An application of the shift-invert Lanczos algorithm to the non-equilibrium Green function method

Kotaro Uzawa (Kyoto U.)

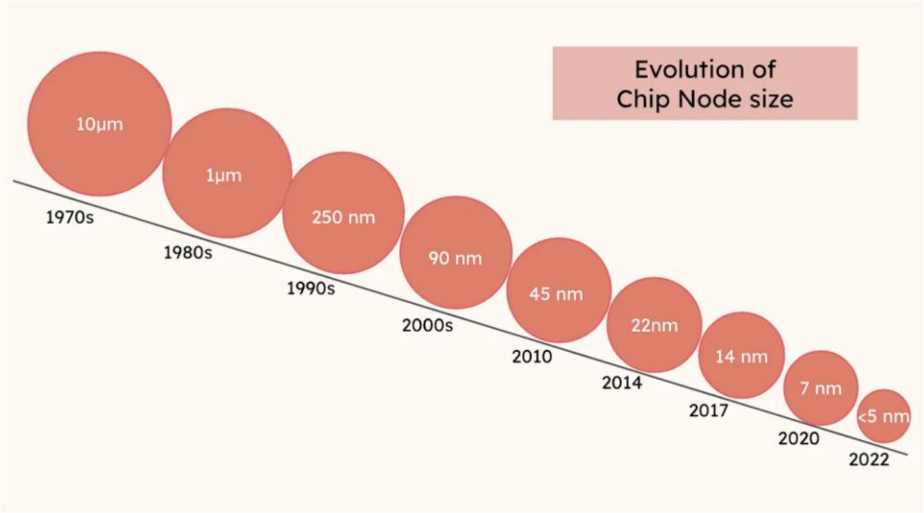
K. Uzawa and K. Hagino, arXiv:2408.06554

Non-Equilibrium Green Function (NEGF) method

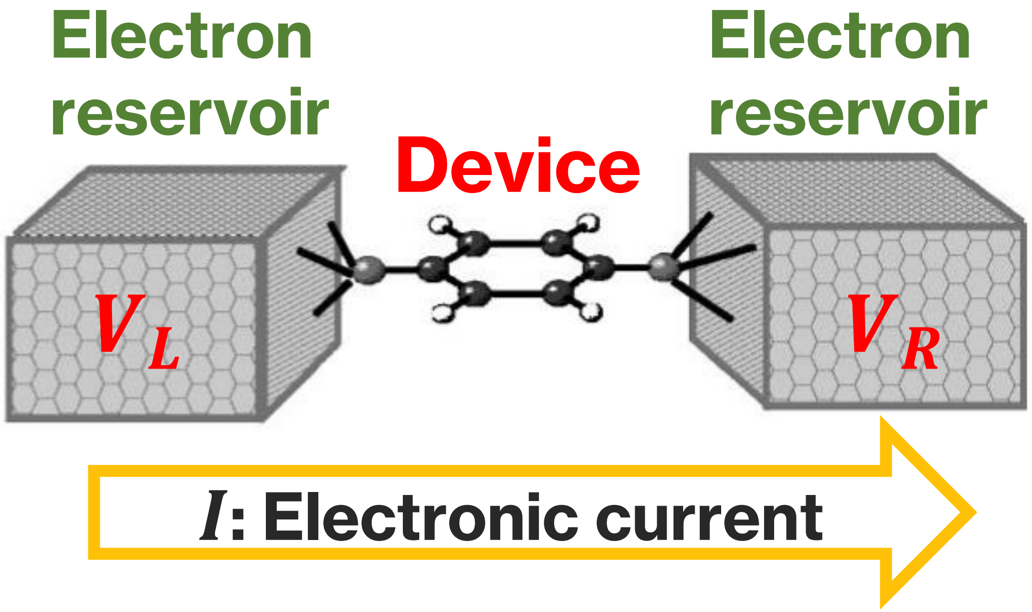
✓ **With the time, the size of semiconductors continues to decrease**

⇒ Quantum effects become important in the semiconductor design

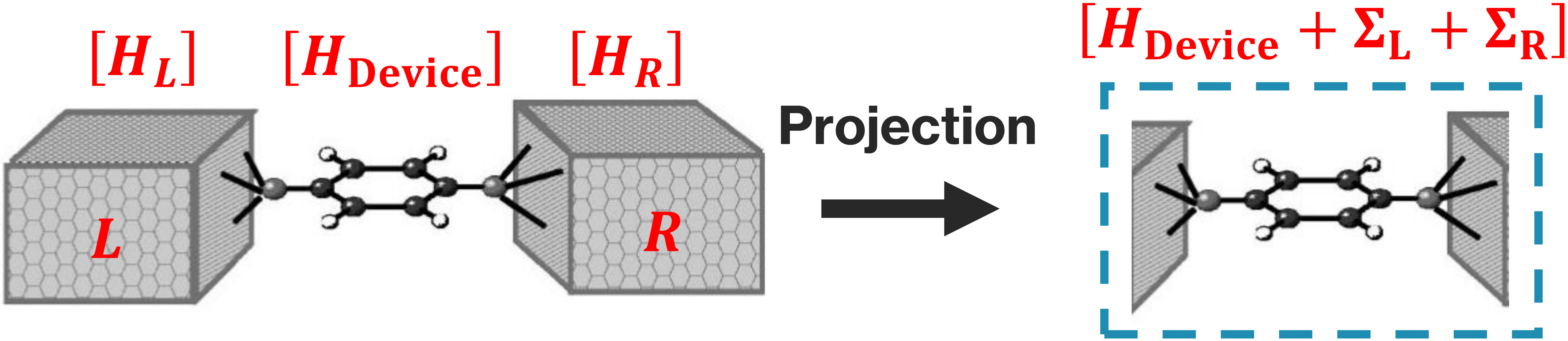
✓ **NEGF method describes electron transports in nano-devices based on its microscopic Hamiltonian!**



https://abhisheksingh-4899.medium.com



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



(Σ_{L} and Σ_{R} are self energies)

- **Introduce Green's functions $G(E)$**

$$G(E) = (E - H_{\text{Device}} - \Sigma_{\text{L}} - \Sigma_R)^{-1}$$

- **Calculate transmission coefficient $T_{L\to R}$**

$$T_{L\to R}(E) = \mathrm{Tr}\left[\Gamma_{\text{L}} \mathrm{G(E)} \Gamma_R \mathrm{G(E)}^{\dagger}\right]$$

