

Application of the non-equilibrium
Green function method
to induced fission reactions

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Abstract

Nuclear fission is a process in which a heavy nucleus splits into two smaller nuclei. Fission plays an important role in many fields, such as nuclear engineering, r-process nucleosynthesis, or radioisotope beam production. Therefore, a precise and reliable theoretical calculation of nuclear fission, especially neutron-induced fission, is highly required. However, even though more than 80 years have passed since the discovery of fission, its microscopic theory has not been established. It is because fission is not only a large-amplitude motion, which is difficult to treat theoretically, but also causes complex interactions between collective and single-particle motions.

To establish a microscopic theory of induced fission reactions, we have developed a novel approach to induced fission based on the non-equilibrium Green's function (NEGF) method. The NEGF method has been widely applied to calculate the electronic properties of a transistor using its microscopic Hamiltonian. Focusing on the fact that a transistor's Hamiltonian and a Hamiltonian of fissioning nuclei have a similar structure, and the conductance of transistors is equivalent to the fission cross-section, application of the NEGF method to nuclear fission is considered to be effective.

In this thesis, we will first review the theoretical foundation of our model, which is based on the generator coordinate method and S-matrix theory.

Then, we will analyze the fluctuation of fission decay channels. Following Porter and Thomas' idea that the distribution of decay widths becomes the chi-squared distribution and its degrees of freedom correspond to the number of decay channels, we analyze the distribution of transmission coefficients of fission channels. Thereby, we discuss the microscopic origin of the degrees of freedom in fission channels.

Next, we will propose a novel approach to reduce the numerical costs of the NEGF method. The main idea is that according to the distribution of fission width, fission channels can be described by a small number of degrees of freedom, and if these essential parts are calculated efficiently, the numerical costs of the NEGF method will be reduced. To realize such efficient calculation, we will apply the shift-invert Lanczos method and demonstrate its effectiveness.

In the above chapters, we have restricted the model space to reduce numerical costs; therefore the results have not been fully realistic. In the following chapter, we will execute a calculation of fission cross sections with more realistic model space including finite seniority configurations and carefully

check the convergence of the results to the model parameters. Thereby we will discuss the applicability of our model and future challenges.

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1 Introduction

1.1 History of nuclear fission

Nuclear fission is a process in which a heavy nucleus splits into two smaller nuclei. In 1938, O. Hahn and F. Strassmann discovered that isotopes of Barium were emitted from Uranium targets under neutron bombardment [1]. In 1939, L. Meitner and O. R. Frisch pointed out that an atomic nucleus has the possibility of dividing itself into two smaller fragments based on the liquid drop model [2]. The important point was that in high Z nuclei the surface tension overcomes the coulomb repulsion slightly, and a small gain of energy by neutron absorption makes this system divide itself. In the same year, N. Bohr and J. Wheeler published an article in which they refined Meitner and Frisch’s picture and calculated the competition between the surface tension and the Coulomb force by expanding the nuclear shape using the spherical harmonics [3]. In addition, they introduced the transition state theory to calculate fission decay rates. This work established the theoretical foundation of nuclear fission, which remains valid until now. On the other hand, the quantum mechanical treatment of nuclear fission was started in Strutinsky’s paper in 1967 [4], in which he introduced nuclear shell effects to the liquid-drop model energy. Thereby, an asymmetry of fission fragment distributions was explained, and this work still remains the foundation of modern microscopic nuclear fission models.

Until now, numerous studies of nuclear fission have been done from experimental and theoretical viewpoints. However, there remain many unresolved problems about fission mechanisms, and especially the understanding of the microscopic mechanism of nuclear fission has been far from complete, as mentioned in the recent review paper [5]. This point will be discussed in detail later.

1.2 Topics related to nuclear fission

Fission plays an important role in many fields of nuclear physics. One example is the r-process nucleosynthesis [6, 7, 8]. In astrophysical environments where neutron flux is high, the neutron capture rates overcome the competing beta-decay rates, and neutrons are captured sequentially by the target nuclei. The resultant neutron-rich nuclei undergo β^- decay and are transformed into nuclei around the beta-stable line, though its yield is different from the one of

the s-process. In r-process yields, the 2nd peak around $A = 130$ is observed, and it is considered to originate from the fission fragment of neutron-rich actinide nuclei generated in the r-process [9, 10]. Therefore, in the numerical simulations of the r-process nucleosynthesis, the resultant yield is known to be sensitive to the input parameter of the fission properties [9, 10].

As another example, a synthesis of superheavy elements can be referred to [11, 12]. In the laboratory, superheavy elements are produced by heavy-ion collision experiments. The evaporation residue cross-sections can be factorized into the products of a fusion probability, a survival probability against quasi-fission, and a survival probability against fission. Compared with the fusion probability, the uncertainties of quasi-fission probability and fission probability are large partly due to the lack of theoretical understanding of these processes.

Nuclear fission is also important in the nuclear engineering field [13, 14]. To calculate neutron transport in the nuclear reactor, the Boltzmann equation is solved, where the fission cross sections of fuel nuclei are inputted [15]. In addition, the neutron-capture reaction competes with the fission reaction. Thereby, the fission-to-capture ratio becomes an important indicator of neutron multiplication rate. This quantity is sensitive to the internal structure of the many-body Hamiltonian and is used as a touchstone of a theoretical fission model [16].

Theoretically, nuclear fission itself is an interesting and challenging problem [5, 17, 18]. In the fission process, the shape of the nucleus changes drastically. It is one example of a large-amplitude motion, where a wave function is largely changed, and perturbation theory or linear response theories are not applicable. It complicates the theoretical treatment of fission. In addition, in the fission dynamics, the interplay between macroscopic and microscopic degrees of freedom should be appropriately treated. For example, the collective inertia is known to be sensitive to pairing interaction [17]. Additionally, energy transfer between macroscopic and microscopic degrees of freedom can be considered as a dissipation. It is phenomenologically included as a friction term in the equation of motion of the macroscopic coordinate, though there are many challenges in consistent treatments of macroscopic and macroscopic motions.

1.3 Motivation

As discussed above, the understanding of nuclear fission is not only an interesting problem as a quantum many-body problem but also important in related fields of science and engineering. To advance our understanding of nuclear fission, in this thesis, we formulate a theoretical fission model based on the microscopic degrees of freedom. A microscopic model has the strong advantage that it does not require any fitting parameters except for the nucleon-nucleon interaction terms in principle. Therefore, microscopic models are suitable for describing the fission process of unstable nuclei which are difficult to study experimentally, though important in r-process nucleosynthesis [6, 7, 8].

Thanks to the rapid growth of computational power including large-scale supercomputer systems, microscopic models of fission have greatly advanced since the onset of the 21st century. Most of those models are formulated based on the mean-field theory and its extensions. This is because the computational cost of mean-field theory increases moderately with respect to the nucleon number which is more than 200 for the actinoid nuclei.

Our theoretical model is also based on the Hartree-Fock approximation and the generator coordinate method (GCM) [19]. The application of the GCM leads to the possibility of overcoming the problem that the time-dependent Hartree-Fock theory fails to describe quantum tunneling of the fission barrier due to the lack of many-body correlation. In addition, our GCM-based framework has another advantage that the GCM Hamiltonian can be connected to a reaction theory in a transparent way. In the following, we apply S-matrix theory and derive a formula connecting the internal Hamiltonian and fission cross-section. Microscopic derivation of fission cross-section is a significant advantage of our theoretical approach, and we mainly focus on this quantity in the following discussion.

1.4 Outlines

This thesis is organized as follows. In chap. 2, we introduce theoretical concepts that are necessary to understand our approach. In chap. 3, we explain the theoretical foundations of our microscopic fission model. In chap. 4, we apply our framework to neutron-induced fission of ^{236}U and analyze the fluctuation of fission probability. Thereby, we explain a small number of the degrees of freedom of fission decay channels based on the GCM many-body

wave functions. In chap. 5, because our theoretical approach requires a high computational cost for the calculation of the Green functions, we apply the shift-invert Lanczos method to our fission model and overcome the problem of high computational cost. In chap. 6, we calculate the fission-to-capture branching ratio with a fully realistic model space and discuss the applicability of our model to realistic cases. In chap. 7, we summarize this thesis and discuss future directions.

2 Basic concepts of nuclear fission

In this chapter, we review the important concepts of nuclear fission. Though there have been many theoretical works on nuclear fission, we select essential topics to understand our theoretical framework explained in chap. 3.

2.1 The liquid drop model and fission barriers

Following the paper of Hahn and Strassmann [1], Meitner and Frisch pointed out that in the Uranium nucleus the surface tension and the Coulomb force are almost balanced, and by an external disturbance, the Coulomb force overcomes the surface tension that makes the system undergo fission. Bohr and Wheeler theoretically refined this discussion based on the liquid drop model and spherical harmonic expansion of the shape of the liquid drop [3]. In the liquid-drop model, a binding energy $B(N, Z)$ is parametrized as

$$B(N, Z) = a_V A - a_S A^{2/3} B_{\text{surf}} - a_C \frac{Z^2}{A^{1/3}} B_{\text{Coul}}, \quad (1)$$

where A is the nucleon number, and a_V , a_S , and a_C are the volume, surface, and Coulomb coefficients, respectively. The factor B_{surf} is the ratio of the surface energy for the deformed nucleus to the spherical nucleus, and B_{Coul} is defined in the same way. Then the fissility parameter x is defined as a ratio of the Coulomb and the surface force,

$$x \equiv \left(a_C \frac{Z^2}{A^{1/3}} \right) / (2a_S A^{2/3}), \quad (2)$$

which indicates how easily fission occurs. Using the fissility, the dimensionless deformation energy B_{def} is calculated as

$$B_{\text{def}} \equiv (a_S A^{2/3} B_{\text{surf}} + a_C \frac{Z^2}{A^{1/3}} B_{\text{Coul}}) / (a_S A^{2/3} + a_C \frac{Z^2}{A^{1/3}}) = (B_{\text{surf}} - 1) + 2x(B_{\text{Coul}} - 1). \quad (3)$$

Next, to calculate the explicit expressions of B_{surf} and B_{Coul} , we parametrize the nuclear shape r as

$$r(\theta) = R[1 + \alpha_2 P_2(\theta)], \quad (4)$$

where R is a radius of considered nuclei without deformation, and P_2 is the 2nd Legendre polynomial. Using deformation parameters α_2 , the surface and

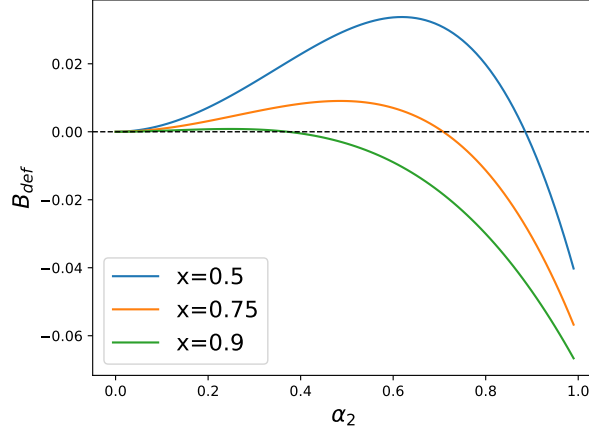


Figure 1: Deformation energy B_{def} as a function of α_2 with different x .

Coulomb energy ratios become [20]

$$B_{\text{surf}} = 1 + \frac{2}{5}\alpha_2^2 - \frac{4}{105}\alpha_2^3 - \frac{66}{175}\alpha_2^4 + \dots \quad (5)$$

and

$$B_{\text{Coul}} = 1 - \frac{1}{5}\alpha_2^2 - \frac{4}{105}\alpha_2^3 + \frac{51}{245}\alpha_2^4 + \dots \quad (6)$$

Therefore, B_{def} reads

$$B_{\text{def}} = \frac{2}{5}(1-x)\alpha_2^2 - \frac{4}{105}(2x+1)\alpha_2^3 + \frac{510x-462}{1225}\alpha_2^4 + \dots \quad (7)$$

Due to the coefficients of α_2^2 , if x exceeds one, the nucleus becomes unstable against quadrupole deformation. In fig. 1, we plot $B_{\text{def}}(\alpha_2)$ with different x , and it is confirmed that the fission barrier disappears as x approaches one.

2.2 Transition state theory

As discussed in the previous subsection, the liquid-drop model gives the foundation of static properties of nuclear fission. To describe fission dynamics, the authors of ref. [3] applied the transition state theory. In this theory, a microcanonical ensemble is assumed for fissioning nuclei which have excitation energy E . The fission decay width $\Gamma_{\text{fis}}(E)$ and the number of decaying

nuclei per unit time N_{decay} are related as

$$\rho(E)dE\Gamma_{\text{fis}}(E)/\hbar = N_{\text{decay}}. \quad (8)$$

Here $\rho(E)$ is the level density of compound states. Then, under the assumption that the degrees of freedom are separated into the collective motion and the others, we calculate N_{decay} . Here we use q and p for a collective coordinate and its conjugate momentum. In the direction of q there is a potential barrier and the states above the barrier are called transition states. We count the number of flux passing through the transition states,

$$\int_0^{p^*} v(dp/h)\rho^*(E - E_f - K)dE, \quad (9)$$

where v is the velocity of the collective motion, E_f is the height of the fission barrier, and ρ^* is the level density of the transition states. $(dp/h)\rho^*(E - E_f - K)dE$ represents the number of the quantum states with the momentum p in internal dp and the kinetic energy K in $dK = d(vp/2) = vdp$. Substituting $dK = vdp$, eq. (9) becomes,

$$\frac{dE}{h} \int_0^{E-E_f} dK \rho^*(E - E_f - K). \quad (10)$$

Assuming that the backscattered flux is negligibly small and comparing eq. (8) with eq. (10), the fission width becomes

$$\Gamma_{\text{fis}} = \frac{1}{2\pi\rho(E)} \int_0^{E-E_f} dK \rho^*(E - E_f - K). \quad (11)$$

Notice that we have applied the microcanonical ensemble to the compound states, and this derivation is justified only when $\rho(E)$ are sufficiently large.

2.3 The Gaussian Orthogonal Ensemble and the chi-squared distribution

In neutron-induced reactions, especially neutron-induced fission, a nucleus after absorbing a neutron is highly excited. Such a highly excited state is called a compound nucleus. Regardless of nuclides, compound nuclei show common properties in the distribution of the level densities (the Wigner distribution) or the decay widths (the Porter-Thomas distribution) [21]. However, a microscopic calculation of such highly excited nuclei is difficult due

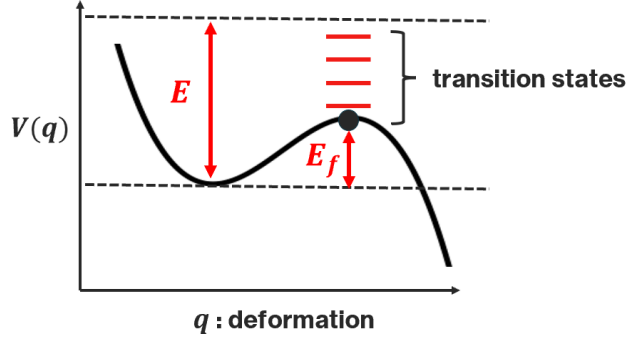


Figure 2: A schematic image of the transition state theory. q and $V(q)$ are the deformation parameter and the potential energy. E_f is the height of the fission barrier. There are transition states above the fission barrier and their number is integrated up to the excitation energy E .

to the complex configuration mixing. As an alternative method, Wigner introduced the Gaussian orthogonal ensemble (GOE) to describe the statistical properties of compound nuclei, which is one type of random matrix [22, 23, 24]. The matrix elements of a GOE Hamiltonian are given as

$$(H_{\text{GOE}})_{i,j} = vr_{i,j}(1 + \delta_{i,j}), \quad (12)$$

where $r_{i,j}(= r_{j,i})$ is a random number sampled from the standard normal distribution, and v is the size of the matrix elements. This Hamiltonian matrix represents the situation where all configurations interact randomly.

The eigensolution of a GOE matrix well reproduces the statistical properties of compound nuclei. In experiments, the distribution of level spacings of compound nuclei is known to be well fitted by the Wigner distribution [25],

$$P(x) = \frac{\pi}{2}x \exp(-\pi x^2/4). \quad (13)$$

Fig. 3 shows the distribution of the level spacings calculated by the GOE Hamiltonian with 2500 dimensions and $v = 1$, which is also well fitted by the Wigner distribution. At $x = 0$, $P(x)$ becomes zero, and it reflects the effects of the level repulsion due to the mixing of basis configurations.

In addition, the eigenvector of a GOE Hamiltonian has an important statistical property: the components of each eigenvector follow the Gauss distribution in the large matrix-size limit. Fig. 4 shows the distribution of

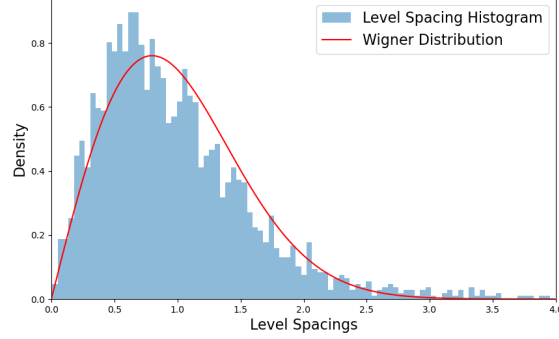


Figure 3: The distribution of level spacings calculated by diagonalizing the GOE Hamiltonian with 2500 dimensions and $\nu = 1$. The level spacings are normalized by dividing by their average.

the components of a certain GOE eigenvector, which follows well the Gauss distribution. This property is a foundation of the following discussion about the statistical properties of decay widths. In ref. [26], Porter and Thomas pointed out that the distribution of the neutron width Γ_n of ^{236}U is well fitted by the chi-squared distribution with $\nu = 1$,

$$P_\nu(x) = \frac{\nu}{2\Gamma(\nu/2)} \left(\frac{\nu x}{2}\right)^{\nu/2-1} e^{-\nu x/2}. \quad (14)$$

The variable of the chi-squared distribution Q is the sum of the squares of the variables $X_1, X_2, \dots, X_\nu$ following the independent normal distributions,

$$Q = \sum_i^\nu X_i^2. \quad (15)$$

Keeping in mind this property, we consider the decay of a compound nucleus. To this end, we introduce a decay width matrix Γ which has ν diagonal matrix elements γ , i.e.,

$$\Gamma = \begin{pmatrix} \gamma & & & \\ & \ddots & & \\ & & \gamma & \\ & & & 0 \\ & & & & \ddots \end{pmatrix}. \quad (16)$$

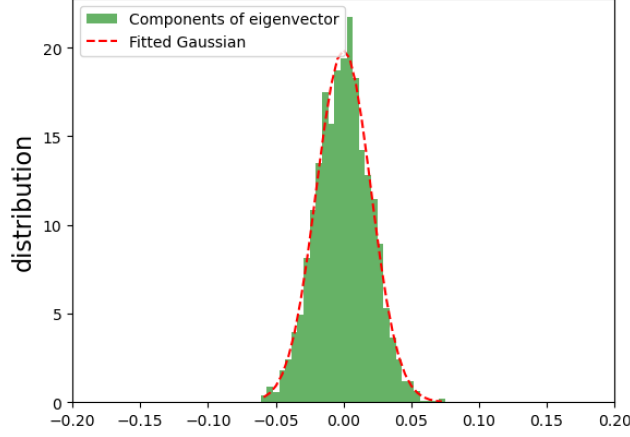


Figure 4: The distribution of the components of a certain GOE eigenvector fitted by the Gauss distribution. The result does not depend on which eigenvectors are chosen.

Then we solve eigenvalue problem for the non-Hermite Hamiltonian $H_{\text{GOE}} - \frac{i}{2}\Gamma$. Typically, the size of decay width γ is much smaller than the size of the GOE matrix elements v . Therefore a perturbative treatment of the imaginary part is justified. The imaginary part of the eigenenergy E_k is calculated as

$$-2\text{Im}(E_k) = \langle k|\Gamma|k\rangle = \sum_{i=1}^{\nu} |\langle i|k\rangle|^2, \quad (17)$$

where $|i\rangle$ is the basis used in eq. (12) and $|k\rangle$ is the one eigenstates. Due to the properties of the GOE matrix, $\langle k|\Gamma|k\rangle$ follows the chi-squared distribution with ν degrees of freedom. Note that the number of the decay channel is equal to the degrees of freedom ν . In low-energy neutron reactions on ^{235}U targets, neutron channels are closed except for the one elastic channel. Therefore, the values of Γ_n are distributed according to the chi-squared distribution with $\nu = 1$ [26], and it is consistent with the above discussion.

