mu(Q) | \Psi_\mu(Q') \rangle \sim e^{-1}$$

dim. =100	42	97	153	125	65	32	100
GOE	18b	22b	26b	29b	33b	37b	GOE
↓ Γ_{cap}	many-body config. based on UNEDF1 (HF basis, E* < 4 MeV)						↓ Γ_{fis}

714x714 Hamiltonian matrix

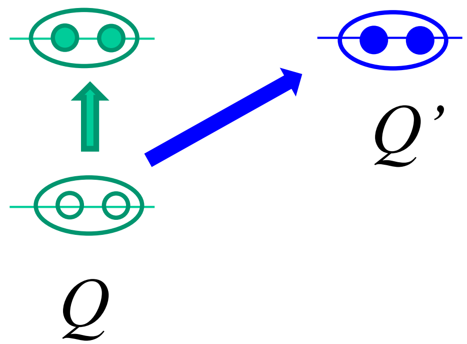
Application to low-energy fission of ^{236}U

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



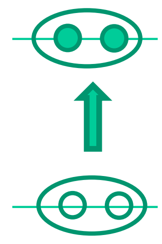
✓ overlap: $\langle\Psi_\mu(Q)|\Psi_\mu(Q')\rangle \sim e^{-1}$

✓ pairing: $v_{\mathsf{pair}} = -GP^\dagger P$

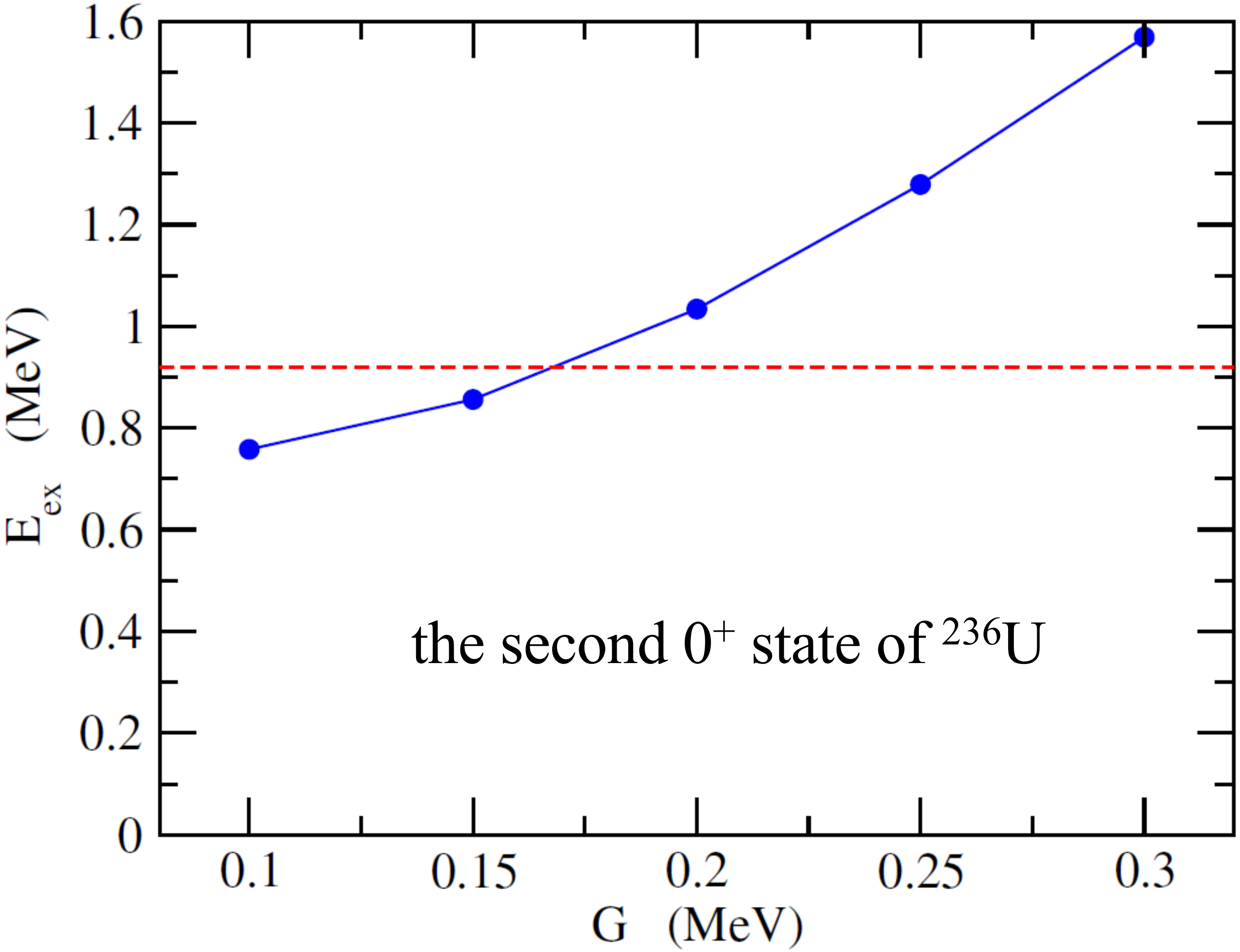


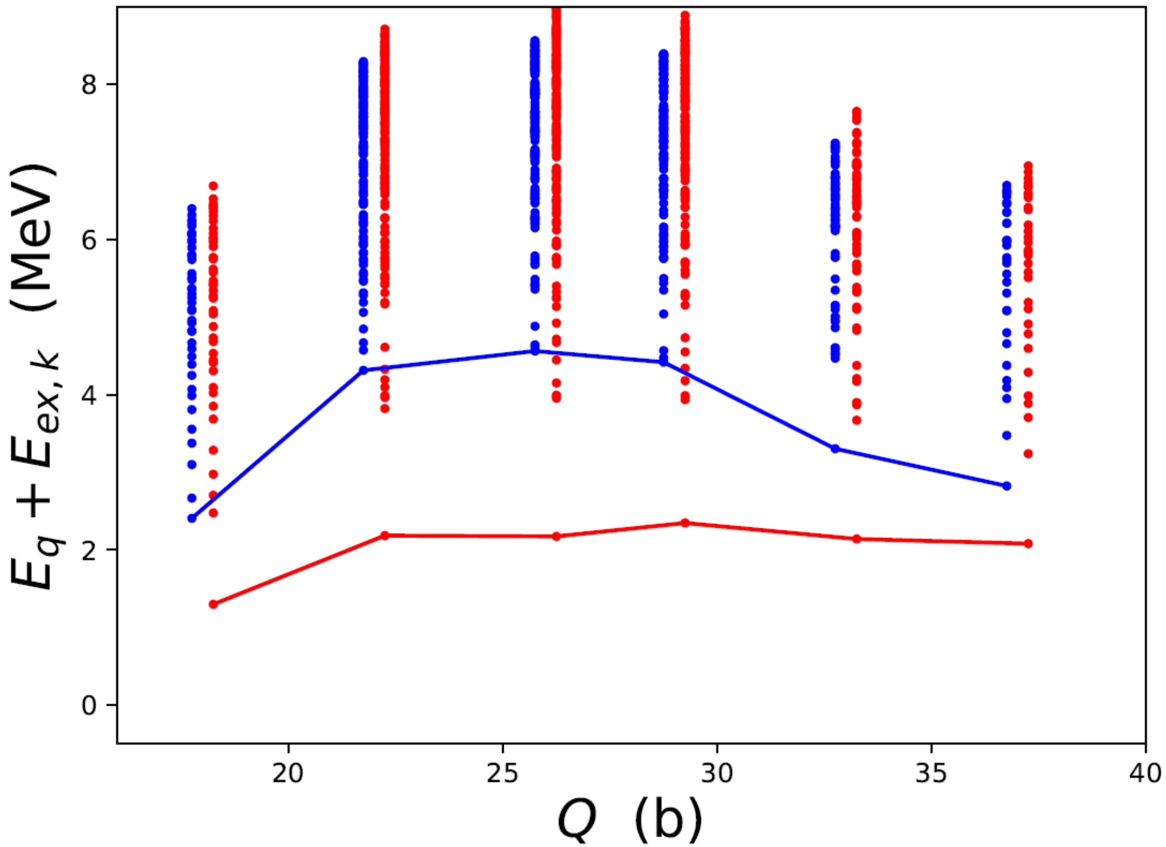
$$H = \sum_k \epsilon_k a_k^\dagger a_k - G P^\dagger P$$

