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On the Convergence Issue for Multi-Poles Conversion from Reich-Moore Formalism

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Abstract - *Multi-poles representation of resonance parameters is one of the most prospecting methods which can be applied in On-The-Fly Doppler broadening cross sections in resolved resonance range with high performance. However, there is numerical instability issue occurring in converting the non s-wave poles for higher angular momentum states from Reich-Moore resonance formula. This paper presents some preliminary solutions including implementation of simultaneous root finding method, restart capability, shift factor approximation cancelation along with arbitrary precision, to achieve the convergence of more poles for the higher orbital angular momentum.*

I. INTRODUCTION

R-Matrix is the most typical theory describing complicated resonance phenomenon of neutron induced reaction cross sections in so-called resolved resonance range (RRR for short). Some approximated forms of R-Matrix formula, i.e., Single-level Breit-Wigner, Multi-level Breit-Wigner, Reich-Moore, are commonly applied in the latest version of the-state-of-art ENDF-formatted neutron sub-library to accurately illustrate resonance parameters in MF=2 data block [1]. However, the R-Matrix based resonance parameters need to be reconstructed into point-wise cross sections and then used in SIGMA1 kernel to generate temperate dependent cross sections for Monte Carlo neutron transport code with very high modeling fidelity. Efficiency of the given approach is not acceptable especially in the On-The-Fly Doppler broadening situation. Another approach to generate resonance cross section is Multi-Pole formalism, which was recently implemented by MIT. The mathematical manipulations of the R-Matrix theory results in the given method. In addition, Multi-poles formalism can be directly utilized in analytical Doppler broadening of the cross sections at any target temperatures using Solbrig kernel [2]. Thus, the original ENDF-formatted resonance parameters should be converted into the Multi-Pole parameters. This paper presents the numerical instability of iterative conversion from Reich-Moore formalism and comes up with preliminary practical solution.

II. METHODOLOGY

1. Multi-Poles Representation

The idea of Multi-Pole comes from mathematical converting the Reich-Moore parameters into Adler-Adler parameters in POLLA code, which was initially proposed by R. HWANG in 1987 [3].

According to the R-Matrix theory, the reaction cross section σ_{nx} for the incident neutron channel n, and outgoing channel x in RRR expressed in terms of the collision matrix U_{nx},

$$\sigma_{nx} = \pi k^2 g_n \left|\delta_{nx} - U_{nx}\right|^2 \tag{1}$$

where k is reduced neutron wavelength; g_n is statistical factor dependent on the spin and momentum of compound nucleus; and δ_{nx} is Kronecker delta.

The collision matrix can be represented in terms of the transmission probabilities ρ_{nx}, as shown in Eq. (2).

$$U_{nx} = e^{-2i\phi_l}\left[\delta_{nx} - 2\rho_{nx}\right] \tag{2}$$

where ϕ_l is hard-sphere phase shift with the given orbital angular momentum l.

In the condition that the collision matrix is single-valued and meromorphic in momentum space, the transmission probability can be expressed as follows,

$$\left|\rho_{nx}\right|^2 = \frac{\left|P^{(2N-1)}\left(\sqrt{E}\right)\right|^2}{\left|P^{(2N)}\left(\sqrt{E}\right)\right|^2} = \sum_{\lambda}\left(\frac{r_{\lambda x}}{p_\lambda - \sqrt{E}} + \frac{r_{\lambda x}^*}{p_\lambda^* - \sqrt{E}}\right) \tag{3}$$

$$\rho_{nn} = \frac{P^{(2N-1)}\left(\sqrt{E}\right)}{P^{(2N)}\left(\sqrt{E}\right)} = \sum_{\lambda}\left(\frac{r_{\lambda n}}{p_\lambda - \sqrt{E}}\right) \tag{4}$$

where $P^{(2N)}\left(E\right)$ is a polynomial of order $2N$; p_λ and r_{nx} are poles and residues, respectively for the specific resonance peak λ; the superscript "*" means complex conjugate of poles and residues.

2. Conversion from R-Matrix Formalism

In order to convert Reich-Moore parameters into Multi-Poles, R. Hwang constructed an equivalent equation, which roots being poles, and residues can be easily calculated at corresponding poles [4].

$$F(u)=\left[\prod_{\lambda}\left[E_{\lambda}-u^{2}-\frac{i}{2}\Gamma_{\gamma\lambda}\right]q^{(l)}(u)\right]\det|I-K|=0 \quad (5)$$

where $u=\sqrt{E}$ stands for momentum space; $(I-K)$ is channel matrix, being represented in the Eq. (6), below.

$$(I-K)_{nx}=\delta_{nx}-\frac{i}{2}\sum_{\lambda}\frac{\Gamma_{n\lambda}^{1/2}(E)\Gamma_{x\lambda}^{1/2}(E)}{E_{\lambda}-u^{2}-\frac{i}{2}\Gamma_{\gamma\lambda}} \quad (6)$$

Moreover, the function $q^{(l)}(z)$ depends on orbital angular momentum, as shown in Eq. (7).

$$q^{l}(u)=\begin{cases}1 & \text{, if } l=0\\ 1+(k_0au)^{2} & \text{, if } l=1\\ 9+3(k_0au)^{2}+(k_0au)^{4} & \text{, if } l=2\end{cases} \quad (7)$$

$$k_0=2.196771\times10^{-3}\frac{A}{A+1} \quad (8)$$

where A is atomic mass in amu unit; and a is channel radius of target nuclide.

