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The Impact of Intermediate Structure on the Average Fission Cross Sections

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This paper discusses two common approximations used to calculate average fission cross sections over the compound energy range: the disregard of the W_{II} factor and the Porter-Thomas hypothesis made on the double barrier fission width distribution. By reference to a Monte Carlo-type calculation of formal R-matrix fission widths, this work estimates an overall error ranging from 12% to 20% on the fission cross section in the case of the ^{239}Pu fissile isotope in the energy domain from 1 to 100 keV with very significant impact on the competing capture cross section. This work is part of a recent and very comprehensive formal R-matrix study over the Pu isotope series and is able to give some hints for significant accuracy improvements in the treatment of the fission channel.

I. CONTEXT AND PURPOSE

The reported accuracy on the fission cross section of the major actinides in current evaluated libraries, such ENDF/B-VII.1 [1], is typically smaller than a few percent within the compound nuclear energy range (from neutron threshold energy up to second chance fission) since the relevant model parameters have been fine-tuned to reproduce a large body of consistent experimental data sets. However, those evaluated files show, in terms of competitive radiative capture and inelastic channels, usually poor accuracy. We might argue this is essentially due to the lack of associated experimental data but another reason lies in the use during the evaluation process of pragmatic fission cross section models which do not guarantee a high degree of confidence in the prediction of other partial cross sections. Among the various ad-hoc hypotheses made for the treatment of the fission channel in a standard evaluation, the most frequently adopted simplification is to disregard the statistical properties of the compound nucleus levels in the second well of the double-humped fission barrier. This paper emphasizes the existence of the so-called class-II state width fluctuation correction factor, W_{II}, and quantifies its impact on calculated fission cross sections for both a fertile and fissile nuclide of plutonium. The correction due to this W_{II} factor is, in particular, compared with both the sub-barrier tunneling fission decay probability reduction and the in-out-going channel width fluctuation correction factor of standard Hauser-Feshbach theory [2]. This paper concludes with an estimate of the impact of the intermediate structure in terms of width fluctuation correction factors on the other partial cross sections.

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II. STANDARD HAUSER-FESHBACH FORMULATION

Average neutron-induced reaction cross-sections are commonly computed using standard Hauser-Feshbach theory [2]. The average fission cross section $\bar{\sigma}_{nf}$ for a given (J, π) at neutron energy E_n reads

$$\bar{\sigma}_{nf}(E_n) = \sigma_n(E_n) \times \bar{P}_f \times W_{nf}, \qquad (1)$$

where σ_n is the neutron-induced compound nucleus formation cross section, $\bar{P}_f$ is the average fission decay probability and W_{nf} the customary in-out-going channel width fluctuation correction factor. The superscripts J^π are omitted along the lines in the equations for clarity.

III. FORMAL R-MATRIX AND EIGENSTATE CLASSIFICATION

A variable η, describing the collective elongation of the system along the fission path, was proposed by Lynn [3]. The Hamiltonian operator is expanded such that

$$H = H_\eta + H_{int}(\zeta; \eta_0) + H_c(\eta, \zeta; \eta_0), \qquad (2)$$

where H_{int} is the term that governs the excitation of all other degrees of freedom, noted ζ, at a fixed elongation η_0 and H_c, the coupling Hamiltonian describing the interaction between the η mode and the other modes of excitation. The eigenfunctions and eigenvalues of H_{int} and H_η are respectively the $(\chi_\mu, \varepsilon_\mu)$ and $(\phi_\nu(\eta), \varepsilon_\nu)$ pairs. It is convenient to expand the eigenstates X_λ of the formal R-matrix states λ of the internal region in terms of product pairs of the quasi-vibrational functions $\phi_\nu(\eta)$ with the intrinsic functions χ_μ defined at some special deformation values η_0 such that

$$X_\lambda^{\eta_0} = \sum_{\nu\mu} C_{\lambda(\nu\mu)} \phi^{\eta_0}_{\nu(\mu)} \chi_\mu. \quad (3)$$

The formal R-matrix compound nucleus eigenstates X_λ, which can be qualified asymptotically as either of quasi-class-I (corresponding to ground-state) or quasi-class-II (fission isomer) depending on the location of the largest vibrational amplitude, contain a mixture of pure class-I and class-II states (with $C_{\lambda(\nu\mu)}$, the admixture coefficients of each class into the formal states λ). The X_λ are to be obtained from the diagonalization of H (Eq. (2)), which implies the determination of the sub-matrix mixing elements $\langle X^{(I)}_{\lambda_I} | H_c | X^{(II)}_{\lambda_{II}} \rangle$ (or the reciprocal elements) characterizing the residual interaction between the λ_I and λ_{II} compound nucleus states.