$$P = a_k^\dagger a_{\bar{k}}^\dagger$$



Q





dim.
=100 | 42 | 97 | 153 | 125 | 65 | 32 | 100

GOE | 18b | 22b | 26b | 29b | 33b | 37b | GOE

Γ_{cap}

many-body config. based on UNEDF1
(HF basis, E* < 4 MeV)

Γ_{fis}

Application to low-energy fission of ^{236}U

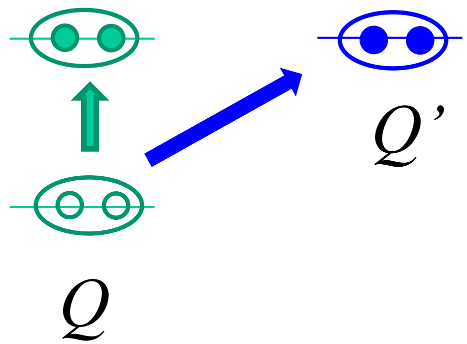
G.F. Bertsch and K.H., Phys. Rev. C107, 044615 (2023).

GOE | 18b | 22b | 26b | 29b | 33b | 37b | GOE

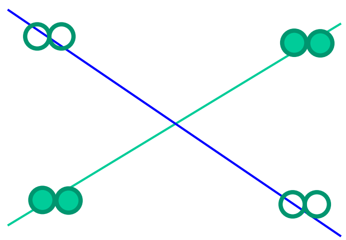
Γ_{cap} — many-body config. based on UNEDF1 — Γ_{fis}

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

✓ pairing: $v_{\text{pair}} = -G P^\dagger P$



✓ diabatic:

