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RECENT ADVANCES IN UTILIZATION OF THE R-MATRIX PARAMETERS FOR REACTOR APPLICATIONS*

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Abstract: A simplified version of the rigorous pole representation of cross sections has been developed to facilitate utilization of the newly released ENDF/B VI resonance data based on the Reich-Moore parameters for reactor applications. The procedure is equivalent to the extraction of the Humblet-Rosenfeld-type parameters and the associated 'background' term explicitly from the rigorous pole and residue parameters which, in turn, are converted from a given set of the Reich-Moore parameters. The computational efficiency and its amenability to the existing reactor codes are significantly enhanced by the introduction of the pertinent analytic continuation in place of the smooth 'background' term via the non-linear least square fitting. The method has been successfully applied to all major nuclides examined and the results are presented.

Introduction

Two special features of the newly released ENDF/B VI resonance data that will have profound impacts on the cross section processing codes for reactor applications are the dramatic expansion of the resolved energy regions and the availability of the R-Matrix parameters based on the Reich-Moore formalism[2] for most major nuclides of practical interest. While the availability of the new resonance data has all but eliminated the long-standing difficulties attributed to the lack of sufficient resolved resonance information and the inadequacy of the Breit-Wigner single level representation for the closely spaced resonances, one obvious question of great practical concern is the compatibility of the new resonance representation with the existing reactor methodologies based almost exclusively on the traditional formalisms.

To facilitate the efficient utilization of the new R-matrix data, a simplified version of the rigorous pole representation described previously[3] has been developed so that the rigor of the Reich-Moore cross sections and the traditional feature of Doppler broadening via the Voigt profile essential to many existing codes can be preserved simultaneously. Extensive calculations have been carried out to demonstrate the viability of the proposed method and the results will be presented.

Natural extension of Rigorous Pole Representation

The theoretical justification of the rigorous pole representation is based on the rationale that the collision matrix must be single-valued and meromorphic in the momentum space. Any function that exhibits such properties must be a rational function according to the well known theorem in complex analysis. Thus, one obtains via partial fraction[3],

$$\sigma_x = \frac{1}{E}\sum_{\ell,J}\sum_{\lambda=1}^{N}\sum_{j=1}^{2(\ell+1)} \mathrm{Re}\left\{R^{(x)}_{\lambda,J,j,\lambda}\cdot\frac{(-i)}{p_\lambda^{(2)*}-\sqrt{E}}\right\} \quad (1)$$

where x denotes the type of reaction under consideration and N is the total number of known R-matrix resonances. The genuine energy independent pole and residue parameters can be obtained from any given set of the Reich-Moore parameters using the WHOPPER code.[3] The expression leads immediately to the well-known Voigt profiles when subject to Doppler-broadening. However, the presence of $2(\ell+1)$ terms for each resonance to be evaluated in momentum domain is obviously undesirable from the point-of-view of computing efficiency, storage requirement and its amenability to existing codes. In the following discussion, it will be shown how the problem can be alleviated.

The $2(\ell+1)N$ poles for a given ℓ and J defined in Eq. 1 can be divided into two distinct classes. There are 2N s-wave-like poles with distinct spacings while the remaining $2\ell N$ poles are closely spaced independent of how well separated the input Reich-Moore resonances are. Such characteristics can be best visualized by examining the denominator of the rational function leading to Eq. 1.

$$P_{2(\ell+1)N}(\sqrt{E}) = P_{2N}^{(1)}(\sqrt{E})\cdot P_{2N}^{(2)}(\sqrt{E}) \quad (2)$$

where $P_{2N}^{(1)}(\sqrt{E})$ is a polynomial with its complex coefficients strongly dependent on the input resonance parameters whereas the coefficients of $P_{2N}^{(2)}(\sqrt{E})$ are dominated by terms involving $k_o a$ with a = channel radius and $k_o = 2.197 \times 10^{-3}[A/1+A)]$.

