Microscopic description of induced fission based on the generator coordinate method

"Fundamentals in density functional theory (DFT2022)"
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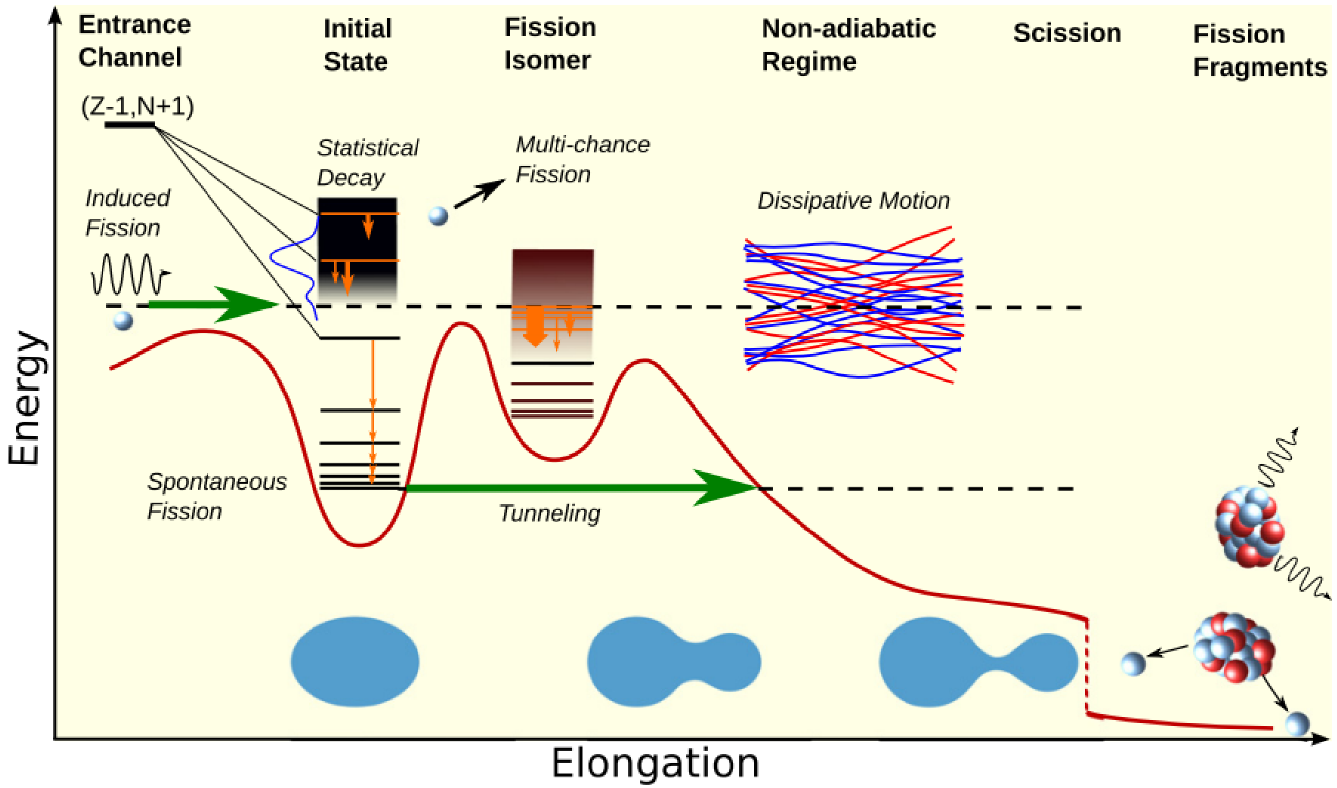
Introduction: Induced Fission



M. Bender et al., J. Phys. G: Nucl. Part. Phys. 47 113002 (2020) .

Phenomenological model: The statistical model, Transport theoretical approach …

Microscopic approach: Density Functional Theory or Generator Coordinate Method

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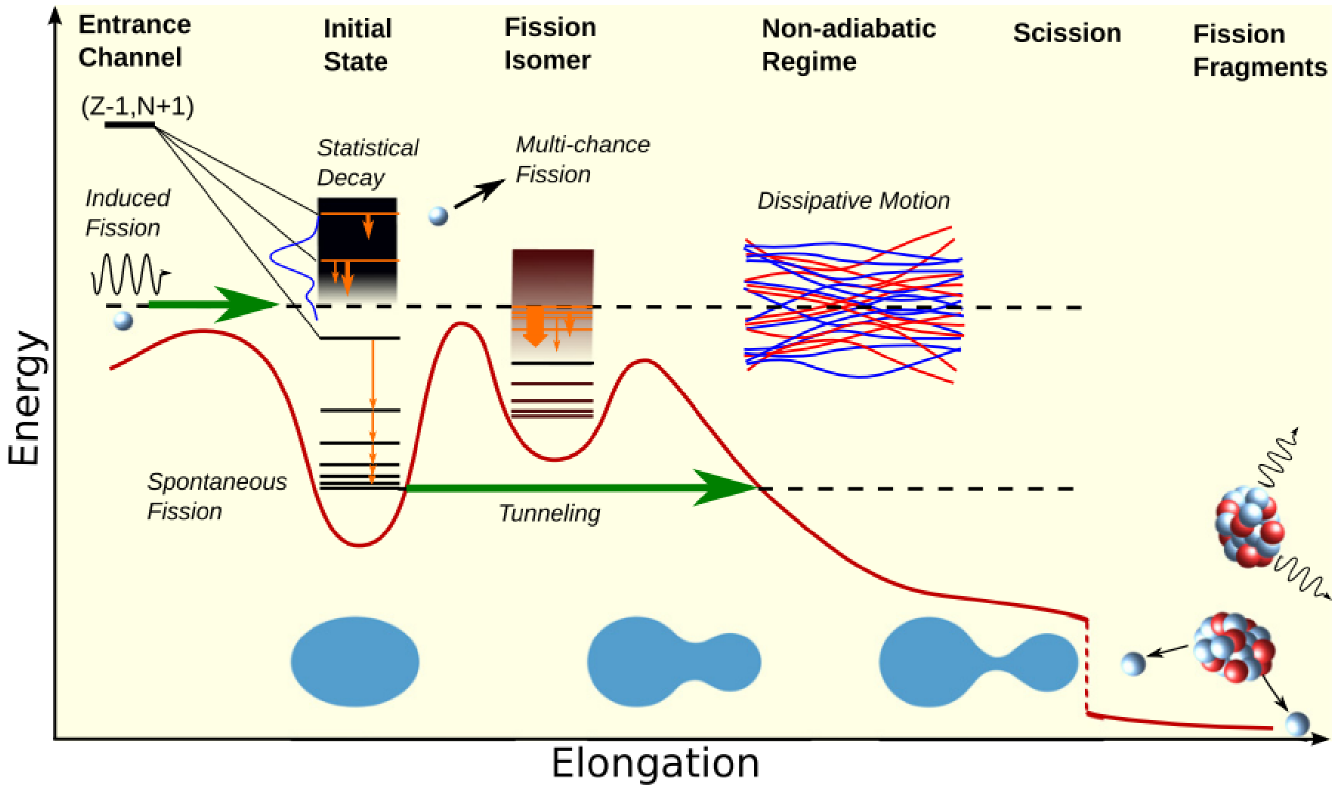