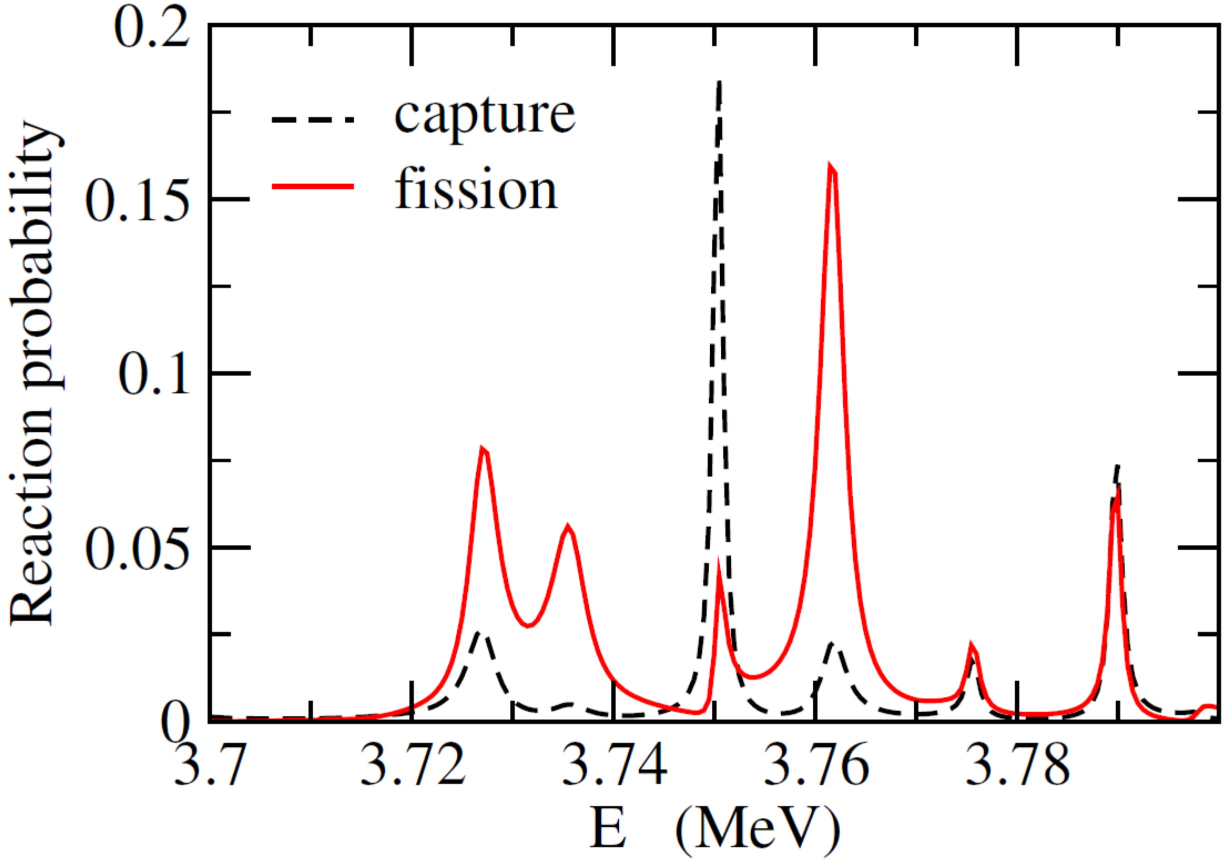


$$\frac{\langle \Psi_\mu(Q) | H | \Psi_\mu(Q') \rangle}{\langle \Psi_\mu(Q) | \Psi_\mu(Q') \rangle} \sim E_\mu(\bar{Q}) - h_2(\Delta Q)^2$$

