Double-humped barrier effects in the R-matrix for fitting of fissile isotope

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Abstract. The Reich--Moore approach has been extensively used in the resolved resonance energy range (RRR) for a wide range of isotopes. The approximation was suggested for cross-section representation of fissile isotopes since experimental fission width distribution according to given resonance spin and parity showed that only a few degrees of freedom (DoF) was involved during the fission process. Experimental cross-section data in RRR were successfully reproduced, and the interference in fission channels were well described. The fitting of the fission cross-section data was done according to one or two fission channels for a given resonance spin (J) and parity (π). Using the two-fission channel representation, channel interference effects observed on cross-section data for fissile heavy isotopes were adequately treated but only on a phenomenological basis. Indeed, this approach is physically unsatisfactory since no fission penetrability is involved in reduced fission channel width evaluation, and therefore no actual connection between R-matrix fission channel widths and Aage Bohr transition fission channels can be made neither in terms of individual barrier height or by the shape. This paper intends to address model deficiency by including 'fluctuating' fission barrier penetrability as a function of resonance spin and parity.

1 Introduction

The concept of fission channels has been around since the discovery of the fission process. From the inception of papers like those of Bohr-Wheeler (Niels Bohr) and Aage Bohr (son of Niels Bohr) the use of the terminology has been emphasized. The interpretation between the two papers is distinct. While Bohr-Wheeler refers to the number of transition states available with a given excitation, from the Aage Bohr viewpoint [1] the idea is that the transition states are saddle-point states, where the nuclear angular momentum should be concentrated on simple collective modes of motion (even-even (e–e) fissioning nuclei). Aage Bohr concluded that only few fission channels would be available on the fission process and nowadays one refers to them as the Bohr fission channels. The measured fission cross-sections asymmetries, also named interferences in the fission channels, support the Aage Bohr assumptions.

In the R-matrix formalism [2], the notion of entrance and exit channels is explicitly shown in the R-matrix elements as

$$R_{cc'} = \frac{\gamma_{cc'}\gamma_{c'c}}{E_\lambda - E}$$

(1)

where $\gamma_{cc'}$ and $\gamma_{c'c}$ are, respectively, the entrance (c) and exit (c') reduced amplitudes for eigenstate $\lambda$. The observed partial width $\Gamma_{cc'}$ is expressed as

$$\Gamma_{cc'}^{1/2} = \gamma_{cc'}\sqrt{2P_c}$$

(2)

where $P_c$ is the penetrability for the entrance channel c (of the neutron in present case). Similar expression is derived for the fission channels except that the penetrability is chosen constant and for convenience set to unity with $P_c = 1$, that is,

$$\Gamma_{cc'}^{1/2} = \gamma_{cc'}\sqrt{2}$$

(3)

The observation that the fission process is a few channels led Reich and Moore (RM) to come up with a brilliant idea, referred nowadays as the reduced R-Matrix formalism to account for the interference effects in the calculated fission cross section. It is also simply referred to as the Reich–Moore (RM) approach [3], which were primarily introduced to deal with the $^{235}$U fission cross section. The RM parameterization of the fission cross section resulted in excellent results in reproduction the experimental data. In the RM representation of the fission cross section, two fission widths are used and no mentioning to fission
penetrability is made which is assumed to be one. The RM R-matrix elements are

\[ R_{cc'} = \frac{\gamma_{cc'}\gamma_{cc'}}{E_A - E - i\frac{\Gamma_A}{2}}, \]  

(4)

where \( \Gamma_A \) represents a sum over all the gamma channels.

It is worth noting that in the fitting of the fission cross section based on the R-matrix resonance parameters, no relation to any fission barrier potential is assumed. The rational in the present study is to investigate the viability and benefit of connecting the knowledge of the fission barrier potential to the cross-section fitting.

2 Fission barrier potential shape

From an historical point of view, the absence of penetrability in R matrix for the fission channel width was a good compromise for e-e fissioning nuclei. Indeed the compound nucleus (CN) fission probability reaches its maximum (Figure 1; \(^{236}\)U CN) at the neutron separation energy (\( S_n \)) and the RRR of the actinides is short enough (\( S_n \) to a few keV above) to encounter little variation of the fission penetrability \( \gamma_{cc} \). Therefore, by standard RM fission cross-section fitting, the main goal of nuclear data evaluation is reached with a fair reproduction of the measured fission cross section. In this framework, using two fission widths per resonance brings the ultimate flexibility for the best \( \chi^2 \) (minimization of the difference between the calculation and measurement). However, the overall fission penetrability is embedded in the fitted value of \( \gamma_{cc} \) (Equation (3)) and biases the analysis of the statistical distribution of the reduced fission width amplitudes.

