Nuclear Fission and the Non-Equilibrium Green’s Function Method :A Novel Microscopic Approach

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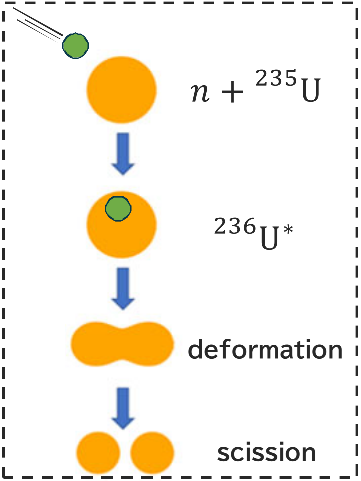
Based on KU and K. Hagino PRC 112 014326 and KU arXiv:2604.17790

Nuclear Fission

- ✓ In fission process,
  a heavy nucleus splits into two smaller fragments

- ✓ Fission process are categorized into
  induced fission and spontaneous fission

- ✓ Understanding nuclear fission requires:
  - shell structure of highly deformed nuclei
  - many-body dynamics with dissipation
    and large-amplitude deformation



Difficult Problem!

Fission of Neutron-Rich Nuclei

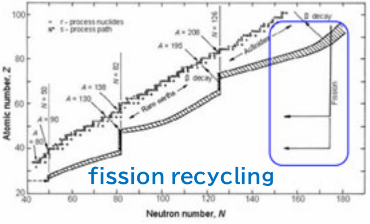
- ✓ Fission of neutron-rich nuclei is crucial in r-process nucleosynthesis
- ✓ In neutron-induced fission of neutron-rich nuclei:
  - low-S_n (neutron separation energy)
  - low-E (excitation energy)
  - low-ρ (level density)

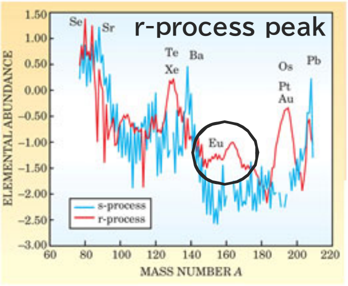
⇩

Breakdown of statistical treatment
(Hauser–Feshbach, Langevin, etc.)

Theoretical Challenge!

r-process path





J.J. Cowan and F.K. Thielemann, Physics Today, 57, 10, 47 (2004).

Theoretical Approach for Nuclear Fission

To describe nuclear fission,
Time-Dependent Hartree-Fock (TDHF) is widely used.

However:

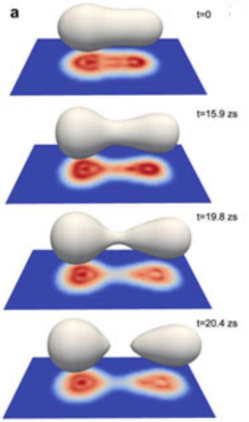
- lack of quantum tunneling of fission barrier
- inconsistency with scattering boundary conditions

(⇒ fission cross section σ_f cannot be obtained)

⇩

Requirement for a new microscopic fission theory overcoming the above problems

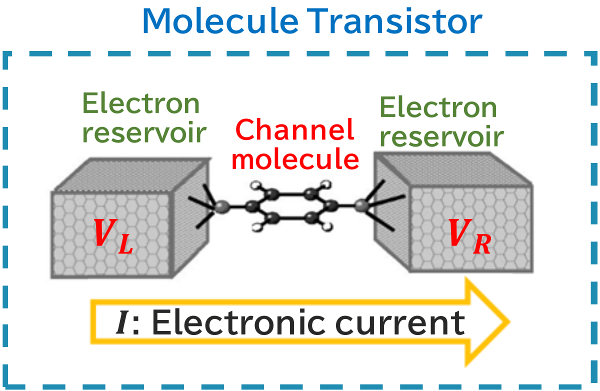
TDHF calculation



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

Non-Equilibrium Green Function (NEGF) method

✓ NEGF method describes electron transports in nano-devices based on the microscopic Hamiltonian



Similar setups are found in

- Solid-state transistor
- Spintronics devices
- Mesoscopic physics experiment with quantum dots

P. S. Damle et al., Phys. Rev. B 64, 201403.

✓ Total Hamiltonian $\boldsymbol{H}$:

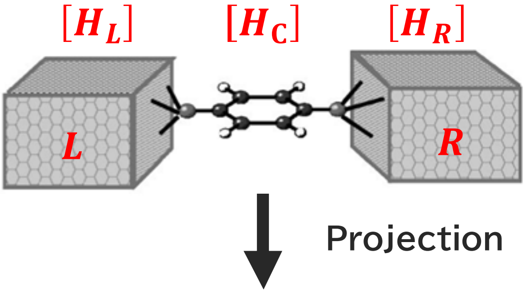
$$H = \begin{pmatrix} H_L & V_L & 0 \\ V_L^\dagger & H_C & V_R \\ 0 & V_R^\dagger & H_R \end{pmatrix}$$

✓ Introduce Green functions $G(E)$:

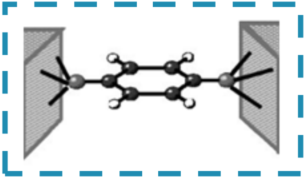
$$G(E) = (E - H_{\mathrm{eff}})^{-1}$$

✓ Using $G(E)$, conductance C is derived:

$$C = \frac{2e^2}{h} \mathrm{Tr}\left[\Gamma_{\mathrm{L}} G(E) \Gamma_R G^\dagger(E)\right]$$