✓ Γ_{cap}: exp. data (scaled according to N_{GOE}), Γ_{fis}: insensitivity

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

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



$\Gamma_{\text{in}} = 0.01$ MeV

$\Gamma_{\text{cap}} = 0.00125$ MeV

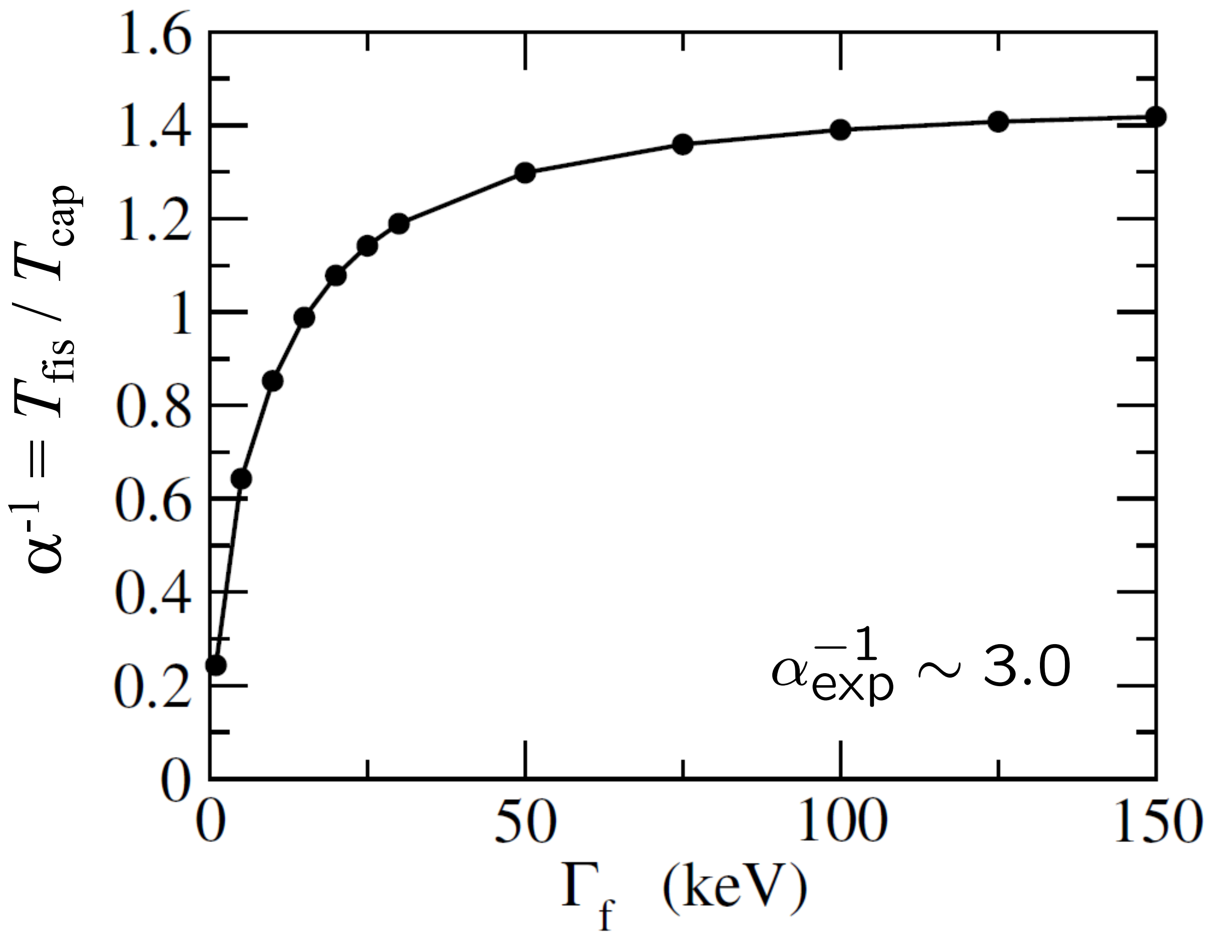
$\Gamma_{\text{fis}} = 0.015$ MeV

energy average

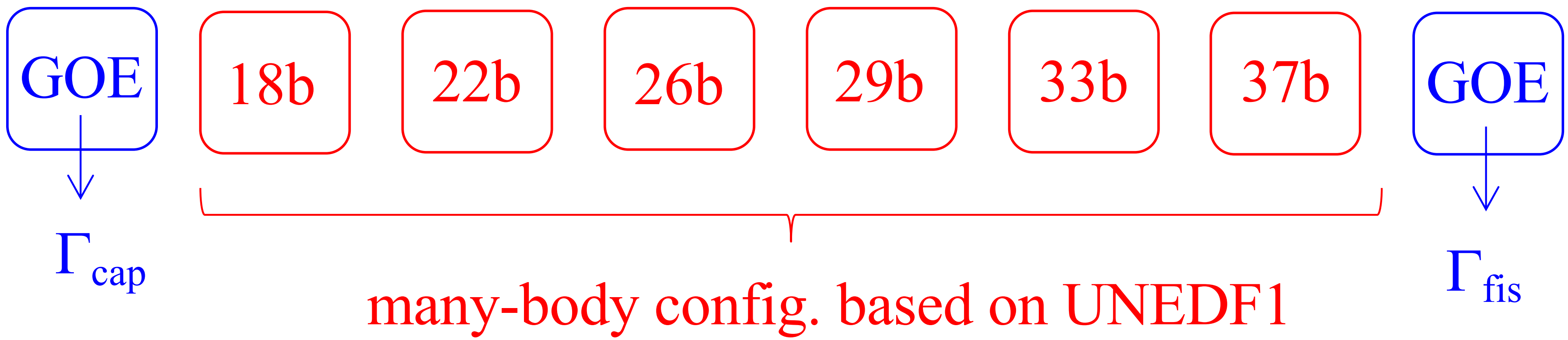
$$\alpha^{-1} = \frac{\int_{\Delta E} T_{\mathsf{fis}}(E')dE'}{\int_{\Delta E} T_{\mathsf{cap}}(E')dE'}$$