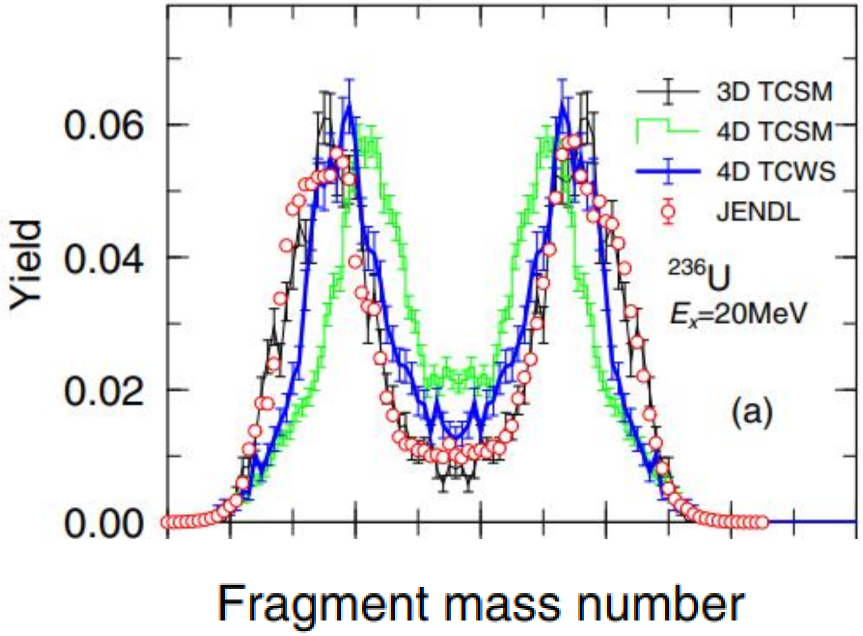

C. Ishizuka et al., Phys. Rev. C 96, 064616 (2017).

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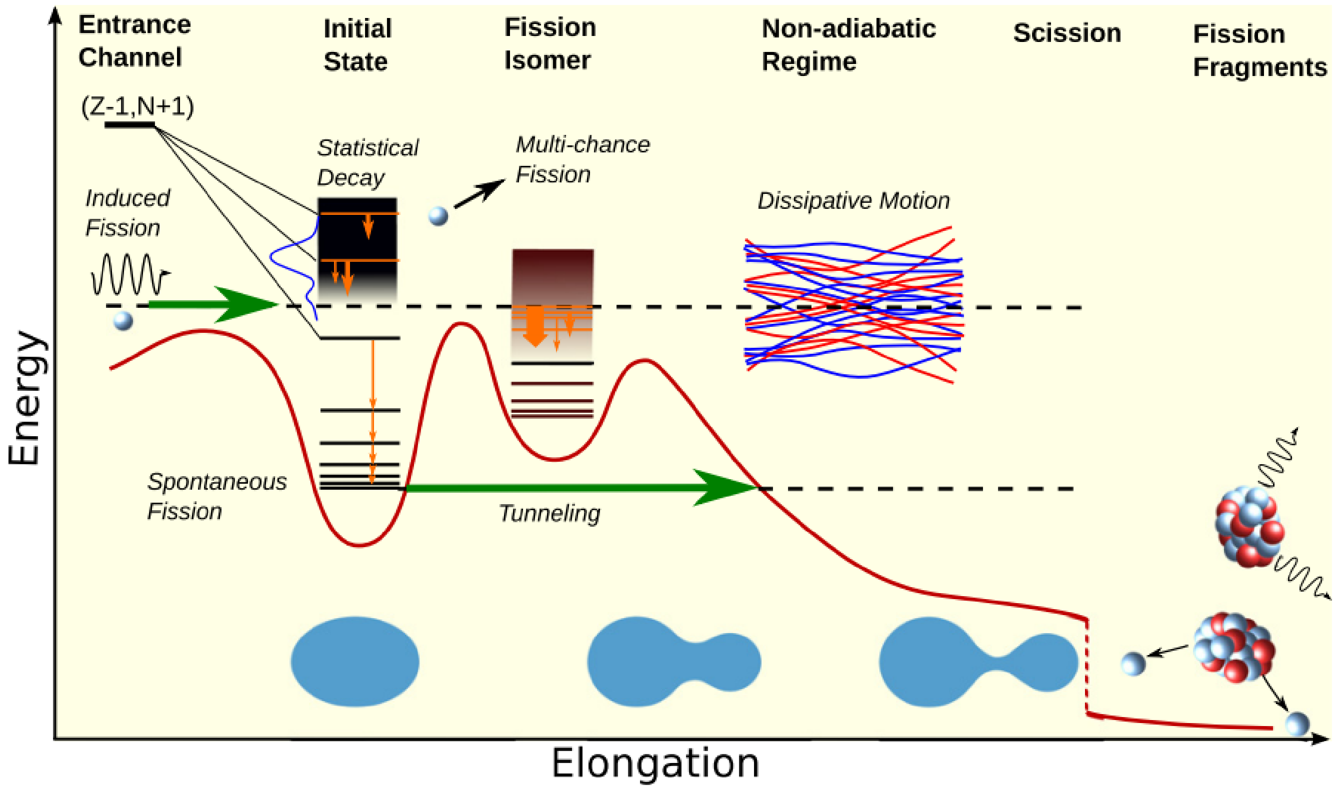
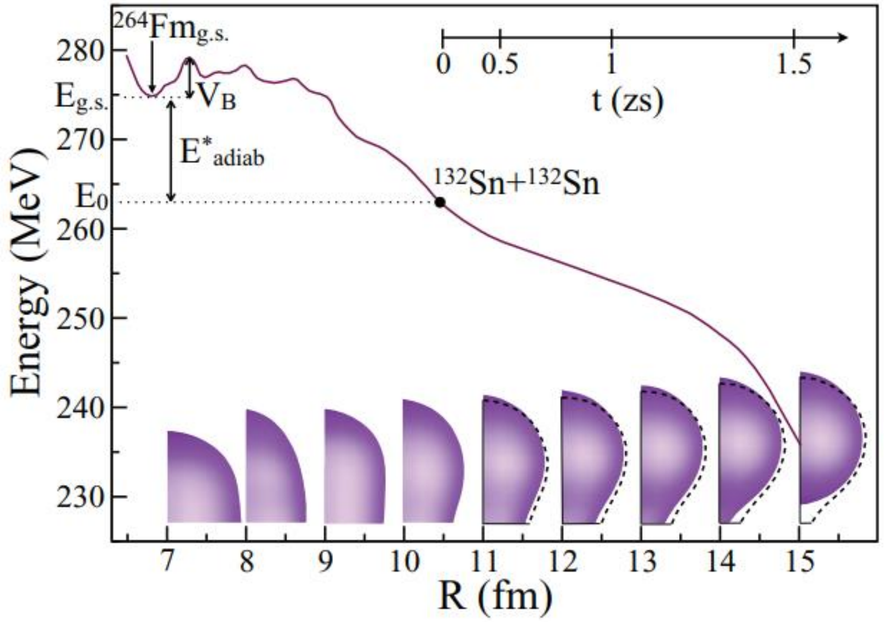




C. Simenel and A. S. Umar Phys. Rev. C 89, 031601(R) (2014).

Phenomenological model: The statistical model, Transport theoretical approach …

Microscopic approach: Density Functional Theory or Generator Coordinate Method

Motivation

Understanding of microscopic mechanism of fission
&
Unified theory for the various fission phenomena
(induced fission, cluster decay, and so on)

↓

Approach based on GCM and CI(configuration interaction)

Advantages

✓Treat spontaneous and induced fission in the same framework

✓Combination with reaction theories (K-matrix theory, R-matrix theory...)