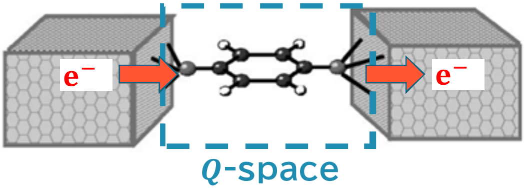


$$H_{\mathrm{eff}} = [H_{\mathrm{C}} + \Sigma_{\mathrm{L}} + \Sigma_{\mathrm{R}}]$$



(Σ_{L} and Σ_{R} are self energies
$\Gamma_{\mathrm{L(R)}} = -2\mathrm{Im}(\Sigma_{\mathrm{L(R)}})$)

nano-device simulations



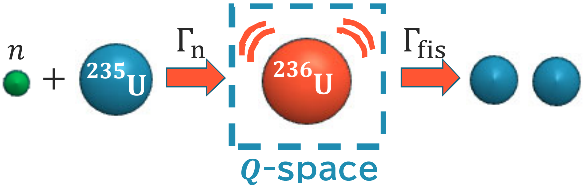
$$T_{L,R} = \mathrm{Tr}\left[\Gamma_L G \Gamma_R G^\dagger\right]$$

Transmission coef.

$$C = (2e^2/h) T_{L,R}$$

conductance

induced fission reactions



$$T_{n,fis} = \mathrm{Tr}\left[\Gamma_n G \Gamma_{fis} G^\dagger\right]$$

Transmission coef.

$$\sigma_{n,fis} = (\pi/k_n^2) T_{n,fis}$$

fission cross-section

Y. Alhassid et al., Ann. Phys. 4124 (2021) 168381.

Development of fission study based on the Non-Equilibrium Green function

- Schematic induced fission model based on Configuration-Interaction
  (G.F. Bertsch PRC 101, 034617 (2020))

- The equivalence between the model in PRC 101, 034671
  and the NEGF method in electronic systems was pointed out
  (Y. Alhassid et al., Ann. Phys. 4124 (2021) 168381)

- Toy model studies by G.F. Bertsch, K. Hagino and H. A. Weidenmüller
  (JPSJ 90 11405, PRE 104 L052104, PRC 105 034618, JPSJ 93 064003 etc.)

- Application to $^{235}\mathrm{U}(n,\mathrm{fis})$ with the model space limitation
  (G.F. Bertsch and K. Hagino, PRC 109 054606, KU and K. Hagino, PRC 110 014321)

- Application to $^{235}\mathrm{U}(n,\mathrm{fis})$ or $^{236}\mathrm{U}(\gamma,\mathrm{fis})$ without the above model space limitation
  (KU and K. Hagino, PRC112 (2025) 014326, KU arXiv:2604.17790)

Theoretical Formulation for nuclear fission

First, we prepare many-body basis

In nuclear fission, both excitation and deformation are important

⇩

Superpose Hartree-Fock w.f. $|HF(Q,E)\rangle$ (generalization of GCM)

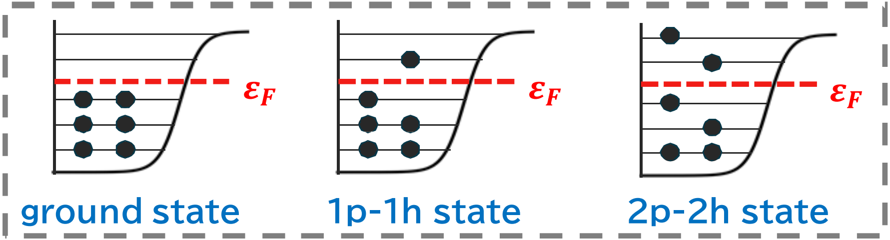
$$|\Phi\rangle = \int dQ dE f(Q,E) |HF(Q,E)\rangle$$

Hartree-Fock state

(Q : deformation)

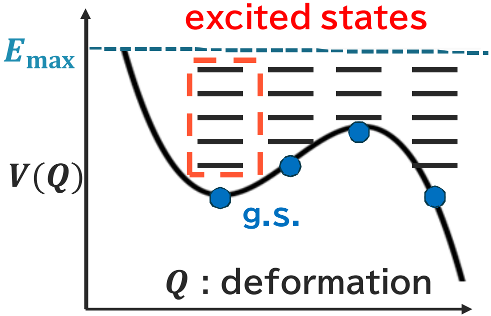
(E : excitation energy)