Figure 2 shows the double-humped fission barrier potential shape typical of an e-e fissioning nucleus that is mimicked here using an extension of the Reich–Moore formalism. At excitation energy well above the fission barrier, Hauser–Feshbach (HF) theory [5] assumes statistical equilibrium among all degrees of freedom in the CN. The latter hypothesis is valid for e-e fissioning nuclei as the \(^{236}\)U since \( S_A \) and \( V_B \) are significantly below \( S_n \). The question of the discrete structure of the class-II states (lying in the second well), which have local impact on the transmission factor across the overall fission barrier, is more sensitive for fertile heavy isotopes than for the here-studied fissile nuclei. The latter point is not addressed in this paper.

One recalls that in the HF theory, the total fission average transmission coefficient for a specific \( \alpha_B \) outer saddle transition state (Fig.2) reads,

\[ T_f(\alpha_B) = \frac{T_A T_B(\alpha_B)}{T_A + T_B}, \]  

(5)

where the \( T_A(\alpha_A) \) and \( T_B(\alpha_B) \), the individual barrier coefficients, are commonly calculated using the Hill–Wheeler approximation [6] across given \( \alpha_A \) inner and \( \alpha_B \) outer transition states. \( T_A \) and \( T_B \) are the sum over the possible transition states at each saddle, respectively.

![Fig. 2. Schematic representation of the deformation potential energy of the \(^{236}\)U fissioning nucleus as a function of its elongation (\( \varepsilon \)). \( V_A \) and \( V_B \) are, respectively, the fundamental (or ground state) heights at the inner and outer barrier deformation.](image)

Present work aims to include explicit fission barrier penetrability dependence in the fission width expression as \( \sqrt{T_f} = \gamma_{cc} \sqrt{2P_f} \) with \( P_f \equiv T_f \). Indeed \( T_f \), the statistical transmission coefficient across the fission barrier is not the conventional external penetration factor of the formal R-matrix theory [7] but expresses the degree of tunnelling thru the potential energy surface at the saddle point. By selecting the relevant set of discrete transition states at each saddle as a function of the spin (\( J \)), parity (\( \pi \)) and spin projection (\( K \)) along the elongation axis of the fissioning nucleus, one can calculate the total fission penetrability (Eq.(5)).
corresponding to a set of transition states of same (J,K,π) and associated to a fission partial width in the extended RM formalism. In the case of the $^{235}\text{U}$ e-e fissioning nucleus, only a limited number of (J,K,π) transition states of collective/rotational nature exists at each saddle for excitation energies below the nucleon pair breaking energy ($V_{AB} \approx 1.4\text{MeV}$). Above this energy, excitations of individual nucleons combined with the CN collective excitations increase the density of transition states for each saddle. In the present attempt, only a discrete transition states sequence has been used, assuming that level densities relevant to above the nucleon pair breaking energy, have no significant impact on the trend observed in fitting the $^{235}\text{U}$ neutron-induced fission cross section over the RRR [0-2.25keV].

![Image 330x249 to 552x387](https://doi.org/10.1051/epjconf/202328403015)

Fig. 3. Fission transmission coefficient for given (J,K,π) transition states sequence as a function of neutron energy over the [0 – 10 keV] range for the ($n+^{235}\text{U}$) reaction. Legends are labelled by (J, K); the resonance spin and band-head spin projection characterizing a transition state. Transition states are of negative parity for s-wave resonances.