$$\propto (\text{conductance})$$

$$\Sigma_{\text{L}} = \Delta_{\text{L}} - \frac{i}{2}\Gamma_{\text{L}}$$

$$\Sigma_{\text{R}} = \Delta_{\text{R}} - \frac{i}{2}\Gamma_{\text{R}}$$

Nuclear Fission

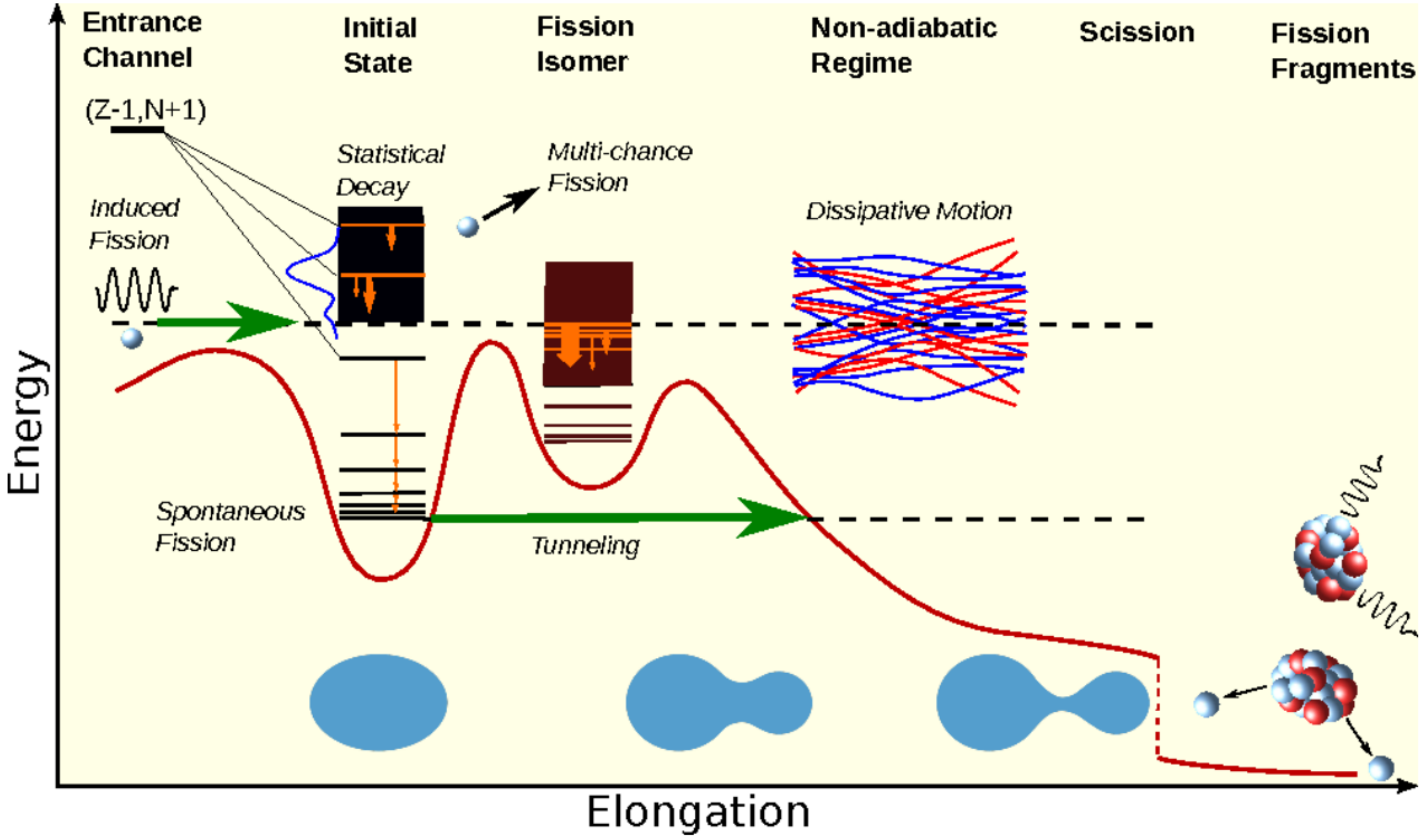
Michael Bender et al., J. Phys. G: Nucl. Part. Phys. 47 113002

✓ **A process of a heavy nucleus splitting into two smaller nuclei**

✓ **It prays an important role in**

- **nuclear energy**
- **nucleosynthesis**
- **RI beam production ...**

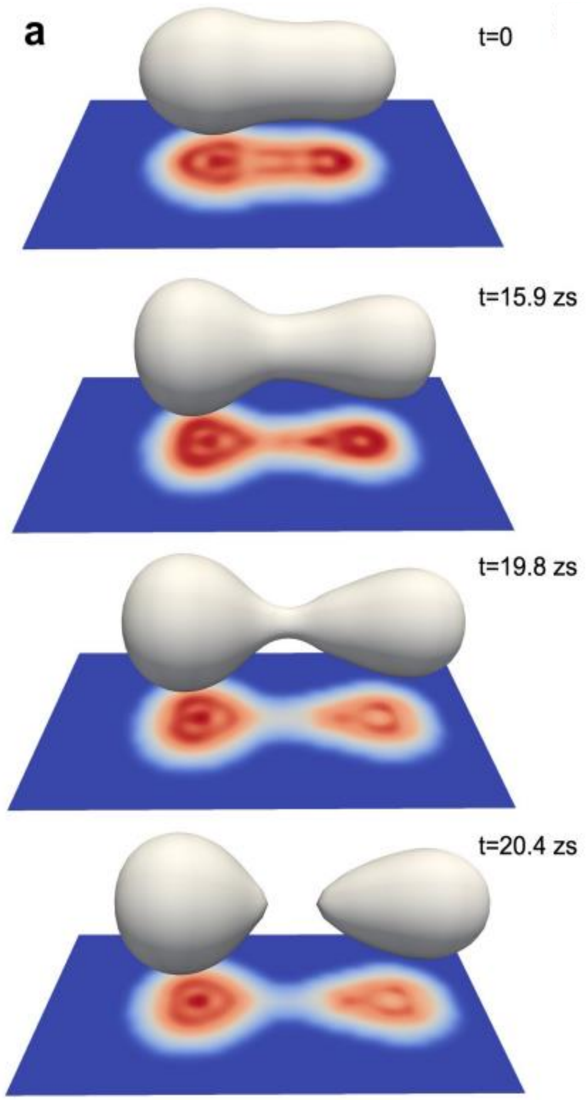
✓ **Its microscopic description is extremely difficult !**



Difficulties of microscopic description of fission come from ...

① Fission is a large-amplitude motion

(✕ Perturbation or Linear response theory)



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

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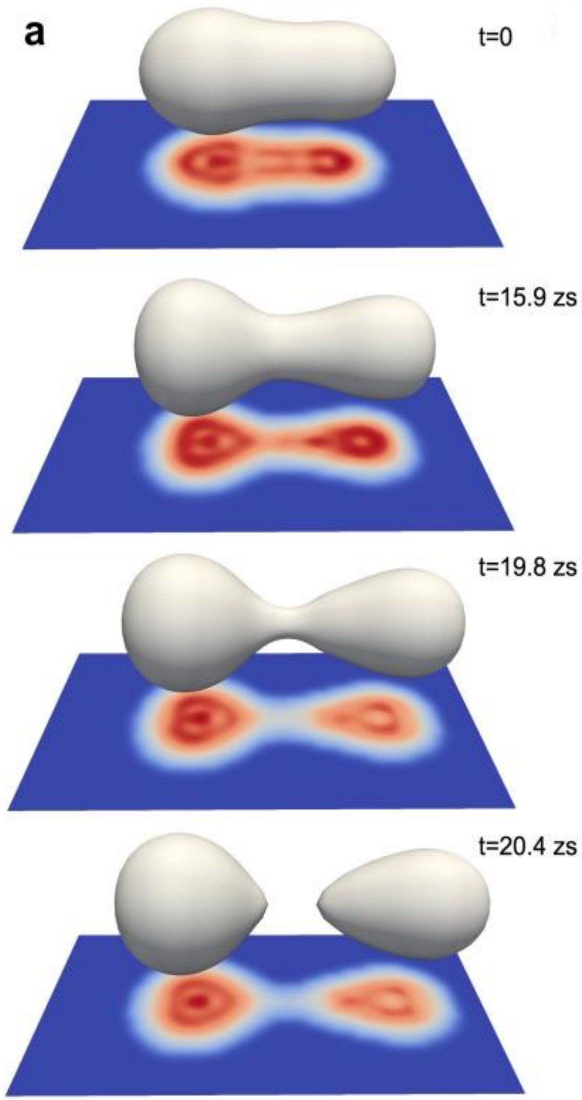

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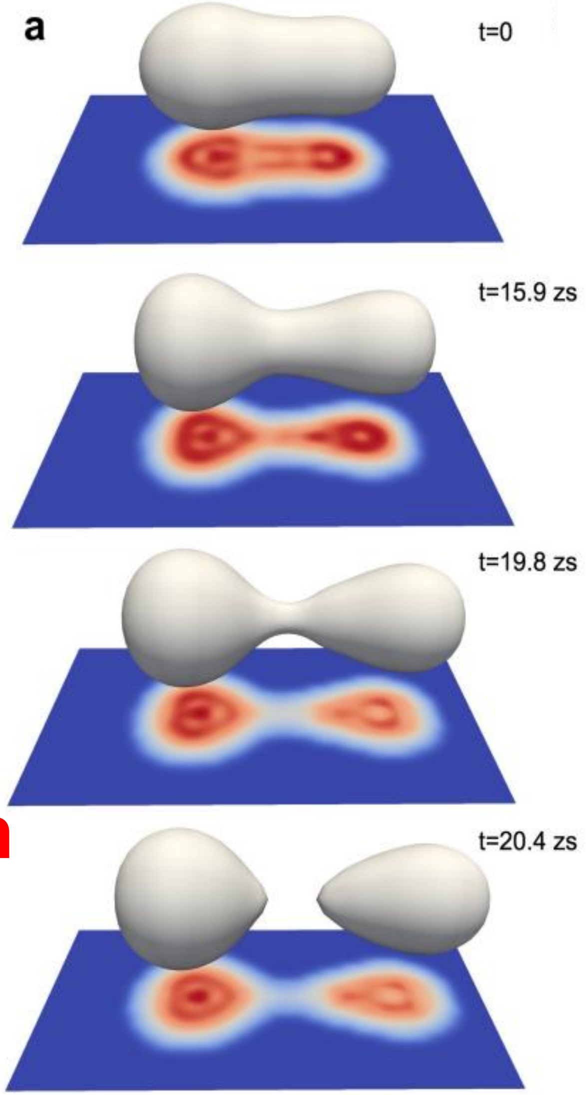