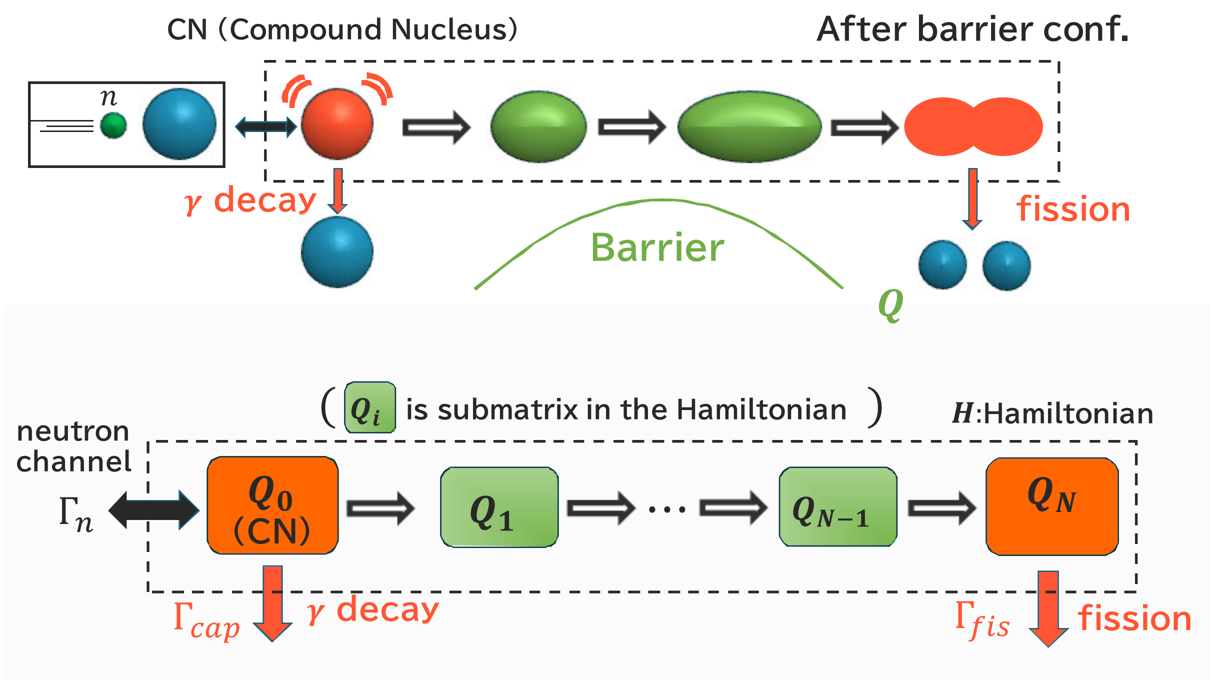
- ✓ particle-hole excited states are generated from reference states



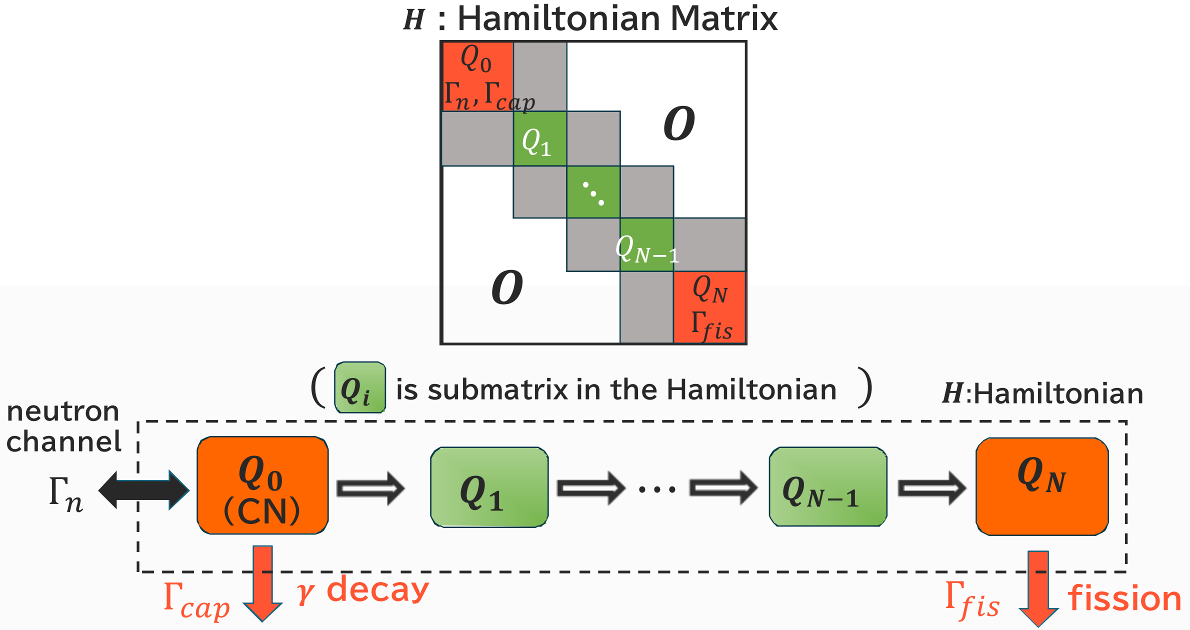
- ✓ At each Q, we generate excited states (up to $E_{\max}$)

$$|\Phi\rangle = \int dQdEf(Q,E)|HF(Q,E)\rangle$$



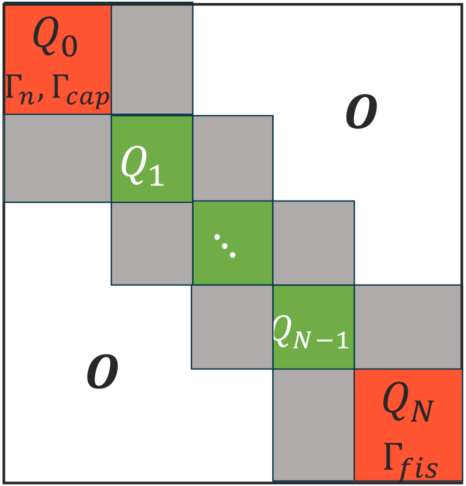


CN (Compound Nucleus)
After barrier conf.
n
γ decay
fission
Barrier
Q
(Q_i is submatrix in the Hamiltonian)
H:Hamiltonian
neutron channel
Γ_n
Q_0 (CN)
Q_1
Q_{N-1}
Q_N
Γ_{cap}
γ decay
Γ_{fis}
fission