Extension of the GCM ansatz

In GCM, we superpose mean-field wavefunction $|\Phi(Q)\rangle$

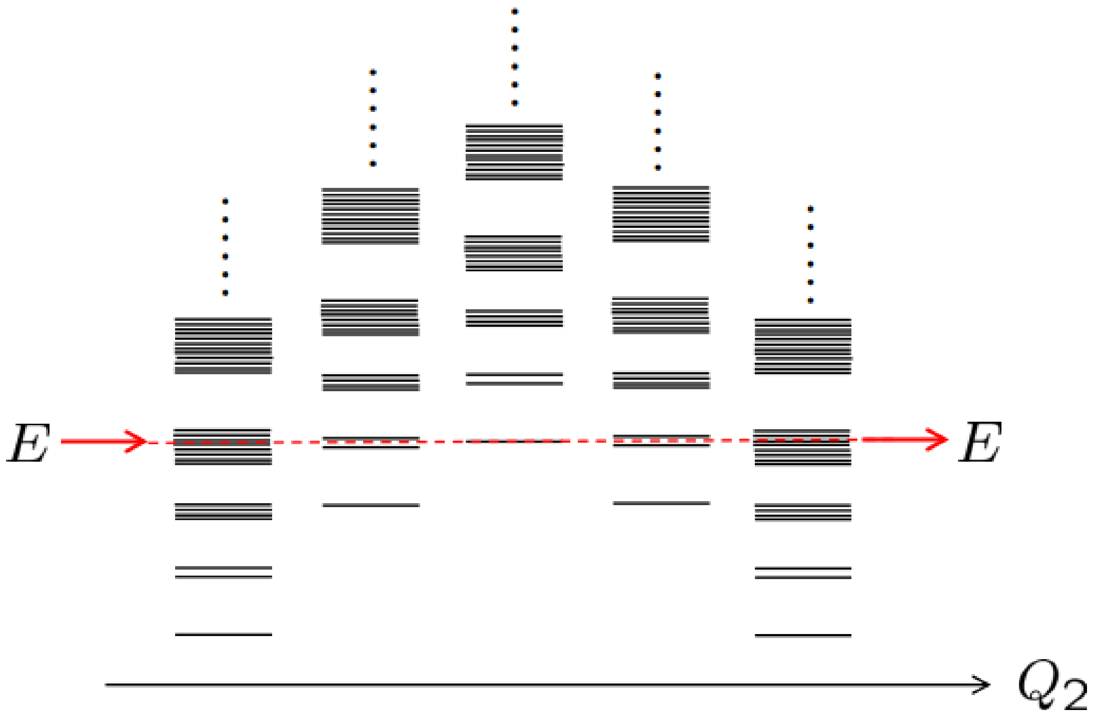
$$|\Psi\rangle = \int dQ\, f(Q)|\Phi(Q)\rangle$$

We extend GCM ansatz and superpose

excited states $|\Phi_i(Q)\rangle = \prod_{ph} a_p^\dagger a_h |\Phi(Q)\rangle$

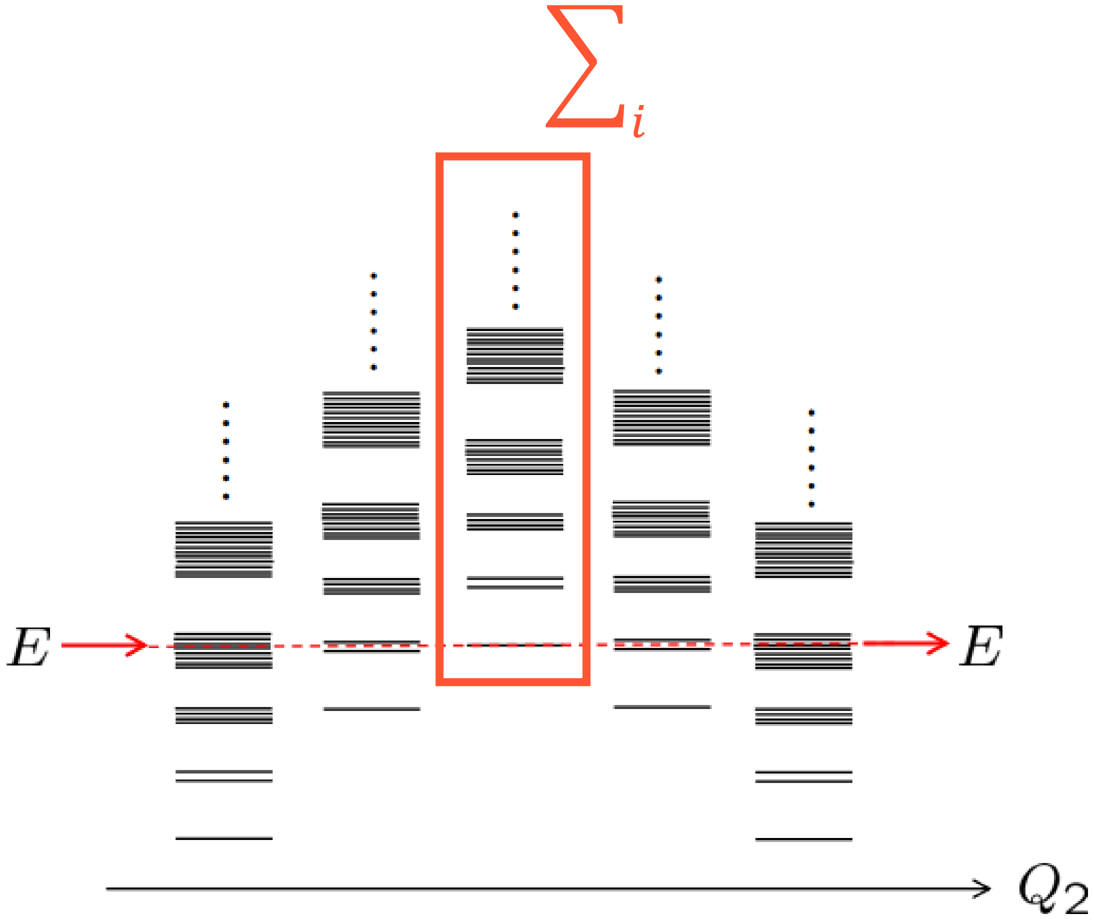
$$|\Psi\rangle = \underline{\sum_i} \int dQ\, f_i(Q)|\Phi_i(Q)\rangle$$