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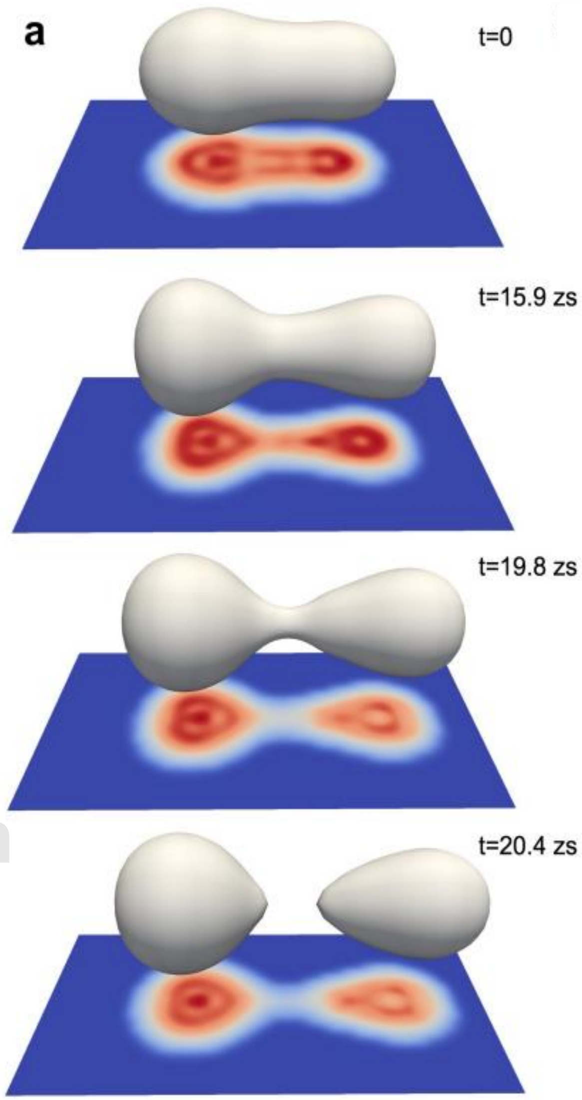


G. Scamps and C. Simenel, Nature 564 382 (2018).

We approach nuclear fission using Non-Equilibrium Green Function method !

Theoretical Formulation

First, we prepare many-body basis

In nuclear fission, both excitation and deformation are important

⇩

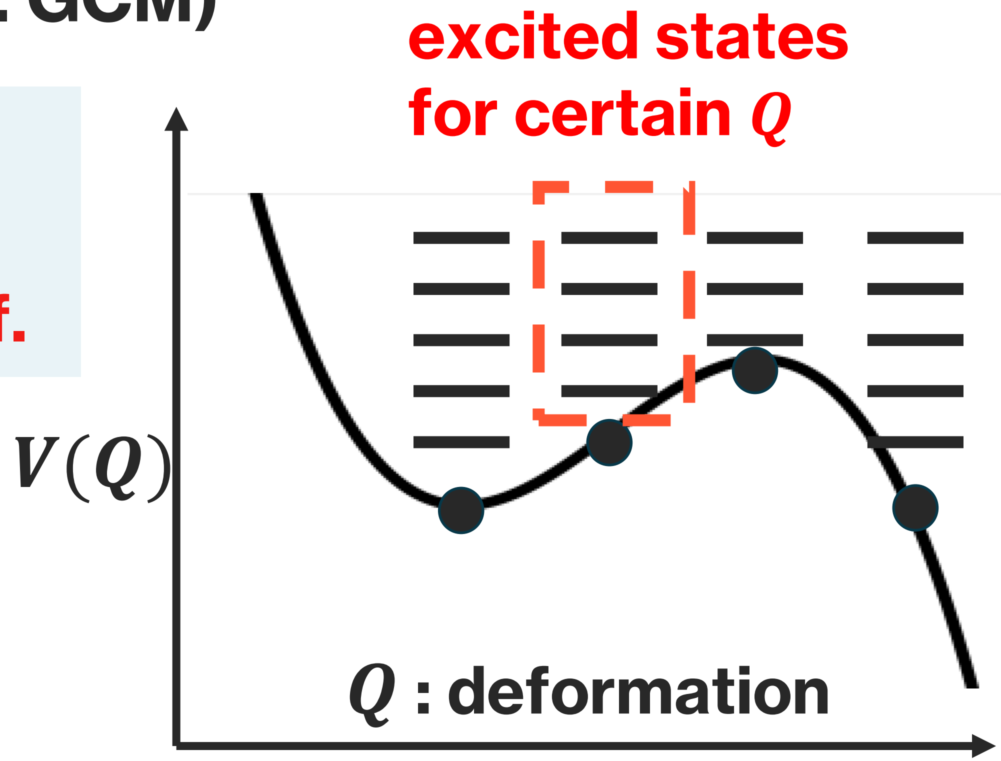
Superpose Hartree-Fock w.f. $|HF(Q, E_i)\rangle$ (i.e. GCM)

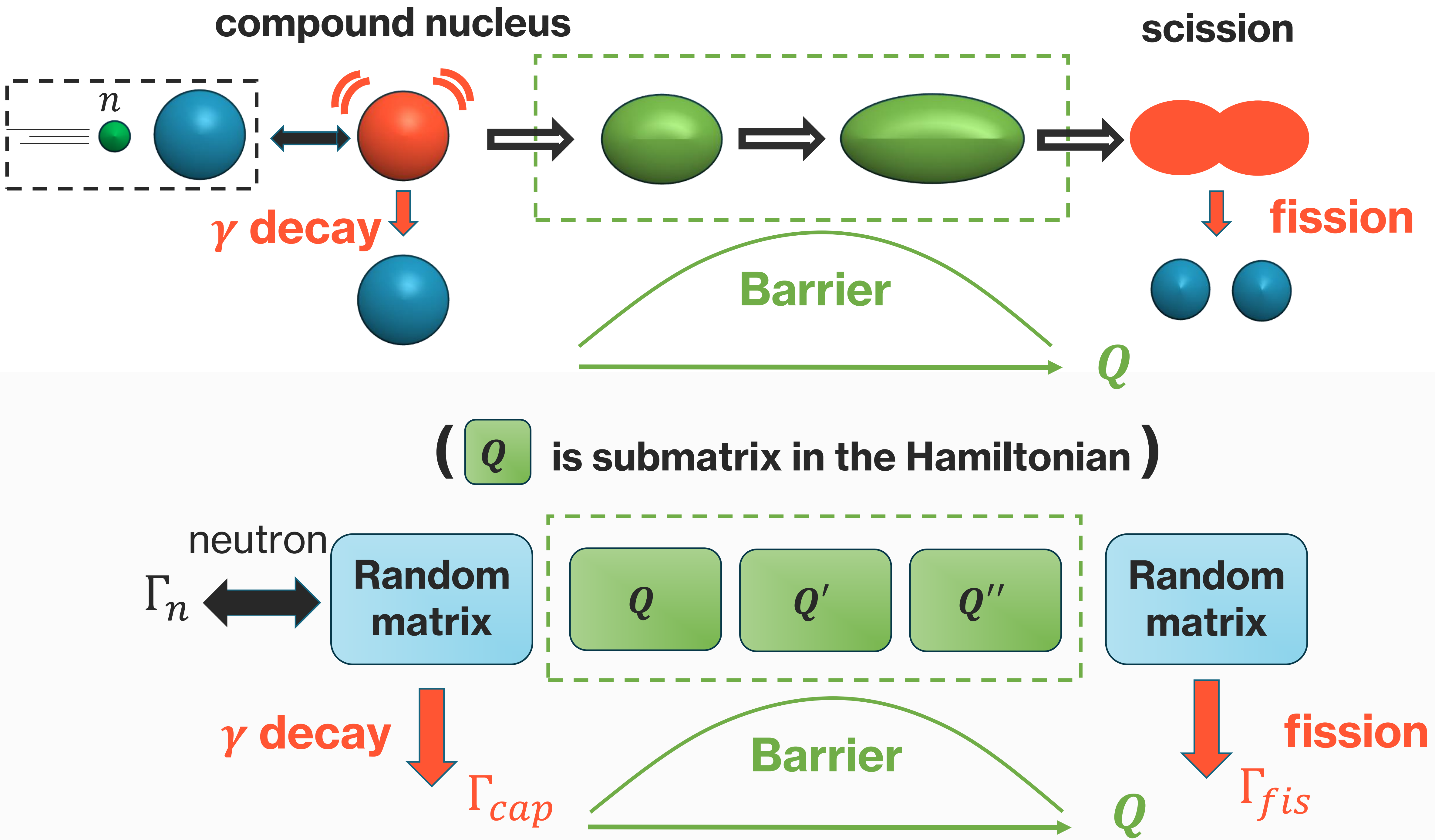
$$|\Psi\rangle_{\text{GCM}} = \sum_i \int dQ\, f(Q, E_i)|\text{HF}(Q, E_i)\rangle$$

Hartree-Fock w.f.