H : Hamiltonian Matrix
Q_0
Γ_n, Γ_{cap}
Q_1
Q_{N-1}
Q_N
Γ_{fis}
O
O
(Q_i is submatrix in the Hamiltonian)
H:Hamiltonian
neutron channel
Γ_n
Q_0 (CN)
Q_1
Q_{N-1}
Q_N
Γ_{cap} γ decay
Γ_{fis} fission

H : Hamiltonian Matrix



Green's function

$$G(E) = \left[EN - H + \frac{i}{2}\Gamma\right]^{-1}$$

(E: excitation energy)

Fission Cross section

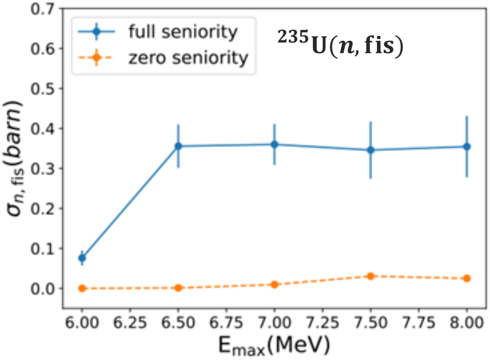
$$\sigma_{n,fis} = \frac{\pi}{k_n^2}\mathrm{Tr}[\Gamma_n G(E) \Gamma_{fis} G^{\dagger}(E)]$$

Fission Cross Section $\sigma_{n,fis}$ is obtained without approximation

✓ In our previous work, $^{235}\mathrm{U}(n,\mathrm{fis})$ was analyzed using NEGF method

⇒ $\sigma_{n,fis}(E_n = 10\mathrm{keV})$ agrees with experimental data within one order of magnitude

(Promising result, but further improvement is also required)



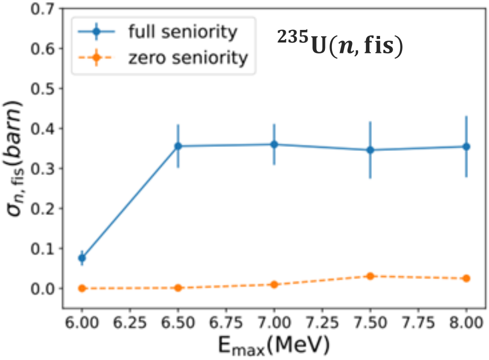
- ✓ $\sigma_{n,fis}(E_n = 10\mathrm{keV})$ converges with respect to E_{max}.
- ✓ Experimental data:

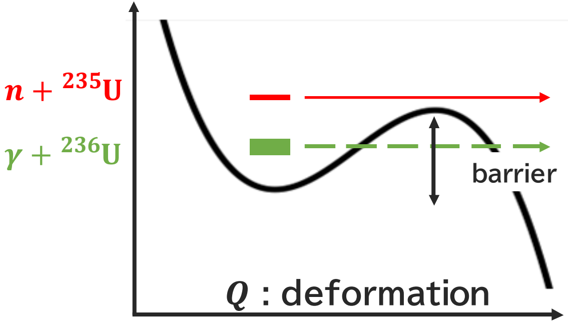
  $\sigma_{n,fis}(E_n = 10\mathrm{keV}) = 3.116$ barn
- ✓ Green function theory:

  $\sigma_{n,fis}(E_n = 10\mathrm{keV}) = 0.354$ barn

K. Uzawa and K. Hagino, PRC 112, 014326 (2025).

✓ As the next step, to test the applicability of the NEGF method in the sub-barrier region, we investigate $^{236}\mathrm{U}(\gamma, \mathrm{fis})$ reaction





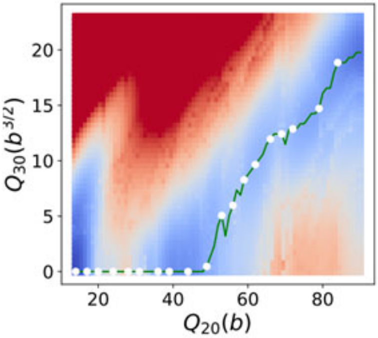
K. Uzawa and K. Hagino, PRC 112, 014326 (2025).

Application to photo induced fission $^{236}\mathrm{U}(\gamma, f)$

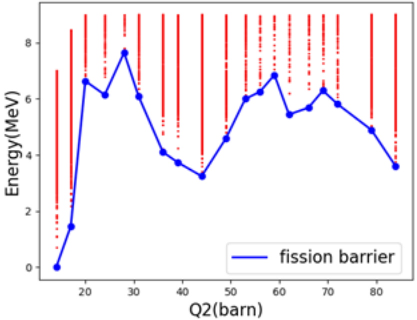
- Static mean-field calculation for $^{236}\mathrm{U}$

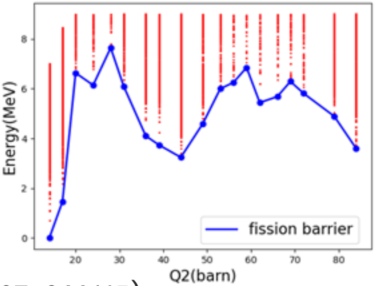
⇒ potential energy and fission path are obtained with SkyAx code
(UNEDF1 Skyrme functional is applied)