$\Delta E = 0.5$ MeV

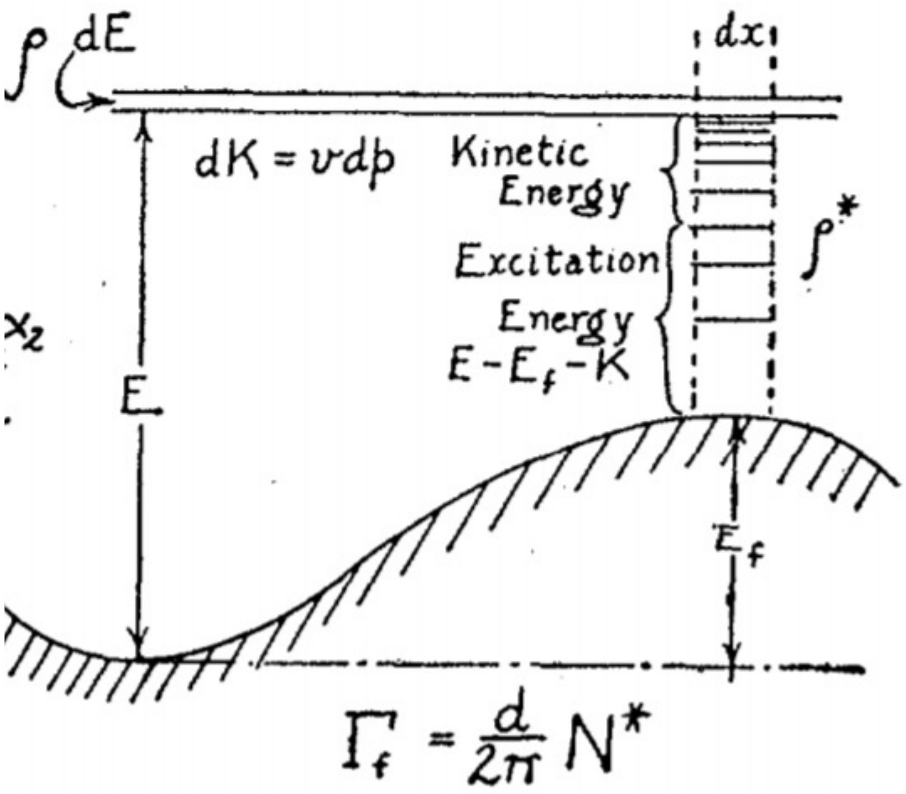
insensitivity property



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



the transition state theory

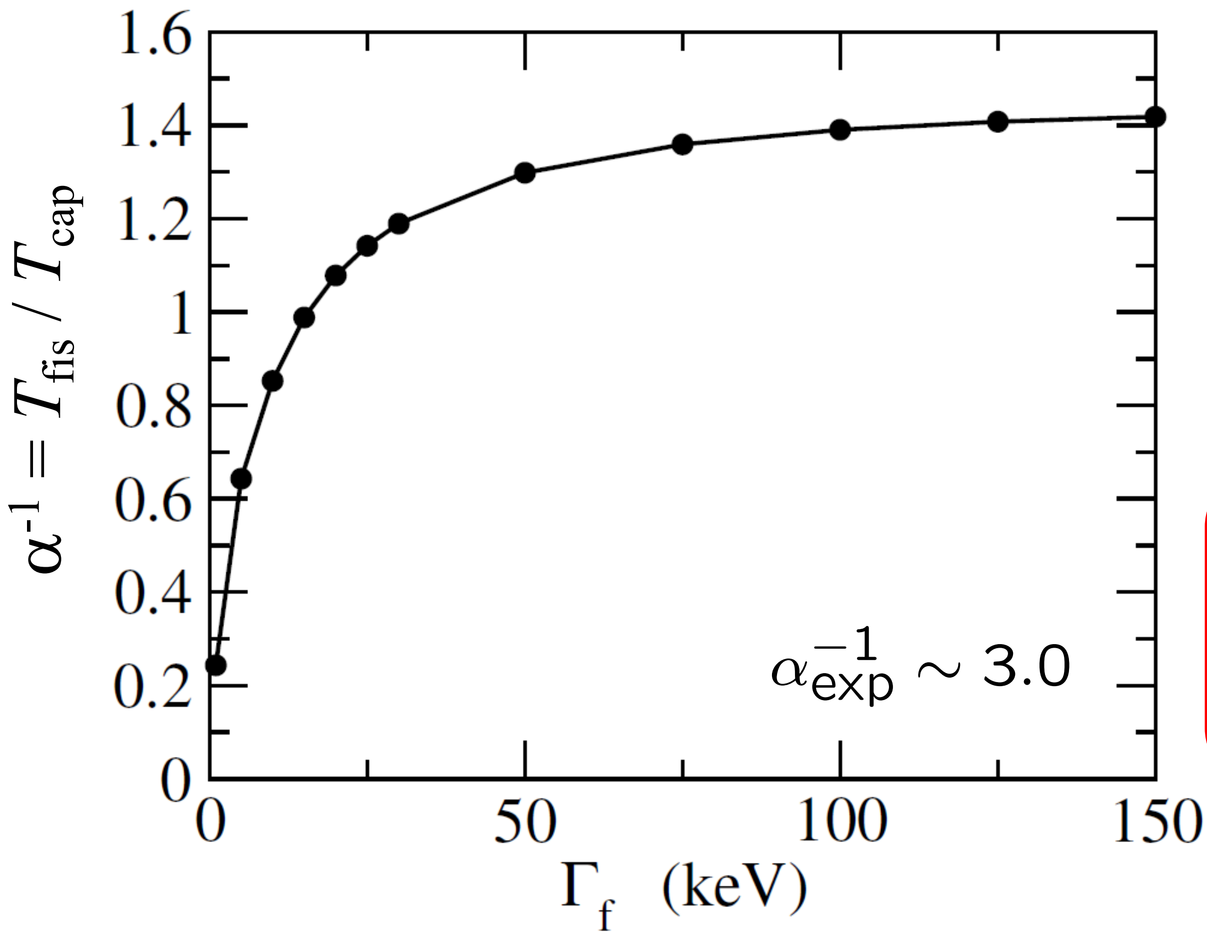


N. Bohr and J.A. Wheeler, Phys. Rev. 56, 426 (1939)

$$\Gamma_f = \frac{1}{2\pi\rho_{\rm gs}(E^*)}\int_0^{E^*-B_f}\rho_{\rm sd}(E^*-B_f-K)dK \rightarrow \frac{1}{2\pi\rho_{\rm gs}(E^*)}\sum_c T_c$$

