

# Microscopic description of induced fission in a configuration interaction approach

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**Abstract.** Even though more than 80 years have passed since the discovery of fission, its microscopic understanding has still been unclear. To clarify the underlying mechanics of induced fission, we analyze the distribution of a fission width using a microscopic framework based on a configuration-interaction approach. The distribution is known to follow a chi-squared distribution, which is characterized by the effective number of decay channels,  $\nu$ . We introduce an effective Hamiltonian for the space of compound nucleus states and estimate  $\nu$  from the rank of the imaginary part of the effective Hamiltonian. Applying the model to  $^{235}\text{U}(n,f)$ , we successfully reproduce the empirical value of  $\nu = 2.3 \pm 1.1$ . We also find that  $\nu$  is insensitive to the number of fission channels, which is consistent with an experimental finding.

## 1 Introduction

Nuclear fission was discovered in 1938 [1], and in the following year, 1939, Bohr and Wheeler explained its mechanism based on the liquid-drop model [2]. That is, fission takes place by overcoming a fission barrier, which is formed as a consequence of the competition between the surface and the Coulomb energies. The basic idea of such macroscopic picture has still been valid until now, and many dynamical fission models assume a nuclear shape evolution in a potential energy surface. On the other hand, a microscopic understanding of nuclear fission has still been unclear [3]. In a fission process, collective and single-particle degrees of freedom interact with each other in a complex way, which makes a microscopical treatment of a fission process formidably difficult. In recent years, with the help of developments of the nuclear many-body theory and computing powers, there have been many attempts to microscopically understand nuclear fission [3].

One of the most important quantities in nuclear fission is the distribution of a fission width. The distribution of decay widths of a compound nucleus is known to follow a chi-squared distribution, which is characterized by the degrees of freedom,  $\nu$  [4]. The parameter  $\nu$  contains information on a decay channel, and, if the output channels are independent of each other,  $\nu$  is equivalent to the number of open channels [4]. In the case of fission of actinide nuclei,  $\nu$  was found to be  $O(1)$  [4, 5]. Notice that this value is considerably smaller than the number of output channels, which are characterized by quantum numbers and excitation energies of fission fragments. Porter and Thomas explained this discrepancy based on the transition state theory [2], for which  $\nu$  was proven to be identical to the number of transition states.

In this paper, we shall analyze a smallness of  $\nu$  based on a microscopic fission model. Our model is based on the configuration-interaction approach with single-particle levels constructed with the constrained density functional theory with several nuclear shapes [6, 7]. We shall analyze a fission decay process of a compound nucleus state by constructing an effective Hamiltonian from our model Hamiltonian. This method provides a distribution of decay widths itself, and this is suitable for analyzing the degrees of freedom in a fission channel. We mention that this is the first microscopical analysis of a distribution of a fission width. While the value of  $\nu$  has been understood phenomenologically by now based on the transition state theory, the present work will offer insights into how a fission process takes place at a microscopic level.

## 2 Method

To describe coherently a collective deformation and single-particle excitations during a fission, we follow the idea of the generator-coordinate method (GCM) [8], in which a many-body wave function is constructed as,

$$|\Psi\rangle = \int dQ \sum_{\mu} f(Q, E_{\mu}) |Q, E_{\mu}\rangle. \quad (1)$$

Here  $|Q, E_{\mu}\rangle$  denotes a mean-field wave function labeled by the deformation parameter  $Q$  and the particle-hole excitation energy  $E_{\mu}$ . Using such GCM basis, the Hamiltonian matrix is represented as  $H_{k\mu, k'\mu'} = \langle Q_k, E_{\mu} | H | Q_{k'}, E_{\mu'} \rangle$ . For residual interactions, we employ a monopole pairing interaction,

$$H_{\text{pair}} = -G \sum_{i \neq j} a_i^{\dagger} a_i^{\dagger} a_j a_j, \quad (2)$$