$Q_{20} - Q_{30}$ potential



particle-hole excited states
above the fission barrier





GCM kernels

✓ Calculate GCM kernels H and N with basis $|Q, E_\mu\rangle$

$$H_{ij} = \langle Q, E_\mu | H | Q', E_{\mu'} \rangle$$

$$N_{ij} = \langle Q, E_\mu | Q', E_{\mu'} \rangle$$

✓ N_{ij} is approximated as（cf. G. F. Bertsch and K. Hagino, PRC 107, 044615）

$$\langle Q, E_\mu | Q', E_{\mu'} \rangle = \langle Q | Q' \rangle \delta_{\mu,\mu'}$$

（$\mu = \mu'$ means the same configuration）

✓ For H_{ij}, the following residual interactions are applied

1. monopole pairing interaction: $H_{\text{pair}} = -G \sum_{i \neq j} a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{j}} a_j.$

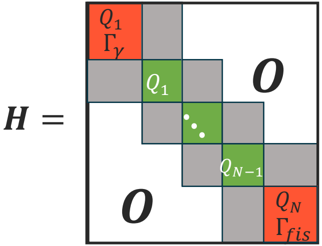
2. random interaction: $H_{\text{ran}} = v \sum r_{ijkl} a_i^\dagger a_j^\dagger a_l a_k,$ (r_{ijkl} is random number)

3. diabatic interaction: $\frac{\langle Q, E_\mu | v_{db} | Q', E_{\mu'} \rangle}{\langle Q, E_\mu | Q', E_{\mu'} \rangle} = \frac{E(Q, E_\mu) + E(Q', E_{\mu'})}{2} + h_2 \ln(\langle Q, E_\mu | Q', E_{\mu'} \rangle).$

Decay width matrices

✓ Determine decay width matrices Γ_γ and Γ_{fis}

- Γ_γ: γ absorption and γ radiation width
- Γ_{fis} : fission width for Q_N configurations



✓ Γ_γ is determined from

empirical gamma strength function $f(E_\gamma)$ and level density $\rho(E)$

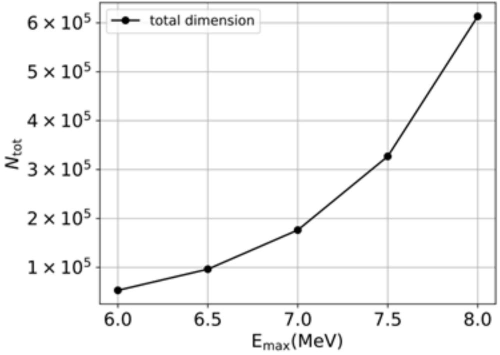
✓ Γ_{fis} is difficult to determine, but σ_f is insensitive to Γ_{fis}.

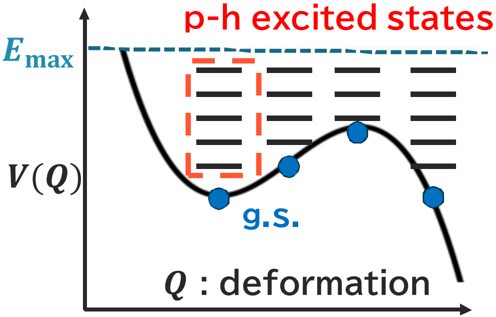
(cf. G. F. Bertsch and K. Hagino, PRC 107, 044615)

✓ Matrix dimension of H, N and $G(E)$ is $O(10^5)$

and matrix inversion is numerically expensive.

$$G(E) = \left[EN - H + \frac{i}{2}\Gamma\right]^{-1} \quad \& \quad T_{n,fis} = \mathrm{Tr}[\Gamma_n G \Gamma_{fis} G^\dagger]$$





PHYSICAL REVIEW E **110**, 055302 (2024)

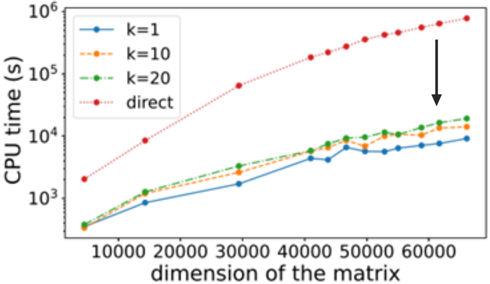
Editors' Suggestion

Application of the shift-invert Lanczos algorithm to a nonequilibrium Green's function for transport problems

K. Uzawa and K. Hagino
Department of Physics, Kyoto University, Kyoto 606-8502, Japan

(Received 12 August 2024; accepted 11 October 2024; published 4 November 2024)

✓ Shift-invert Lanczos method is effective for calculating Green's functions in the context of nuclear fission (discussed in our previous work)



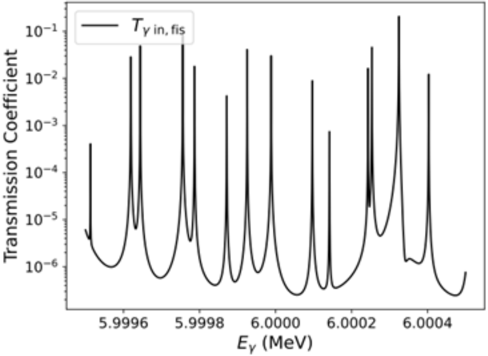
30 times faster

Fission Cross Section

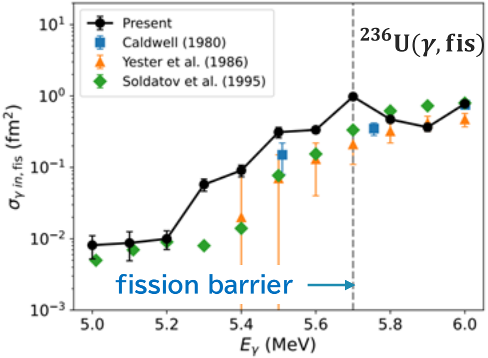
$G(E) = [EN - H + i/2\Gamma]^{-1}$: Green function