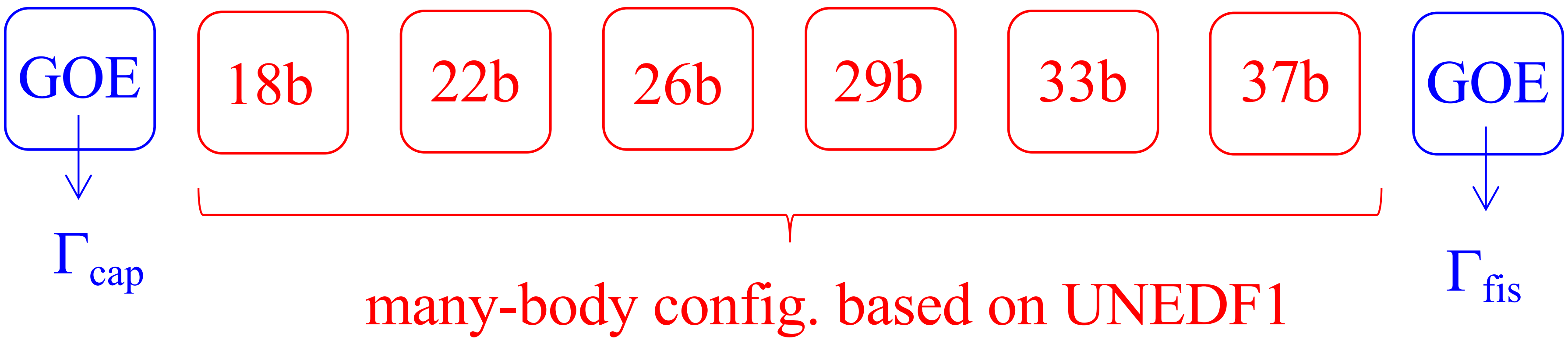
- ✓ decay dynamics: entirely determined at the saddle
- ✓ **does not depend on what will happen after the barrier**

insensitivity property



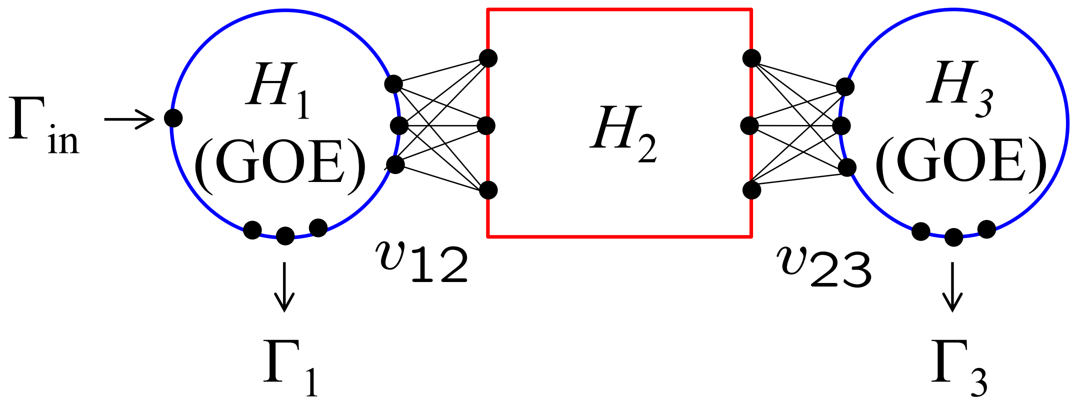
insensitive to Γ_f
(post-barrier dynamics)
→the main assumption of TST

The main assumption of TST is realized for the first time!



An analytic derivation with a Random matrix model

K.H. and G.F. Bertsch, arXiv: 2310.09537 (2023)



$$(H_k)_{ij} = \sqrt{1+\delta_{i,j}}\, v_k r_{ij}$$

$$H = \begin{pmatrix} H_1 & V_{12} & 0 \\ V_{12}^T & H_2 & V_{32}^T \\ 0 & V_{32} & H_3 \end{pmatrix}$$

$$T_{in,3} = \mathrm{Tr}\left(\Gamma_{in} G(E) \Gamma_3 G^\dagger(E)\right)$$

$$\mathcal{T}_3 \equiv 2\pi\rho_3\gamma_3 \gg 1 \rightarrow \langle (V_{32}^T G_3 \tilde{\Gamma}_3 G_3^\dagger V_{32})_{ij} \rangle = 2\pi v_{32}^2 \rho_3 \delta_{ij}$$

$$\rho_k = \frac{N_k^{1/2}}{\pi v_k} \qquad G_3 = (H_3 - i\Gamma_3/2 - E)^{-1}$$

$$\rightarrow \langle T_{\rm in,3} \rangle = \frac{\mathcal{T}_{\rm in}}{\mathcal{T}_1} \sum_i \frac{\Gamma_L \Gamma_R}{E_i^2 + (\Gamma_L + \Gamma_R)^2/4}$$

$$(H_2)_{ij} = E_i \delta_{i,j}$$

$$\Gamma_R = 2\pi v_{32}^2 \rho_3, \quad \Gamma_L = 2\pi v_{12}^2 \rho_1$$

no dependence on γ_3!