excited states *i* at each Q



1. Superpose mean field wave function (GCM ansatz)

$$|\Psi\rangle = \sum_i \int dQ\, f_i(Q) |\Phi_i(Q)\rangle$$



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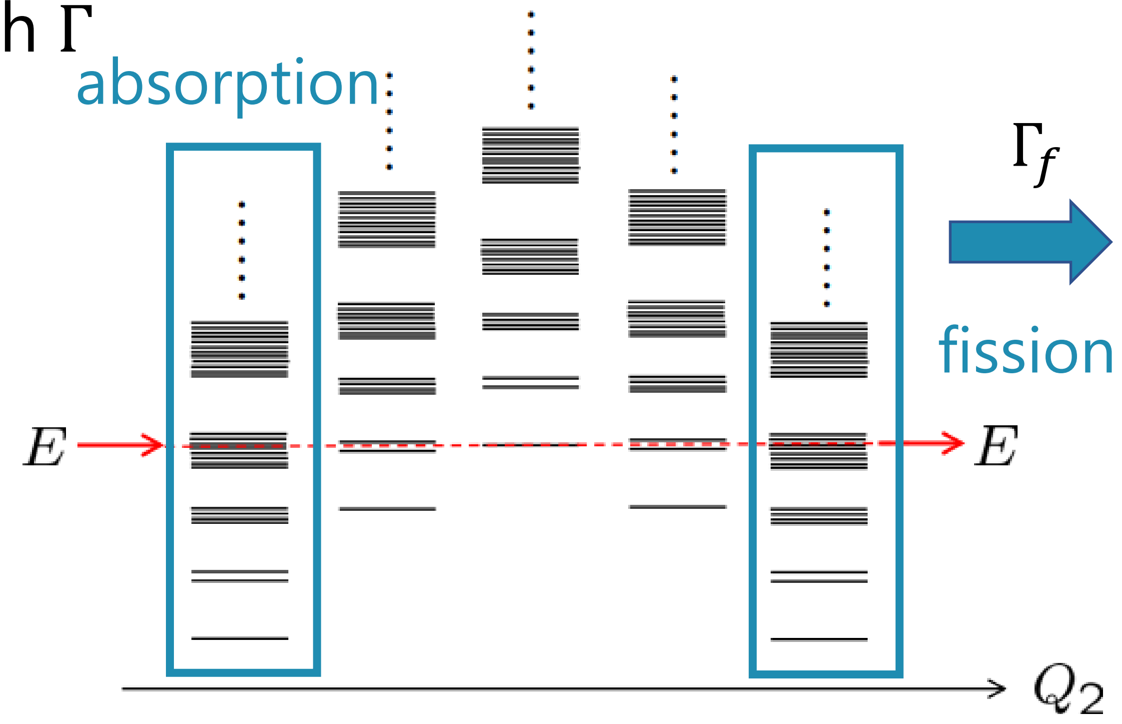
$$|\Psi\rangle = \sum_i \int dQ f_i(Q)|\Phi_i(Q)\rangle$$

2. Calculate GCM kernel and decay width Γ

$$N(Q,Q')_{i,j} = \langle\Phi_i(Q)|\Phi_j(Q')\rangle$$

$$H(Q,Q')_{i,j} = \langle\Phi_i(Q)|\hat{H}|\Phi_j(Q')\rangle$$

$$(\Gamma_j)_{kk'} = \gamma_j N_{kj} N_{k'j}$$



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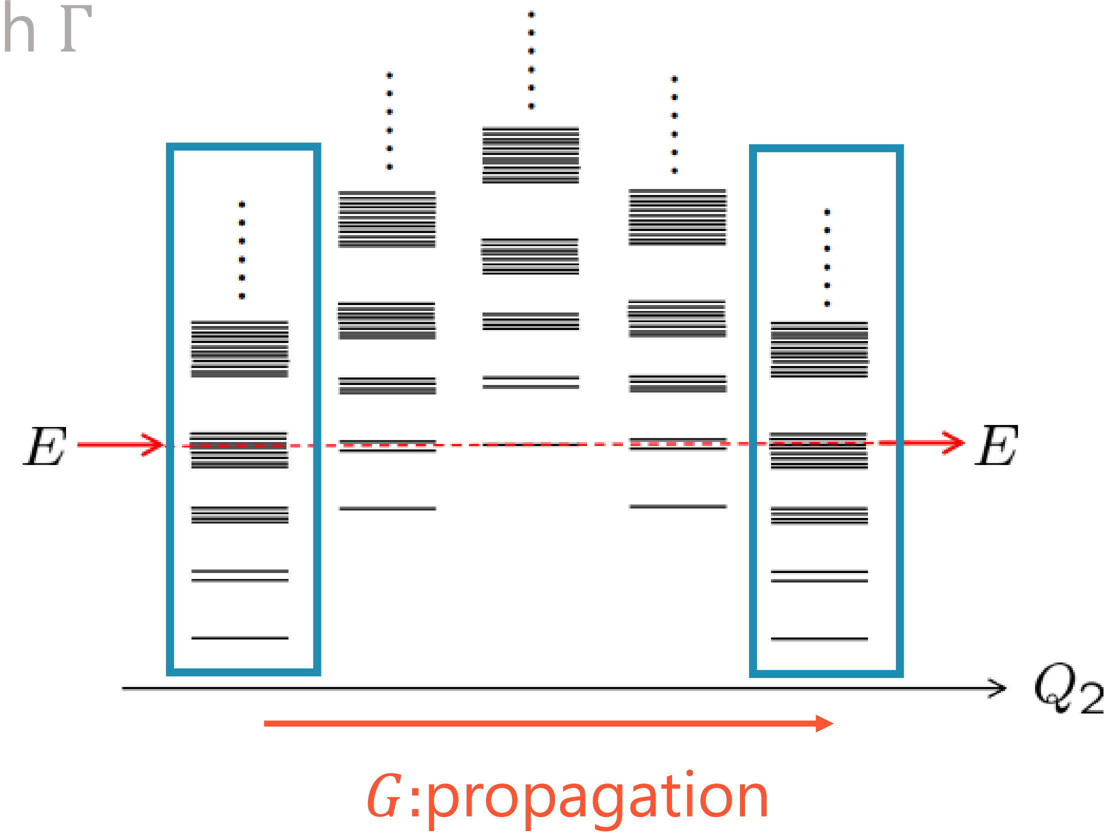
3. Calculate Green's function