$T_{\gamma,fis}(E) = \mathrm{Tr}\left[\Gamma_\gamma G(E) \Gamma_{fis} G(E)^\dagger\right]$: Transmission coefficient

$\sigma_{\gamma,fis}(E) = \frac{3(\pi\hbar c)^2 E}{2\pi E^3} T_{\gamma,fis}$: γ induced fission cross section



Averaging →



KU arXiv:2604.17790.

Fission Cross Section

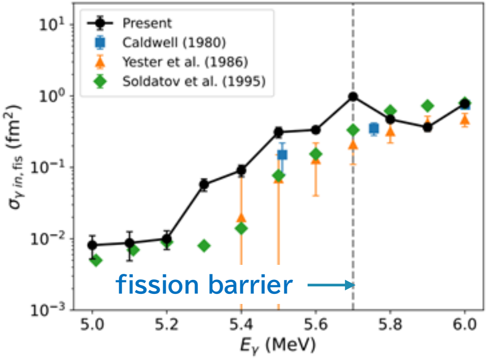
$G(E) = [EN - H + i/2\Gamma]^{-1}$: Green function

$T_{\gamma,fis}(E) = \mathrm{Tr}\left[\Gamma_\gamma G(E) \Gamma_{fis} G(E)^\dagger\right]$: Transmission coefficient

$\sigma_{\gamma,fis}(E) = \frac{3(\pi\hbar c)^2 E}{2\pi E^3} T_{\gamma,fis}$: γ induced fission cross section

Agreement is reasonably good,

even in the sub-barrier region.



KU arXiv:2604.17790.

Eigenchannel Decomposition

✓ We can decompose wave propagation in the fission model space into eigenchannels.

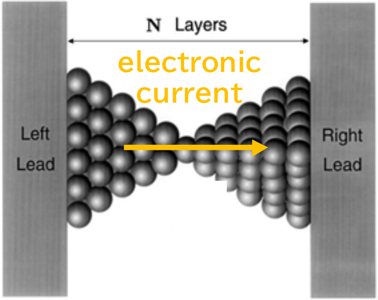
$$G(E) = [E - H]^{-1}$$

$$T_{\gamma,fis}(E) = \mathrm{Tr}\left[\Gamma_\gamma G(E) \Gamma_{fis} G(E)^\dagger\right] = \Sigma_n T_n$$

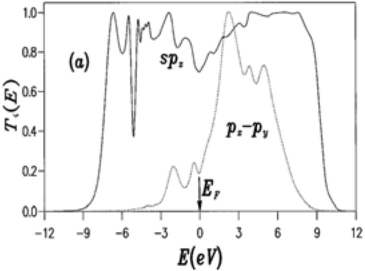
($\sqrt{T_n}$ is eigenvalue of $\left[\Gamma_\gamma^{1/2} G(E) \Gamma_{fis} G(E)^\dagger \Gamma_\gamma^{1/2}\right]$)

J. C. Cuevas et al., Phys. Rev. Lett. 80, 1066 (1988).

Al-atom contact



$T(E)$ in eigenchannels



✓ Apply eigenchannel decomposition for $^{236}\mathrm{U}(\gamma,\mathrm{fis})$ reaction.

Here, resonance average is not performed.

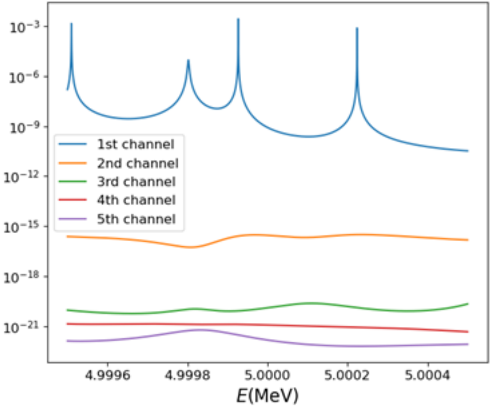
✓ 1st eigenchannels $T_{n=1}$ is dominant

(see the right figure)

⇩ Recall the Bohr-Wheeler transition state formula

Eigenchannel Decomposition	Bohr-Wheeler transition state formula
$T_{\gamma,fis}(E) = \sum_n T_n$	$T_{fis} = \sum_n T_n$
Eigenchannels	Transition states

Fission transmission coefficient $T_n(E)$ for each eigenchannels



KU arXiv:2604.17790.

✓ Apply eigenchannel decomposition for $^{236}U(\gamma,f)$

Here, resonance average is not performed.