2.4 S-matrix dispersion formula

To describe compound nucleus reactions, we need to relate reaction channels and internal configurations. As a first step, we divide the considered model space into P -space and Q -space. Here P -space includes reaction channels,

and Q -space contains mono-nucleus quasi-bound states. The projection operators $\hat{P}$ and $\hat{Q}$ satisfy the following relations,

$$\hat{P} + \hat{Q} = 1, \quad \hat{P}^2 = \hat{P}, \quad \hat{Q}^2 = \hat{Q}, \quad \hat{P}\hat{Q} = \hat{Q}\hat{P} = 0. \quad (18)$$

Inserting the projection operators into the Schrödinger eq.,

$$(E - H)\Psi = 0, \quad (19)$$

we obtain the equations within P -space and Q -space as

$$(E - H_{PP})\hat{P}\Psi = H_{PQ}\hat{Q}\Psi \quad (20)$$

and

$$(E - H_{QQ})\hat{Q}\Psi = H_{QP}\hat{P}\Psi, \quad (21)$$

where $H_{PP} = \hat{P}H\hat{P}$, $H_{QQ} = \hat{Q}H\hat{Q}$, and $H_{PQ} = \hat{P}H\hat{Q}$. H_{QQ} is the Hamiltonian of bound states, and the eigenstates of a compound nucleus are defined as

$$(E_\lambda - H_{QQ})X_\lambda = 0. \quad (22)$$

To calculate the S -matrix, the continuum wavefunctions $\hat{P}\Psi$ are needed. From eqs. (20) and (21), $\hat{P}\Psi$ satisfies

$$(H_{PP} + H_{PQ} \frac{1}{E - H_{QQ}} H_{QP})\hat{P}\Psi = E\hat{P}\Psi. \quad (23)$$

Applying $(E + i\delta - H_{PP})^{-1}$ to eq. (23), we obtain,

$$\begin{aligned} P\Psi^{(+)} &= \psi^{(+)} + \frac{1}{E + i\delta - H_{PP}} H_{PQ} \frac{1}{E - H_{QQ}} H_{QP} P\Psi^{(+)} \\ &= \psi^{(+)} + \frac{1}{E + i\delta - \tilde{H}_{PP}} H_{PQ} \frac{1}{E - H_{QQ}} H_{QP} P\psi^{(+)} \\ &= \psi^{(+)} + \frac{1}{E + i\delta - H_{PP}} H_{PQ} \frac{1}{E - \tilde{H}_{QQ}} H_{QP} P\psi^{(+)}. \end{aligned} \quad (24)$$

Here $\psi^{(+)}$ is a solution of

$$(E - H_{PP})\psi^{(+)} = 0, \quad (25)$$

$\tilde{H}_{PP} = H_{PP} + H_{PQ} \frac{1}{E - \tilde{H}_{QQ}} H_{QP}$, and $\tilde{H}_{QQ} = H_{QQ} + H_{QP} \frac{1}{E - \tilde{H}_{PP}} H_{PQ}$. Using the solution of eq. (24), $\Psi_a^{(+)}$ and its similar incoming solution $\Psi_b^{(-)}$, S matrix elements becomes

$$S_{ab}(E_a)\delta(E_a - E_b) = \langle \Psi_a^{(-)} | \Psi_a^{(+)} \rangle, \quad (26)$$

where

$$S_{ab} = S_{ab}^0 - 2\pi i \langle \psi_a^{(-)} | H_{PQ} \frac{1}{E - \tilde{H}_{QQ}} H_{QP} | \psi_a^{(+)} \rangle. \quad (27)$$

Inserting some complete basis of the Q space, $|\mu\rangle$, S_{ab} becomes

$$\begin{aligned} S_{ab}(E) &= S_{ab}^0(E) - 2i\gamma_{a\mu}^\dagger (E - \tilde{H}_{QQ})_{\mu\nu}^{-1} \gamma_{\nu b} \\ &= S_{ab}^0(E) - 2i\gamma_{a\mu}^\dagger (E\delta_{\mu\nu} - (H_{QQ} + \Delta)_{\mu\nu} - i\pi \sum_c \gamma_{\mu c} \gamma_{c\nu}^\dagger)^{-1} \gamma_{\nu b}. \end{aligned} \quad (28)$$

where $\gamma_{\mu a} = \sqrt{\pi} \langle \mu | H_{QP} | \psi_a^{(+)} \rangle = \sqrt{\pi} \langle \psi_a^{(-)} | H_{PQ} | \mu \rangle$.

Supposing the basis sets $|\mu\rangle$ are many-body configurations, the parameters in eq. (28) are calculated based on a microscopic model. In this case, $\gamma_{\mu a}$ represents the coupling strength between the continuum channel a and the configuration $|\mu\rangle$. The transmission coefficient T_{ab} between channels a and b ($a \neq b$) also becomes [27]

$$\begin{aligned} T_{ab} &\equiv |S_{ab}|^2 \\ &= (2\pi)^2 \left(\sum_{\mu_1, \mu_2} W_{\mu_1, a} G_{\mu_1, \mu_2}^* W_{\mu_2, b} \right) \left(\sum_{\mu_3, \mu_4} W_{\mu_3, a} G_{\mu_3, \mu_4} W_{\mu_4, b} \right) \\ &= \sum_{\mu_1, \mu_2, \mu_3, \mu_4} ((\Gamma_a)_{\mu_1, \mu_3} G_{\mu_2, \mu_1}^\dagger (\Gamma_b)_{\mu_2, \mu_4} G_{\mu_3, \mu_4}) \\ &= \sum_{\mu_1, \mu_2, \mu_3, \mu_4} ((\Gamma_a)_{\mu_1, \mu_3} G_{\mu_3, \mu_4} (\Gamma_b)_{\mu_4, \mu_2} G_{\mu_2, \mu_1}^\dagger) \\ &= \text{Tr}[\Gamma_a G(E) \Gamma_b G^\dagger(E)]. \end{aligned} \quad (29)$$

This trace formula is well known in the electron transport simulation in nano-devices with the non-equilibrium Green function [28, 29, 30, 31, 32, 33]. It suggests that the induced fission reaction can be formulated in a similar way to the electron transport in nano-devices.

2.5 Electron transport in nano-devices

A description of electron transports in electronic many-body systems is an important topic in the design of nano-devices. The non-equilibrium Green function (NEGF) method is an efficient computational method to calculate the electronic properties of nanodevices [34, 35]. The equation (29) can be derived based on the Keldish non-equilibrium Green function formalism [36, 37] and has been applied to describe the electron transport in a nanoscale transistor.

A field effect transistor (FET) includes a source electrode, a channel semiconductor, and a drain electrode, as shown in fig. 5. Both electrodes play the role of the electron reservoir, and are connected to the channel region. If the bias voltage is zero, $V_L = V_R$ and $\mu_L = \mu_R$. Hence the system is in equilibrium. By applying the voltage such that $V_L < V_R$, the electrons in the source tend to flow to the drain through the channel region. The NEGF method gives its conductance as a function of the bias voltage $V_R - V_L$.

In the NEGF method, first, we divide the total Hamiltonian into the three spaces as

$$H = \begin{pmatrix} H_L & V_L & 0 \\ V_L^T & H_C & V_R \\ 0 & V_R^T & H_R \end{pmatrix}. \quad (30)$$

Here H_L , H_C , and H_R correspond to the source, the channel, and the drain regions. Typically the dimensions of H_L and H_R are much larger than the one of H_C since miniaturization of the channel size is required for better performance of transistors. Therefore direct calculation of the side regions requires a lot of numerical costs. We avoid this problem by the construction of the effective Hamiltonian in the channel region,

$$\begin{aligned} H_{\text{eff}}(E) &= H_C + V_L^T \frac{1}{E - H_L + i\epsilon} V_L + V_R^T \frac{1}{E - H_R + i\epsilon} V_R \\ &= H_C + \Sigma_L(E) + \Sigma_R(E). \end{aligned} \quad (31)$$

Here E is the energy of the electrons, which is equal to $eV_R - eV_L$. The important point is that the interaction regions between the source and the channels are localized around its boundaries, and we do not need full information on the Hamiltonian matrix H_L for the calculation of the self energy $\Sigma_L(E)$. The same is true for the drain region. Using the scattering theory, the transmission coefficient from the source to the drain is calculated as [38]

$$T(E) = \text{Tr}[\Gamma_L G(E) \Gamma_R G^\dagger(E)], \quad (32)$$

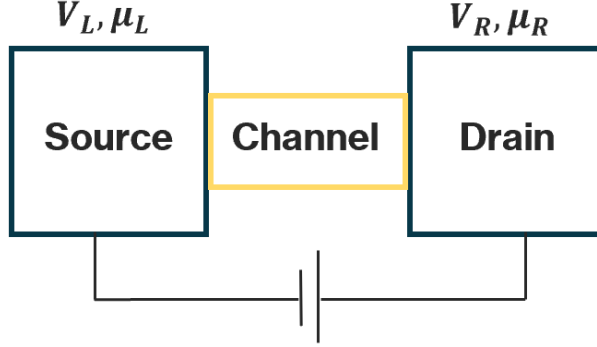


Figure 5: A schematic picture of a field effect transistor. V_i and μ_i ($i = L$ or R) are reservoirs' voltages and chemical potentials.

where

$$G(E) = (E - H_{\text{eff}}(E))^{-1} \quad (33)$$

and

$$\Gamma_{L,R} = i(\Sigma_{L,R} - \Sigma_{L,R}^\dagger). \quad (34)$$

This is the main result of the NEGF calculation. The total current I is also calculated using $T(E)$ as

$$I = \frac{e}{h} \int_{-\infty}^{+\infty} dE T(E) [f_L(E - \mu_L) - f_R(E - \mu_R)], \quad (35)$$

where f_L and f_R are the Fermi-Dirac distribution functions of the reservoirs.

3 Formulation of the NEFG-based fission model

To develop a reliable microscopic model of induced fission, we reformulate the NEGF method in the words of nuclear theory and apply it to neutron-induced fission reactions. For this goal, we need to construct the internal Hamiltonian H and the decay widths Γ_a . Thereafter, we compute the Green function $G(E)$ and transmission coefficients of induced fission reaction, $T_{n,\text{fis}}$, based on eq. (29). This quantity is proportional to the fission cross section as,

$$\sigma_{n,\text{fis}}(E) = \frac{\pi}{k_n^2} T_{n,\text{fis}}(E), \quad (36)$$

where k_n is the wavelength of the incoming neutron. Since there is no other theory that can compute fission cross section microscopically, this point is a prominent advantage of the NEGF approach. The details of these points will be discussed in the following.

3.1 Internal Hamiltonian

In the nuclear fission process, the effects of collective deformation are important. To incorporate it, the GCM has been widely applied [19]. In this method, we prepare many-body states $|Q\rangle$ labeled by the collective parameter Q and superpose them as

$$|\text{GCM}\rangle = \int dQ f(Q) |Q\rangle, \quad (37)$$

where $f(Q)$ is a weight function. $f(Q)$ is determined by solving the Hill-Wheeler equation,

$$\int dQ' \langle Q | H | Q' \rangle f(Q') = E \int dQ' \langle Q | Q' \rangle f(Q'), \quad (38)$$

which is delivered by the variational condition. For the GCM basis $|Q\rangle$, the Hartree-Fock(-Bogoliubov) wavefunctions obtained with the constraints on Q parameter are standardly applied. However, it fails to take into account single-particle excitations. In induced fission reactions, the fissioning mother nucleus is in high temperatures and single-particle excitations become important. To overcome this defect, the GCM can be augmented. In ref. [39], the authors superposed not only the local ground states $|Q\rangle$ but also the

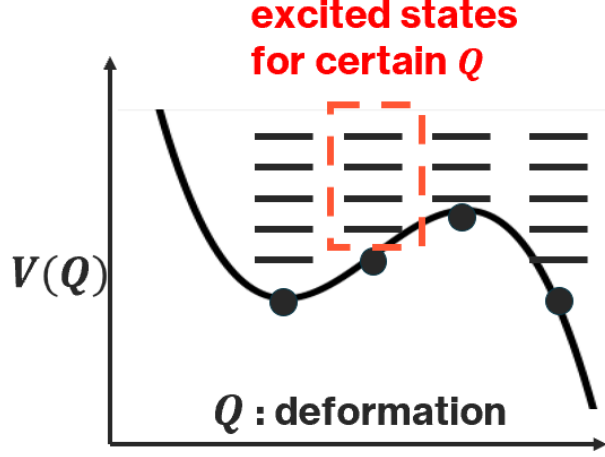


Figure 6: Schematic representation of GCM basis in eq. (39).

two-quasi-particle excited states $\alpha_{i1}^\dagger \alpha_{i2}^\dagger |Q\rangle$. Following them, we construct the GCM wavefunction as

$$|\text{GCM}\rangle = \int dQ \sum_{\mu} f_{\mu}(Q) |Q, E_{\mu}\rangle, \quad (39)$$

where $|Q, E_{\mu}\rangle$ is the Hartree-Fock wavefunction having the expectation value of the quadrupole moment $\langle \hat{Q} \rangle = Q$ and the particle-hole excitation energy E_{μ} . Unlike ref. [39], we incorporate any number of particle-hole pairs up to a certain energy cutoff. Using the GCM basis in eq. (39), we calculate the norm kernel

$$N_{i,i'} = \langle i|i'\rangle = \langle Q, E_{\mu}|Q', E_{\mu'}\rangle, \quad (40)$$

and the Hamiltonian kernel

$$H_{i,i'} = \langle i|H|i'\rangle = \langle Q, E_{\mu}|H|Q', E_{\mu'}\rangle, \quad (41)$$

with $|i\rangle \equiv |Q, E_{\mu}\rangle$. Fig. 6 shows the schematic representation of the GCM basis in eq. (39). At each Q , there are excited states above the local ground states. This is analogous to the microscopic models of electron transport in solid systems, where at each lattice point different electron states are located, and the electronic current flows among them [38].

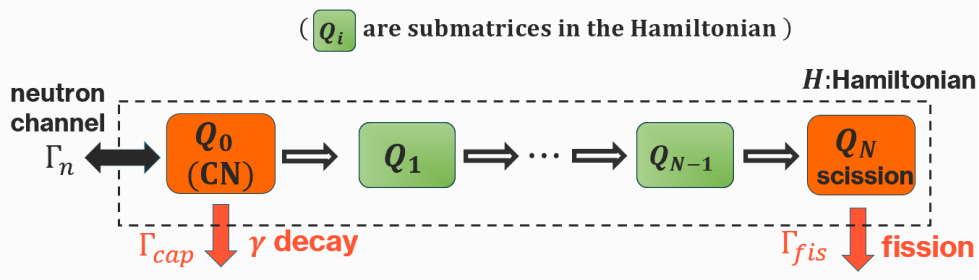


Figure 7: Schematic image of our model. The squares with Q represent the diagonal sub-matrices in the Hamiltonian matrix.

3.2 Decay width matrices

In low-energy neutron-induced reactions, the main decay channels of a compound nucleus are neutron channels, capture channels, and fission channels. Neutron emissions and gamma decay are considered to occur in compound nucleus configurations. On the other hand, fission occurs in scission configurations. In our model, we regard the diagonal sub-block of the Hamiltonian matrix labeled with the smallest Q as compound nucleus configurations. Similarly, the diagonal sub-block with the largest Q is considered as scission configurations. Therefore, the former sub-block includes the neutron width Γ_n and the capture width Γ_{cap} , and the later sub-block has the fission width Γ_{fis} . Fig. 7 shows the schematic image of this structure (see also fig. 10).

In principle, we can calculate these decay widths microscopically. However, our main purpose is to understand fission mechanism, and we take the value of Γ_n and Γ_{cap} from the Reference Input Parameter Library (RIPS) [40]. The values of decay widths taken from this library are energy-averaged ones. Therefore the decay width matrices have the same averaged values in their diagonal parts and the off-diagonal elements should be zero. Regarding the fission width, the insensitivity of the fission cross section to the size of Γ_{fis} is known [16]. Therefore, we check the convergence of results to the value of Γ_{fis} and use a value that ensures convergence.

3.3 Transmission coefficients

To calculate transmission coefficients $T_{n,\text{cap}}$ and $T_{n,\text{fis}}$ based on the trace formula,

$$T_{n,j} = \text{Tr}[\Gamma_n G(E) \Gamma_j G^\dagger(E)] \quad (j = \text{cap or fis}), \quad (42)$$

we need the Green function matrix,

$$G(E) = (EN - H + \frac{i}{2}\Gamma)^{-1}. \quad (43)$$

Here N and H are the overlap matrix and the Hamiltonian matrix defined in eqs. (40,41), E is the excitation energy of the target nuclei, being the sum of the neutron separation energy S_n and the neutron kinetic energy E_n , and $\Gamma = \Gamma_n + \Gamma_{\text{cap}} + \Gamma_{\text{fis}}$ is the total width. By inverting the matrix $(EN - H + \frac{i}{2}\Gamma)$, the Green function is calculated. However, it requires huge numerical costs when applied to nuclear fission because the dimension of the matrix becomes very large. In the case of neutron-induced fission of ^{235}U , the dimension was estimated to be $O(10^6)$ [16].

To overcome this problem, we will apply the method introduced in ref. [41], in which the Green function is efficiently calculated by using the Hamiltonian's block-tridiagonal structure. In addition, we have developed a novel method of computing the Green function using the shift-invert Lanczos method [42]. This method has the advantage of not requiring the block-tridiagonal structure, and its detail will be explained in chap. 5.

After calculating the Green functions, the capture cross section and the fission cross section are derived using eq. (36). Thereby we numerically compare the results with experimental data.

4 Analysis of fluctuations in fission reactions

The NEGF approach was applied to neutron-induced fission as a preliminary calculation in ref. [16]. In that paper, only neutron seniority-zero configurations in ^{236}U were included for the model space because this approach requires matrix inversion calculation of a large dimensional Hamiltonian matrix. In addition, the second fission barrier was not taken into account, and fission was assumed to occur just after the first fission barrier. Therefore, in this chapter, we enlarge the model space and include both neutron and proton excitations and the double barriers.

With the extension of the model space, we will analyze the distribution of fission width. As discussed in sec. 2.3, the distribution of decay widths is characterized by the chi-squared distribution with the degrees of freedom ν [22, 26], which reflects the number of open exit channels. On the other hand, it has been known that the distribution of the fission widths is characterized by a small values of ν , despite the fact that the number of fission decay channels is about the order of 10^{10} in low-energy neutron-induced fission [43]. For example, in the analysis of $^{235}\text{U}(n, f)$ reaction, the distributions of the fission widths were well-fitted by the chi-squared distribution with $\nu = 2$ [44].

The small values of ν have been explained based on the transition state theory: fission takes place through a few transition states above a fission barrier, and the number of degrees of freedom corresponds to the number of open transition states [26]. However, the derivation of transition state theory relies on the macroscopic classical model, and there is still no explanation of the small value of ν based on the quantum theory of many-body systems. Thus, in this chapter, we discuss the origin of the small ν based on the NEGF fission model. The contents in this chapter are summarized in ref. [45]

4.1 GCM bases

We apply the theoretical framework detailed in sec. 3 to neutron-induced fission of ^{235}U . First, we prepare many-body basis for the GCM calculation. We solve the Skyrme-Hartree-Fock equation with the constraint on the mass quadrupole moment $Q_{20} \equiv Q$ (The details of the Hartree-Fock calculation are summarized in Appendix. B). As a solver of the Skyrme-Hartree-Fock equation, we apply the Skyax code [46], in which the equation is solved in the cylindrical coordinate space. As a Skyrme energy functional, we apply the

UNEDF1 parameter set [47], which was parametrized to reproduce the energy of fission isomers of the actinide nuclei. Fig. 8 shows the potential energy surface of ^{236}U as a function of the quadrupole moment and the octupole moment. The ground state is located around $Q_2 = 14b$ and $Q_3 = 0$. By fixing the value of Q_2 and optimizing the energy in the Q_3 direction, we can determine the fission path as shown in fig. 8. Up to the first fission barrier, the deformation is parity symmetric, and after the first barrier Q_3 becomes finite.