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



4. Obtain transmission coefficient $T_{ab}(E)$ using the Datta formula

$$T_{ab}(E) = \mathrm{Tr}(\Gamma_a G(E) \Gamma_b G^\dagger(E))$$

$$T_{ab} \equiv |S_{a,b}|^2$$

Transition probability from channel a to b

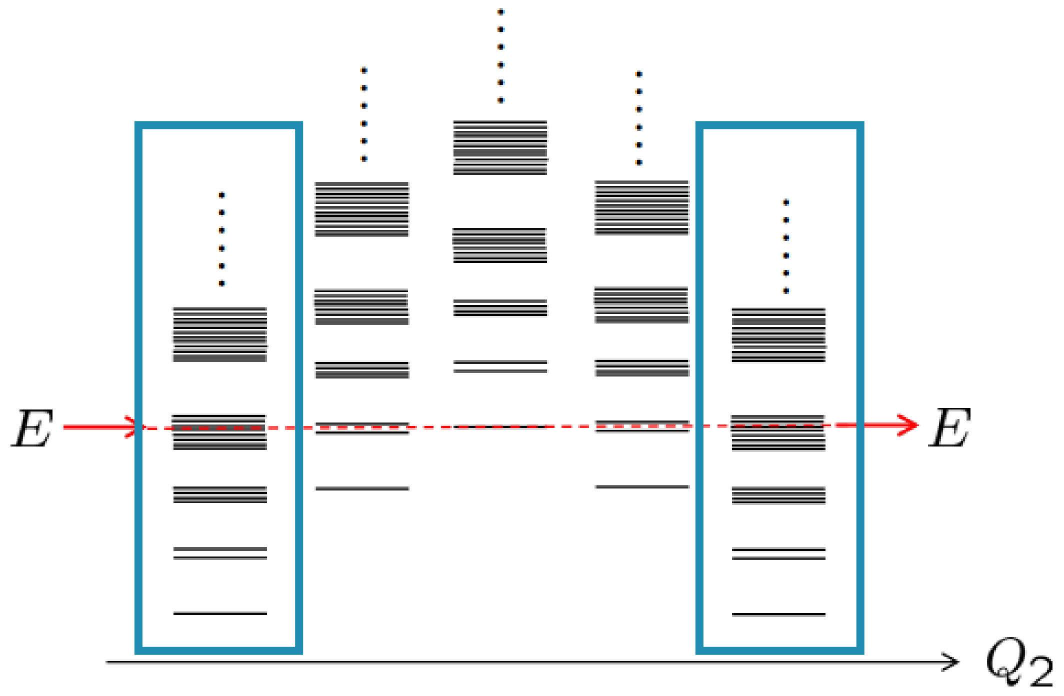
Neutron absorption (channel a)

↓

Formation of the compound nucleus

↓

Fission or Capture (channel b)



Γ_a:input channel Γ_b:output channel

G:propagation

Hamiltonian and model space

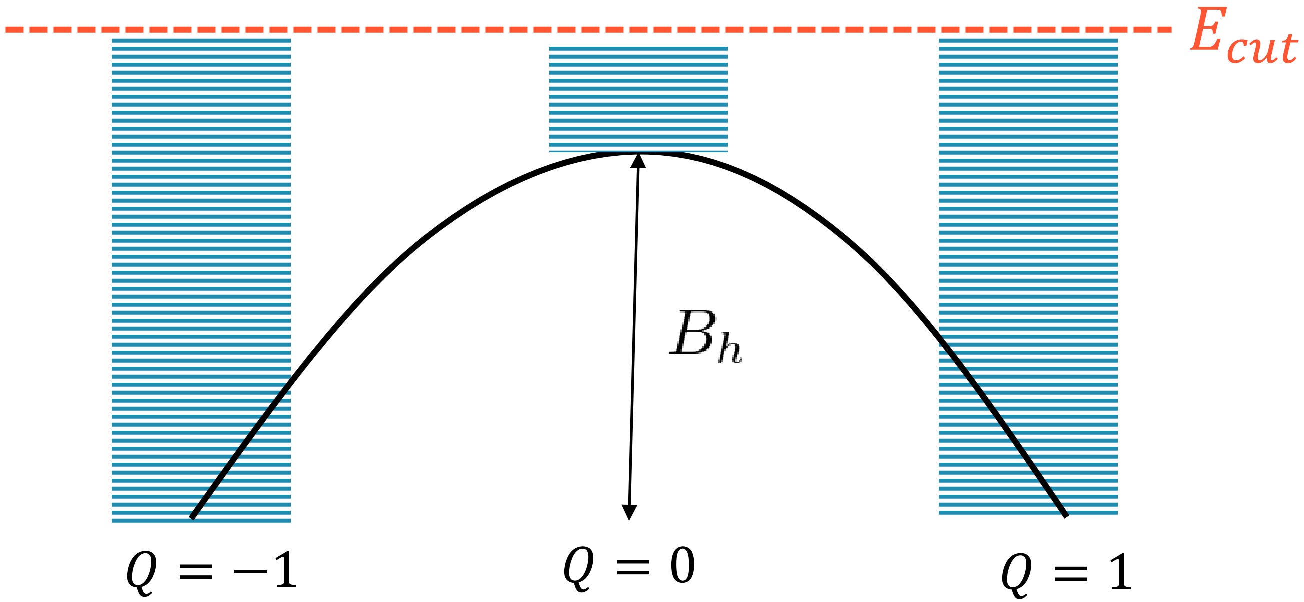
$$H = V(Q) + H_{ph} + H_{ran} + H_{pair}$$

Fission barrier

$$V(Q) = \begin{cases} 0 & (Q = -1, 1) \\ B_h (> 0) & (Q = 0) \end{cases}$$

Particle-hole excitation

$$H_{ph} = d \sum_{\alpha : n_\alpha > 0} a_\alpha^\dagger a_\alpha + d \sum_{\alpha : n_\alpha \leq 0} a_\alpha a_\alpha^\dagger$$



Hamiltonian and model space

$$H = V(Q) + H_{ph} + H_{ran} + H_{pair}$$

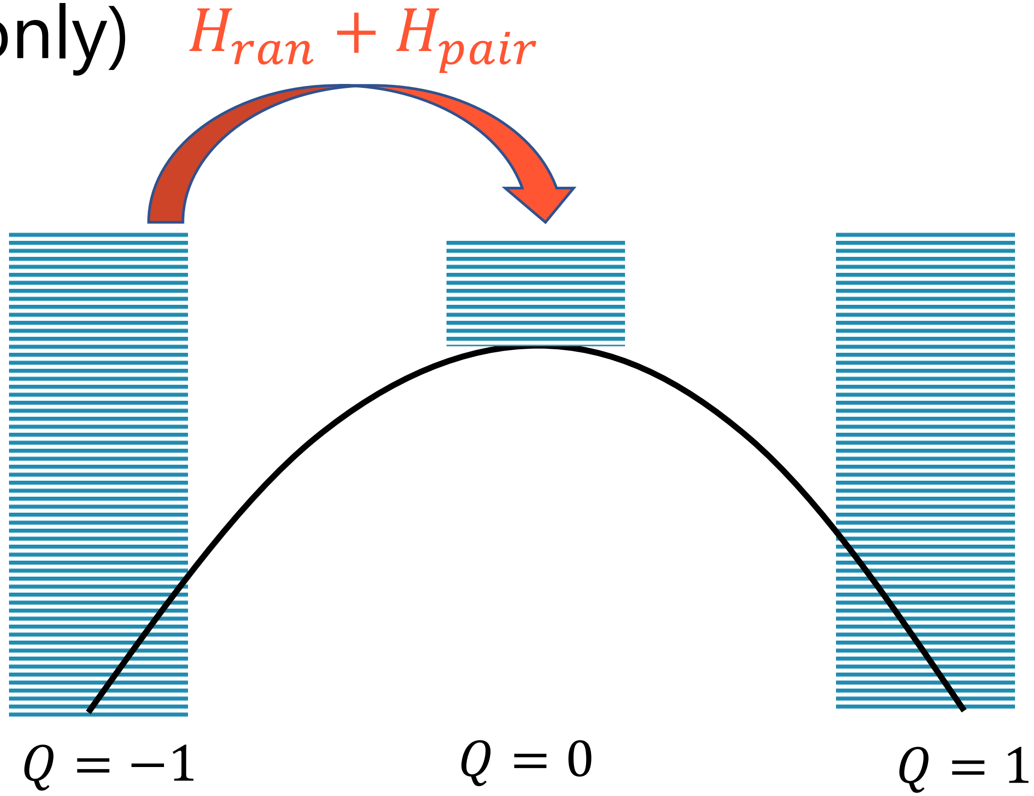
Random interaction (proton-neutron only)

$$H_{ran} = v_{np} \sum r a^{\dagger}_{\alpha 1} a^{\dagger}_{\alpha 2} a_{\alpha 3} a_{\alpha 4}$$

random number

Pairing interaction

$$H_{pair} = -G\mathrm{P}^{\dagger}\mathrm{P} \quad (\mathrm{P} = \sum_{\nu} a_{\bar{\nu}} a_{\nu})$$