### 3 Transmission coefficient profile as a function of given (J,K,π) transition state

The ($n+^{235}\text{U}$) reaction in the RRR neutron energy involves two distinct sets of s-wave resonances of 3$^-$ and 4$^-$ $J^\pi$, respectively. Partial or total opening of fission related to those resonances implies the existence of transition states at each saddle carrying the same $J^\pi$ but possibly of a different K band head number. In a first stage, a plausible set of discrete transition states has been constructed that is based on an axially symmetric inner barrier model with a choice of distant values for ($V_a, V_b$) = (5.2, 5.7)MeV. As alternative, Fig. 1 shows a calculation with close values. Transition states at each saddle are built assuming $\gamma$-vibrations with $K^\pi = 2^+$, mass-asymmetry vibrations with $K^\pi = 0^+$, bending vibrations with $K^\pi = 1^-$ with respective rotational band members, $J^\pi = 2^+, 3^-, 4^-$, etc.; $J^\pi = 1^+$; 3$^-$, 5$^+$, etc.; $J^\pi = 1^-$, 2$^-$, 3$^-$, etc. It reveals that 3$^-$ resonances imply at first, transition states of the $K^\pi = 0^+$ and $K^\pi = 1^-$ bands whereas 4$^-$ resonances rely solely on the $K^\pi = 1^-$ band. However, as energy increases, combinations of two primary vibrations support additional band heads for resonances 3$^-$ and 4$^-$; Finally, four distinct sets of (J, K, π) for each type of s-wave resonance lie within the pairing energy gap. The energy dependence over the RRR of the corresponding transmission coefficients is shown in Figure 3. One observes very little variation of the fission penetrability magnitude for given (J, K, π) over the [0-10 keV] energy range. The latter magnitude spans over the 0.1-0.6 range and justifies the use of independent partial fission channel widths. Another argument to have distinct channel widths is to discriminate the components in the fission cross section as a function of the nature of the vibration (1 phonon mass-asymmetry (m.a), 1 phonon bending, combination of 2 phonons (gamma+m.a), etc.). The extended RM based on four partial fission channel widths, is now substituted to the conventional RM formalism (with two phenomenological fission channel widths per resonance). In practice, the present approach requires fitting four fission widths for 3$^-$ resonances; number reduced to three for 4$^-$ resonances since the fission penetrability of the (J=4, K=4, π=−) channel is zero (Fig. 3).

### 4 Extended Reich–Moore fits of the neutron-induced fission cross section

![Image](https://doi.org/10.1051/epjconf/202328403015)

Fig. 4. Preliminary extended RM SAMMY fit of the spin polarized neutron-induced fission cross-section measurement by Moore et al. [10] according to $J^\pi = 3^-$. The experimental data are corrected for residual background.

A preliminary fit of the newly defined fission partial widths for the ($n+^{235}\text{U}$) fission cross section in the [0-100] eV neutron-incident energy range was achieved using the SAMMY code [8]. The difficulty lies in the fission width amplitude interferences reinforced by the augmented number of fission partial widths; knowing that the $\chi^2$ is commonly of high quality in the various evaluations of the fission cross section [9]. Another difficulty is a correct estimation of prior values for the fission reduced width amplitudes (Eq.(2)) signs of which are unknown. To minimize the fitting issue, polarized (neutron and target) fission cross-section
measurements by Moore et al. [10] were fitted that include resonance spin-discriminated data. Figures 4 and 5 show a preliminary fit of the fission cross section associated with each s-wave resonance spin within the resolved energy range [50-75] eV compared to the observation.

Fig. 5. Same as Fig. 4 but for J = 4.

5 Conclusion and perspectives

For one of the first times, a fit of the neutron-induced energy-resolved resonance fission cross section of an e-e CN nucleus has been performed using an extension of the RM formalism towards the fission channel. In the present approach, the question of the discrete structure of the class-II states modifying locally, less sensitive for fissile than for fertile heavy nuclei, was not treated. The present goal was twofold. First, to include explicitly the energy dependence of the double-humped barrier penetrability in the fission partial widths (Γ_{1/2}) expression. Second, to connect each fission partial width to a unique set of transition states identified by their (I, K, π) quantum numbers. This statement led for the (n+235U) fission cross section to the introduction of more physical fission partial widths, four in number both for s-wave 3- and 4- resonances. By fitting sequentially the 3- and 4- partial fission cross sections measured by Moore et al. [10] and finally the sum of the two, the correlation between resonances of distinct spins and sharing the same K band head (same rotational band) across the penetrability of the fission barrier, is implicitly recovered. However, the new fit with four fission partial reduced width amplitudes per resonance (rather than two with the usual RM formalism) is more challenging because of the increased strength of the interferences between the fission channels. Beyond that difficulty, refined treatment (explicit formulation) of reduced width amplitude correlations (γ_{3/2} = 3Kπ × γ_{4/2} = 4Kπ) between resonances of distinct spins that share the same K, is a possible target for the future.

References

2. A.M. Lane and R.G. Thomas, Rev. Mod. Phys. 30, 257 (1958)
3. C.W. Reich and M.S. Moore, Phys. Rev. 111, 929 (1958)
4. O. Bouland, Phys. Rev. 100, 064611 (2019)
5. W. Hauser and H. Feshbach, Phys. Rev. 87, 366 (1952)