sensitivity test

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

$h_2 \to 2h_2$
$G_{pair} = 0.2$ MeV
$h_2 = 0.3$ MeV
$\to \alpha^{-1} = 1.10$

⟸

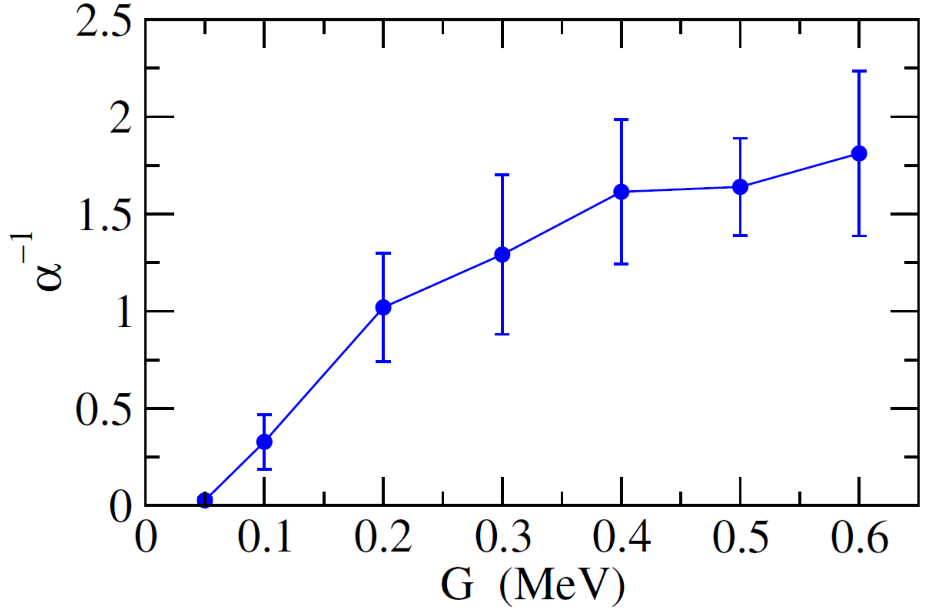
base set
$G_{pair} = 0.2$ MeV
$h_2 = 0.15$ MeV
$\to \alpha^{-1} = 0.95$

⟹

$G_{pair} \to G_{pair}/2$
$G_{pair} = 0.1$ MeV
$h_2 = 0.15$ MeV
$\to \alpha^{-1} = 0.37$

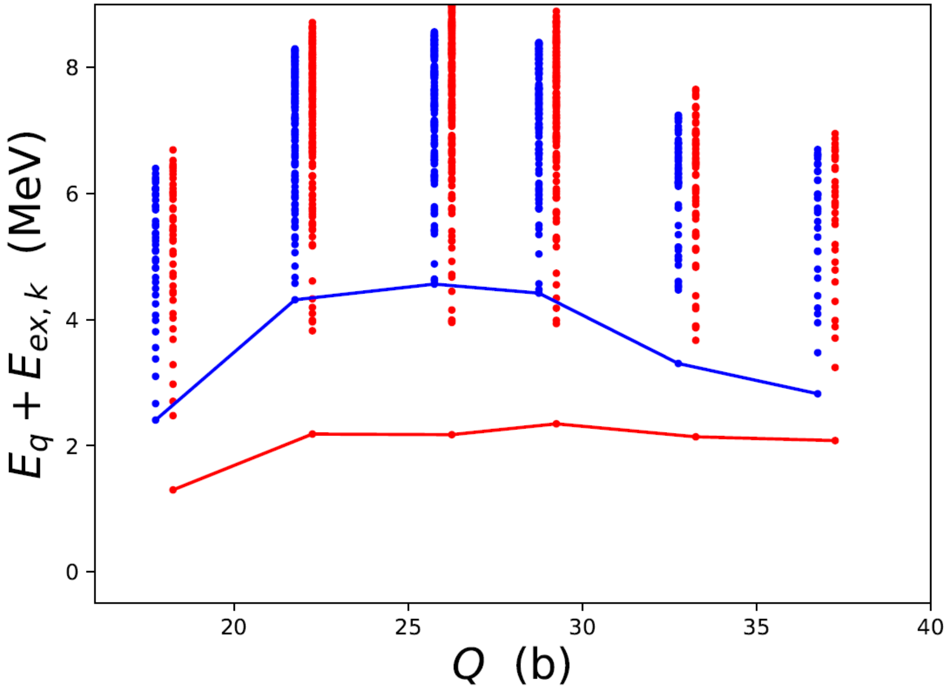
$h_2 \to 0$
$G_{pair} = 0.2$ MeV
$h_2 = 0.0$ MeV
$\to \alpha^{-1} = 0.13$

cf. $\alpha^{-1}_{exp} \sim 3.0$



- sensitive to the pairing, though less than in spontaneous fission
- h_2 effect is not negligible, but insensitive to h_2 when it is large