Neutron width :

$$(\Gamma_n)_{kk'} = \gamma_n \Sigma_{i:Q=-1} N_{ik} N_{ik'}$$

Fission width:

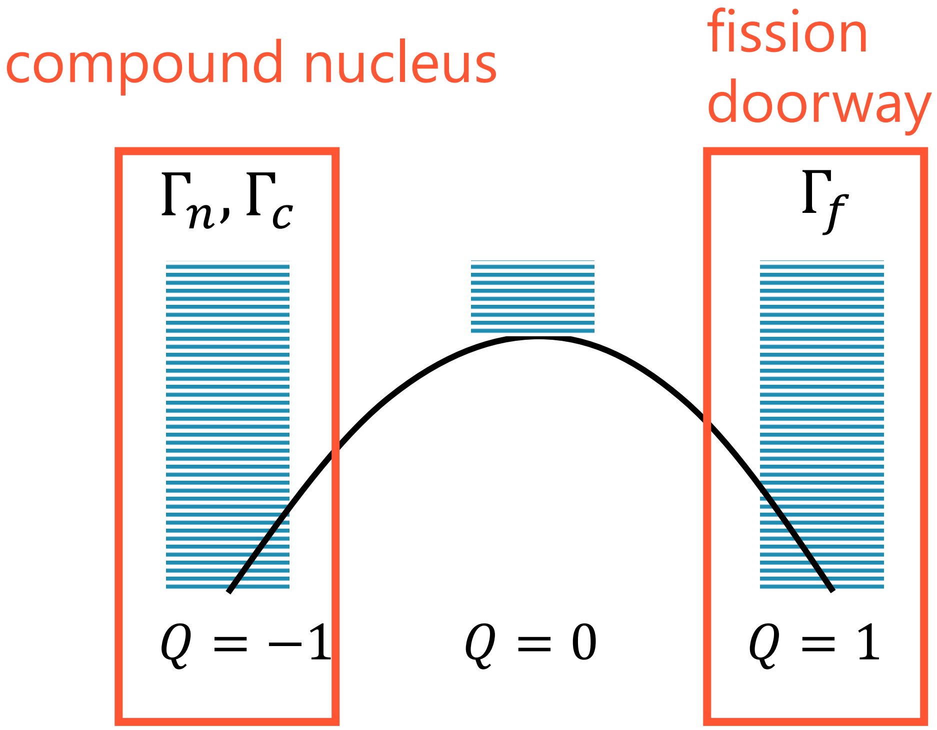
$$(\Gamma_f)_{kk'} = \gamma_f \Sigma_{i:Q=1} N_{ik} N_{ik'}$$

Capture width:

$$(\Gamma_c)_{kk'} = \gamma_c \Sigma_{i:Q=-1} N_{ik} N_{ik'}$$

$Q = -1$: compound nucleus $\Rightarrow \Gamma_n,\ \Gamma_c$

$Q = 1$: fission doorway states $\Rightarrow \Gamma_f$



Overlap kernel

GCM basis $|Q\rangle$ is not orthogonal basis

Overlap kernel $N(Q, Q')$ represents the size of non-orthogonality

$$\langle Q|Q'\rangle = N(Q, Q') = \exp(-\lambda(Q - Q')^2)$$

Applying generalized Wick's theorem to the overlap between excited states

Result

Result 1. Effects of the pairing on the induced fission

In low energy induced fission,

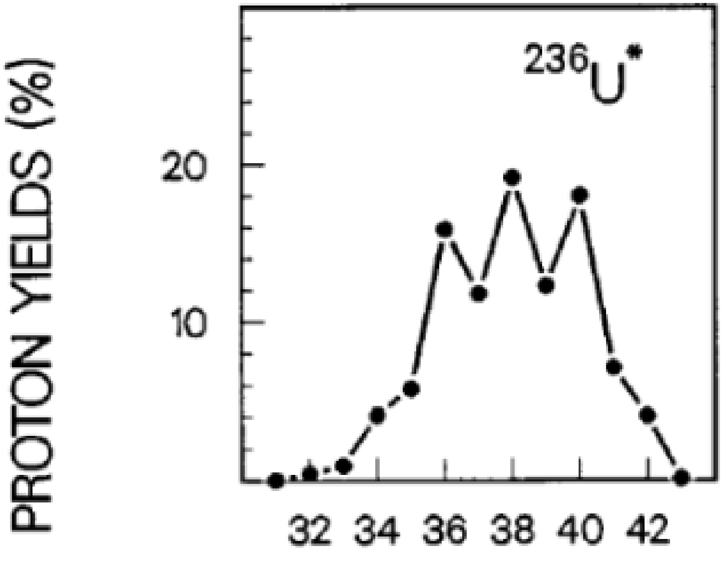
pairing does not completely vanish

Result 2. Effects of the ono-orthogonal basis

DFT generates non-orthogonal GCM basis

(c.f. R-matrix approach by Lynn)

Even-odd effects



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J. P. Bocquet and R. Brissot, Nucl. Phys. A 502, 213 (1989).