Thus, $P_{2N}^{(2)}(\sqrt{E})$ reflects the higher order energy dependence of the penetration and shift factors and its roots are barely distinguishable. In addition, the magnitude of their imaginary components becomes of the order of $1/k_o a$ in the limit of small neutron widths. Such characteristics had already been illustrated analytically for the cases of a single level in Ref. 3. The sum of these pole terms involving poles with exceedingly large 'width' (or imaginary part) can be considered as the background contribution to the cross section with weak $\sqrt{E}$ dependence.

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In contrast, the roots of $P_{2N}^{(1)}(\sqrt{E})$ are distinct and always appear in pairs with their real components opposite in signs but not necessarily equal in magnitude spanning over $(\sqrt{E_{min}} \le \sqrt{E} \le \sqrt{E_{max}}$ and $-\sqrt{E_{max}} \le \sqrt{E} \le -\sqrt{E_{min}})$ on the real axis of the momentum domain. Let $p_\lambda^{(1)}$ and $p_\lambda^{(2)}$ be poles with positive and negative real components, respectively. It is important to note that the actual interval of interest in computing cross sections is half of the interval taken to be $(\sqrt{E_\ell} \le \sqrt{E} \le \sqrt{E_u})$ where E_u $(< E_{max})$ and $E_\ell (> E_{min})$ are the upper and lower resolved region boundaries, respectively. Because of their short range nature of fluctuation, all terms involving $p_\lambda^{(2)}$ constitute another smooth component to σ_x that reflects the contributions from the tails of outlying poles outside the interval of practical interest.

Let $q_\ell^{(x)}(\sqrt{E})$ denote the contributions from those $2\ell N$ terms involving poles with giant 'width'. By taking advantage of the characteristics of poles described above, Eq. 1 can be cast into the same form as that of Humblet-Rosenfeld.[4]

$$\sigma_x = \frac{1}{E}\sum_\ell \Re e\left\{\sum_J \sum_{\lambda=1}^{N}\left[R_{\ell,J,1,\lambda}^{(x)} \cdot \frac{2(-i)\sqrt{E}}{(p_\lambda^{(1)*})^2 - E}\right] + s_\ell^{(x)}(\sqrt{E}) + q_\ell^{(x)}(\sqrt{E}) \cdot \delta_\ell\right\} \quad (3)$$

where

$$s_\ell^{(x)}(\sqrt{E}) = \sum_J \sum_{\lambda=1}^{N}\left[\frac{R_{\ell,J,2,\lambda}^{(x)}(-i)}{p_\lambda^{(2)*} - \sqrt{E}} - \frac{R_{\ell,J,1,\lambda}^{(x)}(-i)}{(-p_\lambda^{(1)*}) - \sqrt{E}}\right]; \quad (4)$$

$$\delta_o = 0,\ \delta_\ell = 1 \text{ for } \ell > o$$

Hence, for a given range of practical interest, the rigorous pole representation can be viewed as a combination of a 'fluctuating' term consisting of N poles with $\Re e\, p_\lambda^{(1)} > 0$ expressed in the energy domain consistent with the traditional formalisms and two 'non-fluctuating' terms attributed to the tails of outlying poles with negative real component and the poles with extremely large 'width' (or $|\Im m\, p_\lambda^{(j)}|$) for $\ell>0$ states respectively. The striking behavior of the 'fluctuating' and 'non-fluctuating' components have been confirmed in recent calculations for all major nuclides specified by the Reich-Moore parameters in the ENDF/B VI files.