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(see the right figure)

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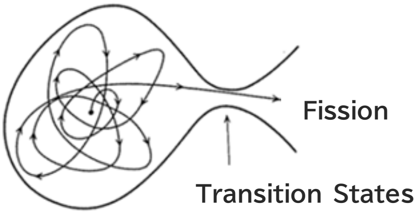
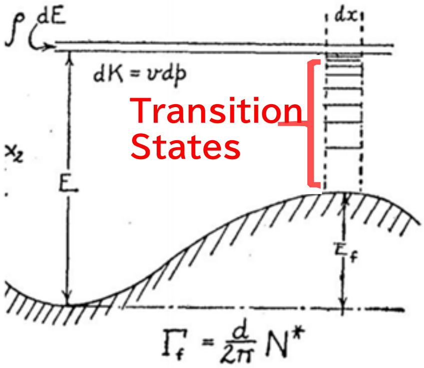
Eigenchannel Decomposition	Bohr-Wheeler transition state formula
$T_{\gamma,fis}(E) = \sum_{n} T_n$	$T_{fis} = \sum_{n} T_n$
Eigenchannels	Transition states





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

Summary

- Induced fission reactions have been described within the NEGF framework.

- The NEGF calculation successfully reproduces the fission cross section, $\sigma_{\gamma,fis}$, even in the tunneling region.

- Eigenchannel analysis shows that the fission probability is dominated by a single channel, consistent with the transition-state picture.

Backup

Note

- S-matrix dispersion formula (H. Feshbach(1952))

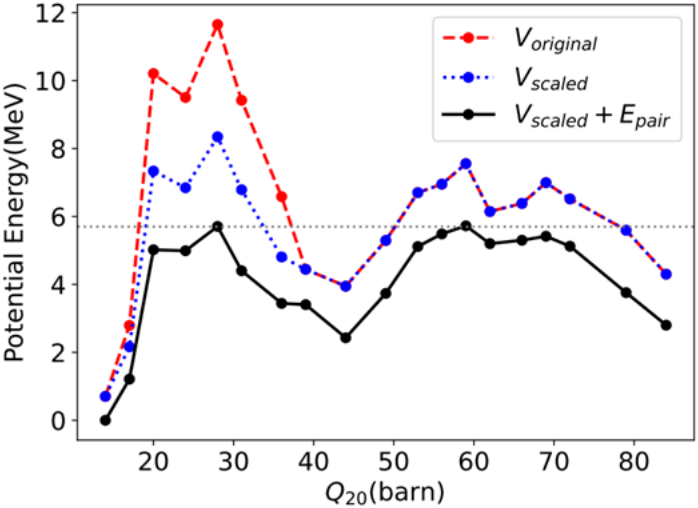
$$S_{ab}(E) = S^0_{ab}(E) - 2i\gamma^\dagger_{a\mu}\left(E - H + i/2\Gamma\right)^{-1}_{\mu\nu}\gamma_{\nu b}$$
$$= S^0_{ab}(E) - 2i\gamma^\dagger_{a\mu}G(E)_{\mu\nu}\gamma_{\nu b}.$$

direct compound nucleus reaction

- Trace formula for T (transmission coefficient)

$$T_{ab} = |S_{ab}|^2$$
$$= \left(2\sum_{\mu_1\mu_2}\gamma_{a\mu_1}G_{\mu_1\mu_2}\gamma_{\mu_2 b}\right)^*\left(2\sum_{\mu_3\mu_4}\gamma_{a\mu_3}G_{\mu_3\mu_4}\gamma_{\mu_4 b}\right)$$
$$= \mathrm{Tr}\left[\Gamma_a G \Gamma_b G^\dagger\right], \qquad (\Gamma_a)_{ij} = 2\gamma_{ai}\gamma_{aj}.$$

✓ Fission barrier is scaled to reproduce experimental barrier height



✓ Residual interactions for GCM calculation

(Skyrme interaction is not used)

- Monopole pairing interaction:

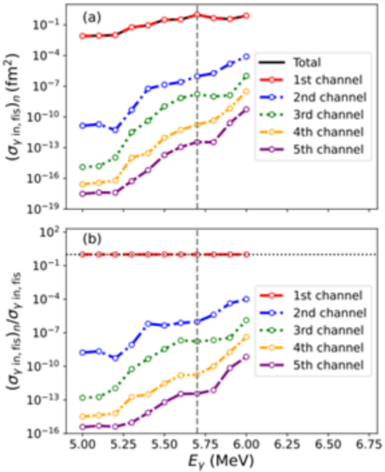
$$H_{\rm pair} = -G \sum_{i \neq j} a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{j}} a_j .$$

- Random interaction: (r_{ijkl} is random number)

$$H_{\rm ran} = v {\sum}' r_{ijkl} a_i^\dagger a_j^\dagger a_l a_k ,$$

- Diabatic interaction: $\frac{\langle Q, E_\mu | v_{db} | Q', E_{\mu'} \rangle}{\langle Q, E_\mu | Q', E_{\mu'} \rangle} = \frac{E(Q, E_\mu) + E(Q', E_{\mu'})}{2} + h_2 \ln(\langle Q, E_\mu | Q', E_{\mu'} \rangle).$

✓ eigenchannel decomposition with energy average

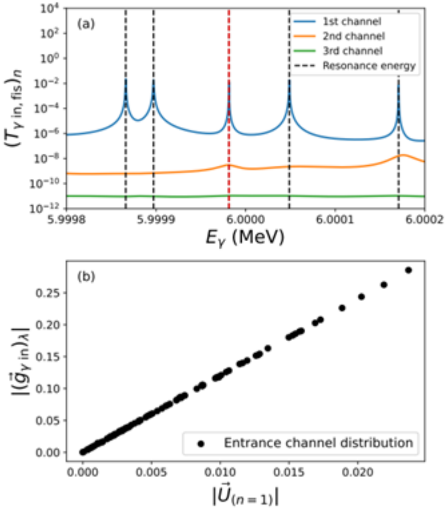


✓ distribution of $\vec{U}$ is corelated to

the GCM collective function $g = N^{1/2} f \quad (Hf = ENf)$

$$
\begin{aligned}
T_{ab} &= \mathrm{Tr}\left[\Gamma_a G(E) \Gamma_b G^\dagger(E)\right] \\
&= \mathrm{Tr}\left[\Gamma_a^{1/2} G(E) \Gamma_b G^\dagger(E) \Gamma_a^{1/2}\right] \\
&= \mathrm{Tr}\left[t t^\dagger\right] \\
&= \sum_n |t_n|^2,
\end{aligned}
$$