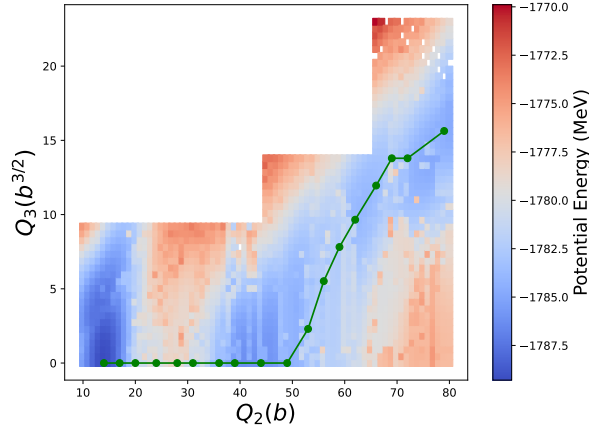


Figure 8: The potential energy of ^{236}U as a function of Q_2 and Q_3 . The upper-left corner of the figure is blank because the shape of the fissioning nucleus is parity symmetric with small Q_2 . The green solid line shows the fission path determined from the potential energy surface.

In numerical calculations of the GCM, generator coordinates are discretized. Following the previous work [16], we discretize the coordinate Q with the criterion that the overlap between the nearest neighbor local ground state becomes $\langle Q|Q' \rangle = e^{-1}$. The range of Q is from $Q = 14b$, where ground states are located to $Q = 83b$ just after the second fission barrier. Fig. 9 shows the potential energy curve along the fission path in the blue line as a function of Q . 13 reference points are selected after the discretization, and we can confirm the first and second fission barriers around $Q_2 = 30b$ and $Q_2 = 60b$, respectively.

From the reference states $|Q\rangle$, we generate many particle-hole excited

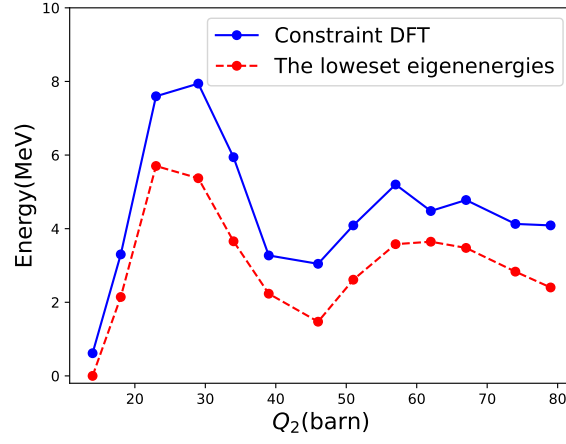


Figure 9: The blue solid line shows the potential energy of ^{236}U along the fission path as a function of the quadrupole moment, Q_2 . It is scaled by a factor of 0.71 (see the main text). The red dashed line shows the lowest eigenenergy after diagonalizing each Q -block, off-diagonal elements of which are the residual pairing interaction. The origin of the energy is set at the lowest eigenvalue at $Q_2=14\text{b}$.

states as

$$a_{p(Q)}^\dagger a_{h(Q)} |Q\rangle, a_{p(Q)}^\dagger a_{p'(Q)}^\dagger a_{h(Q)} a_{h'(Q)} |Q\rangle, \dots \quad (44)$$

These excited states are labeled by its particle-hole excitation energy E_μ as $|Q, E_\mu\rangle$. In the previous work, neutron particle-hole excitation up to 4 MeV was taken into account [16]. Here we extend the model space to include both proton and neutron excitations. The energy cutoff is set to 5 MeV for both proton excitation and neutron excitation at each Q . On the other hand, the seniority quantum number of the configurations is restricted to zero as in the previous work [16]. This is because the inclusion of finite seniority configurations increases numerical cost drastically. Even in the seniority zero case, the dimension of the Hamiltonian becomes 6.6×10^4 as shown in table 1, and it requires a huge numerical cost for the calculation of the Green function.

$Q_2(\text{barn})$	14	18	23	29	34	39	46	51	57	62	67	74	79	83	total
dim.	N_{GOE}	2520	9794	15088	11577	2774	2940	3021	3150	2196	3752	2871	4420	N_{GOE}	$64103 + 2N_{\text{GOE}}$

Table 1: The dimension of the diagonal submatrices labeled by Q_2 in the Hamiltonian (see fig.10). N_{GOE} is the dimension of the GOE matrices, and $N_{\text{GOE}} = 1000$ is used in this chapter.

4.2 GCM kernels

The next step is the calculation of the off-diagonal elements of the norm kernel and the Hamiltonian kernel. Based on the Gaussian overlap approximation, the off-diagonal term of the norm kernel between configurations at Q and Q' decreases exponentially with the square of $\Delta Q = Q' - Q$. Therefore, we neglect the off-diagonal term between blocks separated by more than two blocks, making the norm kernel and the Hamiltonian kernel block-tridiagonal (see fig. 10). We will refer to the diagonal sub-blocks as Q -blocks. This treatment also corresponds to the tight-binding approximation in solid state systems.

In the actual calculations of the norm kernel, the off-diagonal matrix elements between diabatically connected configurations are set to be e^{-1} , and other elements are set to zero. This treatment greatly reduces memory usage when the matrices are stored in a sparse matrix format. Due to this treatment, the Hamiltonian matrix also becomes sparse.

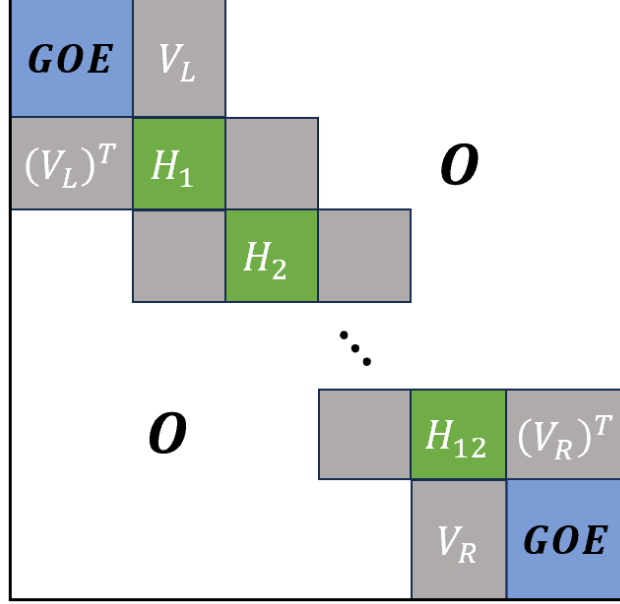


Figure 10: A schematic illustration of the Hamiltonian matrix.

In the calculation of the Hamiltonian kernel, as residual interactions, we apply a monopole pairing interaction,

$$H_{\text{pair}} = -G \sum_{i \neq j} a_i^\dagger a_i^\dagger a_j^\dagger a_j, \quad (45)$$

and a diabatic interaction, [48]

$$\frac{\langle Q, E_\mu | v_{ab} | Q', E_{\mu'} \rangle}{\langle Q, E_\mu | Q', E_{\mu'} \rangle} = \frac{E(Q, E_\mu) + E(Q', E_{\mu'})}{2} + h_2 \ln(\langle Q, E_\mu | Q', E_{\mu'} \rangle). \quad (46)$$

The pairing interaction connects configurations in the adiabatic way: the deformation causes the band crossing, and the pairing interaction is necessary to connect the ground state configurations before and after the crossing [49]. On the other hand, the diabatic interaction connects diabatically connected configurations complementarily. The monopole pairing strength G is determined to reproduce the excitation energy of the first excited 0^+ state of ^{236}U , which becomes $G = 0.16$ MeV. Regarding h_2 , the value of h_2 is microscopically estimated in ref. [16], and we use the same value, $h_2 = 1.5$ MeV.

The red line in fig. 9 shows the lowest eigenvalue obtained by diagonalizing each Q -blocks. The height of a fission barrier is sensitive to the pairing interaction, and we have to compare the red line in fig. 9 the experimental fission barrier heights, not the blue line. To reproduce the barrier height 5.7 MeV [44], we scale the blue solid line in fig. 9 by a factor 0.71. Then we diagonalize the Hamiltonian for each Q -block. Thereby, the top of the red dashed line in fig. 9 is located at 5.7 MeV. As we have mentioned, in the calculation of the Skyrme-Hartree-Fock equation, the axial symmetry is assumed. On the other hand, the height of the first fission barrier is lowered by the triaxial deformation [50], which may be the cause of the overestimation.

4.3 GOE matrices

The left-end Q block at $Q = 14b$ can be regarded as compound states, which is well described by a GOE matrix. The GOE is characterized by two parameters, the dimension of the matrix N_{GOE} and the size of the matrix elements v in eq. (12). In the following calculation, we set $v = 0.317$ MeV and $N_{\text{GOE}} = 1000$ with some arbitrariness. In addition, we shift the central energy of the GOE matrix by adding the constant matrix. This energy corresponds to the excitation energy of the compound nucleus and depends on the setup. The Q -block after the second fission barrier corresponds to the doorway state to the fission decay, and it is highly excited. Therefore we also replace the block at $Q = 83b$ with a GOE matrix with the same parameter with the GOE matrix at $Q = 14b$.

4.4 Width matrices

The left-end GOE matrix includes neutron and capture decay widths. In low-energy neutron reactions, one neutron channel is open [26]. Therefore the matrix Γ_n has one diagonal component γ_n in the first diagonal component. It gives the chi-squared distribution with the degrees of freedom one as explained in sec. 2.3. On the other hand, there are multiple capture channels, and Γ_{cap} has the following structure,

$$\Gamma_{\text{cap}} = \begin{pmatrix} \tilde{\Gamma}_{\text{cap}} & 0 & & \\ 0 & 0 & & \\ & & \ddots & \\ & & & 0 \end{pmatrix}, \quad (47)$$

where $\tilde{\Gamma}_{\text{cap}} = \gamma_{\text{cap}} I$, with I being the unit matrix with the dimension N_{GOE} . Regarding fission width, since the right-end GOE configurations are the doorway states of fission, Γ_{fis} is given by

$$\Gamma_{\text{fis}} = \begin{pmatrix} 0 & & & \\ & \ddots & & \\ & & 0 & 0 \\ & & 0 & \tilde{\Gamma}_{\text{fis}} \end{pmatrix}, \quad (48)$$

where $\tilde{\Gamma}_{\text{fis}} = \gamma_{\text{fis}} I$. Here we have assumed that Γ_{cap} and Γ_{fis} do not have off-diagonal parts. Using the reduced width amplitude $g_{a,i}$, the decay width matrix is represented as $(\Gamma_a)_{i,j} = g_{a,i} g_{a,j}$. When the system is highly excited, the configurations interact in a complex way, and the value of $(\Gamma_a)_{i,j}$ becomes zero on average for $i \neq j$. In our setup, the left-end and right-end GOE matrices correspond to the compound states and scission configuration. Therefore this treatment is justified.

To determine the size of decay widths γ_a ($a = n, \text{cap}, \text{ or fis}$), we employ compound nucleus phenomenological formula [16],

$$T_a = 2\pi\rho\gamma_a. \quad (49)$$

Here T_a is the transmission coefficient for channel a , and ρ is the level density of the compound states. In $n + {}^{235}\text{U} \rightarrow {}^{236}\text{U}^*$ reaction, T_n is parametrized as

$$T_n = 2\pi S_0 E_n^{1/2}, \quad (50)$$

where S_0 is the s -wave neutron strength function, and E_n is incident neutron energy in eV units. S_0 is about 10^{-4} and we take $E_n = 10$ keV. Thereby $T_n = 0.063$. Using $\rho = 31.8 \text{ MeV}^{-1}$, γ_n becomes 0.01 MeV. On the other hand, the empirical value of T_{cap} is about 0.25 [16]. Applying the same formula in eq. (49), γ_{cap} is estimated to be 0.00125 MeV.

The determination of γ_{fis} is more difficult. The value of γ_{fis} determined by the S-matrix theory or the R-matrix theory referring to the experimental data is not the fission width for the scission configurations but for the compound configurations. In addition, in a theoretical view as well, its value has rarely been investigated [51]. However, it is known that the transition probability $T_{n,\text{fis}}$ is insensitive to the size of γ_{fis} [16]. It can be understood based on the transition state picture. In this theory, the decay rate of fission is mainly determined by the information of the saddle, and details after the fission

barrier do not change the decay rate. It is because the flux passing through the barrier is assumed not to be backscattered. The insensitivity to γ_{fis} implies the validity of this assumption. In the calculation below, we use $\gamma_{\text{fis}} = 0.015$ MeV referring ref. [16], which value is within the insensitive range.

4.5 Calculation of the Green function

According to the discussion above, the Hamiltonian kernel has the following structure,

$$H = \begin{pmatrix} \tilde{H}_{\text{GOE}}^{(L)} & (V^{(L)})^T & & & \\ V^{(L)} & H_1 & V_{1,2} & & O \\ & V_{2,1} & H_2 & V_{2,3} & \\ & & & \ddots & \\ O & & & V_{11,12} & H_{12} & (V^{(R)})^T \\ & & & & V^{(R)} & \tilde{H}_{\text{GOE}}^{(R)} \end{pmatrix}. \quad (51)$$

Here O is zero matrix, and $\tilde{H}_{\text{GOE}}^{(L)}$ and $\tilde{H}_{\text{GOE}}^{(R)}$ are the GOE matrices including the decay width. H_i are diagonal block components (Q -blocks), and $V_{i,j}$, $V^{(L)}$, and $V^{(R)}$ are the off-diagonal matrices connecting neighboring configurations. We assume that the matrix elements of $V^{(L)}$ and $V^{(R)}$ follow the Gaussian distributions with the variances set to be $v_a = 0.02$ MeV and $v_b = 0.03$ MeV, respectively. These values are close to the strength of the particle-hole random interaction 0.025 MeV which was estimated by the overlap of the single particle orbitals [52].

The structure of the overlap kernel is similar to the Hamiltonian as

$$N = \begin{pmatrix} I^{(L)} & O & & & O \\ O & I_1 & S_{1,2} & & \\ & S_{2,1} & I_2 & S_{2,3} & \\ & & & \ddots & \\ O & & & S_{11,12} & I_{12} & O \\ & & & & O & I^{(R)} \end{pmatrix}, \quad (52)$$

where I is the identity matrix, and $S_{k,k'}$ represents the overlap between neighboring Q -block configurations. Therefore, the matrix $(EN - H)$ also has the same block-tridiagonal structure. We can utilize this special structure for the

inversion calculation of the Green function $G(E)$ as we explain in appendix C.

4.6 The fission to capture branching ratio

Let us now numerically evaluate the branching ratio $\alpha^{-1} = T_{n,\text{fis}}/T_{n,\text{cap}}$. In the experiment, α^{-1} is measured to be about 3 in low energy neutron reaction of ^{235}U [53], and we regard this value as a benchmark of the fidelity of our model. Considering that in experiments cross-sections of neutron reactions are measured within an energy resolution, we calculate energy-averaged transmission coefficients ($a = \text{cap}$ or fis)

$$\langle T_{n,a}(E) \rangle = \frac{1}{\Delta E} \int_{E-\Delta E/2}^{E+\Delta E/2} dE' T_{n,a}(E'), \quad (53)$$

where ΔE is an energy interval. We take $\Delta E = 0.25$ MeV, which satisfies the condition $\Delta E \gg 1/\rho$. Furthermore, we have to take an ensemble average of the transmission coefficients with different samples due to the usage of the random matrices. With 100 samples, the statistical error becomes less than 10 %, and the results following are the ones obtained using 100 samples. Fig. 11 shows the energy and ensemble averaged transmission coefficients for the capture and the fission as functions of the excitation energy. $\langle T_{n,\text{fis}} \rangle$ increases as the energy increases, while $\langle T_{n,\text{cap}} \rangle$ decreases due to the conservation of the total reaction probability. Figure 12 also plots the fission to capture branching ratios, $\alpha^{-1} = \langle T_{n,\text{fis}} \rangle / \langle T_{n,\text{cap}} \rangle$. At $E = 6.5$ MeV, that is close to the neutron separation energy of ^{236}U ($S_n = 6.536$ MeV) [44], α^{-1} is 0.071 in this calculation. This value underestimates the empirical value $\alpha^{-1} \simeq 3.0$ by a factor of about 40. It indicates that one needs to extend the model space by including the finite seniority configurations to reproduce the empirical branching ratio.

4.7 Distribution of P_{fis}

In compound nucleus reactions, the number of decay channels is characterized by the degrees of freedom ν . We examine this quantity using the the distribution and the fluctuation of the fission probability

$$P_{\text{fis}} = T_{n,\text{fis}}/T_n \sim T_{n,\text{fis}}/(T_{n,\text{cap}} + T_{n,\text{fis}}). \quad (54)$$

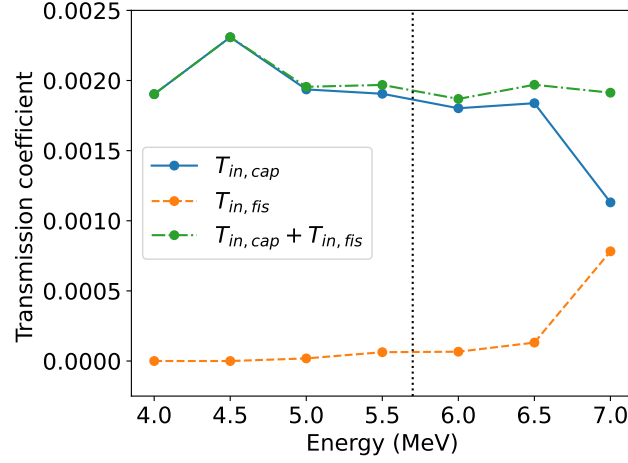


Figure 11: The averaged transmission coefficients for capture $\langle T_{n,cap}(E) \rangle$ (the blue solid line) and for fission $\langle T_{n,fis}(E) \rangle$ (the orange dashed line). The sum of these transmission coefficients is also plotted with the green dot-dashed line. The vertical dotted line shows the height of the fission barrier located at 5.7 MeV.

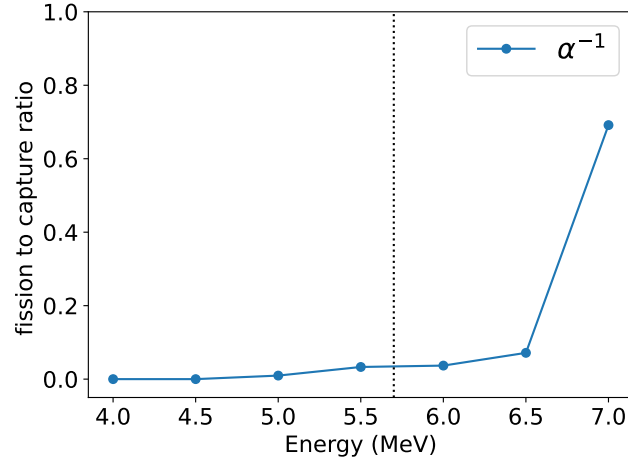


Figure 12: The branching ratio $\alpha^{-1}(E) = \langle T_{n,fis}(E) \rangle / \langle T_{n,cap}(E) \rangle$ as a function of the excitation energy E . The vertical dotted line shows the height of the fission barrier located at 5.7 MeV.

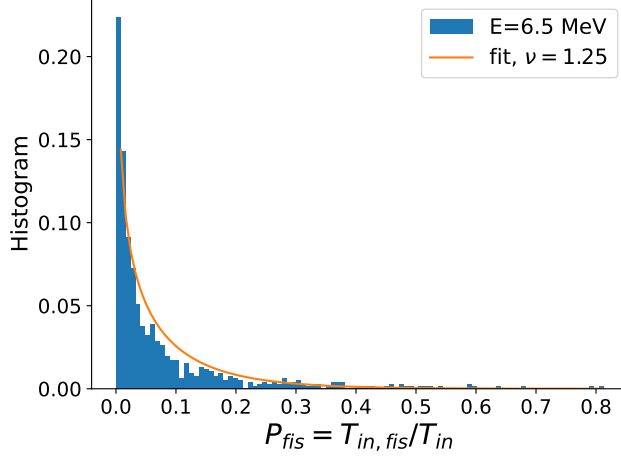


Figure 13: Distributions of $P_{\text{fis}}(E)$ for 1000 samples at $E = 6.5$ MeV. The orange solid line shows a chi-squared distribution with ν determined by the maximum likelihood fit. The value of ν is shown in the inset.