Eq. 3 represents no more than an empty form unless the background terms can be evaluated efficiently. The smooth behavior of these terms clearly suggests that their energy dependence can obviously be reproduced by other simpler functions within the finite interval of practical interest. It is well known in numerical analysis that the rational functions are best suited to approximate a well behaved function within a finite range. Hence, the obvious choice is to set the approximate functions $\hat{s}_\ell^{(x)}(\sqrt{E})$ and $\hat{q}_\ell^{(x)}(\sqrt{E})$ to be rational functions of arbitrary order. If the order of polynomials in the numerator and the denominator are taken to be MM and NN respectively, a total of (MM + NN + 2) complex coefficients (twice as many entries) can be used as the variables to be determined in the non-linear fitting procedure. Because of the extremely well behaved nature of $s_\ell^{(x)}(\sqrt{E})$ and $q_\ell^{(x)}(\sqrt{E})$, the MM and NN required are expected to be very small. One attractive feature of the proposed method is that the rational functions so obtained can be again expressed in the form of pole expansion via partial fraction, i.e.,

$$\hat{s}_\ell^{(x)}(\sqrt{E}) = \frac{P_{MM}(\sqrt{E})}{Q_{NN}(\sqrt{E})} = \sum_{\lambda=1}^{NN}\frac{r_\lambda^{(x)}(-i)}{\alpha_\lambda^* - \sqrt{E}} \quad (5)$$

$$\hat{q}_\ell^{(x)}(\sqrt{E}) = \sum_{\lambda=1}^{NN}\frac{b_\lambda^{(x)}(-i)}{\xi_\lambda^* - \sqrt{E}} \quad (6)$$

if NN > MM.

Conceptually, the procedure is equivalent to determining the analytic continuations of $s_\ell^{(x)}(\sqrt{E})$ and $q_\ell^{(x)}(\sqrt{E})$ for $\sqrt{E_\ell} \le \sqrt{E} \le \sqrt{E_u}$. The pole and residue parameters so obtained can be viewed as 'pseudo' pole parameters. A code (WHOPJR) based on the MINPACK-package[5] has been developed to compute these 'pseudo' pole parameters. To provide sufficient accuracy to cross sections, NN of no greater than 3 is required.

The Doppler-broadening of Eq. 3 and Eq. 5 immediately leads to the similar form defined by the traditional formalisms:

$$\sigma_x(E,T) = \frac{1}{E}\sum_\ell \Re e\left\{\sum_J \sum_{\lambda=1}^{N} 2\sqrt{E} R_{\ell,J,1,\lambda}^{(x)} \frac{\sqrt{\pi}}{\Delta_\Sigma} W\left(\frac{E-\epsilon_\lambda}{\Delta_\Sigma}\right) + \hat{s}_\ell^{(x)}(\sqrt{E},T) + \hat{q}_\ell^{(x)}(E)\cdot\delta_\ell\right\} \quad (7)$$

where

$$\hat{s}_\ell^{(x)}(\sqrt{E},T) = \sum_{k=1}^{NN}\frac{r_k^{(x)}}{\Delta_m}\left[\sqrt{\pi}\, W\left(\frac{\sqrt{E}-\alpha_k^*}{\Delta_m}\right)\right] \quad (8)$$

$$\epsilon_\lambda = [p_\lambda^{(1)*}]^2 \quad (9)$$

$$\psi(x,y) + i\chi(x,y) = \sqrt{\pi}\, y\, W(z) \quad (10)$$

and $\Delta_\Sigma = 2\sqrt{E}\,\Delta_m$ denotes the Doppler width in energy and momentum domains respectively.

Thus, the only difference between Eq. 7 and the traditional formalisms is the presence of the 'background' terms explicitly defined by a handful of 'pseudo' poles with weak energy and temperature dependence. Its compatibility to all ENDF/B format based codes is quite apparent.

Results and Conclusions

Extensive calculations have been carried out in order to demonstrate the viability of the proposed method. The studies include all major actinides and two structural isotopes.