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as well as a diabatic interaction [9],

$$\frac{\langle Q, E_\mu | v_{ab} | Q', E_{\mu'} \rangle}{\langle Q, E_\mu | Q', E_{\mu'} \rangle} = \frac{E(Q, E_\mu) + E(Q', E_{\mu'})}{2} + h_2 \ln(\langle Q, E_\mu | Q', E_{\mu'} \rangle), \quad (3)$$

where  $G$  and  $h_2$  are the interaction strength parameters. The Hamiltonian matrix has diagonal sub-blocks characterized by  $Q$ , which we call  $Q$ -blocks. The left-most and the right-most  $Q$ -blocks correspond to the compound states and the pre-fission configurations, respectively. Both of them are at high excitation energies, and we thus replace them by random matrices based on a Gaussian orthogonal ensemble (GOE), which is characterized by an interaction strength  $v$  and the matrix dimension,  $N_{\text{GOE}}$ . The right-end scission configurations have couplings to the continuum states with two fission fragments, and an imaginary matrix  $-i\Gamma_{\text{fis}}/2$  is added to the Hamiltonian matrix<sup>1</sup>. Then, the Hamiltonian matrix has the following structure,

$$H = \begin{pmatrix} H_{\text{GOE}}^{(L)} & (V^{(L)})^T & & & \\ V^{(L)} & H_1 & V_{1,2} & & O \\ & V_{2,1} & H_2 & V_{2,3} & \\ & & & \ddots & \\ O & & & V_{N-1,N} & H_N & (V^{(R)})^T \\ & & & & V^{(R)} & \tilde{H}_{\text{GOE}}^{(R)} \end{pmatrix}, \quad (4)$$

Here  $O$  denotes the zero matrix, and  $H_{\text{GOE}}^{(L)}$  and  $\tilde{H}_{\text{GOE}}^{(R)}$  are the GOE matrices, the latter having the imaginary part. The overlap matrix  $N_{k\mu, k'\mu'} = \langle Q_k, E_\mu | Q_{k'}, E_{\mu'} \rangle$  has a similar block structure.

Let us write this Hamiltonian as,

$$H = \begin{pmatrix} H_{\text{GOE}}^{(L)} & (V^{(L)})^T \\ V^{(L)} & H_Q \end{pmatrix}, \quad (5)$$

with  $(V^{(L)})^T = ((V^{(L)})^T, O, O, \dots, O)$ . The compound states in  $H_{\text{GOE}}^{(L)}$  decay via fission through the coupling to  $H_Q$ . We incorporate this effect by constructing an effective Hamiltonian as,

$$H_{\text{eff}}(E) = H_{\text{GOE}}^{(L)} - (V^{(L)})^T (H_Q - EN_Q)^{-1} V^{(L)} \equiv H_{\text{GOE}}^{(L)} + \Delta(E) - i\Gamma_{\text{eff}}(E)/2, \quad (6)$$

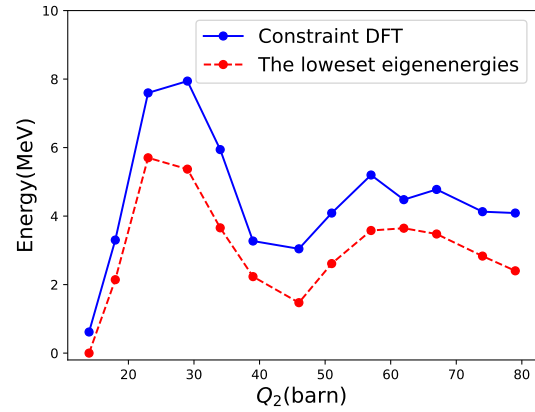
where  $\Delta(E)$  and  $\Gamma_{\text{eff}}(E)$  are the real and the imaginary parts of the self-energy, respectively. When  $\Delta(E)$  can be treated perturbatively, the real part of  $H_{\text{eff}}$  approximately follows GOE, and thus the distribution of the decay width, that is, the imaginary part of the eigenvalues of  $H_{\text{eff}}$ , follows approximately the chi-squared distribution [10]. In this approximation, one could approximately regard the rank of  $\Gamma_{\text{eff}}$  as the degrees of freedom  $\nu$ . In this way, the value of  $\nu$  in the fission channel can be microscopically estimated.

### 3 Results

Let us now apply the formalism to the induced fission of  $^{236}\text{U}$ , for which the empirical value of  $\nu$  is  $2.3 \pm 1.1$  [4]. For

<sup>1</sup>A similar imaginary matrix,  $-i\Gamma_{\text{cap}}/2$ , may be added also to the left-end GOE matrix [6, 7], but this is not relevant to the discussion on the effective Hamiltonian (see below).

the DFT calculations, we employ the Skyrme UNEDF1 functional [11]. We solve the Kohn–Sham equations in the cylindrical coordinate with the Skyax code[12]. The pairing interaction is not taken into account in constructing the GCM basis  $|Q, E_\mu\rangle$ , but it is taken into account as a residual interaction in constructing the Hamiltonian matrix. The strength is set to be  $G = 0.16$  MeV to reproduce the excitation energy of the first excited  $0^+$  state of  $^{236}\text{U}$ . On the other hand, the strength for the diabatic interaction is set to be  $h_2 = 1.5$  MeV [6].