A comment on the Dynamical GCM



Q as a collective coordinate

$$|\Phi\rangle = \int dQ\, f(Q)|\Psi_Q\rangle$$

a (may be) better approach for dynamics:

$$|\Phi\rangle = \int dQ\, dP\, f(Q,P)|\Psi_{QP}\rangle$$

dynamical GCM

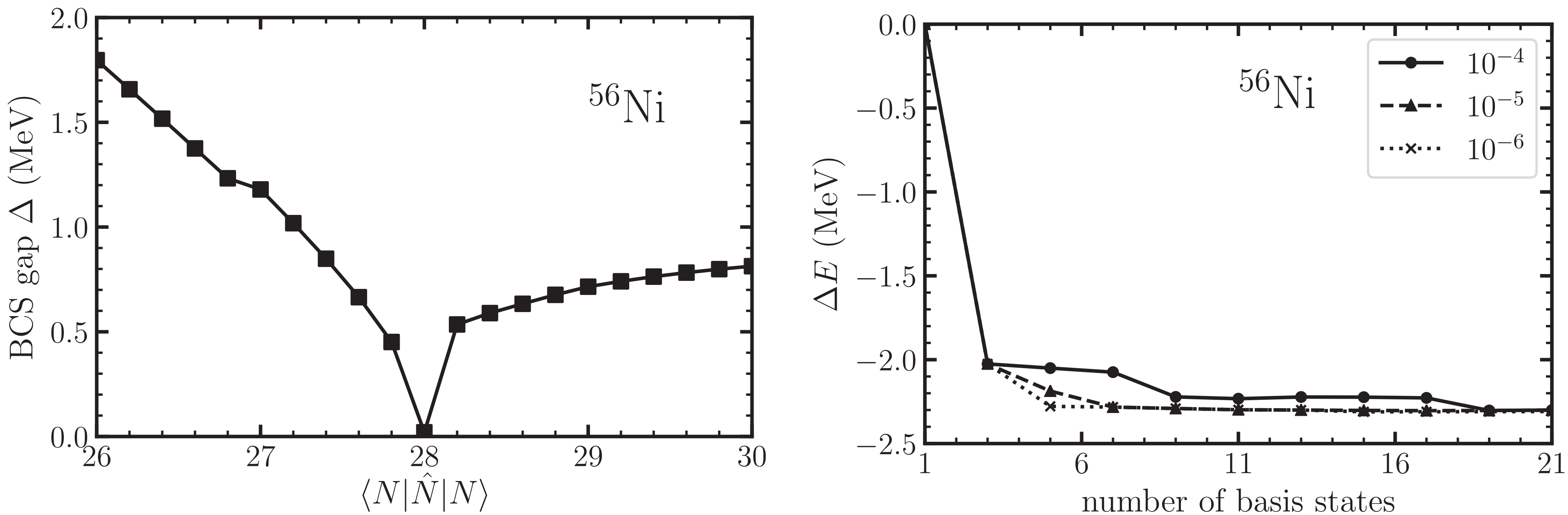
$$|\Psi_{QP}\rangle = e^{iP\hat{Q}}|\Psi_Q\rangle$$

N. Hizawa, K.H., and K. Yoshida,
PRC103, 034313 (2021)
PRC105, 064302 (2022)

A comment on the Dynamical GCM

for a particle number projection: usually $|\Phi_N\rangle = \hat{P}_N|BCS(N)\rangle$

$$|\Phi\rangle = \sum_{N'} f_{N'}\hat{P}_N|BCS(N')\rangle; \quad \langle BCS(N')|\hat{N}|BCS(N')\rangle = N'$$



N. Hizawa, K.H., and K. Yoshida, PRC103, 034313 (2021)

(See J.L. Egido, M. Borrajo, and T. Rodriguez, PRL116, 052502 (2016)
for cranking + angular momentum projection)

A comment on the Dynamical GCM

$$|\Psi_{QP}\rangle = e^{iP\hat{Q}}|\Psi_Q\rangle$$

$$|\Phi\rangle = \int dQ\,dP\,f(Q,P)|\Psi_{QP}\rangle$$

Quadrupole motion of ^{16}O with Gogny D1S

TABLE I. The GCM and the DGCM energy for the quadrupole excitations of ^{16}O with the point sets S_{25}^{GCM} and S_{25}^{DGCM}, respectively. The cut-off for the norm kernel is taken as 10^{-5}.

state	GCM (MeV)	DGCM (MeV)
1	−129.682	−129.765
2	−107.993	−108.140
3	−92.260	−104.475
4	−77.911	−87.019
5	−64.097	−83.059

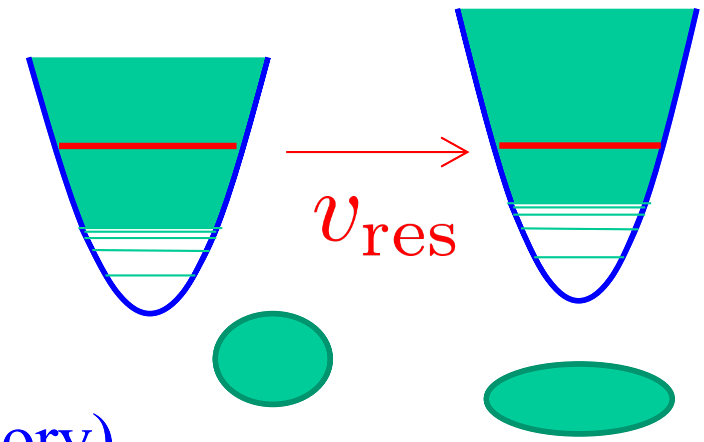
N. Hizawa, K.H., and K. Yoshida, PRC105, 064302 (2022)

Summary

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

✓ neutron seniority-zero configurations only

- insensitivity property (transition state theory)
- an importance of the pairing interaction

Future perspectives:

✓ seniority non-zero config. →pn res. interaction

a test with a schematic model:
K. Uzawa and K. Hagino, PRC108 ('23) 024319

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

✓ role of conjugate momentum (Dynamical GCM)?