The viability of the method can be best illustrated by examining the relative errors in the resulting cross sections with respect to the

directly computed Reich-Moore cross sections. Representative results corresponding to the absorption cross sections of ^{239}Pu and ^{238}U are shown in Fig. 1 and Fig. 2 respectively. These figures show the behavior of the absolute values of relative errors in great detail as a function of $\sqrt{E}$ over the $(\sqrt{E_l} \le \sqrt{E} \le \sqrt{E_u})$. By and large, the relative errors and the cross section values are anti-correlated. The peaks of the former correspond to the valleys of the latter and vice versa. The lower curves represent the inevitable errors attributed to the computations of parameters when all poles defined by Eq. 1 are included. The errors are generally less than 10^{-9} and can reach 10^{-7} as E approaches zero. Thus, Eq. 1 is not only analytically rigorous but also numerically exact for practical purposes. The upper curves show the corresponding errors when the simplified version is used. It is important to note that the results are based on the tolerance limit of 10^{-5} and NN=3 in computing the background terms. The maximum errors are of the order of 10^{-4} near the valleys between resonances (much smaller for fissionable nuclides) and are clearly tolerable in practical applications.

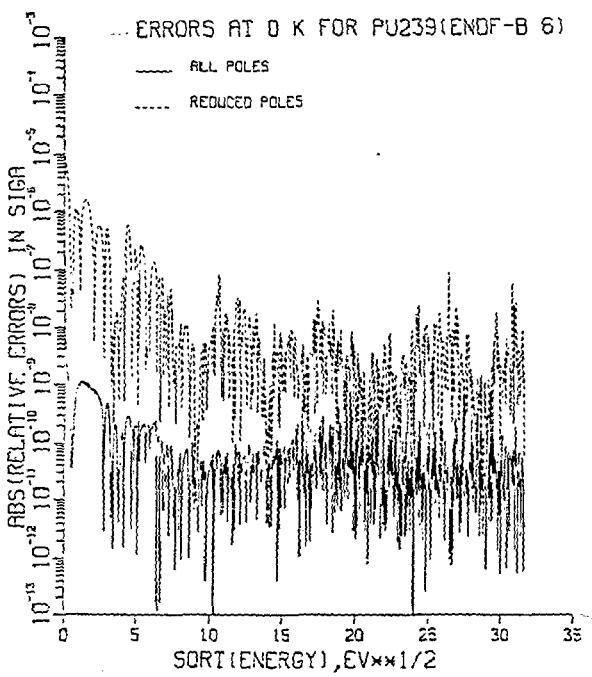

Fig. 1. Relative errors in σ_a of ^{239}U based on the parameters converted from ENDF/B VI data.

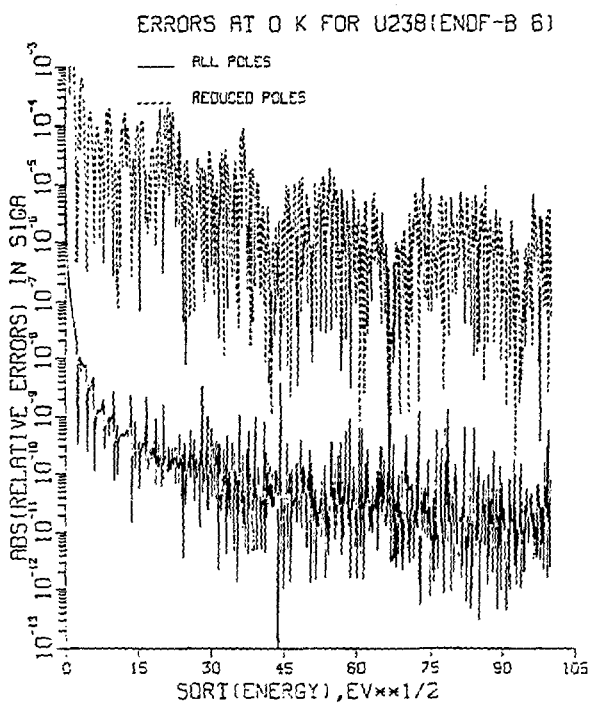

Fig. 2 Relative errors in σ_a of ^{238}U based on the parameters converted from ENDF/B VI data.

It is, therefore, reasonable to conclude that the proposed method is not only readily amenable to methodologies based on the traditional formalisms but also preserves the rigor of the Reich-Moore cross sections. The procedure is being implemented in the MC^2-2 code.[6]

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