(Q : deformation parameter)

(E_i : particle-hole excitation energy)

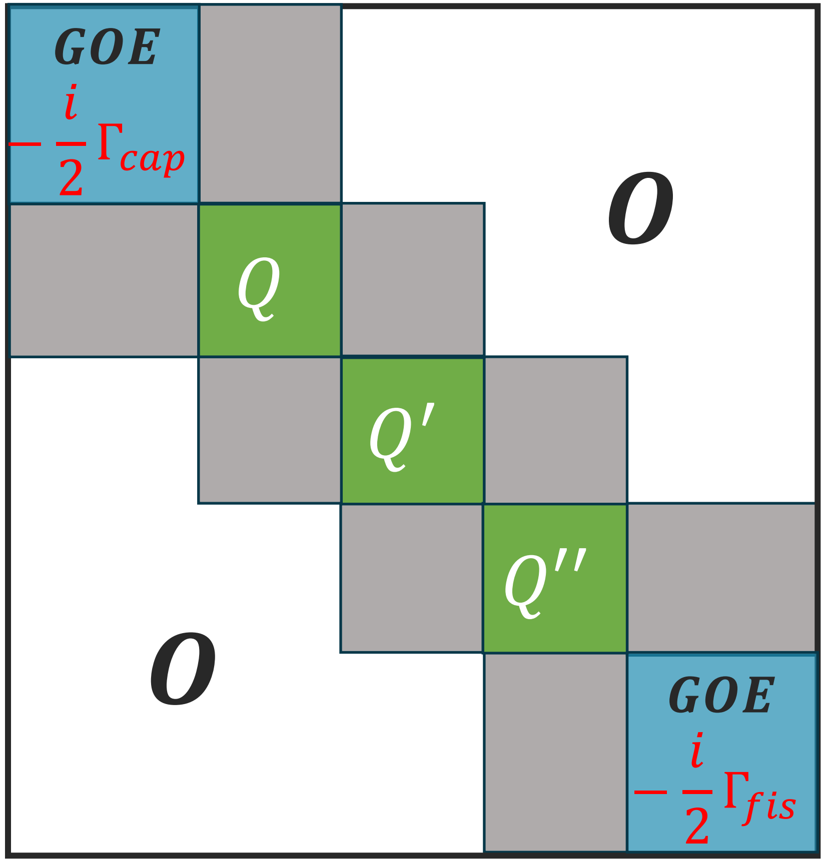




compound nucleus
scission
n
γ decay
fission
Barrier
Q
(Q is submatrix in the Hamiltonian)
neutron
Γ_n
Random matrix
Q
Q'
Q''
Random matrix
γ decay
Γ_{cap}
Barrier
Q
fission
Γ_{fis}

Non-equilibrium Green's function method

H : Hamiltonian Matrix



GOE means
Gaussian Orthogonal Ensemble

&

Green's function

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

(E: excitation energy)
(N: overlap matrix)

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

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

G. F. Bertsch and K. Hagino, PRC 107 044615 (2023).

K. Uzawa and K. Hagino, PRC 110 014321 (2024).

However, the dimension of the Hamiltonian matrix is extremely large

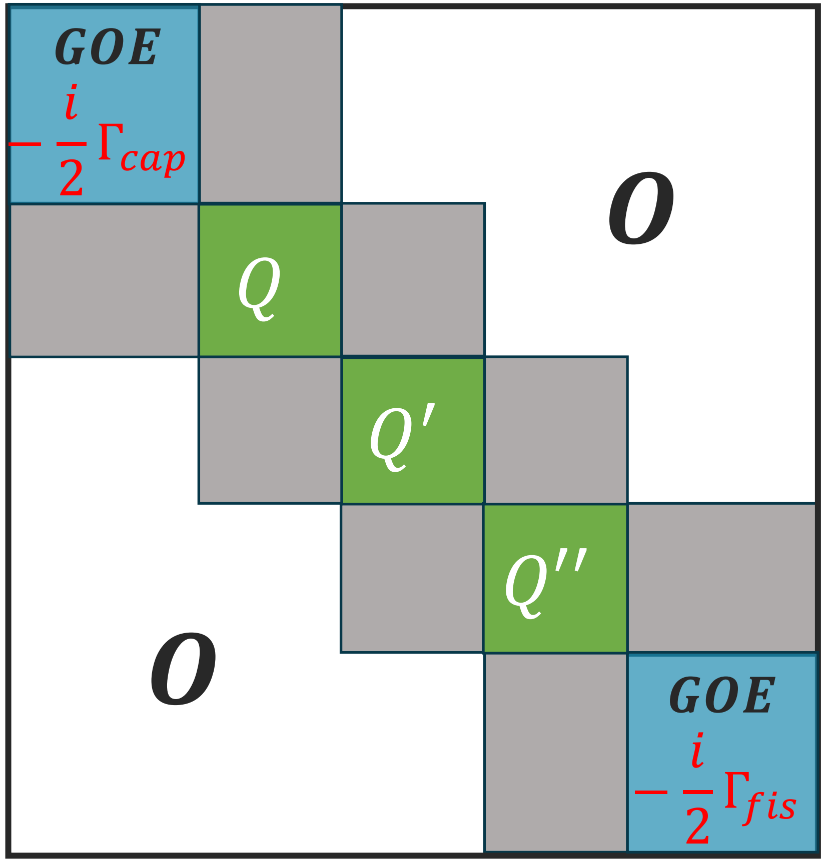
(**In the case of $^{235}\mathrm{U}(n, fis)$ reaction,**
the dimension is $O(10^5) - O(10^6)$)

An inversion of the Green function matrix becomes expensive

Green's function

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

H : **Hamiltonian Matrix**



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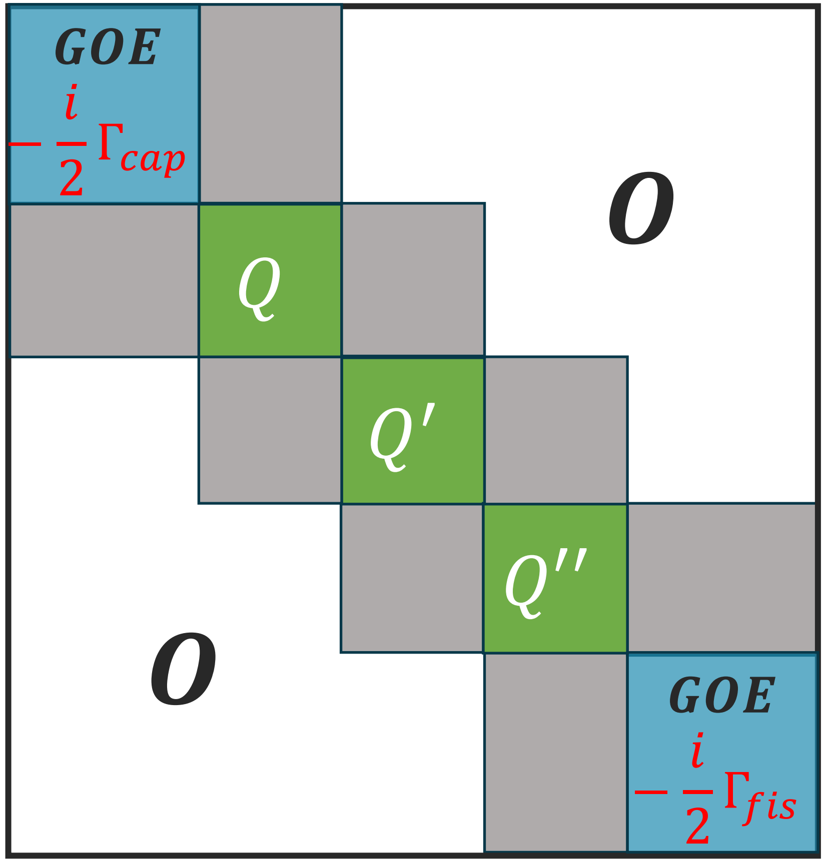
H : Hamiltonian Matrix



⇒ Application of the Lanczos method !