By dividing by T_n , the fluctuation of the input channel is canceled out, and P_{fis} reflects the fluctuation of the fission channel only. The relation $T_n \sim T_{n,\text{cap}} + T_{n,\text{fis}}$ is derived from the conservation of the probability flux, and its validity was numerically confirmed in the appendix in ref. [16].

The distribution of P_{fis} with $E = 6.5$ MeV is shown in fig. 14, which is fitted by the chi-squared distribution given by eq. (13). It is remarkable that the distribution is well-fitted by the chi-squared distribution with the small value of ν . In this model, the apparent number of the fission channels is $N_{\text{GOE}} = 1000$ in eq. (48), and the resultant value of $\nu = 1.25$ is much smaller than it. This value is also consistent with the estimate of Porter and Thomas ($\nu = 2.3 \pm 1.1$) [26].

We also plot the value of ν as a function of the excitation energy E in fig. 14. ν gradually increases as a function of E , which reflects the number of open exit channels increases as the excitation energy increases.

We emphasize that this result is the first indication of the small number of ν in fission channels based on a microscopic approach without the transition state assumption. In the next subsection, we will further discuss the value of ν based on a different approach: the effective Hamiltonian method. Thereby, we try to reinforce the above discussion and clarify the mechanism of the small number of ν .

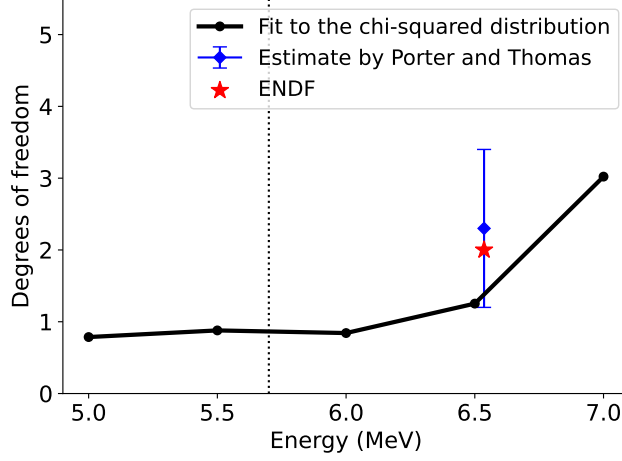


Figure 14: The number of degrees of the freedom ν obtained by fitting the distribution of transmission coefficients for fission to the chi-squared distribution. The blue diamond is the empirical estimate of ν in ref. [26], while the star represents the data from ENDF/B-VIII.0 [54]. The vertical dotted line denotes the height of the fission barrier.

4.8 Effective Hamiltonian H_{eff}

The distribution of P_{fis} close to the chi-squared distribution is explained by the properties of the GOE matrix included in the Hamiltonian in eq. (51). To clarify it, we divide the model space into the compound nucleus configurations (the left-end GOE) and the other spaces as

$$H = \begin{pmatrix} H_{\text{GOE}}^{(L)} & (\vec{V}^{(L)})^T \\ \vec{V}^{(L)} & H_Q \end{pmatrix}, \quad (55)$$

where H_Q is the Hamiltonian in the model space excluding $H_{\text{GOE}}^{(L)}$ and $\vec{V}^{(L)}$ is defined as $\vec{V}^{(L)} = (V^{(L)}, O, O, \dots, O)^T$. In the discussion here, only the fission channels play a role and we set $\Gamma_n = \Gamma_{\text{cap}} = 0$. The overlap kernel N is expressed in the same way,

$$N = \begin{pmatrix} I^{(L)} & O \\ O & N_Q \end{pmatrix}. \quad (56)$$

The effective Hamiltonian for the space of $H_{\text{GOE}}^{(L)}$ is constructed as

$$\begin{aligned} H_{\text{eff}}(E) &= H_{\text{GOE}}^{(L)} + \vec{V}^{(L)}(EN_Q - H_Q)^{-1}(\vec{V}^{(L)})^T \\ &\equiv H_{\text{GOE}}^{(L)} + \Delta(E) - i\Gamma_{\text{eff}}(E)/2. \end{aligned} \quad (57)$$

Here $H_{\text{GOE}}^{(L)} + \Delta(E)$ and $-\Gamma_{\text{eff}}(E)/2$ are the real and the imaginary parts of the effective Hamiltonian, respectively. $\Gamma_{\text{eff}}(E)$ corresponds to the fission width for the compound states. Notice that the fission width in eq. (48) is the width for the fission doorway configurations, not for the compound states.

If $\Delta(E)$ is negligibly small, the real part of $H_{\text{eff}}(E)$ becomes a GOE matrix, and we can apply the discussion in sec. 2.3. That is, the rank of the decay width matrix corresponds to the degrees of freedom. Fig. 15 shows the eigenvalues of Γ_{eff} with $E = 5.5$ MeV and 6.5 MeV for specific random seeds. There is a clear gap between large eigenvalues and negligibly small eigenvalues. It suggests that there are small number of dominant fission modes, and the others do not play a role. The dimension of Γ_{eff} is $N_{\text{GOE}} = 1000$, and the number of the dominant fission mode is significantly smaller than it. These modes are considered to be the microscopic counterparts of transition states.

Next, to understand the small value of ν shown in fig. 14, we analyze the rank of Γ_{eff} as discussed in sec. 2.3. To numerically calculate the rank of Γ_{eff} , we shall set 10^{-2} for the threshold value, which is indicated by the dotted line in fig. 15. Therefore the rank of Γ_{eff} is the number of the singular values larger than the threshold 10^{-2} . Fig. 16 plots the rank of Γ_{eff} as a function of E . It exhibits a similar behavior to fig. 14, and the small number of $\nu = \text{rank}(\Gamma_{\text{eff}})$ is reproduced. At $E = 5.5$ MeV $\text{rank}(\Gamma_{\text{eff}}) \sim 1$. It indicates that the first open channel is around the height of the fission barrier 5.7 MeV, and consistent with the transition state picture.

We also find the insensitivity of $\text{rank}(\Gamma_{\text{eff}})$ to the size of the right-end GOE matrix N_{GOE} , as shown in fig. 16. This is consistent with the experimental finding that the number of apparent fission channels is not related to the degrees of freedom ν .

4.9 Discussion

In the previous subsections, we have shown that the fission channels have a small number of degrees of freedom. To understand its mechanism micro-

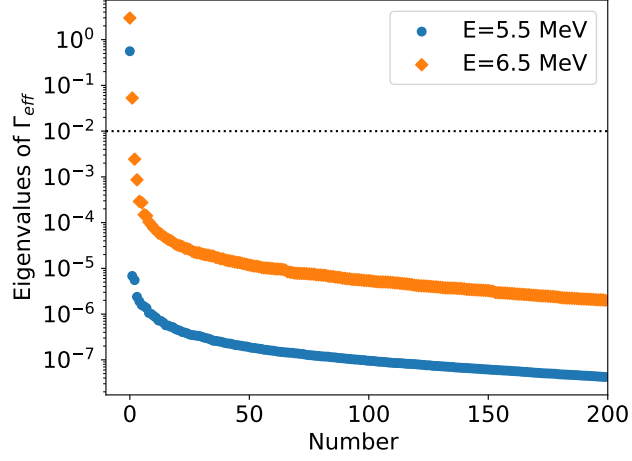


Figure 15: The eigenvalues of Γ_{eff} at $E=5.5$ MeV (the blue circles) and 6.5 MeV (the orange diamonds) for a typical sample. They are plotted in descending order. The dotted line shows the threshold value 10^{-2} used to calculate the rank of Γ_{eff} .

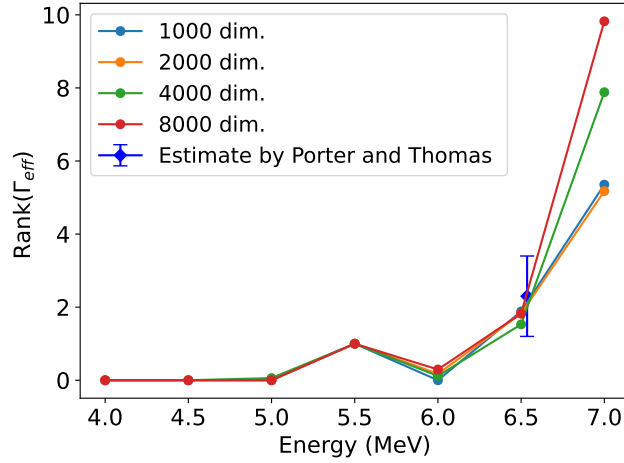


Figure 16: The rank of Γ_{eff} as a function of excitation energy, obtained after averaging over 100 samples. The different lines indicate the results of different dimensions of the right-end GOE matrix. The blue diamond shows the empirical estimate of ν [26].

scopically, we go back to the trace formula in eq. (29). Here Γ_n and Γ_{cap} are reintroduced.

With the setup of our model of the width, the transition probability reads,

$$T_{n,\text{fis}} = \gamma_n \gamma_{\text{fis}} \sum_{j \in \text{fis}} |G_{n,j}|^2. \quad (58)$$

Here the neutron channel n represents a specific configuration in the left-end GOE and the fission channel includes all configurations in the right-end GOE. Then we apply a spectral decomposition of the Green function $G(E)$ as

$$G_{ij}(E) = \sum_{\lambda} f_i^{(\lambda)} \frac{1}{E - (E_{\lambda} - \frac{i}{2}\Gamma_{\lambda})} (f_j^{(\lambda)})^*. \quad (59)$$

Here $f_i^{(\lambda)}$ is a solution of the Hill-Wheeler equation

$$\sum_j (H - E_{\lambda} N)_{ij} f_j^{(\lambda)} = 0, \quad (60)$$

with the GCM kernels in eqs.(40) and (41). In general, the Hamiltonian matrix is not Hermitian, and the Green function should be decomposed using a non-identical left-eigenvector and right-eigenvector. However, in our setup, the imaginary parts in the Hamiltonian are small and can be perturbatively treated. Thus the imaginary part of the eigenvalue Γ_{λ} is given by

$$\Gamma_{\lambda} = \sum_{i,j} (f_i^{(\lambda)})^* (\Gamma_{\text{in}} + \Gamma_{\text{cap}} + \Gamma_{\text{fis}})_{ij} f_j^{(\lambda)}, \quad (61)$$

and we use the eigenvector $f_i^{(\lambda)}$ of the non-perturbative Hamiltonian in eq. (59). Then we substitute eq. (59) into eq. (92), and the transition probability becomes

$$\begin{aligned} T_{n,\text{fis}} = & \gamma_n \gamma_{\text{fis}} \sum_{\lambda} \frac{|f_1^{(\lambda)}|^2}{(E - E_{\lambda})^2 + (\Gamma_{\lambda}/2)^2} \sum_{j \in \text{fis}} |f_j^{(\lambda)}|^2 \\ & + \gamma_n \gamma_{\text{fis}} \sum_{\lambda \neq \lambda'} \sum_{j \in \text{fis}} \frac{f_1^{(\lambda)} f_1^{(\lambda')*} f_j^{(\lambda)} f_j^{(\lambda')*}}{(E - \tilde{E}_{\lambda})(E - \tilde{E}_{\lambda'})^*}. \end{aligned} \quad (62)$$

Based on this expression, we can understand how each eigenstates contribute to the transition process. Taking an ensemble average of $T_{n,\text{fis}}$, the expression

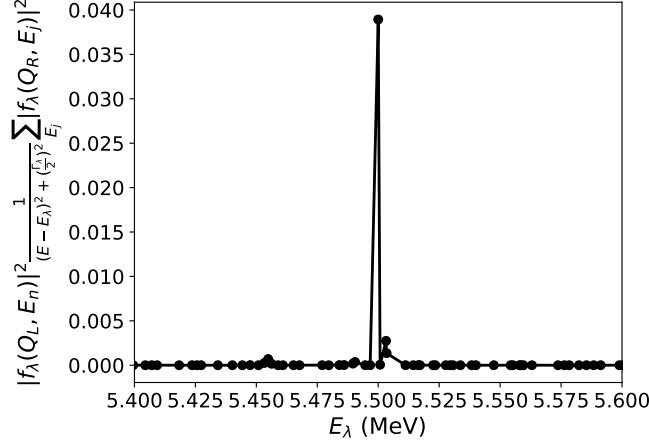


Figure 17: The spectrum decomposition of the transmission coefficient for fission at $E = 5.5$ MeV defined by eq. (63).

becomes simplified. To this end, we notice that $f_k^{(\lambda)}$ follows a Gaussian distribution when k is for the neutron or the fission channels. This is because amplitudes of GOE eigenstates follow in general a Gaussian distribution, and this property is expected to be conserved in our model as long as the couplings between the GOE matrices and the bridge Hamiltonian are not too strong.

The coefficients $f_j^{(\lambda)} f_j^{(\lambda')}$ follow the independent Gauss distributions when $\lambda \neq \lambda'$, and thereby the second term in eq. (82) vanish after the average. Finally, ensemble averaged transmission coefficients for fission becomes

$$\begin{aligned} \langle T_{n,\text{fis}}(E) \rangle &= \gamma_n \gamma_{\text{fis}} \sum_{\lambda} \langle |f_{\lambda}(Q_L, E_n)|^2 \rangle \\ &\times \left\langle \frac{1}{(E - E_{\lambda})^2 + (\Gamma_{\lambda}/2)^2} \right\rangle \left\langle \sum_{\mu} |f_{\lambda}(Q_R, E_{\mu})|^2 \right\rangle, \end{aligned} \quad (63)$$

where Q_L and Q_R denote the left-most and the right-most configurations, respectively. Here $\langle T_{n,\text{fis}}(E) \rangle$ is decomposed into a sum of contributions of each GCM eigenstates λ .

Let us investigate how many eigenstates contribute to the transition probability $T_{n,\text{fis}}$. Fig. 17 plots the contribution of each eigenmodes for $E = 5.5$ MeV as a function of E_{λ} . Due to the Breit-Wigner term acting as an energy window, the eigenstates whose E_{λ} is close to the excitation energy E only

Table 2: The breakdown of eq. (63) at $E = 5.5$ MeV for specific eigenstates, including the dominant eigenmode (at $E_\lambda = 5.4999$ MeV) shown in the bottom panel in fig. 17. The table also lists the value of Γ_λ defined by eq. (91).

E_λ (MeV)	$ f_\lambda(Q_L, E_n) ^2$	$\frac{1}{(E-E_\lambda)^2+(\Gamma_\lambda/2)^2}$	$\sum_\mu f_\lambda(Q_R, E_\mu) ^2$	the product	Γ_λ (MeV)
5.4946	2.56×10^{-9}	3.51×10^4	2.82×10^{-2}	2.58×10^{-6}	4.23×10^{-4}
5.4969	1.30×10^{-5}	9.04×10^4	2.26×10^{-6}	2.68×10^{-6}	5.68×10^{-4}
5.4999	1.17×10^{-7}	6.22×10^6	5.34×10^{-2}	3.89×10^{-2}	8.02×10^{-4}
5.5008	9.54×10^{-9}	1.66×10^6	3.59×10^{-3}	5.68×10^{-5}	5.39×10^{-5}
5.5032	1.41×10^{-7}	6.57×10^4	2.96×10^{-1}	2.74×10^{-3}	4.45×10^{-3}

contribute to $T_{n,\text{fis}}$. The breakdown of each term in eq. (63) for five eigenstates around the dominant eigenmode is shown in table 2. One can see that the components both at the left-most and the right-most Q are relatively large for the dominant eigenmode as compared to those for the other eigenmodes. This is a necessary condition to have a large transmission coefficient, as is evident from eq. (63).

4.10 Rank of the matrix Γ_{eff}

In the previous subsection, we have discussed the smallness of degrees of freedom, ν , in terms of the spectrum decomposition of the Green function. Here we present an alternative explanation of the smallness of ν based on the rank of Γ_{eff} . As shown in fig. 16, Γ_{eff} has a low-rank structure, and the value of rank corresponds to the degrees of freedom in the fission channels. Here we analytically evaluate the rank of Γ_{eff} to explain the smallness of ν .

From eq. (57), Γ_{eff} is given by,

$$(\Gamma_{\text{eff}})_{i,j} = 2 \sum_{kl} V_{ik} \text{Im}((G_Q)_{kl}) (V^T)_{lj}, \quad (64)$$

where G_Q denotes the Green function corresponding to H_Q ,

$$G_Q = (EN_Q - H_Q)^{-1}, \quad (65)$$

and V is simple expression of $V^{(L)}$. Then we decompose G_Q into its eigen-

states λ as

$$(G_Q)_{kl} = \sum_{\lambda} O_{k\lambda} (\tilde{G}_Q)_{\lambda} O_{\lambda l}^T. \quad (66)$$

Here, $(\tilde{G}_Q)_{\lambda}$ denotes the eigenvalue of G_Q and O is defined as $O = (\vec{f}_1, \vec{f}_2, \dots, \vec{f}_N)$ with the column-vectors $\vec{f}_{\lambda}$ representing the GCM weight functions. Substituting eq. (66) into eq. (65), Γ_{eff} reads

$$\begin{aligned} (\Gamma_{\text{eff}})_{ij} &= \sum_{\lambda, E_{\mu}, E_{\mu'}} V_{i, (Q_1, E_{\mu})} f_{\lambda}(Q_1, E_{\mu}) \\ &\times \frac{\Gamma_{\lambda}}{(E - E_{\lambda})^2 + (\frac{\Gamma_{\lambda}}{2})^2} f_{\lambda}(Q_1, E_{\mu'}) V_{j, (Q_1, E_{\mu'})}, \end{aligned} \quad (67)$$

where Q_1 is the first Q -block in Q space at $Q = 18b$ and E_{μ} denotes the label for the configurations at Q_1 . The rank of a matrix VAV^T is known to be equal to the rank of the symmetric matrix A [55], and thereby the rank of the matrix Γ_{eff} is equal to the rank of $\sum_{\lambda} A_{\lambda}$, defined as

$$(A_{\lambda})_{\mu, \mu'} = f_{\lambda}(Q_1, E_{\mu}) \frac{\Gamma_{\lambda}}{(E - E_{\lambda})^2 + (\frac{\Gamma_{\lambda}}{2})^2} f_{\lambda}(Q_1, E_{\mu'}). \quad (68)$$

Applying the relation

$$\text{rank} \left(\sum_{\lambda} A_{\lambda} \right) \leq \sum_{\lambda} \text{rank}(A_{\lambda}), \quad (69)$$

one can analyze the rank of each A_{λ} separately. Furthermore A_{λ} is rank-1 matrix and it has only one nonzero eigenvalue a_{λ} . It is equal to $\text{Tr}(A_{\lambda})$ and evaluated as

$$\begin{aligned} a_{\lambda} &= \sum_k |f_{\lambda}(Q_1, E_k)|^2 \frac{\Gamma_{\lambda}}{(E - E_{\lambda})^2 + (\frac{\Gamma_{\lambda}}{2})^2} \\ &\simeq \left(\sum_k |f_{\lambda}(Q_1, E_k)|^2 \right) \frac{\gamma_{\text{fis}}(\sum_{E_l} |f_n(Q_R, E_l)|^2)}{(E - E_{\lambda})^2 + (\frac{\Gamma_{\lambda}}{2})^2}. \end{aligned} \quad (70)$$

In the last line, we apply the perturbative expression of Γ_{λ} in eq. (91). This expression is analogous to eq. (63). In eq. (70), only the eigenstates which

have enough amplitude at both $Q = Q_1$ and $Q = Q_R$ and whose eigenenergy is close to E contributes to the rank of Γ_{eff} .