A. Class-I and class-II Level Properties

By nature class-I states, of mean spacing D_I, exhibit very small fission widths. By contrast class-II states exhibit much larger fission widths and a larger mean spacing ($D_{II} \approx 50 \times D_I$ at S_n). Class-II neutron widths can be neglected since the compound nucleus is originally formed in the ground-state (first well) and because neutron emission from the second well is much less probable than fission. Therefore, class-I and class-II total widths, $\Gamma_{\lambda_I(tot)}$ and $\Gamma_{\lambda_{II}(tot)}$ respectively, are constructed from

$$\begin{aligned} \Gamma_{\lambda_I(tot)} &\approx \Gamma_{\lambda_I(n)} + \Gamma_{\lambda_I(n')} + \Gamma_{\lambda_I(\gamma)}, \\ \Gamma_{\lambda_{II}(tot)} &\approx \Gamma_{\lambda_{II(\downarrow)}} + \Gamma_{\lambda_{II(\uparrow)}} + \Gamma_{\lambda_{II}(\gamma)}, \end{aligned} \quad (4)$$

where $\Gamma_{\lambda_{II}(\uparrow)}$ and $\Gamma_{\lambda_{II}(\downarrow)}$ are respectively the class-II fission and coupling widths whose definitions are introduced in the next paragraph.

B. Concept of class-II Level Partial Widths

Using first order definition of Moldauer's transmission coefficient [4], we define the inner barrier transmission coefficient, T_A, as the average over neighboring class-II states of the class-II coupling width, $\Gamma_{\lambda_{II}(\downarrow)}$. Reciprocally, the outer fission barrier transmission coefficient, T_B, can be expressed as function of the average of the class-II fission width, $\Gamma_{\lambda_{II}(\uparrow)}$ as

$$T_A = 2\pi \frac{\langle \Gamma_{\lambda_{II(\downarrow)}} \rangle_{II}}{D_{II}}, \; T_B = 2\pi \frac{\langle \Gamma_{\lambda_{II(\uparrow)}} \rangle_{II}}{D_{II}}. \quad (5)$$

Besides, the class-II state coupling width is also established by the average of the squared coupling matrix mixing elements, $\langle X^{(I)}_{\lambda_I} | H_c | X^{(II)}_{\lambda_{II}} \rangle$, connecting a selected class-II state, λ_{II}, with its neighbouring class-I levels, λ_{I_i}, across the inner fission barrier, such that

$$\Gamma_{\lambda_{II(\downarrow)}} = 2\pi \big\langle \langle \lambda_{II} | H_c | \lambda_I \rangle^2 \big\rangle_I / D_I. \quad (6)$$

IV. DERIVED AVERAGE FISSION CROSS SECTION FORMULATION

In presence of a double-humped fission barrier, two cases are generally considered for calculating the average fission probability, $\bar{P}_f = \langle T_f \rangle / T_{total}$. At excitation energies well above fission barrier energy, we commonly assume statistical equilibrium among all degrees of freedom in the compound nucleus. Under this hypothesis, the overall fission transmission coefficient across a specified Bohr [5] outer fission barrier channel μ is

$$T_f(\mu) = (T_A T_B(\mu))/(T_A + T_B), \quad (7)$$

where T_A and T_B are the total fission transmission coefficients over respectively barriers A and B which, are calculated commonly from the well-known Hill-Wheeler expression [6]. At sub-barrier and near-barrier excitation energies, the detailed structure of class-II levels has significant impact on T_f. If the bulk of the strength of T_f is concentrated in a narrow energy interval about a class-II level, the average fission probability will vary strongly in the vicinity of this level. In the neighborhood of a single class-II level and on the assumption of uniform class-I and class-II level spacings (so-called "picket fence model"), Lynn and Back [10] have worked out an average formulation of $\bar{P}_f$ corresponding to barrier tunneling with moderately weak class-I -II coupling such that

$$\bar{P}_f = \left[1 + \left(\frac{T_I}{T_f} \right)^2 + \left(\frac{2T_I}{T_f} \right) \coth \left(\frac{T_A + T_B}{2} \right) \right]^{-1/2} \quad (8)$$

with T_I, being the total class-I transmission coefficient including all open reactions within first well.

Under both the hypothesis of Eq. (7) and the concept developed in Section III B, we can express the average over neighboring class-II states of the overall fission barrier transmission coefficient, T_f, as

$$\langle T_f \rangle_{\lambda_{II}} \approx \left\langle \frac{T_A T_B}{T_A + T_B} \right\rangle_{\lambda_{II}} = \frac{2\pi}{D_{II}} \left\langle \frac{\Gamma_{\lambda_{II}\downarrow} \Gamma_{\lambda_{II}\uparrow}}{\Gamma_{\lambda_{II}}} \right\rangle_{\lambda_{II}}, \quad (9)$$

where $\Gamma_{\lambda_{II}}$ represents the total width of a single class-II state. Since we intuitively expect that statistical fluctuations of the class-II partial fission widths exhibit an independent Porter-Thomas distribution [7] (characterized by a number of Degrees of Freedom (DoF), ν_f, set to unity) across each fully open outer Bohr fission channel and, the coupling width distribution across the inner Bohr fission channels (considered as a whole - meaning an aggregate of channels) to belong to the chi-squared family (characterized by an effective DoF value, $\nu_f^{\rm eff}$), we anticipate that correlations between coupling and fission class-II width