# 生成座標法のバリア透過過程への適用

「理論と実験で拓く中性子過剰核の核分裂」@理研RIBF 2023/2/17

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## **Introduction: Induced Fission**

Phenomenological model: The statistical model, Transport theoretical approach ... Microscopic approach: Density Functional Theory, Generator Coordinate Method ...



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

## **Introduction: Induced Fission**

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

#### **Motivation**

- fast neutron ( $E_n > 1 \text{ MeV}$ )
- barrier top fission ( $E^* \sim 6 \text{ MeV}$ )
- neutron-rich nuclei
- spontaneous fission ( $E^* = 0$ )



# Unified theory for the barrier transmission problem & Microscopic understanding of nuclear fission Configuration Interaction (CI) approach based on GCM

## **Extension of the GCM ansatz**

Superpose mean-field wavefunction  $|\Phi(Q)\rangle$ in Generator coordinate method (GCM)

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

Extend usual GCM ansatz and superpose p-h excited states

$$\Phi_i(Q)\rangle = a_p^{\dagger}a_h |\Phi(Q)\rangle, \ a_{p'}^{\dagger}a_p^{\dagger}a_{h'}a_h |\Phi(Q)\rangle \dots$$

#### p-h excited states



1. Superpose mean field wave function (GCM ansatz)

$$|\Psi\rangle = \sum_{i} \int dQ f_{i}(Q) |\Phi_{i}(Q)\rangle$$

p-h excited states



1. Superpose mean field wave function (GCM ansatz)

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

#### 2. Calculate GCM kernel and decay width $\Gamma$

$$N(Q,Q')_{i,j} = \langle \Phi_i(Q) | \Phi_j(Q') \rangle$$
$$H(Q,Q')_{i,j} = \langle \Phi_i(Q) | \hat{H} | \Phi_j(Q') \rangle$$
$$(\Gamma_j)_{kk'} = \gamma_j (N^{\frac{1}{2}})_{jk} (N^{\frac{1}{2}})_{jk'}$$



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3. Calculate Green's function

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



G: propagation

4. Transmission coefficient  $T_{ab}(E)$  obtained by the Datta formula

$$|S_{a,b}(E)|^2 \equiv T_{a,b}(E) = \operatorname{Tr}(\Gamma_a G(E) \Gamma_b G^{\dagger}(E))$$





## **Hamiltonian and model space**

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

✓ Deformation Energy

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

 $\checkmark$  Particle-Hole excitation

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



#### **Hamiltonian and model space**

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

 $H_{ran} + H_{pair}$ 



## **Overlap kernel**

Mean-field w.f.  $|\Phi_i(Q)\rangle$  is not orthogonal in general

Overlap kernel  $N_{i,j}(Q,Q')$  express size of non-orthogonality

$$N_{i,j}(Q,Q') = \langle \Phi_i(Q) | \Phi_j(Q') \rangle \simeq \exp(-\lambda(Q-Q')^2) \delta_{i,j}$$

We assume the form of Gaussian Overlap Approximation ( $\lambda = 1$ ) and  $a_{\mu}(Q) \simeq a_{\mu}(Q')$ 

Neutron width :  

$$\left( \Gamma_n \right)_{kk'} = \gamma_n \Sigma_{i:Q=-1} \left( N^{1/2} \right)_{ik} \left( N^{1/2} \right)_{ik'}$$
Capture width:  

$$\left( \Gamma_{cap} \right)_{kk'} = \gamma_{cap} \Sigma_{i:Q=-1} \left( N^{1/2} \right)_{ik} \left( N^{1/2} \right)_{ik'}$$
Fission width:  

$$\left( \Gamma_{fis} \right)_{kk'} = \gamma_{fis} \Sigma_{i:Q=1} \left( N^{1/2} \right)_{ik} \left( N^{1/2} \right)_{ik'}$$

Q = -1: compound nucleus  $\Rightarrow \Gamma_n$ ,  $\Gamma_{cap}$ 

Q = 1 : fission doorway states  $\Rightarrow \Gamma_{fis}$ 

#### Datta's formula

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



#### **Diabatic interaction**

$$\langle \Phi_i(Q) | \sum \epsilon_\mu a_\mu^\dagger a_\mu | \Phi_j(Q') \rangle = - [h_2] \langle \Phi_i(Q) | \Phi_j(Q') \rangle (Q - Q')^2$$
  
size of diabatic int.