The Lanczos method

Solve eigenvalue eq. of matrix A

$$A\vec{x} = \lambda\vec{x} \quad (A \text{ is a symmetric } N \times N \text{ matrix})$$

We introduce a subspace called Krylov subspace ($\vec{q}$ is arbitrary vector)

$$\mathrm{span}\{\vec{q}, A\vec{q}, A^2\vec{q}, \dots, A^{n-1}\vec{q}\}$$

$Ax = \lambda x$ is solved in the Krylov subspace,

and few specific eigenstates are calculated with $O(n^2N)$

(direct diagonalization requires $O(N^3)$)

Spectral decomposition of Green's function

$$G(E)_{\mu\mu'} = \sum_\lambda f_\lambda^*(\mu') \frac{1}{E-E_\lambda} f_\lambda(\mu)$$

$$(Hf_\lambda = E_\lambda N f_\lambda)$$

(E_λ : eigenenergy
f_λ : eigenvector)

Substituting it, fission probability $T_{n,fis}(E)$ becomes

$$T_{n,\mathrm{fis}}(E) = \mathrm{Tr}[\Gamma_n G(E) \Gamma_{\mathrm{fis}} G^\dagger(E)] = \gamma_n \gamma_{\mathrm{fis}} \sum_{\lambda\lambda'} \frac{f_\lambda^{(a)} f_{\lambda'}^{(a)*} f_\lambda^{(b*)} f_{\lambda'}^{(b)}}{(E-E_\lambda)(E-E_{\lambda'})^*}$$

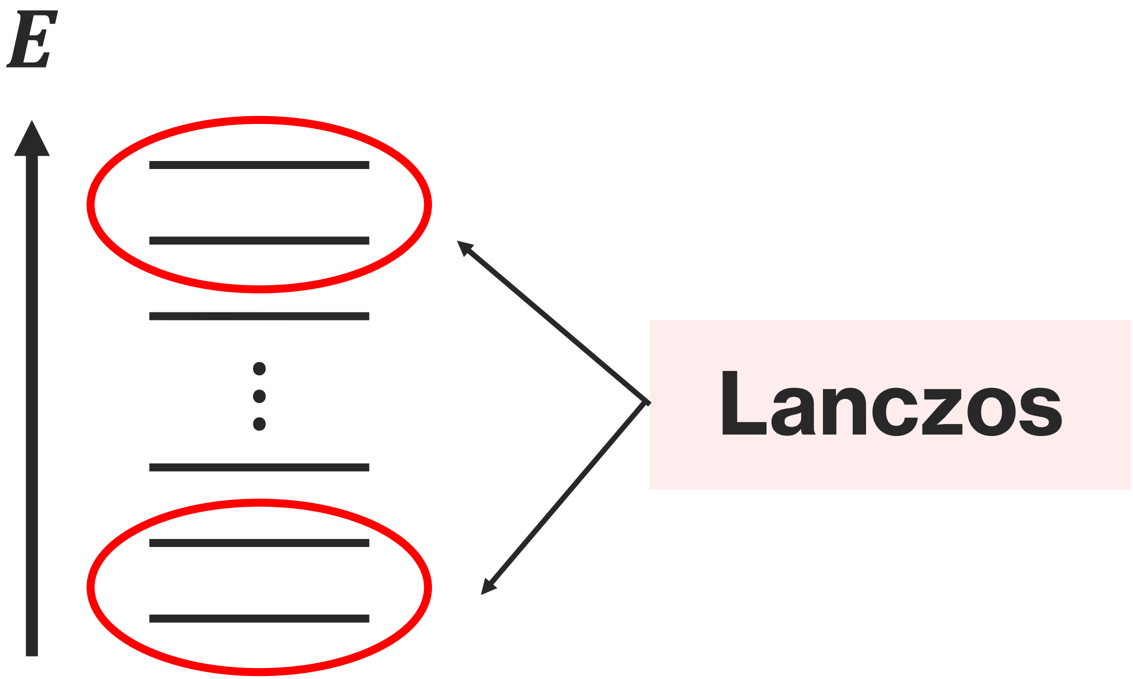
Eigenstates with $E_\lambda \simeq E$ are dominant !

(due to $\frac{1}{(E-E_\lambda)(E-E_{\lambda'})^*}$ factor)

◆ Our approach

Calculate eigenstates $|\lambda\rangle$ with $E_\lambda \simeq E$ using the Lanczos method

However, the Lanczos method gives eigenstates around the ground state



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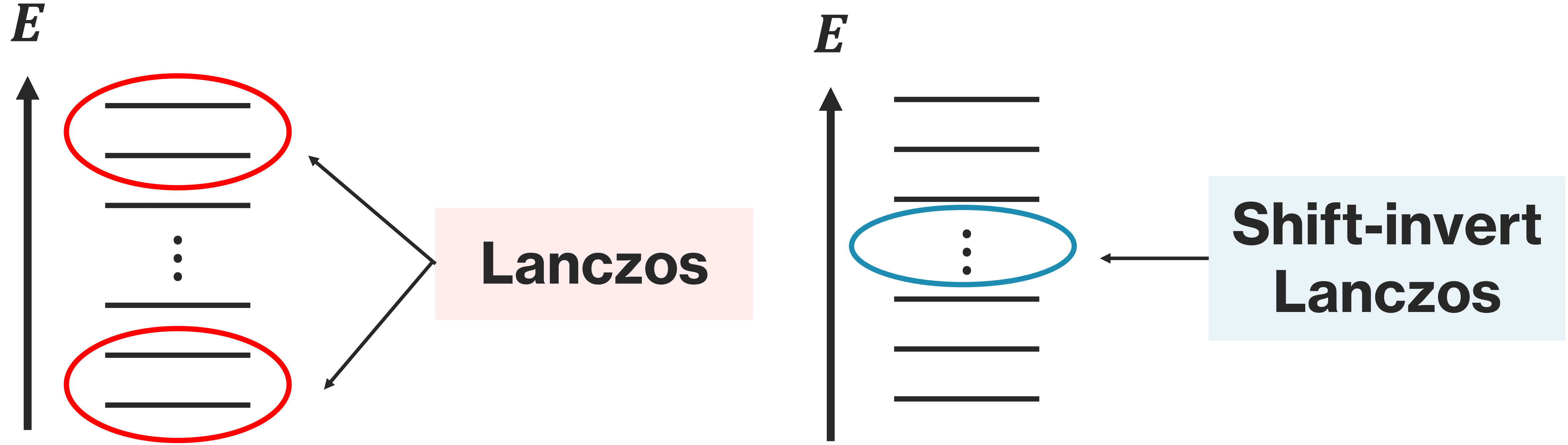
⇒ Shift-invert Lanczos method



Shift-invert transformation

$$Hf = ENf$$

$\Downarrow - \sigma N$

$$(H - \sigma N)f = (E - \sigma)Nf,$$

$\Downarrow \times (E - \sigma)^{-1}(H - \sigma N)^{-1}$

$$(H - \sigma N)^{-1}Nf = (E - \sigma)^{-1}f.$$

Applying the Lanczos method to the last eq.

- ✓ Eigenvalue E is transformed into $(E - \sigma)^{-1}$
- ✓ Lanczos method calculates eigenstates with large eigenvalues

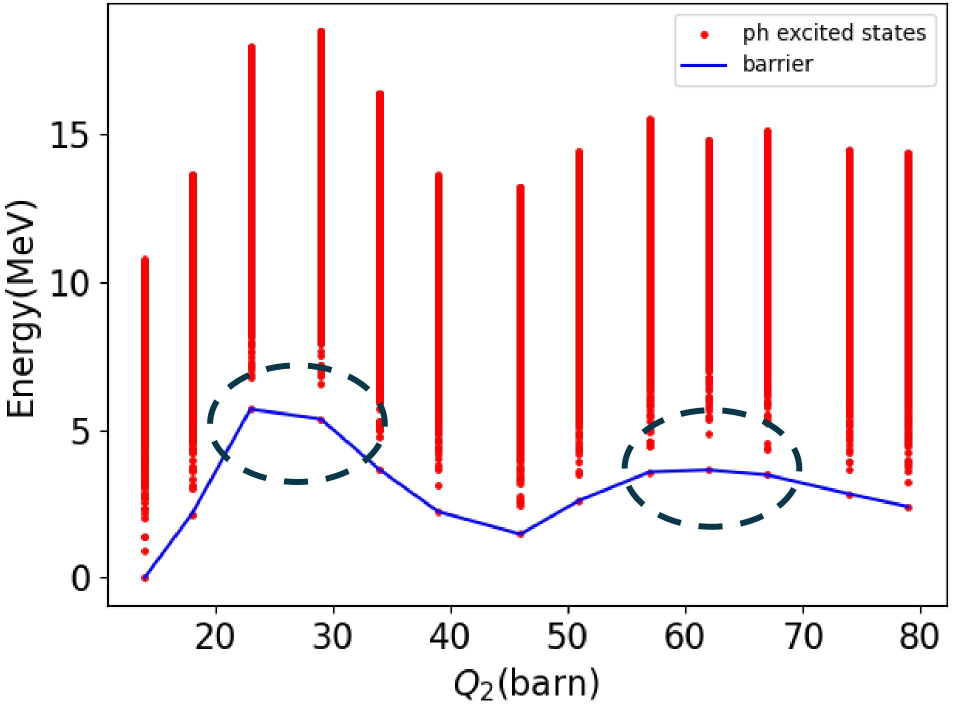
  ⇒ the eigenvalue $E \simeq \sigma$ is obtained !