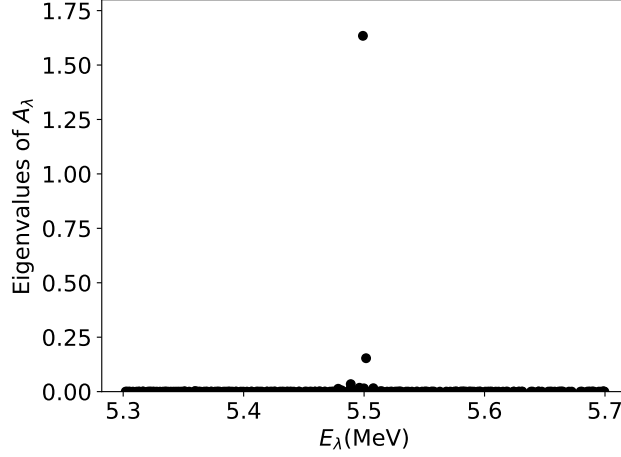


Figure 18: Eigenvalues of A_n defined in eq. (68) as a function of eigenenergy E_n .

The eigenvalues of A_λ , that is, a_λ for our model at $E = 5.5$ MeV are shown as a function of E_λ in fig. 18. One can see that most of a_λ are almost zero, and only two of them have significant values. That is, only two matrices of A_λ have rank 1 while the rest may be regarded to have rank 0. Therefore effectively $\sum_\lambda \text{rank}(A_\lambda)$ is 2, which provides the upper limit of $\text{rank}(\Gamma_{\text{eff}})$ as $\text{rank}(\Gamma_{\text{eff}}) \leq 2$. This is a direct proof why the $\text{rank}(\Gamma_{\text{eff}})$ is small as shown in fig. 14.

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

The NEGF method is a powerful tool to describe the transport properties in fermionic many-body systems. On the other hand, NEGF methods require a significant numerical cost, especially for calculations of the Green function. To overcome this problem, many numerical methods have been proposed [56, 57, 58]. However, the applicability of these methods is limited by the structure of the considered Hamiltonian, such as the block-tridiagonal structure.

In this section, we discuss the applicability of the Lanczos method to the NEGF method. Applying the spectrum decomposition of the Green function, we can transform the calculation of the Green function to the eigenvalue problem. On the other hand, the Lanczos method is known to be an efficient tool to solve eigenvalue problems. Therefore, there is a possibility that it reduces the numerical cost of the NEGF method without assuming special structures of the Hamiltonian matrix, and we demonstrate it.

The contents in this chapter are summarized in ref. [42]

5.1 The Lanczos algorithm

Consider the eigenvalue problems for a Hamiltonian H ,

$$H\psi = E\psi. \quad (71)$$

The numerical cost of the direct diagonalization increases cubically to the dimension of the Hamiltonian. On the other hand, the dimension of the Hamiltonian increases exponentially to the number of particles considered, and it complicates the numerical approach to many-body systems.

The Lanczos algorithm is a powerful method to overcome these problems. If one is interested in the eigenstates only around the ground state, this method calculates a small set of these eigenstates efficiently. For example, in nuclear spectroscopy, if we are interested in transitions among low-lying states, the application of the Lanczos to the Hamiltonian in many-particle many-hole configuration space is a promising way to calculate these levels and transitions.

In this algorithm, first, we introduce the Krylov subspace

$$\text{span}\{\vec{q}, H\vec{q}, H^2\vec{q}, \dots, H^{n-1}\vec{q}\}. \quad (72)$$

Here $\vec{q}$ is an arbitrary initial vector and n is the dimension of the subspace. Usually, n is much smaller than the dimension of H . Then the original Hamiltonian H can be tridiagonalized in this subspace in the following way. First, we prepare the initial Lanczos vector, $\vec{v}_0 = \vec{q}/|\vec{q}|$. Then we start the Lanczos iteration with $\beta_0 = 0$ and $\vec{v}_{-1} = 0$,

$$\alpha_k = (H\vec{v}_k, \vec{v}_k), \quad (73)$$

$$\vec{w} = H\vec{v}_k - \beta_k\vec{v}_{k-1} - \alpha_k\vec{v}_k, \quad (74)$$

$$\beta_{k+1} = |\vec{w}|, \quad (75)$$

and

$$\vec{v}_{k+1} = \vec{w}/\beta_{k+1}. \quad (76)$$

Using the matrix

$$V = (\vec{v}_0, \vec{v}_1, \dots, \vec{v}_{n-1}), \quad (77)$$

the original Hamiltonian H is projected into the Krylov subspace as

$$T = V^\dagger H V. \quad (78)$$

Here T is the tridiagonal matrix,

$$T = \begin{pmatrix} \alpha_0 & \beta_1 & & & \\ \beta_1 & \alpha_1 & \beta_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \beta_{n-2} & \alpha_{n-2} & \beta_{n-1} \\ & & & \beta_{n-1} & \alpha_{n-1} \end{pmatrix}, \quad (79)$$

and the eigenvalues of T approximate the eigenvalues of H . The eigenvector of T , $\tilde{\psi}$ is related to the eigenvector of H , ψ as $\psi = V\tilde{\psi}$.

The initial vector $\vec{q}$ can be decomposed using ψ_i , the eigenvectors of H ,

$$\vec{q} = \sum a_i \psi_i. \quad (80)$$

Then the other vectors in eq. (72) reads,

$$H^m \vec{q} = [\sum a_i (E_i)^m \psi_i], \quad (81)$$

where E_i is the eigenvalue for ψ_i . Thereby the eigenstates with large absolute value of the eigenvalue are dominately selected, and the approximate eigenvalues of H are obtained in order of the magnitude of the eigenvalues.

5.2 The shift-invert Lanczos algorithm

Notice that the equation of the transmission coefficients in the spectral decomposed representation is given by,

$$T_{a,b} = \gamma_a \gamma_b \sum_{\lambda} \frac{|f_a^{(\lambda)}|^2 |f_b^{(\lambda)}|^2}{(E - E_{\lambda})^2 + (\Gamma_{\lambda}/2)^2} + \gamma_a \gamma_b \sum_{\lambda \neq \lambda'} \frac{f_a^{(\lambda)} f_a^{(\lambda')*} f_b^{(\lambda)} f_b^{(\lambda')*}}{(E - \tilde{E}_{\lambda})(E - \tilde{E}_{\lambda}')^*}. \quad (82)$$

This equation suggests that due to the energy dominator those eigenstates whose eigenvalue E_{λ} is close to the excitation energy E dominantly contribute to the transition process. This motivates calculating these dominant eigenstates and approximating $T_{a,b}$ by these selected states. However, there is a problem that the Lanczos algorithm can only calculate eigenstates around the ground states or the top of the spectrum, though in general the eigenstates around the excitation energy E are neither of those. In the case of neutron-induced fission, an excitation energy is typically $6 \sim 8$ MeV, and there are amount of states between the ground state and the considered excited states.

To avoid this difficulty, we apply the shift-invert Lanczos method [59]. In this method, the original eigenvalue problem $H\psi = E\psi$ is first transformed to

$$(H - \sigma I)\psi = (E - \sigma)\psi, \quad (83)$$

where σ is a real parameter and I is the identity matrix. Then we apply $(E - \sigma)^{-1}(H - \sigma I)^{-1}$ to the both sides of eq. (83), and we obtain

$$(H - \sigma I)^{-1}\psi = (E - \sigma)^{-1}\psi. \quad (84)$$

Here the original eigenvalue problems is transformed into the eigenvalue problem of the matrix $(H - \sigma I)^{-1}$, and the eigenvalues around σ have large absolute values due to the form of $(E - \sigma)^{-1}$. Thereby applying the Lanczos iteration to the matrix $(H - \sigma I)^{-1}$ we can efficiently calculate the eigenstate whose eigenenergy is close to σ .

Remembering the Lanczos iteration in sec. 5.1, we do not need the inversion matrix $(H - \sigma I)^{-1}$ itself, but the Lanczos vector multiplied by the inversion matrix, $(H - \sigma I)^{-1}\vec{v}_k$. This can be done by solving the linear equation,

$$(H - \sigma I)\vec{x} = \vec{v}_k \quad (85)$$

using the LU factorization or other methods. This series of procedures is called the shift-invert Lanczos method, and it has been implemented in

ARPACK [60], which is a numerical software library written in FORTRAN 77. In the next subsections, we apply this method to the NEGF formalism and demonstrate its effectiveness.

5.3 GOE+barrier+GOE model

As a first example, we apply our method to a simple model Hamiltonian. It has been used to model and discuss the transition state dynamics in refs. [61, 62, 63]. The model Hamiltonian is given by

$$H = \begin{pmatrix} H_1 & V_1 & 0 \\ V_1^T & B_h & V_2^T \\ 0 & V_2 & H_2 \end{pmatrix}. \quad (86)$$

Here H_1 and H_2 are random matrices sampled from the GOE. As discussed in sec.2.3, the GOE matrix is parametrized by the two parameters, v and N_{GOE} . In the calculation shown below, we take $N_{\text{GOE}} = 100$ and $v = 0.1$ in the units of the typical energy scale of the system for both H_1 and H_2 . In this subsection, all quantities related to energy are scaled in a similar way to the typical energy scale of the system. B_h is a real scalar number and represents the height of a potential barrier. In the following, we take $B_h = 2$. The vectors V_1 and V_2 connect the GOE matrices and the barrier configuration. The elements of V_1 and V_2 are random numbers sampled from the normal distribution with a mean value of zero and a standard deviation of 0.1.

We assume that H_1 is connected to two different kinds of external channels, the input channel Γ_{in} and the left output channels Γ_{L} . On the other hand, H_2 is assumed to connect to the right output channels Γ_{R} . In the problem of neutron induced fission reactions, Γ_{in} , Γ_{L} , and Γ_{R} correspond to a neutron channel, capture channels, and fission channels, respectively. The decay matrices corresponding to these channels are given by,

$$(\Gamma_{\text{in}})_{k,k'} = \gamma_{\text{in}} \delta_{k,1} \delta_{k',1}, \quad (87)$$

$$\Gamma_{\text{L}} = \begin{pmatrix} \gamma_{\text{L}} I & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (88)$$

and

$$\Gamma_{\text{R}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \gamma_{\text{R}} I \end{pmatrix}. \quad (89)$$

For the size of the decay matrices, we take $\gamma_{\text{in}} = 1.25 \times 10^{-3}$, $\gamma_{\text{L}} = 3.25 \times 10^{-3}$, and $\gamma_{\text{R}} = 1 \times 10^{-3}$, which are much smaller than the real parts of the Hamiltonian matrix elements, $v = 0.1$ in eq. (86). Since the values of γ are small, one can perturbatively treat the decay matrix $\Gamma = \Gamma_{\text{in}} + \Gamma_{\text{R}} + \Gamma_{\text{L}}$ to evaluate the eigenstates of the non-Hermitian matrix $H - i\Gamma/2$. That is, we first solve the Schrödinger equation without the imaginary part as

$$Hf_{\lambda} = E_{\lambda}Nf_{\lambda}, \quad (90)$$

and then evaluate the imaginary part of the eigenvalues approximately as

$$\Gamma_{\lambda} = \sum_i |(f_{\lambda})_i|^2 \Gamma_{ii}. \quad (91)$$

A similar simplified treatment of the decay matrices was employed in the previous chapter.

In our setup, the trace formula (42) is transformed to

$$T_{\text{in,R}} = \gamma_{\text{in}}\gamma_{\text{R}} \sum_{j \in \text{R}} |G_{1,j}|^2. \quad (92)$$

and

$$T_{\text{in,L}} = \gamma_{\text{in}}\gamma_{\text{L}} \sum_{j \in \text{L}} |G_{1,j}|^2. \quad (93)$$

Then applying the spectrum decomposition of the Green function, $T_{a,b}$ reads,

$$T_{a,b} = \gamma_a\gamma_b \sum_{\lambda} \frac{|(f_{\lambda})_a|^2 |(f_{\lambda})_b|^2}{(E - E_{\lambda})^2 + (\Gamma_{\lambda}/2)^2} + \gamma_a\gamma_b \sum_{\lambda \neq \lambda'} \frac{(f_{\lambda})_a (f_{\lambda'})_a^* (f_{\lambda})_b^* (f_{\lambda'})_b}{(E_{\lambda} - E)(E_{\lambda'} - E)^*}. \quad (94)$$

In our approach, we calculate k eigenstates around the excitation energy E by setting $\sigma = E$ in the shift-invert Lanczos method and use these k eigenstates to calculate $T_{a,b}$ by reducing the summation in eq. (94) as

$$\sum_{\lambda} \rightarrow \sum_{\lambda=1}^k. \quad (95)$$

The dimension of the Hamiltonian in eq. (86) is 201, and we can easily calculate the inverse matrix $(E - H)^{-1}$ in a direct way. Then we compare the transmission coefficients obtained by the direct method to those with the shift-invert Lanczos method.

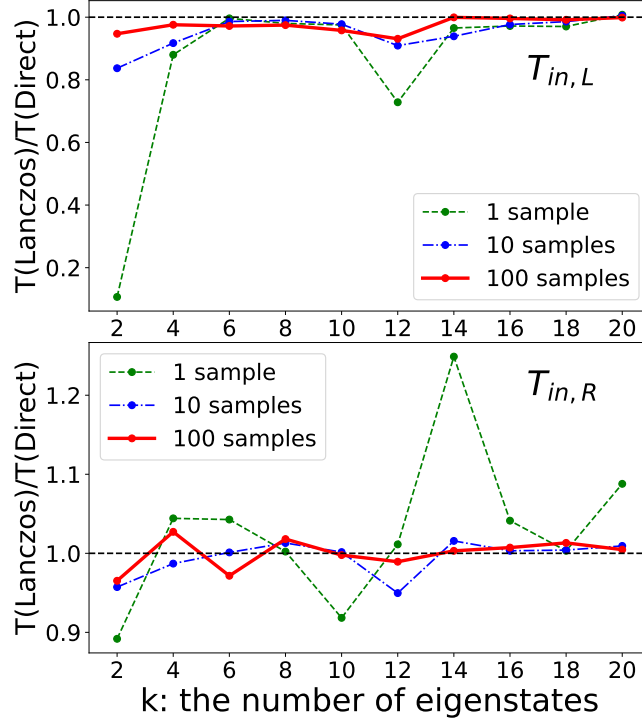


Figure 19: The ratio of transmission coefficients for the Hamiltonian in eq. (86) calculated by the direct matrix inversion and the shift-invert Lanczos approach. The number of eigenstates k included in the shift-invert Lanczos calculation is shown on the horizontal axis. Calculations for $T_{in,L}$ and $T_{in,R}$ are shown in the upper and lower panels, respectively.

Since the Hamiltonian in eq. (86) includes the random matrices, we need to take an ensemble average to calculate physical quantities. The ratio of the ensemble averaged transition probabilities at $E = 0$ calculated with the shift-invert Lanczos method to those with the direct method is shown in fig. 30. The horizontal axis in fig. 30 is the number of the eigenstates k used in the summation in eq. (95). In the cases with 1 sample, the transition coefficients obtained with the shift-invert Lanczos method do not converge even with large values of k . As the sample number increases, the ratios become close to one. With 100 samples, the error becomes less than 1% for both $T_{in,L}$ and $T_{in,R}$ at $k = 20$.

Next, we consider a case where γ_{in} , γ_L , and γ_R are no longer smaller than

the real part of the Hamiltonian, which corresponds to the case that the resonances are overlapping with each other. In this case, the perturbative treatment of Γ in eq. (91) is not justified, and one needs to solve the eigenvalue equation for the Hamiltonian $H - \frac{i}{2}\Gamma$ itself. The Lanczos algorithm is only applicable to the symmetric or Hermite Hamiltonian, and instead we have to use the Arnoldi algorithm, which is a generalization of the Lanczos algorithm [60]. In the Arnoldi algorithm, the original Hamiltonian matrix H is transformed into a Hessenberg matrix as

$$\tilde{H} \equiv QHQ^\dagger = \begin{pmatrix} h_{11} & h_{12} & h_{13} & \dots & h_{1n} \\ h_{21} & h_{22} & h_{23} & \dots & h_{2n} \\ 0 & h_{32} & h_{33} & \dots & h_{3n} \\ & \ddots & \ddots & & \vdots \\ & & & h_{n-1,n} & h_{n,n} \end{pmatrix}, \quad (96)$$

where the matrix Q is constructed by aligning the Arnoldi vectors $\vec{q}_i$. $\tilde{H}$ approximates the original Hamiltonian in the Krylov subspace and its eigenvalues approximate the original ones.

We apply the shift-invert Arnoldi algorithm to the Hamiltonian $H - \frac{i}{2}\Gamma$ and calculate the right eigenvector $\vec{f}_\lambda$, the left eigenvector $\vec{\tilde{f}}_\lambda$ and its complex eigenvalues $E_\lambda - \frac{i}{2}\Gamma_\lambda$. Then we substitute them into eq. (82) directly and calculate the transition probabilities $T_{\text{in,L}}$ and $T_{\text{in,R}}$. Figure. 20 shows the results for $\gamma_{\text{in}} = \gamma_{\text{L}} = \gamma_{\text{R}} = 0.1$, while the other parameters are set to be the same as before. One can confirm that the transmission coefficients with the Arnoldi algorithm are converged to those with direct calculations when the value of k is large enough. The number of k required is larger compared to the case with the smaller decay widths shown in fig. 30. The slower convergence can be easily understood with eq. (82), which indicates that more eigenstates contribute to the transition process with larger values of widths.

5.4 ^{236}U with seniority zero configurations

Next, we apply the same approach to a case of neutron-induced fission of ^{236}U . The setup of the Hamiltonian is the same as the one used in chapter 4. We use the UNEDF1 parameter set to solve the Skyrme-Hartree-Fock eq. and calculate the reference states along the fission path labeled by Q_2 . Then we generate many-particle many-hole excited states at each Q_2 , calculate the

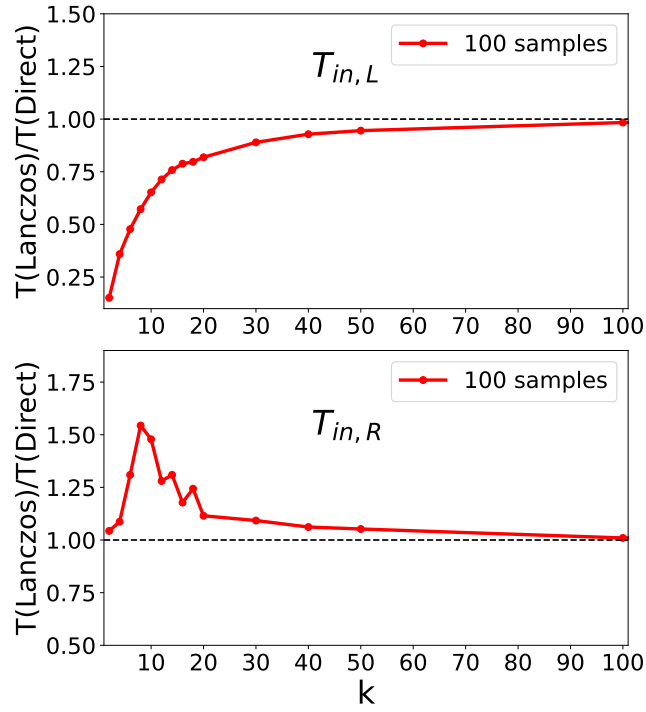


Figure 20: The ratio of transmission coefficients with the larger value of the width parameters (see the main text). The horizontal axis k is the number of eigenstates obtained by the shift-invert Arnoldi method.

Hamiltonian kernel and the norm kernel following the GCM procedure, and replace the first and the last Q -blocks with the GOE matrices. Finally, we add the decay matrices to the Hamiltonian kernel and calculate the transition probability $T_{n,\text{cap}}$ or $T_{n,\text{fis}}$. Notice that in this case, we have to solve the generalized eigenvalue problems

$$Hf = ENf \quad (97)$$

to calculate the eigenstates. The shift-invert Lanczos method is known to be applicable to the generalized eigenvalue problems by simply replacing the identity matrix I with the overlap matrix N in eqs. (83, 84).

The following calculations were performed using a single node equipped in Yukawa-21 supercomputer at the Yukawa Institute for Theoretical Physics (YITP), Kyoto University. We apply the ZGETRF and ZGETRI subroutines included in LAPACK [64] for the calculations of the matrix inversion. On the other hand, the ARPACK library is used for the calculation of the shift-invert Lanczos algorithm [60].

Fig. 21 shows the ratios of the transition probabilities calculated with the shift-invert Lanczos method to those with the direct method. By taking an ensemble average with 100 samples, the error of our approach is smaller than 3% for both capture and fission, as shown by the red lines. Moreover, one can also observe that the result is almost converged with $k = 10$. That is, we need only as small as 10 eigenstates to represent the Green function, whose dimension is 66103.