Result 1. Effects of Pairing

Calculate $T_{n,f}(E)$ with different G

$$H_{pair} = -G\mathrm{P}^{\dagger}\mathrm{P}$$

For simplicity, we use orthogonal basis here

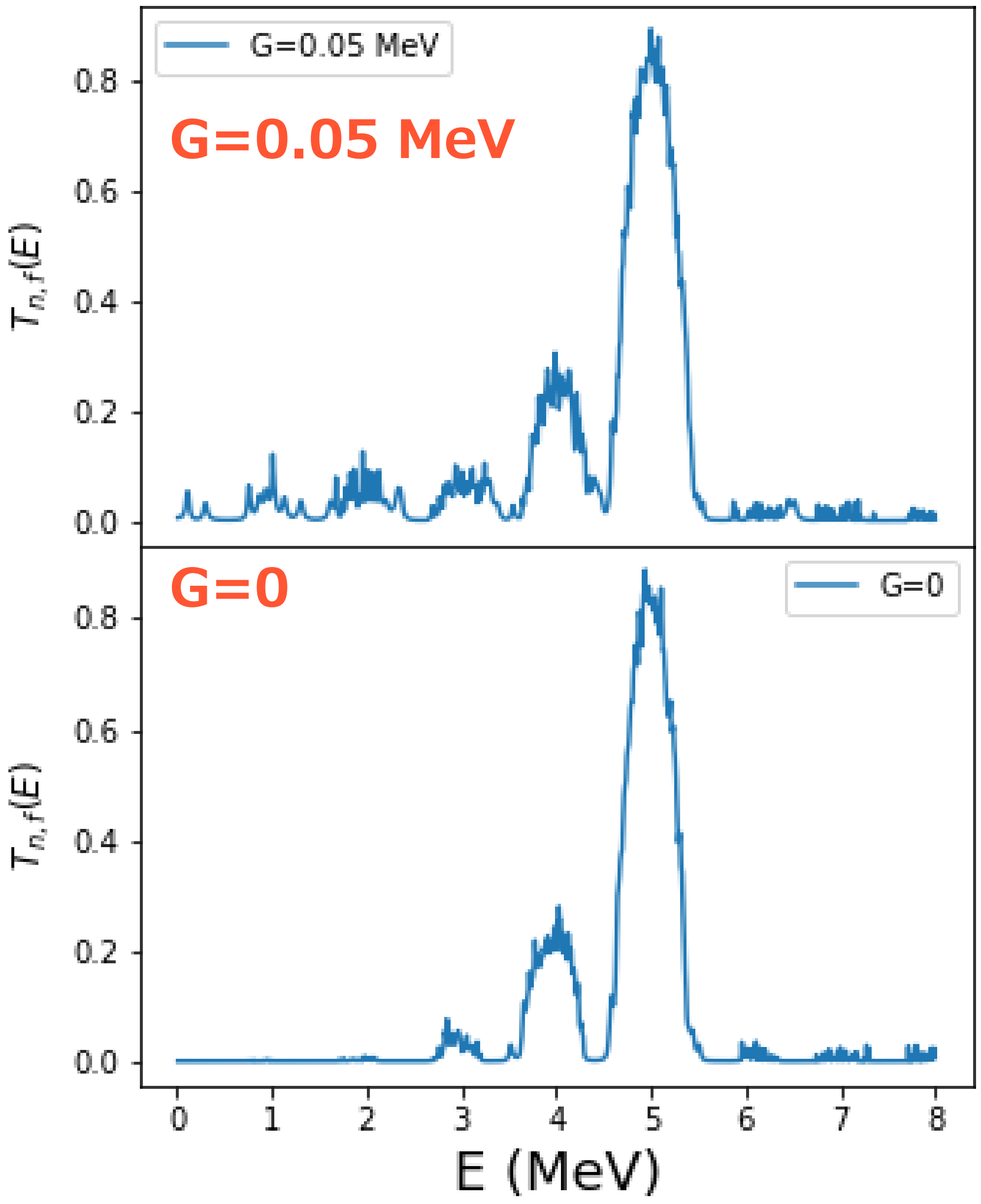
Pairing strength : $0 \leq G \leq 0.05$ MeV

Random interaction : $v_{np} = 0.03$ MeV

Barrier height : $B_h = 4$ MeV

Energy scale : $d = 1$ MeV

Decay width : $\gamma_n = 0.001$ MeV, $\gamma_f = 0.1$ MeV



Energy averaged transmission coefficient $\langle T_{n,f} \rangle$

$$\langle T_{n,f} \rangle = \frac{1}{1\mathrm{MeV}} \int_{E^*-0.5}^{E^*+0.5} T(E)\, dE$$

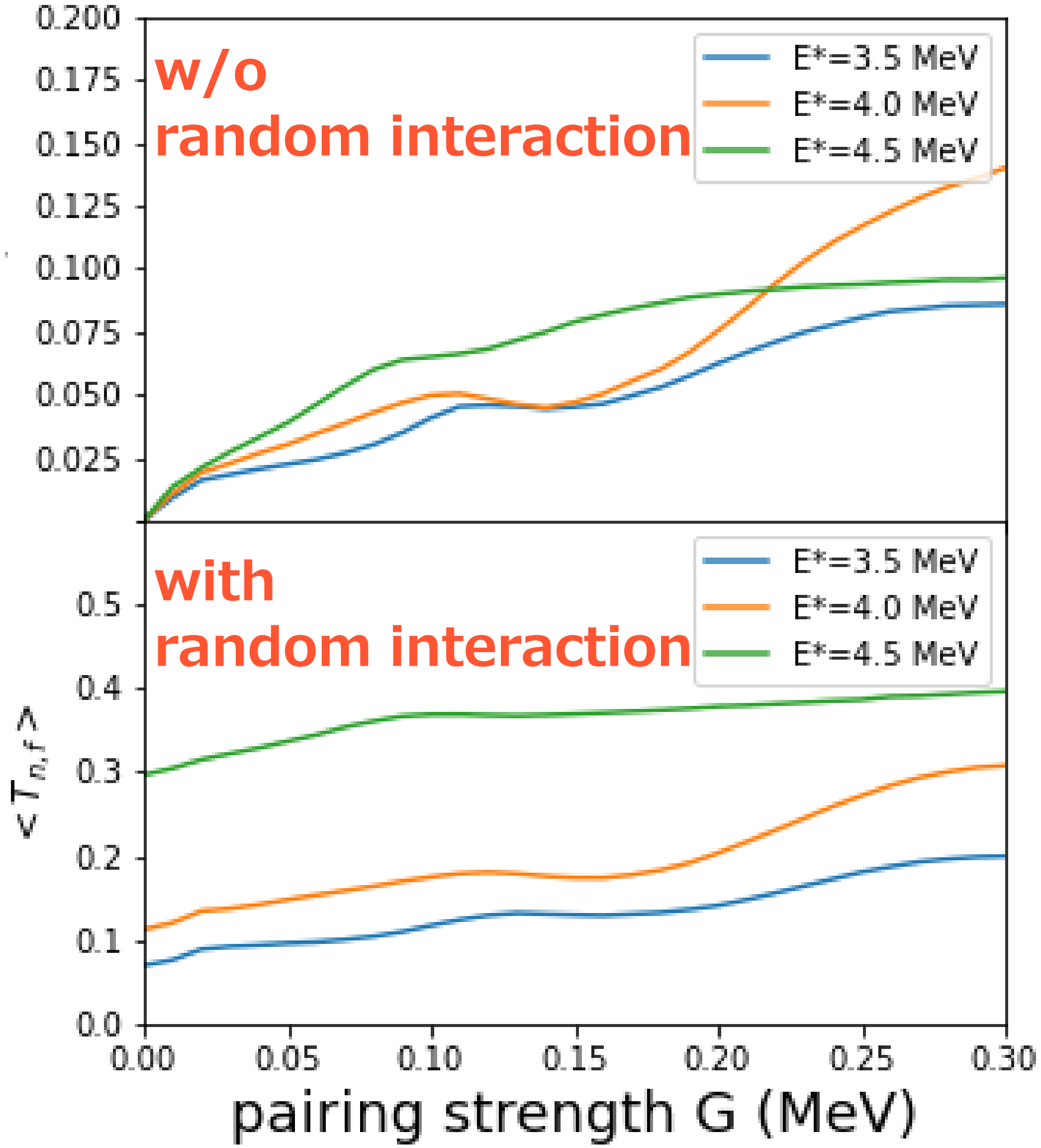
・w/o random interaction:

⇒Pairing increase fission probability

・ w random interaction (realistic):