Application to $^{235}\mathrm{U}(n,f)$

Solve Skyrme-Hartree-Fock equation for $^{236}\mathrm{U}$

⇒Calculate fission barrier and particle-hole excited states

fission barrier & ph excited states



Hamiltonian matrix (its dimension is 66103)

$$H = \begin{pmatrix} H^{(L)}_{\mathrm{GOE}} & V_L & & & & & \\ V_L^T & H_1 & V_{1,2} & & & O & \\ & V_{2,1} & H_2 & V_{2,3} & & & \\ & & & \ddots & & & \\ O & & & V_{11,12} & H_{12} & V_R \\ & & & & V_R^T & H^{(R)}_{\mathrm{GOE}} \end{pmatrix}$$

GCM calculation

✓ **Calculate Hamiltonian matrix H_{ij} and overlap matrix N_{ij} (GCM)**

$$H_{ij} = \langle Q, E | \hat{H} | Q', E' \rangle \text{ and } N_{ij} = \langle Q, E | Q', E' \rangle$$

✓ **As residual interactions, we apply**

constant pairing interaction and diabatic interaction

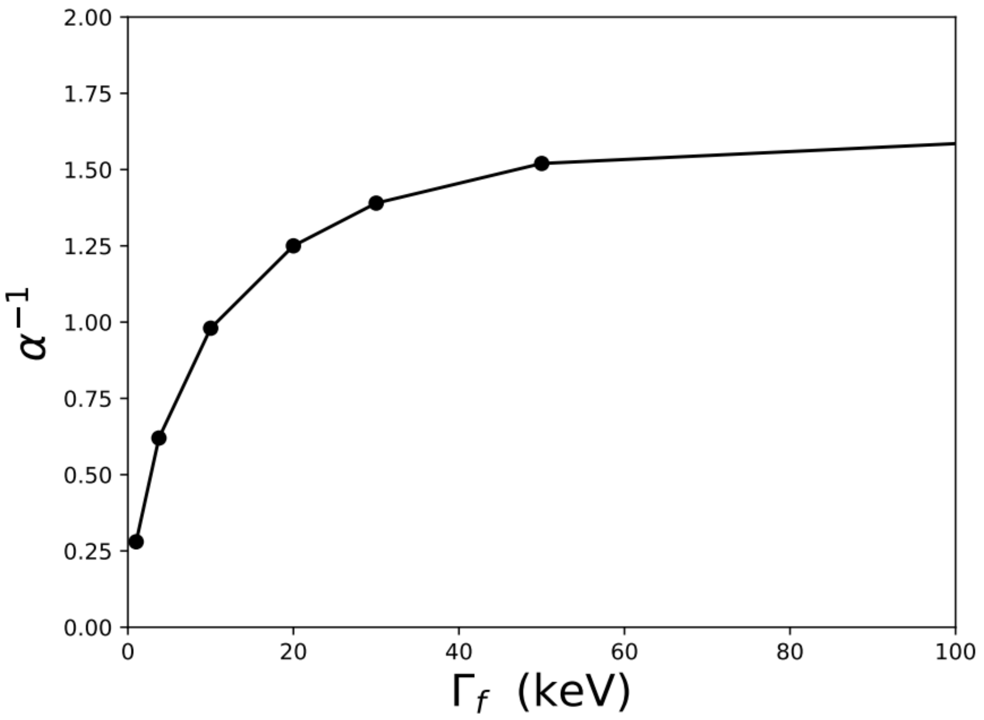
$$H_{pair} = -G\mathrm{P}^\dagger \mathrm{P} \quad (\mathrm{P} = \textstyle\sum_\nu a_{\bar{\nu}} a_\nu)$$

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

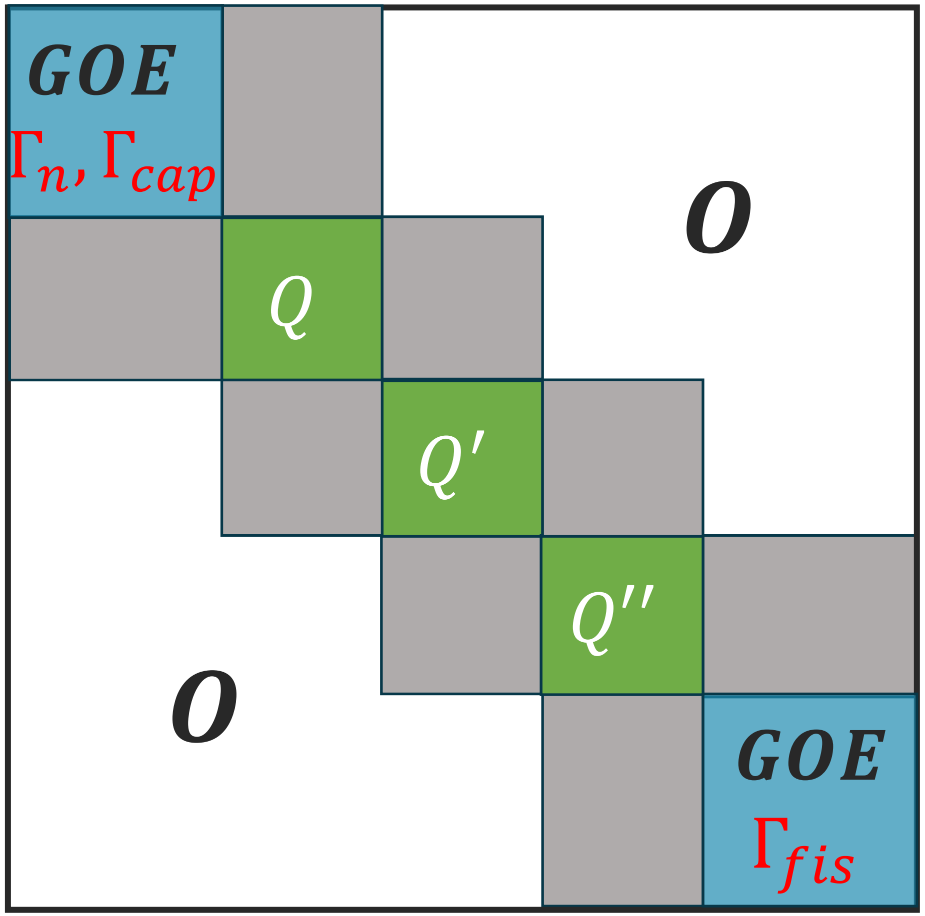
Decay widths

✓ Γ_n and Γ_{cap} are fitted to empirical values in the RIPL library

✓ σ_{fis} is known to be insensitive to the fission width Γ_{fis} (fixed to 125 keV)



H : Hamiltonian Matrix



G. F. Bertsch and K. Hagino, PRC 107 044615 (2023).

K. Uzawa and K. Hagino, PRC 108 024319 (2024).

Calculate fission probability $T_{n,fis}$

$$T_{n,\mathrm{fis}}(E) = \gamma_n \gamma_{\mathrm{fis}} \sum_{\lambda\lambda'} \frac{f_\lambda^{(a)} f_{\lambda'}^{(a)*} f_\lambda^{(b*)} f_{\lambda'}^{(b)}}{(E-E_\lambda)(E-E_{\lambda'})^*}$$

$\begin{pmatrix} E_\lambda : \text{eigenenergy} \\ f_\lambda : \text{eigenvector} \end{pmatrix}$