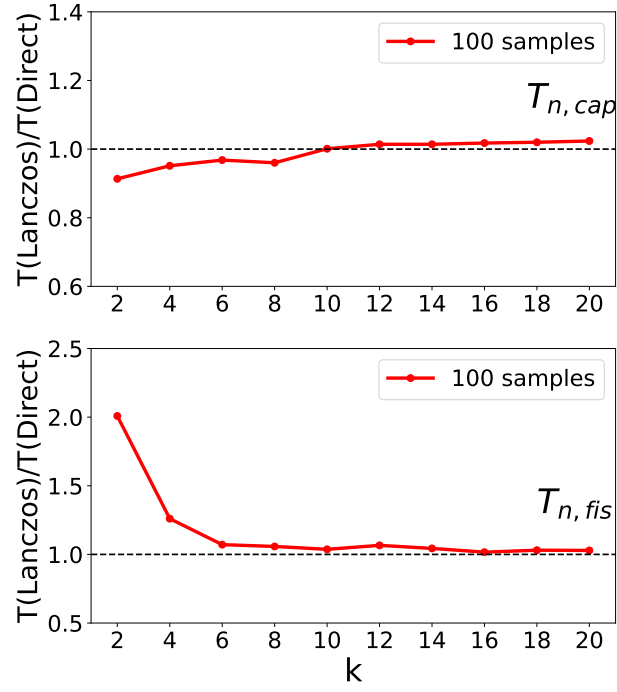


Figure 21: Similar to fig. 30, but for the transmission coefficients in $^{235}\text{U}(n, f)$ reaction at $E=6.5$ MeV. In the shift-invert Lanczos calculation, we set $\sigma = 6.5$ MeV.

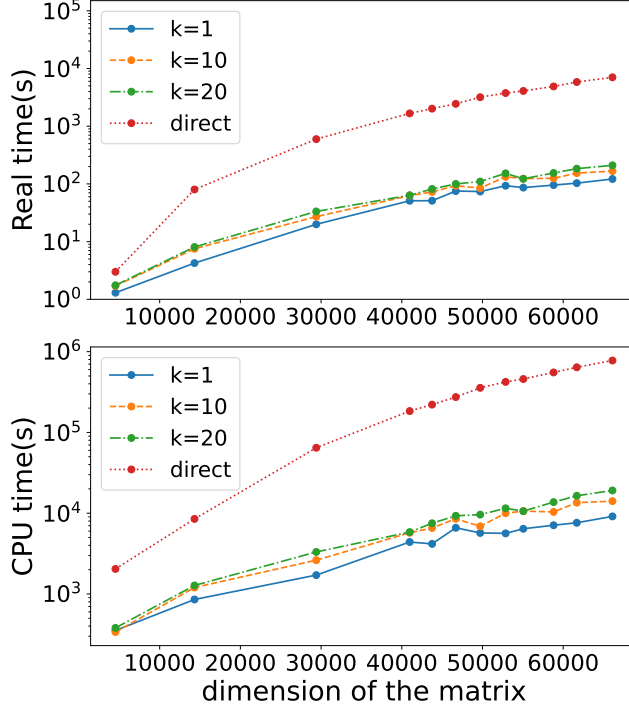


Figure 22: (The upper panel) The real computational time for the shift-invert Lanczos method and the direct matrix inversion. To draw this figure, the left-end and the right-end GOE matrices are fixed and the number of intermediate Q -blocks is increased one by one. The quantity k in the legend denotes the number of eigenvectors calculated with the shift-invert Lanczos method. See the text for details of the numerical calculations. (The lower panel) Similar to the upper panel, but for the CPU times.

Next, we discuss the computation times needed to compute the Green function,

$$G(E) = \left(EN - \left(H - \frac{i}{2}\Gamma \right) \right)^{-1}. \quad (98)$$

In the following calculations, we fix the left-end and the right-end GOE matrices and increase the number of the intermediate subblocks H_i and $V_{i,i+1}$ one by one. We measure the needed times for the matrix inversion or the shift-invert Lanczos calculation. The upper and lower pannes in fig. 22 show the real times and the CPU times as a function of the matrix dimension,

Table 3: The computational times required to compute the Green function with the direct matrix inversion method and with the shift-invert Lanczos method.

	dimension	direct	shift-invert Lanczos		
			$k=1$	$k=10$	$k=20$
Real time(s)	4520	3.59	1.18	1.51	1.89
	43753	2.01×10^3	5.11×10	7.26×10	8.17×10
	66103 (full)	7.03×10^3	1.22×10^2	1.67×10^2	2.10×10^2
CPU time(s)	4520	2.04×10^3	3.35×10^2	3.42×10^2	3.81×10^2
	43753	2.21×10^5	4.17×10^3	6.57×10^3	7.51×10^3
	66103 (full)	7.77×10^5	9.14×10^3	1.41×10^4	1.93×10^4

respectively. As shown in the panels, the shift-invert Lanczos method reduces the computational times with any value of k . For the dimension of 66103, the shift-invert Lanczos method is faster by a factor of about 34.0 in real time and about 40.3 in the CPU time as compared to the direct matrix inversion. The computation times are also summarized in table 3.

6 Realistic model space calculations with finite seniority configurations

In the previous chapters, we have taken into account seniority zero configurations only due to the restriction of the numerical cost. Even in this case, the dimension of the Hamiltonian is about 66 thousand, and the repeated calculation of the Green function requires a huge numerical cost. In addition, we have replaced the left-end and right-end Q blocks with the GOE matrices. Due to this treatment, we have to introduce the parameters of interaction strength by hand. It introduces uncertainty to the resultant transmission coefficients, and it is desirable to remove it for a reliable calculation. If we remove these two restrictions and take into account realistic model spaces including the compound nucleus configurations, the dimension of the Hamiltonian becomes the order of 10^5 to 10^6 [16]. Consequently, the numerical costs become huge. In this chapter, we tackle this problem and execute a realistic calculation of the transmission coefficients.

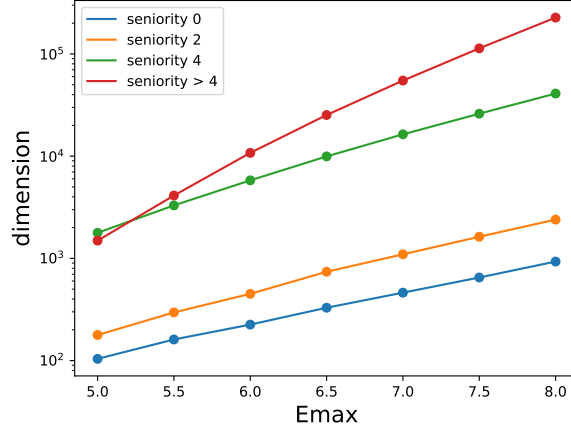


Figure 23: The number of configurations with different seniority numbers whose particle-hole excitation energy is lower than $E_{\max}$. The particle-hole excited configurations are generated from the Hartree-Fock wave function of ^{236}U at $Q_2 = 14$ b. We use the UNEDF1 parameter set for the Hartree-Fock calculation.

6.1 Inclusion of finite seniority configurations

The seniority quantum number is defined as the number of particles not forming the Kramers pair. Fig. 23 shows the number of configurations of ^{236}U whose excitation energy is under E_{max} . The particle-excited states are generated from the ground state at $Q = 14b$, and the lines in the figure correspond to configurations with different seniority numbers. This figure clearly shows that incorporating only seniority zero configurations is insufficient for a realistic description of nuclear fission. In addition, the proton-neutron particle-hole interaction is known to be important in a transport coefficient of induced fission [65]. However, this interaction can not be included unless finite seniority configurations are incorporated.

The inclusion of finite seniority configurations increases the size of the Hamiltonian matrix and makes numerical calculation difficult. To mitigate numerical difficulty, we introduce energy cutoff in a Q -dependent manner. With the deformation energy $V(Q)$ and the particle-hole excitation energy of configuration i at Q , $E_i(Q)$, we take into account configurations satisfying the condition,

$$E_i(Q) + V(Q) \leq E_{\text{max}}, \quad (99)$$

where the energy cutoff E_{max} is constant. Compared to the energy cutoff criterion in chap. 4, configurations dominantly contributing to nuclear fission are incorporated avoiding the increase of the matrix dimension.

Then we discretize the fission path and generate particle-hole excited configurations from reference states. As the discretization criterion, we have taken into account the neighboring reference states satisfying $\langle Q_i | Q_{i+1} \rangle \sim e^{-1}$, in chapters 4 and 5. To execute more reliable calculations, we have to precisely determine the value of overlap.

We use the same fission path shown in fig. 8 and discretize it with different overlap sizes. Next, we calculate the Hamiltonian matrix elements and the overlap matrix. As residual interactions, we apply the monopole pairing interaction, the diabatic interaction, and the particle-hole random interaction,

$$H_{\text{ran}} = v_{\text{ran}} r \sum_{ijkl} a_i^\dagger a_j^\dagger a_l a_k, \quad (100)$$

where r is a random number sampled from the standard distribution. The value of v_{ran} was estimated microscopically in ref. [52], and we apply $v_{\text{ran}} = 0.025$ MeV for proton-neutron channels and $v_{\text{ran}} = 0.02$ MeV for neutron-neutron and proton-proton channels, respectively.

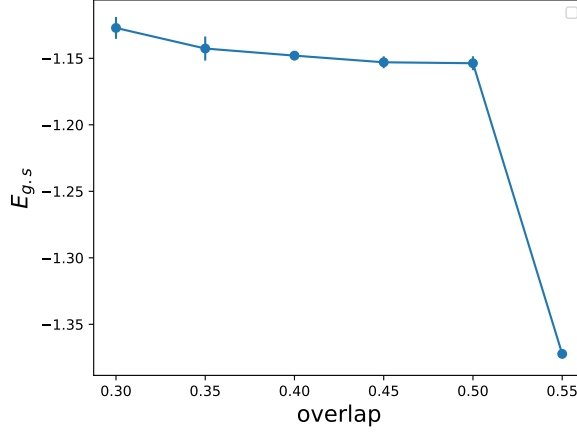


Figure 24: The GCM ground state energy with different overlaps between neighboring reference states. The energy cutoff of the GCM basis is $E_{\max} = 7$ MeV, and the details of other parameters are explained in the main text.

Then we solve the the Hill-Wheeler eq. and examine the convergence of GCM ground energies. Fig. 24 shows the obtained GCM ground energies with different overlap size. The energy gradually decreases as the overlap increases, though it suddenly decreases between 0.5 and 0.55. It signifies the numerical instability due to the overcompleteness of the GCM basis. Therefore, in the following calculations, we use 0.5 as the size of the neighboring overlap.

6.2 Description of the compound nucleus configurations

In the previous chapters, we have replaced the parts of the Hamiltonian matrix with the GOE matrices. However, due to the usage of the GOE matrices, we have to introduce phenomenological parameters, the dimension of the GOE matrix and the size of the GOE matrix elements, and it introduces uncertainty to our theoretical calculations. In addition, in neutron-induced fission reactions of neutron-rich nuclei, which are important in the r-process nucleosynthesis, the excitation energy of the mother nucleus is not high enough to form a compound nucleus. In this case, the usage of the GOE matrix is not justified.

Therefore, in this chapter, we directly calculate the Hamiltonian matrix for compound nucleus configurations (left-end) and fission doorway configurations (right-end) from the Hartree-Fock wave functions. For the calculation of the compound nucleus and fission doorway configurations, the particle-hole excited states are taken into account up to $E_{\max}$ in eq. (99).

The Hamiltonian submatrices corresponding to the compound nucleus and fission doorway configurations include decay width matrices. Unlike previous chapters, compound nucleus configurations and fission doorway configurations have finite overlaps between other basis functions. Consequently, the decay width matrices should be modified from the diagonal ones used in chap. 4.4. The width matrices are defined as [52]

$$(\Gamma_n)_{i,j} = \gamma_n N_{n,i} N_{n,j}, \quad (101)$$

$$(\Gamma_{\text{cap}})_{i,j} = \gamma_{\text{cap}} \sum_{k \in \text{cap}} N_{k,i} N_{k,j}, \quad (102)$$

and

$$(\Gamma_{\text{fis}})_{i,j} = \gamma_{\text{fis}} \sum_{k \in \text{fis}} N_{k,i} N_{k,j}, \quad (103)$$

where N is the overlap matrix. This form of decay width matrices is determined to make decay width matrices diagonal after the Löwdin transformation, and the detail is discussed in appendix A. The neutron channel n and the capture channels are a single configuration and multiple configurations respectively in the left-end Q -block. The excitation energy of these configurations should be around $E_n + S_n$. The fission channels are the all configurations in the fission doorway states.

In the previous chapters, we estimated the size of the decay widths γ_i using these equations,

$$T_i = 2\pi\rho\gamma_i, \quad (104)$$

$$T_n = 2\pi S_0 E_n^{1/2}, \quad (105)$$

and

$$T_{\text{cap}} = 0.25. \quad (106)$$

However, these formulas should be used with the assumption of the complete compound nucleus formation, and this is not the case in our model. Fig. 25 shows the distribution of the component of the eigenvector having eigenenergy around 6.546 MeV. This eigenstate is obtained by diagonalizing

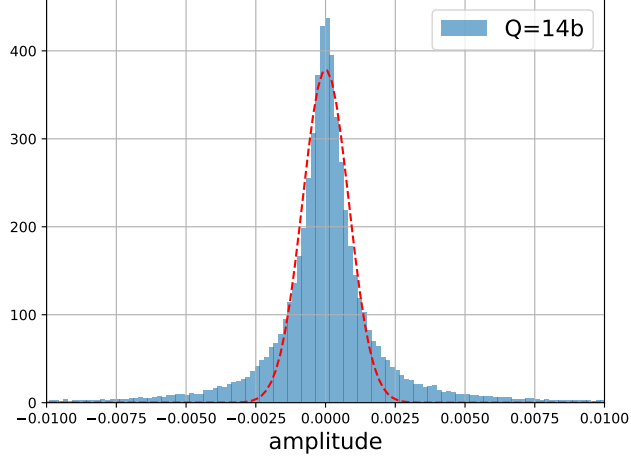


Figure 25: The distribution of coefficients of an eigenvector at $Q = 14$ b. The red lines shows the result of the Gaussian fitting.

the first diagonal submatrix in the total Hamiltonian matrix, which includes the particle-hole excitation configurations at $Q = 14$ b up to $E_{\text{max}} = 7$ MeV. This distribution is not perfectly fitted by the Gauss distribution contrary to the eigenvector of the GOE matrix (see fig. 4). All matrix elements of the GOE matrix have non-zero characters. However, the Hamiltonian matrix for the configurations we take is not dense but sparse due to the two-body nature of the residual interactions. Therefore, its behavior deviates from the GOE matrix. Similar results were reported in the studies applying the embedded GOE matrix [66]. Hence, the eq. (104) can not be applied directly, and we make modifications to that formula. In the following calculation, we assume the linear relationship of T_i and Γ_i as

$$T_i = f_{GOE} 2\pi \rho \gamma_i, \quad (107)$$

and rescale γ_n and γ_{cap} by the factor f_{GOE} . Thereby, we determine the value of f_{GOE} which reproduces the results in the case of the GOE matrix.

Fig. 26 shows the dependence of $T_{n,\text{cap}}$ on the factor f_{GOE} . The number of the neutron channels is one and that of the capture channels is 77 [44]. In the calculation of $T_{n,\text{cap}}$, we take an energy average of the input channel around the energy $E = S_n + E_n = (6.536 + 0.01)$ MeV with a range of 0.5 keV. Fig. 26 shows that the dependence of $T_{n,\text{cap}}$ on f_{GOE} is well fitted by a quadratic function. On the other hand, using eqs. (105,106) and the GOE

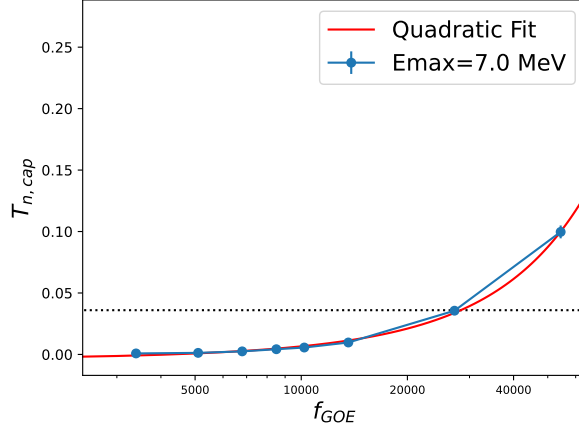


Figure 26: $T_{n,\text{cap}}$ as a function of f_{GOE} . The values of the neutron decay width and the capture decay width are determined by eqs.(105,106,107). On the other hand, Γ_{fis} is set to be zero. The horizontal dotted line indicates $T_{n,\text{cap}} = 0.036$ obtained by the GOE matrix and eq. (104).

matrix, $T_{n,\text{cap}}$ becomes 0.036. Therefore, by interpolation, we determine the value of f_{GOE} with which $T_{n,\text{cap}}$ equals 0.036. In the same way, we determine the value of f_{GOE} with different E_{max} , and the results are summarized in table 4.

On the other hand, the determination of γ_{fis} is relatively simple. In the previous works, the insensitivity of results to the size of γ_{fis} was reported [16, 52]. The insensitivity can be confirmed even in the case with finite-seniority configurations. Fig. 27 shows the values of α^{-1} with different γ_{fis} . The energy cutoff is $E_{\text{max}} = 7$ MeV, and a random seed is fixed in this calculation. This result reproduces the insensitivity reported in ref. [16]. Therefore, in the following calculations, we use $\gamma_{\text{fis}} = 0.15$ MeV, with which the result converges.

6.3 calculation of the transmission coefficients

In order to calculate the transmission coefficients $T_{n,\text{cap}}$ and $T_{n,\text{fis}}$, we have to solve the linear equation,

$$(EN - H)G(E) = I, \quad (108)$$

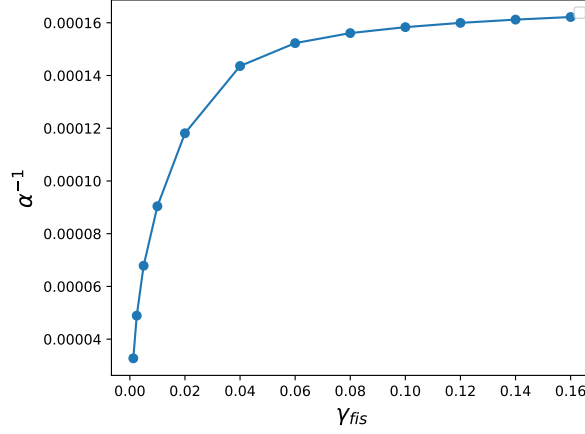


Figure 27: The fission to capture branching ratio α^{-1} with different γ_{fis} . The ensemble average and the energy average are not taken, and the calculation is done with a fixed random seed.

where I is the identity matrix. With the inclusion of the finite seniority configurations, N_{dim} becomes $O(10^5)$. When $N_{\text{dim}} = 5 \times 10^5$, for instance, the memory size of the Hamiltonian matrix becomes $(8+8) \times (5 \times 10^5) \times (5 \times 10^5) = 4\text{T}$ bytes. It exceeds a typical memory capacity of supercomputer systems. Therefore, the usage of sparse matrix formats is almost mandatory. Because we apply residual two-body interactions in the calculation of the Hamiltonian matrix, the Hamiltonian matrix becomes sparse. The percentage of finite matrix elements is about 0.01 %, and the required memory size does not exceed 1G bytes.

In addition, we can notice that the neutron input channel n is single and the corresponding few lines of the Green function are enough for the calculation of the fission probability. If decay matrices are diagonal, the fission transmission coefficient becomes

$$T_{n,\text{fis}} = \gamma_n \gamma_{\text{fis}} \sum_{i \in \text{fis}} |G_{n,i}|^2. \quad (109)$$

Also, the Green function $G(E)$ is a complex symmetric matrix. Therefore it is enough to calculate the single column of the Green function

$$\sum_j (EN - H)_{i,j} G_{j,n} = (0, \dots, 0, 1, 0, \dots, 0)_i^T, \quad (110)$$

where one component of the right-hand side vector corresponding to the channel n is one. Actually, the decay matrices are non-diagonal as defined in eqs. (101-103). However, even in this case, it is enough to make small modifications in eq. (109), and we need to calculate two lines of the Green function matrix to obtain $T_{n,\text{fis}}$. We detail this point in appendix D.