Diabatic interaction connects diabatic configurations (as the name suggests)

Adiabatic configurations are connected by the pairing



Q:deformation



Result 1. Effects of the pairing on the induced fission

Result 2. Role of the diabatic interaction with non-orthogonality

Result 3. Comparison with the Bohr-Wheeler theory



## **Result 1: Effects of the pairing**

$$T_{n,fis}(E)$$

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

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

Apply orthogonal basis for simplicity

Pairing plays a role mainly in the sub-barrier region



parameters: $(v_{np} = 0.03d, B_h = 4d, \gamma_n = 0.001d, \gamma_f = 0.1d)$ 

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

$$\langle T_{n,fis}(E) \rangle = \frac{1}{\Delta E} \int_{E-\Delta E/2}^{E+\Delta E/2} dE' T_{n,fis}(E')$$

- ✓ Pairing enhances transmission probabilities mainly in the sub-barrier region
- ✓ Random interaction smears out coherent pairing interaction



#### **Result 2: Role of the diabatic interaction** $T_{n,fis}(E)$ and $C_{n,fis}(E)$

Non-orthogonality leads to diabatic interaction

$$\frac{\langle nQ|v_{db}|nQ'\rangle}{\langle nQ|nQ'\rangle} = \frac{E(nQ) + E(nQ')}{2} - h_2(Q-Q')^2$$

Define cumulative sum of  $T_{n,fis}(E)$ 

$$C_{n,fis}(E) = \int_{0}^{E} T_{n,fis}(E')dE' .$$

Diabatic transition increases barrier transmission



 $(v_{np} = 0.03d, B_h = 4d, G = 0, \lambda = 1)$ 

Relation between  $\langle T_{n,fis} \rangle$  (*E*) and excitation energy *E* 

$$\cdot \left\langle T_{n,fis} \right\rangle$$
 increases as *E* with finite  $v_{np}$ 

• 
$$\left\langle T_{n,fis} \right\rangle$$
 is insensitive to *E* if  $v_{np} = 0$ 

✓ Transmission by  $h_2$  is insensitive to *E* 

✓ Diabatic transition becomes important relatively in low-energy induced fission



 $(v_{np} = 0.03d, B_h = 4d, G = 0, \lambda = 1)$ 

## **Results 3: Transition state theory**

$$\Gamma_{\rm BW} = \frac{1}{2\pi\rho} \sum_c T_c$$

- $\Gamma_{BW}$ : fission decay width
- $\rho$ : level density of the compound nuclei
- $T_c$ : transmission probability via transition state
- B-W formula assumes
- ➤ mother nucleus is in statistical equilibrium
- transition states determine the fission dynamics
  Justify the assumption microscopic viewpoint



N. Bohr and A. Wheeler, Phys. Rev. 56 426 (1939). Focus on the capture-fission branching ratio  $\alpha^{-1}$ ,

$$\alpha^{-1} = \frac{\int dE' T_{n,fis}(E')}{\int dE' T_{n,cap}(E')}$$

$$\alpha^{-1}$$
 vs  $\gamma_{fis}$ (fission width)



 $(v_{np} = 0.03d, B_h = 4d, G = 0, \lambda = 1)$ 

✓ 
$$\alpha^{-1}$$
 is constant in the BW theory  
✓  $\alpha^{-1}$  increases as  $\gamma_f$  in Q=(-1, 0, 1) case

(not consistent with BW theory)

✓ 7-Q block model reproduces BW theory's results
 ⇒justify the transition state hypothesis microscopically



#### Conclusion

- Apply GCM+CI approach to the barrier transmission problem
- Pairing increases fission probability and competes random interaction
- Diabatic transition enhances fission probability and show insensitivity to E
- Transition states hypothesis is justified microscopically within our approach

#### **Future perspectives**

• Realistic calculation with DFT and development of efficient numerical methods