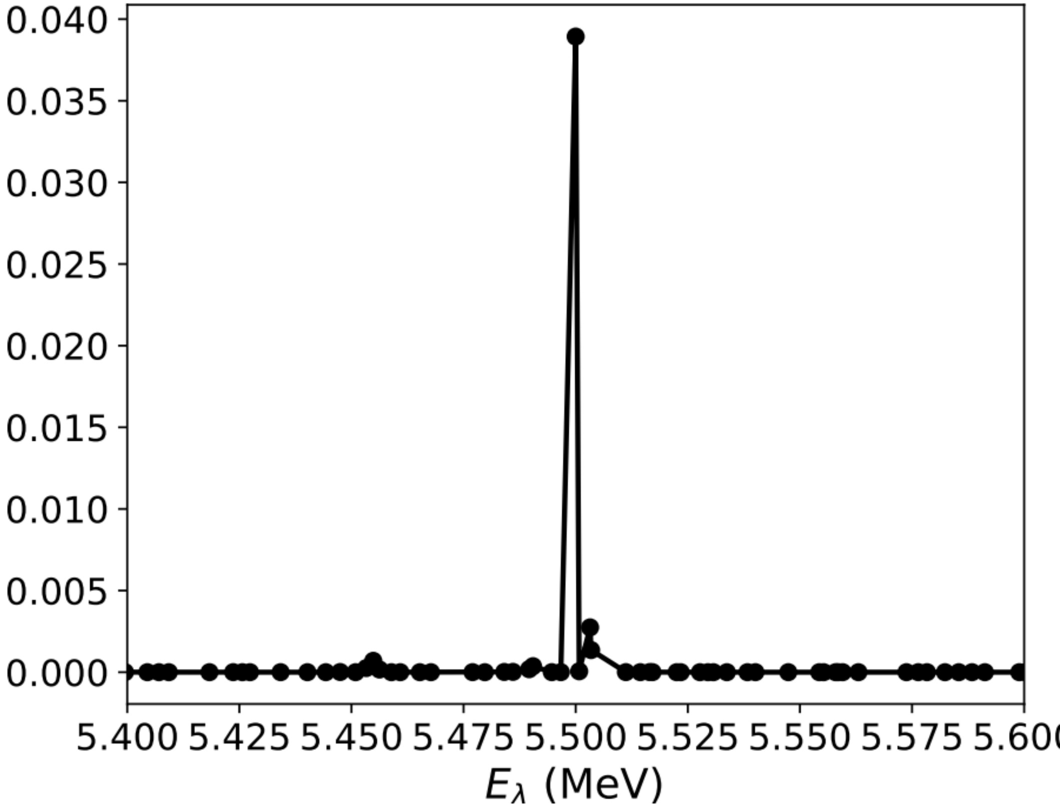
The summation is $\sum_{\lambda=1}^{66103}$.

But, λ with $E_\lambda \simeq E$ is dominant (right figure).

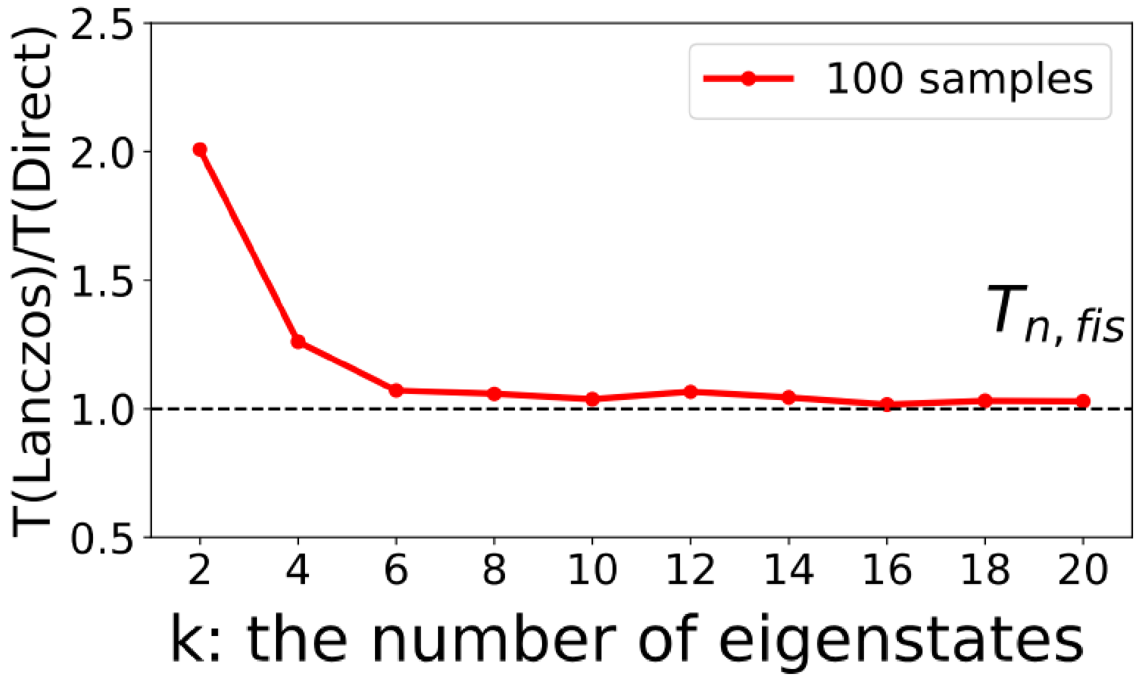
Reduce $\sum_{\lambda=1}^{66103} \to \sum_{\lambda=1}^{k}$.

Here k is the number of eigenstates calculated by shift-invert Lanczos

$$\sum_\lambda \frac{|f_\lambda^{(a)}|^2 |f_\lambda^{(b)}|^2}{|E-E_\lambda|^2} \quad (E = 5.5\mathrm{MeV})$$



The ratio $\frac{T_{\mathrm{n,fis}}\,(\mathrm{Lanczos})}{T_{\mathrm{n,fis}}\,(\mathrm{Direct})}$ **as a function of** k **(# of eigenstates)**