To solve the simultaneous linear equations in eq. (110), instead of the LU decomposition which destroys the sparsity of a matrix, we apply the LSMR algorithm to solve linear equation eq. (110) [67]. This method is mathematically equivalent to the minimal residual method. However, it is more robust than the minimal residual method or other ones. The LSMR algorithm is implemented in SciPy and CuPy libraries, and we use the latter implementation to make use of the NVIDIA A100 GPU equipped in SQUID supercomputer system at Osaka University.

6.4 Results

In a similar way to the previous subsection, we determine the parameters included in our model. First, we generate seniority-zero configurations only up to E_{max} and determine the pairing strength G to reproduce the excitation energy of the second 0^+ state. Then we calculate the fission path and discretize it based on the criterion that $\langle Q_i | Q_{i+1} \rangle \simeq 0.5$. It generates the chain of the Q -blocks: $Q = 14, 17, 20, 24, 28, 31, 36, 39, 44, 49, 53, 56, 59, 62, 66, 69, 72, 79$, and 84. Next, we determine the value of factor f to reproduce experimental fission barrier height, 5.7 MeV [44]. After that, we generate finite seniority particle-hole excited states at each Q , and the size of each Q -blocks are determined. The resultant values of G and f are summarized in table 4, and the sizes of each Q -blocks are also plotted in fig. 28.

Table 4: The determined values of G , f , and f_{GOE} with different E_{max} .

$E_{\text{max}}(\text{MeV})$	G (MeV)	f	f_{GOE}
6.0	-0.1425	0.6810	35070
6.5	-0.1448	0.6905	23954
7.0	-0.1465	0.6980	28288
7.5	-0.1436	0.6973	26476
8.0	-0.1412	0.6949	40964

To calculate transmission coefficients, we have to determine the factor f_{GOE} in eq. (107). f_{GOE} depends on the excitation energy, and we fix

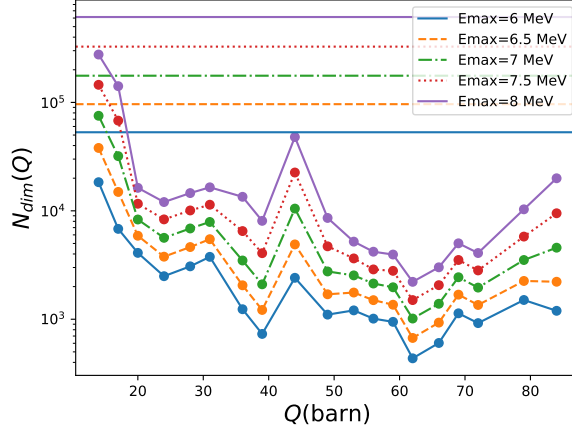


Figure 28: Each lines shows the sizes of Q -blocks at Q with different $E_{\max}$. The horizontal lines show the total sizes of the Hamiltonian matrix with different $E_{\max}$.

$E = S_n + E_n = (6.536 + 0.01)$ MeV here and in the following calculation. As detailed in sec. 6.2, we fit the dependence of $T_{n,\text{cap}}$ on f_{GOE} by the quadratic function and take a value of f_{GOE} giving $T_{n,\text{cap}} = 0.036$. The values of obtained f_{GOE} are summarized in table 4.

Based on the above setup, we calculate the branching ratio $\alpha^{-1} = T_{n,\text{fis}}/T_{n,\text{cap}}$ and check the convergence to the energy cutoff. Fig. 29 shows the calculated α^{-1} with different $E_{\max}$. The value of α^{-1} converges in the region where $E_{\max}$ is greater than 7 MeV. It suggests that the model space is adequate to describe the induced fission with $E = 6.546$ MeV. However, our results underestimate the experimental value $\alpha^{-1} \simeq 3$ by an order of magnitude [53]. Though it is an achievement that values comparable to experimental results were obtained through realistic microscopic calculations for the first time, the improvement of the underestimation should be an important future work.

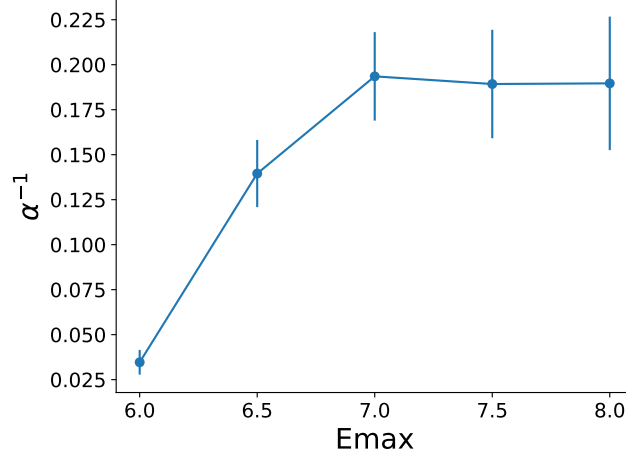


Figure 29: α^{-1} with different $E_{\max}$. The error bars indicate a statistical error, and it is smaller than 20 %.

One of the possible reasons might be the lack of symmetric fission modes. According to the fission yields of $^{235}\text{U}(n, f)$ reaction, even though the symmetric fission mode is not dominant, it contributes to some extent [68]. To incorporate this effect in our model, as a first step, it is possible to consider splitting the fission path into two branches in the $Q_2 - Q_3$ plane. Then, it is desirable to execute full two-dimensional GCM calculation with Q_2 and Q_3 coordinates for the next step. As another direction, one could consider the role of the dynamical effects of the generator coordinate. It is well known that the GCM fails to reproduce the mass of the center of mass motion [19], though the incorporation of the conjugate collective momentum resolves this problem [69]. The importance of the collective momentum in the fission reaction was pointed out in the recent publication [70]. In this reference, the authors discussed that based on the simple Hamiltonian, it will be meaningful to test the role of the collective momentum in a more realistic setup.

7 Conclusion and Outlook

In this thesis, we have discussed a microscopic formulation of neutron-induced fission and its applications. In chap. 1 we have introduced nuclear fission, and in chap. 2, we have reviewed the previous theoretical works being the foundation of our approach. In chap. 3, we have detailed our NEGF approach based on the S-matrix dispersion formula and the generator coordinate method. In chap. 4, we have applied the NEGF approach to the induced fission reaction $^{235}\text{U}(n, f)$, and analyzed the fluctuation of the fission channels. Our calculation has reproduced the small value of the degrees of freedom in the fission channels microscopically for the first time. In addition, by applying the spectrum decomposition of the Green function, we have shown that the number of the GCM eigenstates contributing to the fission corresponds to the degrees of freedom. In chap. 5, to reduce the numerical costs of the NEGF calculation, we have proposed the usage of the shift-invert Lanczos method. Using this method we can calculate the dominantly contributing eigenstates to the fission and well approximate the transmission coefficients. In our demonstration, the error of this approximation is about 1%, and the numerical costs are reduced about 30-40 times. In chap. 6, we have taken into account all seniority configurations and have improved the reliability of our approach. To manage the increase of the numerical costs accompanied with the finite seniority configurations, we have improved the criteria for the energy cutoff, made use of the high-performance GPU, and applied the efficient numerical algorithm of the linear simultaneous equation, the LSMR algorithm. It allowed us to calculate the branching ratio for the large-dimensional Hamiltonian of the order of $O(10^5)$. Although our results underestimate the experimental value of the branching ratio by about one order, it provides a reasonable estimation of it. This point will be improved by the inclusion of the symmetric fission modes or the effects of the conjugate collective momentum.

As a future direction, an application of the NEGF approach to the induced fission of the neutron-rich nuclei is a promising one. In these cases, experimental studies are extremely difficult, and an analysis based on reliable microscopic models is highly desired. Also, in neutron-rich nuclei, the excitation energy of the fissioning nuclei is lower, and studying how the fission mechanism changes with energy and temperature is intriguing. As another future direction, the analysis of the spontaneous fission process based on the eigenmode decomposition is also interesting. In the microscopic studies

of spontaneous fission, adiabatic approximation is widely applied, and this approach is suitable to examine the validity of it.

Acknowledgements

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I am grateful to the members of the nuclear theory group as well. Without their support, it would have been difficult to continue my research.

Finally, I would like to thank my parents for all the support so far.

A Schematic model calculation with finite seniority configurations

In this appendix, we detail the calculation of nuclear fission based on the schematic Hamiltonian. A calculation with finite seniority configuration like sec. 6 requires huge numerical cost. Therefore we apply the simple model Hamiltonian and examine the role of the finite seniority configurations and different types of nucleon-nucleon interactions. The contents in this appendix are summarized in ref. [52]

A.1 Model Hamiltonian

The Hamiltonian for each Q is constructed as

$$H_Q = V(Q) + H_{\text{sp}} + H_{\text{pair}} + H_{\text{ran}}. \quad (111)$$

Here $V(Q)$ is the potential energy, H_{sp} is the single-particle Hamiltonian, H_{pair} is the pairing interaction, and H_{ran} is the random neutron-proton interaction. We use a model with a uniform spectrum of orbital energies with a spacing d for both protons and neutrons. Thus, the single-particle Hamiltonian is given as

$$H_{\text{pair}} = d \sum_{\alpha: n_\alpha > 0} n_\alpha a_\alpha^\dagger a_\alpha + d \sum_{\alpha: n_\alpha < 0} n_\alpha a_\alpha a_\alpha^\dagger. \quad (112)$$

The label α includes the parameter q and an index ν of orbitals, and the conserved quantum numbers, parity π , isospin t_z and angular momentum projection K . To keep the model as simple, K is restricted to $\pm \frac{1}{2}$.

The single-particle excitation energy of many-particle configurations becomes integral multiples of d , $E_{\text{ex}} = kd$. The number of configurations having $\sum K = 0$ and $\sum t_z = 0$ increases exponentially as a function of $\sqrt{E_{\text{ex}}}$ as shown in fig. 30, and it reproduces the empirical forms of level density [40].

About the size of the level spacing d , there are several estimates of d for ^{236}U [52] summarized in table 5. In this appendix, we use 0.5 MeV for the value of d .

For residual interactions, we include both the particle-particle (pp) and particle-hole (ph) types. For the pp interaction, we use a monopole pairing interaction,

$$H_{\text{pair}} = -G_{\text{pair}} \sum_{\nu \neq \nu'} a_{\nu'}^\dagger a_{\bar{\nu}'}^\dagger a_{\bar{\nu}} a_\nu. \quad (113)$$

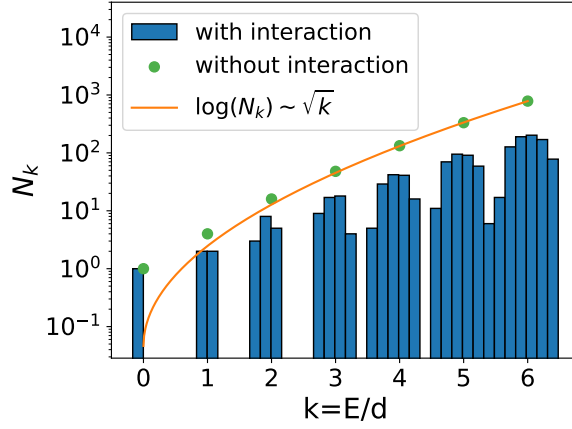


Figure 30: A spectrum of many-body configurations in the uniform spacing model. N_k denotes the number of configurations at the excitation energy $E = kd$. The green circles show the spectrum without the interaction terms, while the orange curve shows its fit to the functional form of $N_k = \exp(a\sqrt{k} + b)$ with $a = 3.97$ and $b = -3.06$. The blue histograms show the interacting spectrum, obtained by diagonalizing the Hamiltonian with $G_{pair} = 0$ and $v_{np} = 0.03d$.

Table 5: Estimated orbital level spacing in ^{236}U .

d (MeV)	Source
0.45	Woods-Saxon well
0.51	FRLDM [71]
0.33	FGM [72]

Empirically, $G_{\text{pair}} = \frac{28}{A}$ has been used [73], and we take $G_{\text{pair}} = 0.3d$ as the baseline value. For the ph type interaction, we employ a random interaction

$$H_{\text{ran}} = -v_{np} \sum'_{\alpha 1, \alpha 2, \alpha 3, \alpha 4} r a_{\alpha 1}^{\dagger} a_{\alpha 2}^{\dagger} a_{\alpha 4} a_{\alpha 3}, \quad (114)$$

where the parameter v_{np} is the strength of the interaction and r is a random number sampled from the standard normal distribution. The sum of α is restricted to the combinations satisfying $K_1 + K_2 = K_3 + K_4$. Ref. [65] suggests that the proton-neutron interaction dominantly contributes to a diffusion process in a deformation parameter space compared with the interactions between identical particles. We therefore take into account only the proton-neutron interaction. The strength of the proton-neutron interaction is summarized in table 6 and we take $v_{np} = 0.03d$ as a base value.

Table 6: Estimates of the neutron-proton interaction strength.

Basis of estimate	v_0 (MeV fm ³)	Citation
G -matrix	530	[65]
sd -shell spectra	490	[74]
β -decay	395,320	[75]

A.2 Couplings between the Q-blocks

The interaction between different Q blocks is suppressed due to the imperfect overlap of basis functions. The size of the suppression is determined by the overlap kernel $N(Qj, Q'j')$. For simplicity, we assume that the change of the single-particle orbital is small, and the configurations with the same j with different Q are connected as

$$N(Qj, Q'j') = N(Q, Q')\delta_{jj'}. \quad (115)$$

$N(Q, Q')$ is the overlap between the same configurations and parametrized based on the Gaussian overlap approximation,

$$N(Q, Q') = \exp(-\lambda(Q - Q')^2). \quad (116)$$

The parameter λ is the measure of the distance between neighboring configurations, and we take $\lambda = 1.0$.

We can calculate the Hamiltonian kernel with the same assumptions. The matrix elements between the configurations belonging to different Q blocks is multiplied by the factor $N(Q, Q')$. In addition, the diabatic interaction should be taken into account for the diabatically connected configurations. The form of this interaction was derived in ref. [48], and the formula reads

$$\frac{\langle qj|v_{db}|q'j\rangle}{\langle q|q'\rangle} = \frac{E(qj) + E(q'j)}{2} - h_2(q - q')^2. \quad (117)$$

The value of h_2 was estimated to be about 1.5 MeV in ref. [16], and we take $h_2 = 3d$ in this model.

A.3 Width matrices

To derive the form of width matrices in a non-orthogonal basis, first, we consider the Green function for the collective Hamiltonian

$$\tilde{H}_{\text{coll}} = N^{-1/2} H N^{-1/2}, \quad (118)$$

where H and N are the Hamiltonian and the norm kernel. The Green function reads

$$\tilde{G}_{\text{coll}}(E) = (EI - \tilde{H}_{\text{coll}})^{-1}. \quad (119)$$

The Green function in the orthogonalized basis is transformed as

$$\tilde{G}_{\text{coll}}(E) = (EI - N^{-1/2} H N^{-1/2})^{-1} = N^{1/2} (EN - H)^{-1} N^{1/2}. \quad (120)$$

The decay width matrix $\tilde{\Gamma}_a$ in the orthogonalized basis is also transformed as

$$(\Gamma_a)_{i,j} = N_{ia}^{1/2} N_{ja}^{1/2} \tilde{\Gamma}_a, \quad (121)$$

which is derived based on the invariance of the transmission coefficients,

$$T_{ab}(E) = \text{Tr}[\tilde{\Gamma}_a \tilde{G}_{\text{coll}}(E) \tilde{\Gamma}_b \tilde{G}_{\text{coll}}^\dagger] = \text{Tr}[\Gamma_a G(E) \Gamma_b G^\dagger(E)]. \quad (122)$$

Therefore in this appendix, we use the form of the decay width matrix

$$(\Gamma_a)_{kk'} = \gamma_a \sum_{l \in a} (N^{1/2})_{kl} (N^{1/2})_{k'l}, \quad (123)$$

which is parametrized by the scalar parameter γ_a .

A.4 Results

In this subsection, we consider a chain of three Q blocks with $Q = -1, 0, 1$. Thus the overlap between neighboring Q blocks is $N(Q, Q \pm 1) = e^{-1}$ by eq. (116). For the barrier, we set $V(Q = \pm 1) = 0$ and $V(Q = 0) = 4d$. The single particle excitation is taken into account up to $E_{\text{cut}} = V(Q) + 5.5d$ in each Q blocks. The neutron and capture channels are coupled to all configurations at $Q = -1$, and likewise the fission channels are coupled to all configurations at $Q = 1$. In the actinide region, the relation $\gamma_n < \gamma_{\text{cap}} < \gamma_{\text{fis}}$ is known, and we set $\gamma_n = 0.001d$, $\gamma_{\text{cap}} = 0.01d$, and $\gamma_{\text{fis}} = 0.1d$.

Fig. 31 shows the transition probability $T_{n,\text{fis}}$ with two different values of v_{np} . Here the pairing interaction G_{pair} is set to be zero. The peaks in fig. 31 are lowered and broadened as v_{np} increases. It is because the random interaction spreads the spectrum as indicated in fig. 30. The proton-neutron random interaction also increases the fission probability as summarized in table 7 below.

Table 7: The average transmission coefficient for fission $\langle T_{n,\text{fis}} \rangle$ and the branching ratio α^{-1} for several sets of interactions. The parameters shown for models I-V are the only ones that differ from the base model.

Model	v_{np}	G_{pair}	h_2	$\langle T_{n,\text{fis}} \rangle$	α^{-1}
base	0.03	0.3	3	0.417	1.62
I		0.0		0.413	1.49
II	0.0			0.372	1.14
III	0.05			0.429	2.27
IV			0.0	0.294	0.739
V	0.0	0.0	0.0	0.172	0.291

Then, fig. 32 shows an average fission-to-capture branching ratio defined as

$$\alpha^{-1}(E) = \frac{\int_{E-0.5d}^{E+0.5d} dE' T_{n,\text{fis}}(E')}{\int_{E-0.5d}^{E+0.5d} dE' T_{n,\text{cap}}(E')}. \quad (124)$$

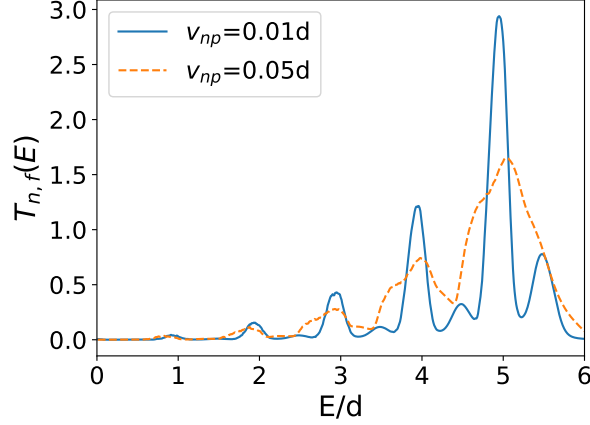


Figure 31: The transmission coefficient $T_{n,\text{fis}}(E)$ with two different values of v_{np} . The pairing interaction $G_{\text{pair}} = 0$, and the other parameters are set to be $\lambda = 1.0$, $h_2 = 3d$, and $B_h = 4d$.

The solid and the dashed lines show the results with $h_2 = 3d$ and $h_2 = 0$, respectively. $\alpha^{-1}(E)$ increases with the excitation energy, and the diabatic interaction increases the branching ratios, being consistent with the result in ref. [16].

Table 7 summarizes the results for several parameter sets. The results of models I, II, and III indicate that both the neutron-proton random interaction and the pairing interaction increase the fission probability, though the probability is more sensitive to the neutron-proton interaction. The model IV tells us that the $T_{n,\text{fis}}$ and α^{-1} significantly decreases without the diabatic interaction. In model V, the transmission coefficient is not zero even though all the interaction strengths are set to zero. This is due to the non-orthogonality of the reference states. By constructing the non-orthogonal basis by the transformation from the orthogonal basis, the transmission is confirmed to become zero [52].