⇒Pairing competes with random interaction

$\langle T_{n,f} \rangle$ vs G



Result 2. Effects of the non-orthogonality

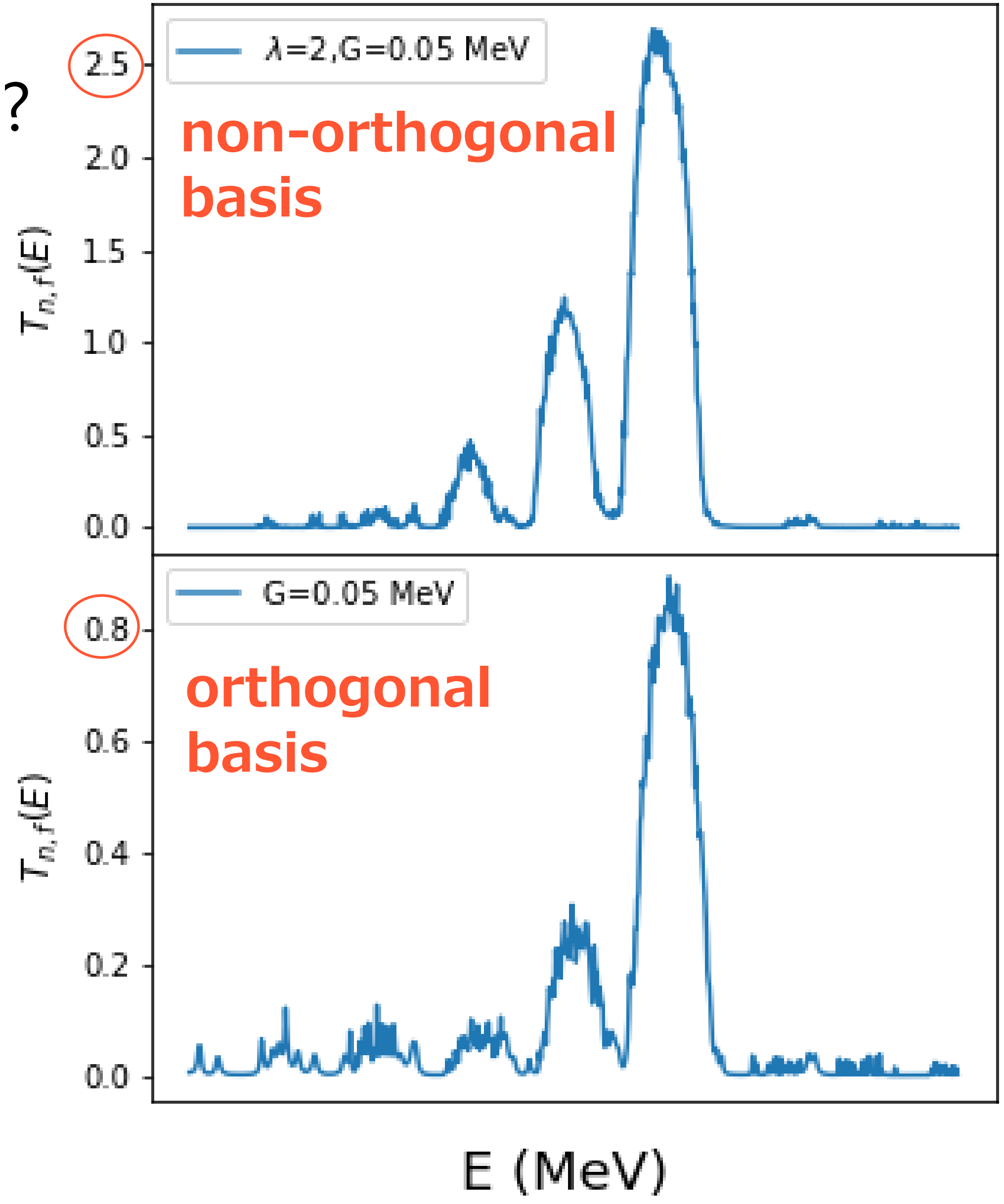
Non-orthogonality enhances fission probability ?

$$\langle Q|Q'\rangle = N(Q,Q') = \exp(-\lambda(Q-Q')^2)$$

Pairing strength: $G = 0.05$ MeV

Random interaction : $v_{np} = 0.03$ MeV

Barrier height : $B_h = 4$ MeV



Relation between $\langle T_{n,f} \rangle$ and barrier height B_h

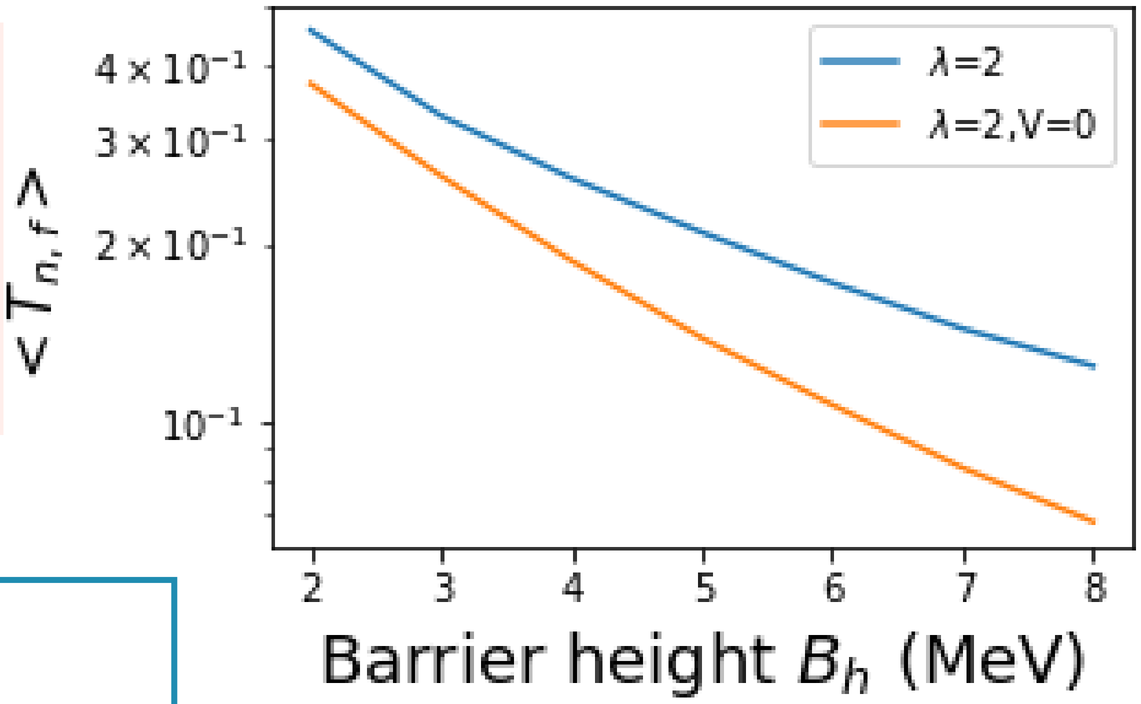
Overlap parameter $\lambda = 2$

- $\langle T_{n,f} \rangle$ decrease exponentially as B_h
- $\langle T_{n,f} \rangle \neq 0$ even if H_{ran}=0 and $H_{pair} = 0$

Transition between compound states (Q=-1) and the fission doorway (Q=1) by the overlap

w residual interaction

w/o residual interaction



Summary

Conclusion

- Apply GCM+CI approach to the barrier transmission problem
- Pairing increases fission probability and competes random interaction
- Non-orthogonality of the basis increases the transmission coefficient

Future perspectives

- Compare with the B-W theory and justify the transition states hypothesis
- Realistic calculation with the basis obtained using DFT