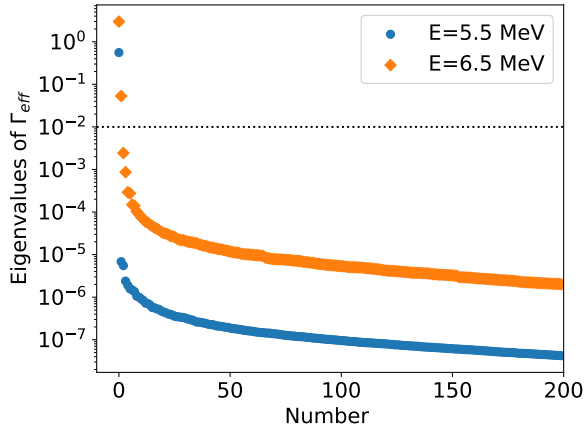


**Figure 1.** The fission barrier of  $^{236}\text{U}$  as a function of the mass quadrupole moment,  $Q_2$ . The blue solid line shows the ground state energy at each  $Q_2$ . This is obtained with the DFT with the Skyrme UNEDF1 functional, after introducing the scaling factor of 0.71. The red dashed line shows the lowest eigenenergies obtained by diagonalizing the Hamiltonian at each  $Q_2$ .

The fission barrier is calculated as a function of the mass quadrupole moment,  $Q_{20} \equiv Q_2$ , see the blue line in Fig. 1. The figure also shows by the red dashed line the lowest eigen-energy at each  $Q_2$  after diagonalizing the Hamiltonian for each  $Q$ -block. Due to the lack of triaxial deformation, the first fission barrier is somewhat overestimated. We thus rescale the fission barrier by 0.71 so that the energy difference between the lowest eigen-energy at  $Q_2 = 14$  b and that at  $Q_2 = 23$  b becomes identical to the experimentally determined barrier height, 5.7 MeV.

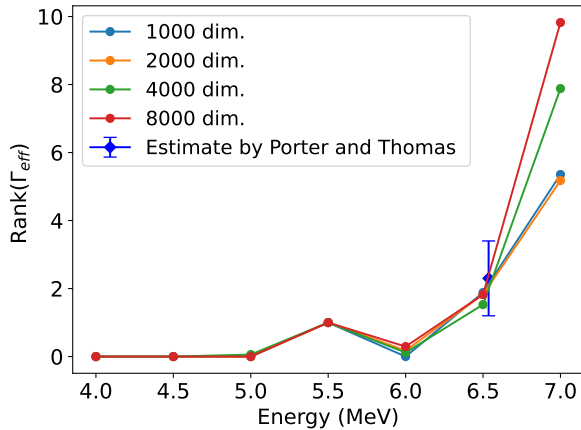
Based on the single-particle levels at each  $Q_2$ , we generate many-particle many-hole excited configurations at each  $Q_2$ . To this end, both proton and neutron excitations are taken into account up to 5 MeV. As we have mentioned, we replace the left-end the right-end configurations at  $Q_2 = 14$  b and 83 b, respectively, by GOE matrices. We take  $N_{\text{GOE}} = 1000$  and  $v = 0.31$  MeV for the GOE matrices, which yield  $\rho = v\pi/N_{\text{GOE}}^{1/2} = 31.8$  MeV<sup>-1</sup>. We assume a diagonal width matrix,  $\Gamma_{\text{fis}} = \gamma_{\text{fis}}\mathbf{1}$ , where  $\mathbf{1}$  is the unit matrix with the dimension of  $N_{\text{GOE}}$ . We arbitrarily take  $\gamma_{\text{fis}} = 0.015$  MeV based on the previous work [6]. Notice that the fission to capture branching ratio has been found insensitive to the size of the fission width[6, 13], and the actual value of  $\gamma_{\text{fis}}$  would not be important.

After we calculate the GCM kernels,  $H$  and  $N$ , the effective Hamiltonian is constructed according to Eq.(6). In



**Figure 2.** Eigenvalues of  $\Gamma_{\text{eff}}$  at  $E=5.5$  MeV (the blue circles) and  $6.5$  MeV (the orange diamonds) for a typical sample. They are plotted in the descending order. The dotted line shows the threshold value  $10^{-2}$  to be used in calculating the rank of  $\Gamma_{\text{eff}}$ .