Then we examine the validity of the transition state hypothesis. The Bohr-Wheeler formula in eq. (11) indicates that the transition states entirely determine the decay rate, and the details after the barrier are unimportant. Fig. 33 shows the branching ratios at $E = 4d$ as a function of γ_{fis} . In the case of the orthogonal basis, the branching ratio is almost insensitive to γ_{fis} , in agreement with the insensitivity property. On the other hand, α^{-1}

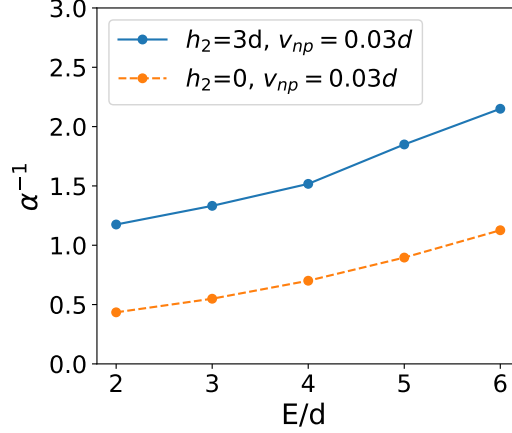


Figure 32: The average fission-to-capture branching ratios as a function of the energy with two different values of h_2 . The random neutron-proton interaction is taken into account with the strength of $v_{np} = 0.03d$, while the pairing interaction is set to be zero.

gradually increases and tends to converge at a large value of γ_{fis} . To check the dependence on the number of Q blocks, we repeat the calculations with $7Q$ blocks ranging from $q = -3$ to $q = 3$. In this case, α^{-1} changes by less than a factor of two within the whole range of γ_{fis} . All of these results indicate that the transition state hypothesis is realized in the microscopic theory.

B Skyrme-Hartree-Fock equation

In this appendix, we explain the Skyrme-Hartree-Fock equation, which has been applied to generate many-body configurations in the main part of this thesis.

In the Hartree-Fock approximation, a many-body Hamiltonian

$$H = \sum_{ij} t_{i,j} a_i^\dagger a_j + \frac{1}{2} \sum_{ijkl} V_{ijkl} a_i^\dagger a_j^\dagger a_l a_k \quad (125)$$

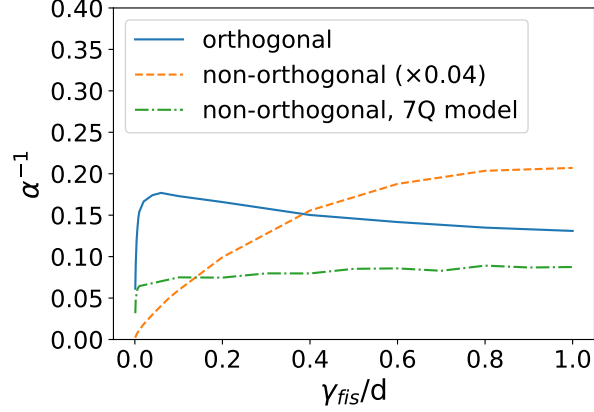


Figure 33: The branching ratios at $E = 4d$ as a function of γ_{fis} . The interaction strengths are $(v_{pn}, G_{\text{pair}}, h_2) = (0.03, 0.3, 3)d$. The solid and the dashed lines show the results of the $3Q$ model, while the dot-dashed line the result of the $7Q$ model. The non-orthogonality of the configurations is neglected in the solid line.

is approximated as

$$\begin{aligned}
 H_{\text{HF}} &= \sum_{ij} \left\{ t_{ij} + \frac{1}{2} \sum_{kl} (V_{ikjl} \langle a_k^\dagger a_l \rangle - V_{ilkj} \langle a_l^\dagger a_k \rangle) \right\} a_i^\dagger a_j, \\
 &\equiv \sum_{ij} h_{ij} a_i^\dagger a_j.
 \end{aligned} \tag{126}$$

where t_{ij} and V_{ijkl} are the kinetic term and a two-body interaction [19]. We defined the single particle Hamiltonian h_{ij} in the last line. The total Hamiltonian becomes the sum of the single-particle Hamiltonians, and the many-body wavefunction becomes the Slater determinant. On the other hand, h_{ij} includes the on-body particle-hole density $\langle a_k^\dagger a_l \rangle$, and it depends on the single particle wavefunctions. Therefore we have to solve the Schrödinger equation for H_{HF} iteratively until the solution converges self-consistently.

As a two-body interaction in eq. (125), we apply the Skyrme interaction

[76] defined as

$$\begin{aligned}
V(i, j) = & t_0(1 + x_0 \hat{P}_\sigma) \delta(\vec{r}_i - \vec{r}_j) + \frac{t_3}{6}(1 + x_3 \hat{P}_\sigma) \delta(\vec{r}_i - \vec{r}_j) \rho^\alpha \left(\frac{1}{2}(\vec{r}_i + \vec{r}_j) \right) \\
& - \frac{t_1}{2}(1 + x_1 \hat{P}_\sigma) ((\nabla_1 - \nabla_2)^2 \delta(\vec{r}_i - \vec{r}_j) + h.c.) \\
& - t_2(1 + x_2 \hat{P}_\sigma) ((\nabla_i - \nabla_j) \delta(\vec{r}_i - \vec{r}_j) (\nabla_i - \nabla_j)) \\
& - it_4(\nabla_i - \nabla_j) \times \delta(\vec{r}_i - \vec{r}_j) (\nabla_i - \nabla_j) (\vec{\sigma}_i + \vec{\sigma}_j). \tag{127}
\end{aligned}$$

Here $t_0, t_1, t_2, t_3, t_4, x_0, x_1, x_2, x_3$ and α are the parameters, and $\hat{P}_\sigma = \frac{1}{2}(1 + \vec{\sigma}_i \cdot \vec{\sigma}_j)$ is the spin-exchange operator. The Skyrme interaction has zero-range spatial parts and it simplifies the treatment of the non-local exchange interactions.

Using the Skyrme interaction, the Schrödinger equation for the single-particle Hamiltonian becomes,

$$\left[-\nabla \frac{1}{2m_q^*(\vec{r})} \nabla + U_q(\vec{r}) + \vec{W}_q(\vec{r}) \cdot (-i\nabla \times \vec{\sigma}) \right] \phi_k(\vec{r}) = \epsilon_k \phi_k(\vec{r}), \tag{128}$$

where ϕ_k is the single-particle wavefunction, the effective mass $2m_q^*$ is written as

$$\frac{1}{2m_q^*(\vec{r})} = \frac{1}{2m} + \frac{1}{4} \left\{ t_1 \left(1 + \frac{x_1}{2} \right) + t_2 \left(1 + \frac{x_2}{2} \right) \right\} \rho - \frac{1}{4} \left\{ t_1 \left(\frac{1}{2} + x_1 \right) - t_2 \left(\frac{1}{2} + x_2 \right) \right\} \rho_q, \tag{129}$$

and the potential term U_q becomes

$$\begin{aligned}
U_q(\vec{r}) = & t_0 \left(1 + \frac{x_0}{2} \right) \rho - t_0 \left(\frac{1}{2} + x_0 \right) \rho_q \\
& + \frac{t_3}{12} \left(1 + \frac{x_3}{2} \right) (\alpha + 2) \rho^{\alpha+1} - \frac{t_3}{12} \left(\frac{1}{2} + x_3 \right) \left(\alpha \rho^{\alpha-1} \sum_q \rho_q^2 + 2\rho^\alpha \rho_q \right) \\
& + \frac{1}{4} \left\{ t_1 \left(1 + \frac{x_1}{2} \right) + t_2 \left(1 + \frac{x_2}{2} \right) \right\} \tau - \frac{1}{4} \left\{ t_1 \left(\frac{1}{2} + x_1 \right) - t_2 \left(\frac{1}{2} + x_2 \right) \right\} \tau_q \\
& - \frac{1}{8} \left\{ 3t_1 \left(1 + \frac{x_1}{2} \right) - t_2 \left(1 + \frac{x_2}{2} \right) \right\} \Delta \rho + \frac{1}{8} \left\{ 3t_1 \left(\frac{1}{2} + x_1 \right) + t_2 \left(\frac{1}{2} + x_2 \right) \right\} \Delta \rho_q \\
& - \frac{t_4}{2} \left\{ \nabla \vec{J} + \nabla \vec{J}_q \right\}. \tag{130}
\end{aligned}$$

Here, the density, the kinetic energy density, and the spin current density are defined as,

$$\rho(\vec{r}) = \sum_k |\phi_k(\vec{r})|^2, \quad (131)$$

$$\tau(\vec{r}) = \sum_k |\nabla \phi_k(\vec{r})|^2, \quad (132)$$

and

$$\vec{J}(\vec{r}) = -i \sum_k \phi_k^*(\vec{r}) [\nabla \phi_k(\vec{r}) \times \vec{\sigma}], \quad (133)$$

respectively. q is the label of the isospin and the term without q is the sum of the neutron and proton term as $\rho = \rho_n + \rho_p$.

We can solve this single-particle Schrödinger equation by diagonalizing the Hamiltonian matrix. Thereby the single-particle wavefunctions and the single-particle Hamiltonian are updated. This procedure is continued until the solution converges. As an alternative way, using the gradient methods and updating the single-particle wavefunctions to minimize the total energy, we can obtain the correct Hartree-Fock wavefunction. In the SkyAx code [46], the latter procedure is adopted.

In the main text, we have used the Hartree-Fock wave functions labeled by the quadrupole moment, $|Q_2\rangle$. Because the derivation of the Hartree-Fock equation is based on the variation, we added the constraint terms to the original Hamiltonian,

$$H'_{\text{HF}} = H_{\text{HF}} + \lambda(\hat{Q}_2 - Q_2) + \frac{C}{2}(\hat{Q}_2 - Q_2)^2, \quad (134)$$

where λ and C are the parameters, $\hat{Q}_2$ is the quadrupole moment operator, and Q_2 is the desired value. Solving the Hartree-Fock equation for H'_{HF} , the Hartree-Fock wavefunction satisfying $\langle \hat{Q}_2 \rangle_{\text{HF}} = Q_2$ is obtained. Within the constraint Hartree-Fock calculation, the usage of the linear and quadratic constraints is called the augmented Lagrangian method and is known to be numerically advantageous compared to the case with only linear or quadratic constraints [77].

C Details of the inversion calculation of the Green function

In this appendix, we detail the calculation of the Green function matrix used in Chapter. 4. The following discussion is mainly based on Ref. [41]. We consider the block tridiagonal matrix A as

$$A = \begin{pmatrix} a_{11} & a_{12} & & & & \\ a_{21} & a_{22} & a_{23} & & & \\ & a_{32} & a_{33} & a_{34} & & \\ & & \ddots & \ddots & \ddots & \\ & & & & a_{NN-1} & a_{NN} \end{pmatrix}. \quad (135)$$

In the calculation of the transition probability T_{ab} , we do not need all matrix elements of the inversion matrix $G \equiv A^{-1}$. First we augment the matrix A with the identity matrix I as

$$[A|I] = \left(\begin{array}{cccccc|cccc} a_{11} & a_{12} & & & & & i_{11} & & & \\ a_{21} & a_{22} & a_{23} & & & & & i_{22} & & \\ & a_{32} & a_{33} & a_{34} & & & & & i_{33} & \\ & & \ddots & \ddots & \ddots & & & & & \ddots \\ & & & & a_{NN-1} & a_{NN} & & & & \end{array} \right). \quad (136)$$

By manipulating the matrix to $[A|I]$ such that A is reduced to the identity matrix I , the augmented matrix is converted to $[I|G]$, where the inversion matrix G is obtained. To do so, the forward and backward block Gaussian elimination method can be applied.

In the block Gaussian elimination step, first, we add the first block row multiplied by the matrix $c_1^L = -a_{21}a_{11}^{-1}$ to the second block row. Thereby,

the block in the (2,1) position becomes zero as,

$$\begin{aligned}
& \left(\begin{array}{ccc|ccc} a_{11} & a_{12} & & i_{11} & & \\ a_{21} + c_1^L a_{11} & a_{22} + c_1^L a_{12} & a_{23} & c_1^L i_{11} & i_{22} & \\ & a_{32} & a_{33} & & i_{33} & \\ & & \ddots & & & \ddots \end{array} \right) \\
&= \left(\begin{array}{ccc|ccc} a_{11} & a_{12} & & i_{11} & & \\ 0 & a_{22} - a_{21} a_{11}^{-1} a_{12} & a_{23} & -a_{21} a_{11}^{-1} i_{11} & i_{22} & \\ & a_{32} & a_{33} & & i_{33} & \\ & & \ddots & & & \ddots \end{array} \right). \tag{137}
\end{aligned}$$

Next, the second row is added to the third row after multiplied by the factor $C_2^L = -a_{32}(a_{22} - a_{21}a_{11}^{-1}a_{12})^{-1}$, and the block in the (3,2) position is erased. This process is continued up to the last row block. Thereby the diagonal blocks of the resulting matrix on the left become,

$$\begin{aligned}
d_{11}^L &= a_{11} \\
d_{22}^L &= a_{22} - a_{21}(d_{11}^L)^{-1}a_{12} \\
d_{33}^L &= a_{33} - a_{32}(d_{22}^L)^{-1}a_{23} \\
&\vdots \\
d_{ii}^L &= a_{ii} - a_{i,i-1}(d_{i-1,i-1}^L)^{-1}a_{i-1,i} \\
&\vdots \\
d_{NN}^L &= a_{NN} - a_{N,N-1}(d_{N-1,N-1}^L)^{-1}a_{N-1,N} \\
&, \tag{138}
\end{aligned}$$

and the multiplication factor is

$$\begin{aligned}
c_1^L &= -a_{21}(d_{11}^L)^{-1} \\
c_2^L &= -a_{32}(d_{22}^L)^{-1} \\
c_3^L &= -a_{43}(d_{33}^L)^{-1} \\
&\vdots \\
c_i^L &= -a_{i+1,i}(d_{ii}^L)^{-1} \\
&\vdots \\
c_{N-1}^L &= -a_{N,N-1}(d_{N-1,N-1}^L)^{-1}. \tag{139}
\end{aligned}$$

Using d^L and c^L , the resultant matrix after the forward Gaussian elimination process is written as,

$$[D^L|J^L] = \left(\begin{array}{cccc|cccc} d_{11}^L & a_{12} & & & i_{11} & & & \\ 0 & d_{22}^L & a_{23} & & c_1^L i_{11} & i_{22} & & \\ & 0 & d_{33}^L & a_{34} & c_2^L c_1^L i_{11} & c_2^L i_{22} & i_{33} & \\ & & \ddots & \ddots & \vdots & \vdots & & \ddots \end{array} \right). \quad (140)$$

In the same way, the backward process is defined and the resultant matrix becomes,

$$[D^R|J^R] = \left(\begin{array}{cccc|cccc} d_{11}^R & 0 & & & i_{11} & c_2^R i_{22} & c_2^R c_3^R i_{33} & \dots \\ a_{21} & d_{22}^R & 0 & & & i_{22} & c_3^R i_{33} & \dots \\ & a_{32} & d_{33}^R & 0 & & & i_{33} & \dots \\ & & \ddots & \ddots & & & & \ddots \end{array} \right). \quad (141)$$

Here, we use the facts

$$AG = 1, D^L G = J^L, D^R G = J^R, \quad (142)$$

the relation

$$(A - D^L - D^R)G = I - J^L - J^R \quad (143)$$

is obtained. This linear equation is represented in the form of the augmented matrix as,

$$[B|F] = [A|I] - [A^L|J^L] - [A^R|J^R], \quad (144)$$

where

$$B = \begin{pmatrix} a_{11} - d_{11}^L - d_{11}^R & & & \\ & a_{22} - d_{22}^L - d_{22}^R & & \\ & & a_{33} - d_{33}^L - d_{33}^R & \\ & & & \ddots \end{pmatrix}, \quad (145)$$

and

$$F = \begin{pmatrix} -i_{11} & -c_2^R & -c_2^R c_3^R & \\ -c_1^L & -i_{22} & -c_3^R & \\ -c_2^L c_1^L & -c_2^L & -i_{33} & \\ & & & \ddots \end{pmatrix}. \quad (146)$$

The green function G is expressed as $G = B^{-1}F$ and B^{-1} is also block diagonal. Therefore, using the factors $g_{ii} = (-a_{ii} + d_{ii}^L + d_{ii}^R)^{-1}$, G becomes,

$$G = \begin{pmatrix} g_{11} & g_{11}c_2^R & g_{11}c_2^R c_3^R & \dots & g_{11}c_2^R c_3^R \dots c_N^R \\ g_{22}c_1^L & g_{22} & g_{22}c_3^R & \dots & g_{22}c_3^R c_4^R \dots c_N^R \\ g_{33}c_2^L c_1^L & g_{33}c_2^L & g_{33} & \dots & g_{33}c_4^R c_5^R \dots c_N^R \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ g_{nn}c_{N-1}^L \dots c_1^L & g_{nn}c_{N-1}^L \dots c_2^L & g_{nn}c_{N-1}^L \dots c_3^L & \dots & g_{nn} \end{pmatrix}. \quad (147)$$

Following this expression, we can calculate the block elements of G by the matrix inversion of the submatrix $(-a_{ii} + d_{ii}^L + d_{ii}^R)$ instead of the full matrix inversion. Another advantage of this expression is calculating the block matrix elements of G selectively. In the neutron fission reaction, we need only the block matrix in the (1,N) position.

D Transmission coefficients with non-orthogonal baiss

We derive the simple expression for the trace formula

$$T_{n\text{fis}} = \text{Tr}[\Gamma_n G(E) \Gamma_{\text{fis}} G(E)^\dagger], \quad (148)$$

when the bases are non-orthogonal and the overlap matrix is not identity. To make the discussion simple, we consider the 3×3 Hamiltonian and the overlap matrix,

$$H = \begin{pmatrix} 0 & V & 0 \\ V & B_h & V \\ 0 & V & 0 \end{pmatrix}, \quad (149)$$

and

$$N = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & n \\ 0 & n & 1 \end{pmatrix}. \quad (150)$$

The first, second, and third bases correspond to a compound nucleus, a barrier configuration, and a fission doorway, respectively. The important point is the second and the third bases are not orthogonal. Therefore Γ_{fis} becomes non-diagonal,

$$(\Gamma_{\text{fis}})_{i,j} = \gamma_{\text{fis}}(N^{1/2})_{3,i}(N^{1/2})_{3,j}. \quad (151)$$

On the other hand, Γ_n is still diagonal,

$$\Gamma_n = \begin{pmatrix} \gamma_n & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (152)$$

Using $a = \frac{1}{2}(\sqrt{1+n} + \sqrt{1-n})$ and $b = \frac{1}{2}(\sqrt{1+n} - \sqrt{1-n})$, $N^{1/2}$ can be expressed as

$$N^{1/2} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & a & b \\ 0 & b & a \end{pmatrix}. \quad (153)$$

Then Γ_{fis} becomes

$$\Gamma_{\text{fis}} = \gamma_{\text{fis}} \begin{pmatrix} 0 & 0 & 0 \\ 0 & b^2 & ab \\ 0 & ab & aa \end{pmatrix}. \quad (154)$$

Therefore,

$$G\Gamma_n = \gamma_n \begin{pmatrix} G_{11} & 0 & 0 \\ G_{21} & 0 & 0 \\ G_{31} & 0 & 0 \end{pmatrix}, \quad (155)$$

and

$$G^\dagger \Gamma_{\text{fis}} = \gamma_{\text{fis}} \begin{pmatrix} 0 & (b^2 G_{21} + ab G_{31})^* & (ab G_{21} + a^2 G_{31})^* \\ 0 & (b^2 G_{22} + ab G_{32})^* & (ab G_{22} + a^2 G_{32})^* \\ 0 & (b^2 G_{23} + ab G_{33})^* & (ab G_{23} + a^2 G_{33})^* \end{pmatrix}. \quad (156)$$

Finally,

$$\text{Tr}[\Gamma_n G(E) \Gamma_{\text{fis}} G(E)^\dagger] = \gamma_n \gamma_{\text{fis}} (b^2 |G_{21}|^2 + 2ab \text{Re}(G_{21} G_{31}^*) + a^2 |G_{31}|^2). \quad (157)$$

The generalization of this expression for arbitral dimension cases is straightforward, and we made use of it in the calculation in chapter 6.

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