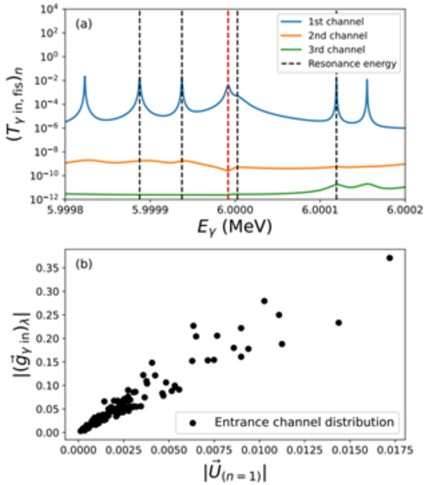
$$
t = U \, \mathrm{diag}(t_1, t_2, \ldots) \, V^\dagger,
$$



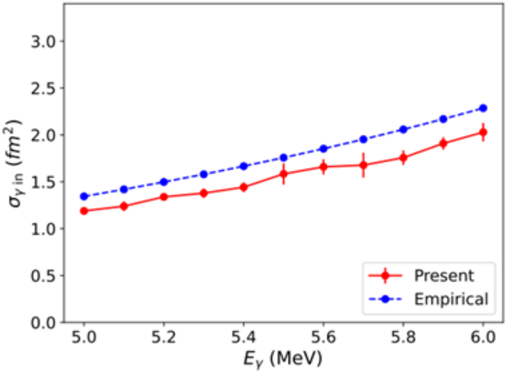
✓ distribution of $\vec{U}$ is corelated to the GCM collective function $g = N^{1/2}f \quad (Hf = ENf)$

$$
\begin{aligned}
T_{ab} &= \mathrm{Tr}\left[\Gamma_a G(E) \Gamma_b G^\dagger(E)\right] \\
&= \mathrm{Tr}\left[\Gamma_a^{1/2} G(E) \Gamma_b G^\dagger(E) \Gamma_a^{1/2}\right] \\
&= \mathrm{Tr}\left[t t^\dagger\right] \\
&= \sum_n |t_n|^2,
\end{aligned}
$$

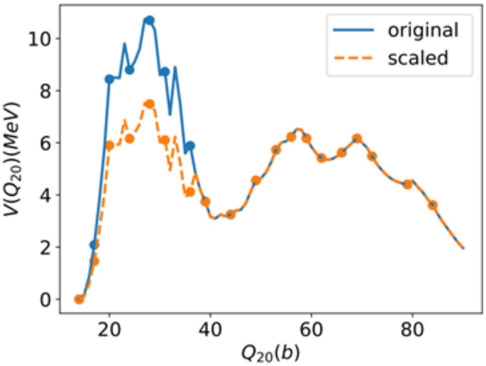
$$
t = U \, \mathrm{diag}(t_1, t_2, \ldots) \, V^\dagger,
$$



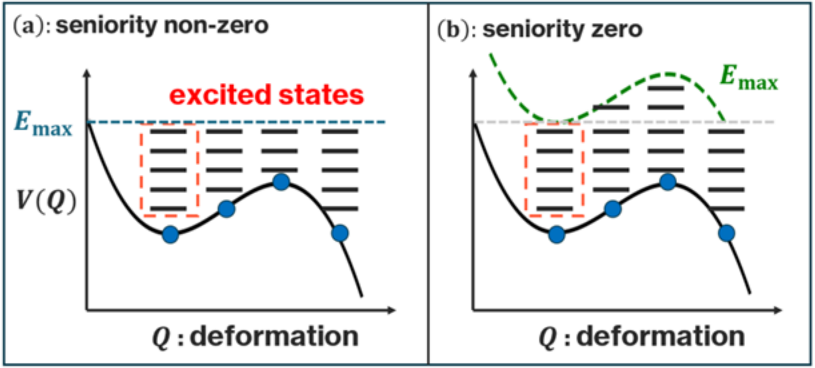
✓ total gamma absorption probability is consistent with phenomenological value



✓ Scaled fission barrier



✓ Model space



(a): seniority non-zero
excited states
E_{max}
$V(Q)$
Q : deformation
(b): seniority zero
E_{max}
Q : deformation

✓ Decay width matrices

$$(\Gamma_n)_{ij} = \bar{\Gamma}_n \, N_{k_n,i}^{1/2} N_{k_n,j}^{1/2},$$

$$(\Gamma_{\text{cap}})_{ij} = \bar{\Gamma}_{\text{cap}} \sum_{k \in Q_k = 14\text{b}} N_{k,i}^{1/2} N_{k,j}^{1/2},$$

$$(\Gamma_{\text{fis}})_{ij} = \bar{\Gamma}_{\text{fis}} \sum_{k \in Q_k = 84b} N_{k,i}^{1/2} N_{k,j}^{1/2},$$