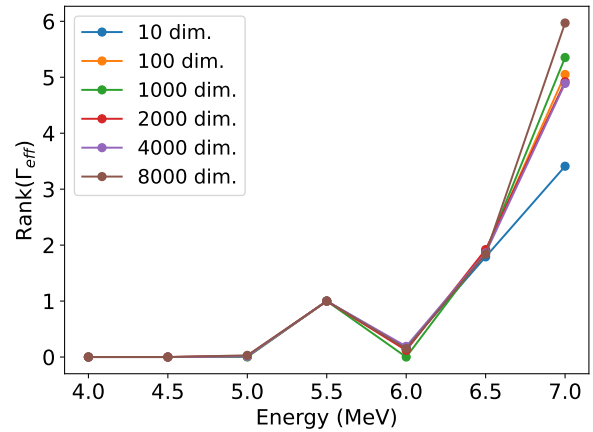
order to numerically determine the rank of  $\Gamma_{\text{eff}}$ , one needs to set a threshold value so that the rank is defined as the number of eigenvalues which are larger than it. To determine the threshold value, we analyze the distribution of the eigenvalues of  $\Gamma_{\text{eff}}$  at  $E=5.5$  and  $6.5$  MeV (see Fig.2). One can see that there is a clear gap, especially at  $E = 5.5$  MeV, between large eigenvalues and negligibly small eigenvalues. In the following calculations, we shall set  $10^{-2}$  for the threshold value, as is indicated by the dotted line in Fig.2.



**Figure 3.** The rank of  $\Gamma_{\text{eff}}$  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  $\nu$  [4].

The energy dependence of the rank so determined is shown in Fig. 3. The blue line shows the result with  $N_{\text{GOE}} = 1000$  as a reference. It is remarkable that our calculation reproduces a small number of  $\nu = \text{rank}(\Gamma_{\text{eff}})$ , the value of which is consistent with the empirical value,  $\nu = 2.3 \pm 1.1$ , at  $E = 6.536$  MeV [4]. Notice that  $\text{rank}(\Gamma_{\text{fis}})$  tends to increase as the excitation energy increases. This reflects the fact that channels gradually open as the exci-

tation energy increases. We also find that at low energies  $\text{rank}(\Gamma_{\text{eff}})$  is insensitive to the size of the right-end GOE matrix, that is,  $N_{\text{GOE}}$ , as shown in Fig. 3. This is compatible with the experimental finding that the number of apparent fission channels is not related to the degrees of freedom  $\nu$ . Moreover, we have also confirmed that  $\text{rank}(\Gamma_{\text{eff}})$  is insensitive to the size of the left-end GOE matrix, as shown in Fig. 4. These results indicate that the conclusion is independent of the dimension of the GOE-matrices. We expect that a similar conclusion is achieved even when a realistic shell-model Hamiltonian is employed instead of GOE-matrices as long as the Hamiltonian matrix is sufficiently chaotic.



**Figure 4.** Similar to Fig. 3, but for the cases where the dimension of the left-end GOE is varied while the dimension of the right-end GOE is fixed to 1000.

## 4 Summary

Using the microscopical fission model based on the DFT and the CI approach, we have discussed the distribution of a fission decay width of compound nucleus states of  $^{236}\text{U}$ . In our model, many-body configurations are generated according to the mass quadrupole moment  $Q_2$ . To analyze the fission decay width of compound nucleus states, we have constructed an effective Hamiltonian which acts on the space of the compound nucleus states, and identified its imaginary part,  $\Gamma_{\text{eff}}$ , as the fission decay width. We have found that  $\Gamma_{\text{eff}}$  has a small number of non-negligible eigenvalues, and thus the rank of  $\Gamma_{\text{eff}}$  is small. As long as the real part of the self-energy is small, the rank of  $\Gamma_{\text{eff}}$  is identical to the effective number of degrees of freedom,  $\nu$ . We have shown that the estimated value of  $\nu$  is consistent with the empirical value,  $\nu = 2.3 \pm 1.1$ . Furthermore, we have also shown that the rank of  $\Gamma_{\text{fis}}$  is insensitive to the dimension of the GOE-matrices. This is consistent with the experimental finding that the apparent number of exit channels is not reflected in the number of degrees of freedom.

We emphasize that this is the first microscopic estimate of the number of degrees of freedom in a fission channel. A more detailed discussion on the correspondence

between  $\nu$  and many-body wavefunctions will be given in a separate publication.

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