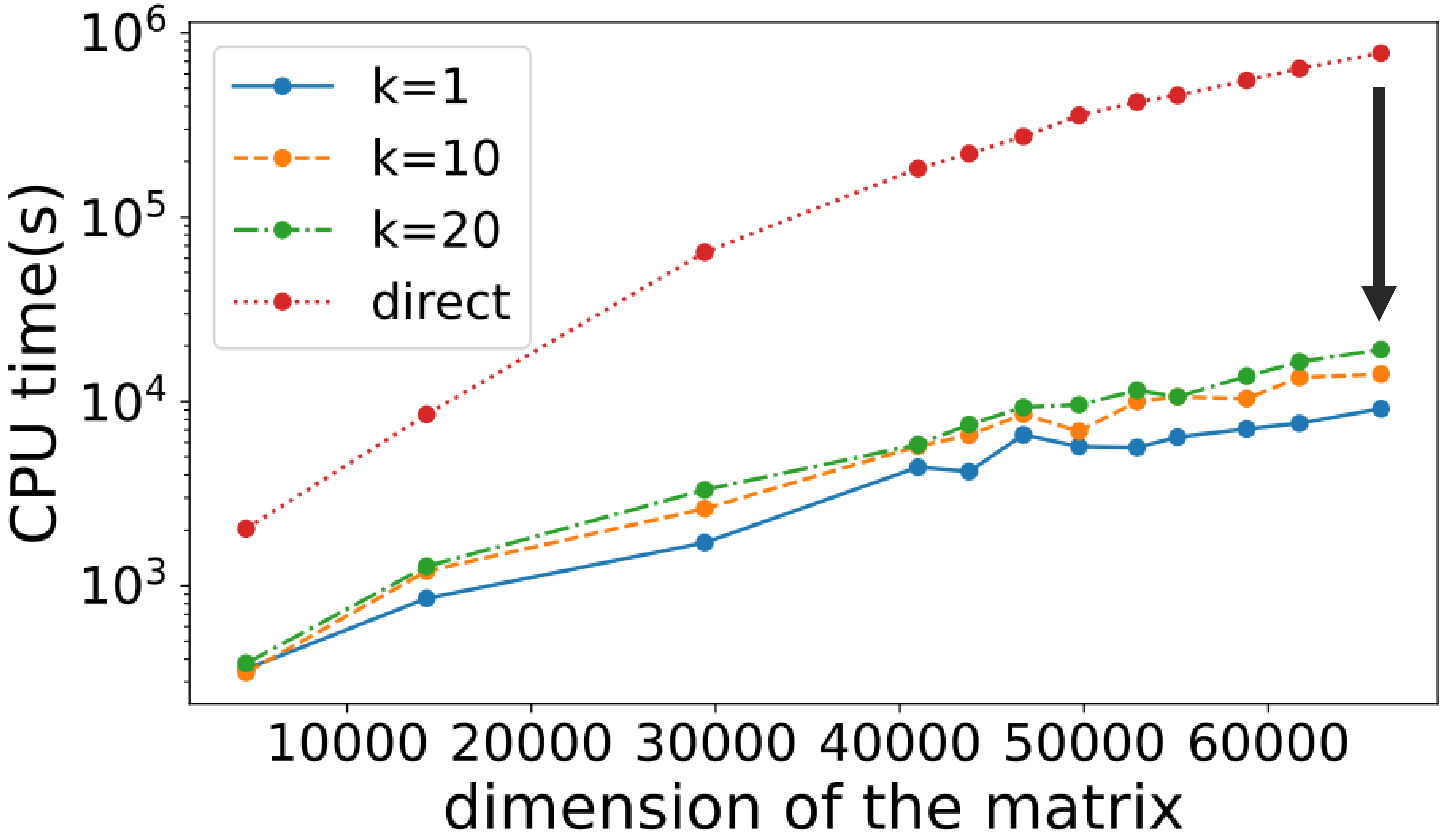


The ratio is close to one with $k \geq 6$**, and the error is about** 1%

The CPU time with different matrix dimensions

Red line : direct matrix inversion $G(E) = (E - H)^{-1}$ with LAPACK

Other lines : the shift-invert Lanczos calculations with ARPACK



30-40 time faster than direct calculations

Summary

- NEGF method is a promising way to describe fission microscopically, but requires huge numerical costs.
- We propose a novel method of calculating $T_{n,fis}(E)$ based on the shift-invert Lanczos + spectral decomposition of $G(E)$
- The error is about 1% and CPU time is about 30-40 time faster.

Shift-Invert Lanczos method is implemented in ARPACK library or SciPy library (scipy.sparse.linalg.eigsh).

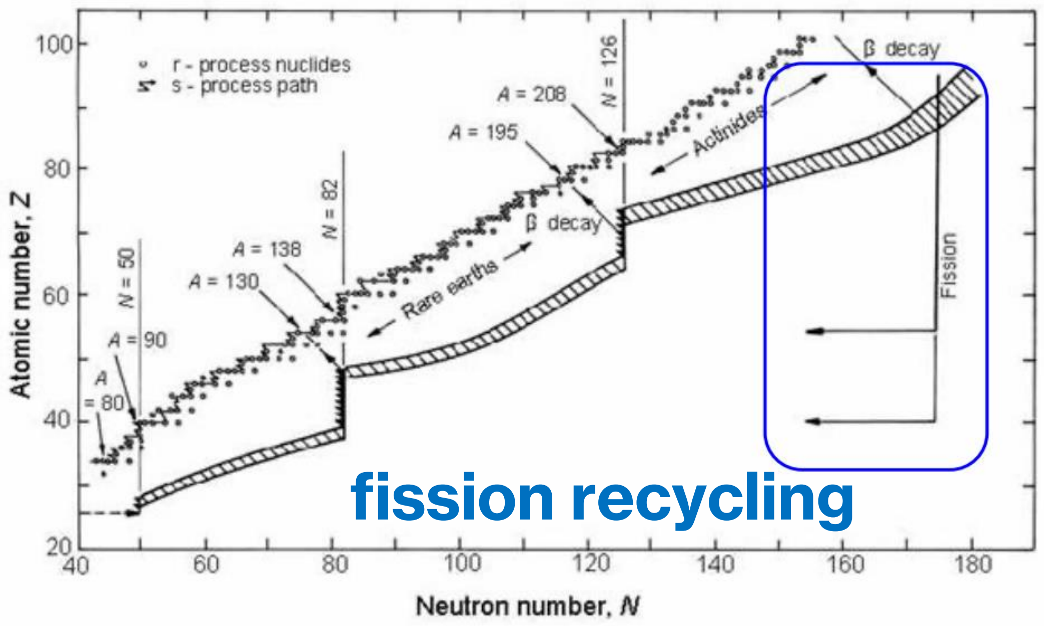
K. Uzawa and K. Hagino, arXiv:2408.06554

Why we need microscopic theory of fission ?

- In r-process, nuclear fission plays an important role (fission recycling)

fission of neutron-rich nuclei

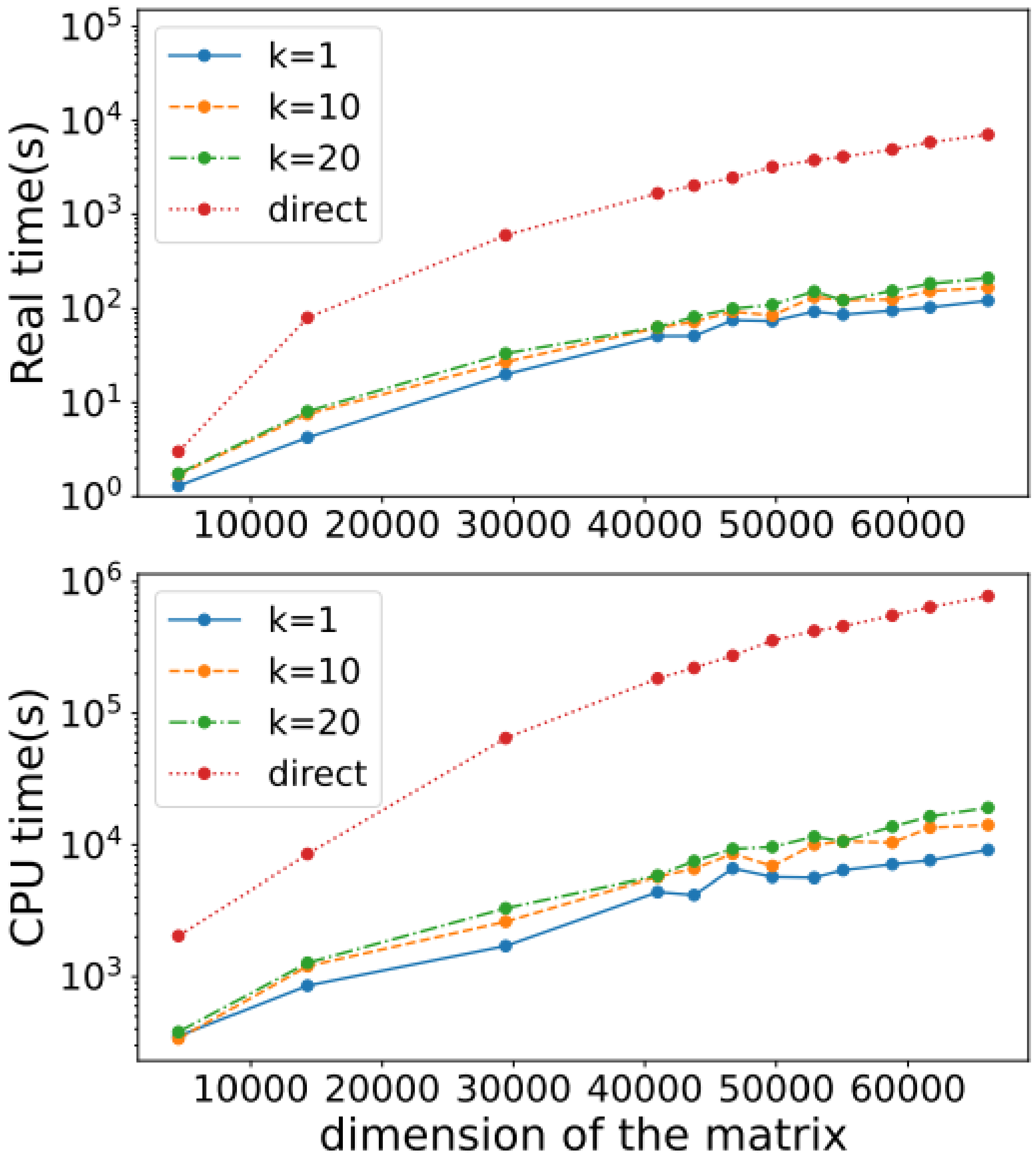
⇒ low S_n, low E^*, and low $\rho(E^*)$



Hauser-Feshbach theory or Langevin eq. may not be applicable...

⇒ Microscopic models without phenomenological assumptions

We apply **the non-equilibrium Green function method** to nuclear fission!



Real time(s)
k=1
k=10
k=20
direct
CPU time(s)
dimension of the matrix