For every single resonance, Eq. (5) simplifies into the complex polynomial of specific order as follows,

$$F(u)=\sum_{k=0}^{2(l+1)}a_k u^{k}=0 \quad (9)$$

where the polynomial order is 2, 4, and 6 for $l=0,1,2$ cases, respectively.

The roots for Eq. (9) are calculated using the Laguerre's method [5-8]. However, strong interferences among resonances expressed in Reich-Moore formalism cause the deviation of poles from the roots of Eq. (9). By considering all the resonances, the order of polynomial $F(u)$ reaches more than 2000, especially in case of the conversion with very dense resonances for many actinides i.e. U-235, U-238, and Pu-239. It is a well-known problem in mathematics to find all the roots of a polynomial of several hundred or thousand order. For solving this problem, the roots for Eq. (9) at every single resonance should be used as initial guesses for Newton-Raphson method.

$$u^{(n)}=u^{(n-1)}-\left.\frac{F(u)}{F'(u)}\right|_{u^{(n-1)}} \quad (10)$$

It was stated by R. Hwang that the some roots become very close to each other for higher angular momenta. Those closely packed poles are determined by the solution of the Eq. (11) under the condition that resonance energy is much larger than the neutron width.

$$q^{(l)}(u)=0 \quad (11)$$

In case of the p-wave orbital angular momentum, there is one pair of poles for every resonance with the dependence shown in Eq. (12).

$$p_{\lambda}\approx\pm\frac{1}{k_0a}i \quad (12)$$

Similarly, for the d-wave, four poles for every resonance will be expected at the location like this.

$$p_{\lambda}\approx\pm\sqrt{\frac{3}{2}}\frac{(-1\pm3i)^{\frac{1}{2}}}{k_0a} \quad (13)$$

Considering the fact that Newton-Raphson method is extremely sensitive to initial guesses, R. Hwang adapted quad precision in numerical computation to obtain multi-poles.

An in-house code for generation of Multi-Poles from R-Matrix based resonance parameters has been developing in UNIST. Currently, the given method allows to calculate poles corresponding to s-wave resonances, and the s-wave-like poles for higher angular momentum resonances. Although the converting method is effective and efficient for many major actinides with only s-wave resonance parameters, i.e., Th-230, U-233,U-235, Pu-239 and Am-241; it confronts numerical instability problem, while processing the resonances with higher angular momentum, i.e. U-238, Ni-60 and etc.

III. NUMERICAL RESULTS

1. Numerical Instability

This chapter presents the instability issue on the conversion of resonance parameters for Ni-60, due to the presence of s-, p-, and d-wave resonances.

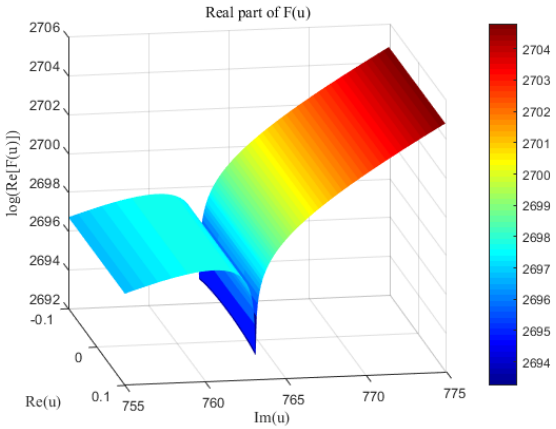

Fig. 1. Real part of $F(u)$ for Ni-60 p-wave resonances.

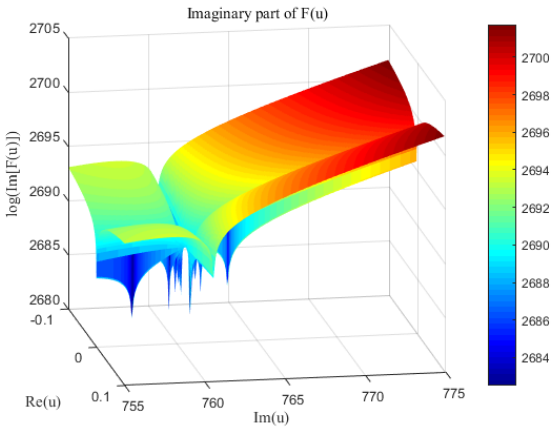

Fig. 2. Imaginary part of $F(u)$ for Ni-60 p-wave resonances.

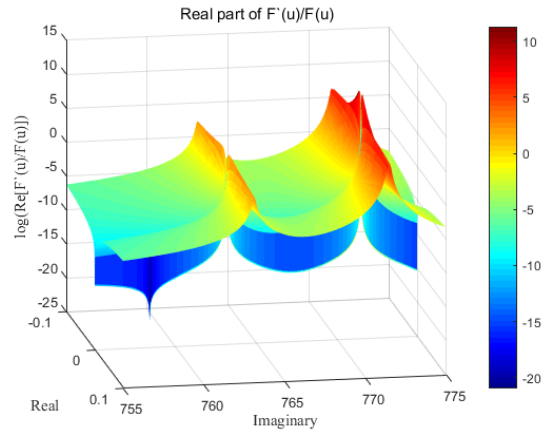

Fig. 3. Real part of $F'(u)/F(u)$ for Ni-60 p-wave resonances.

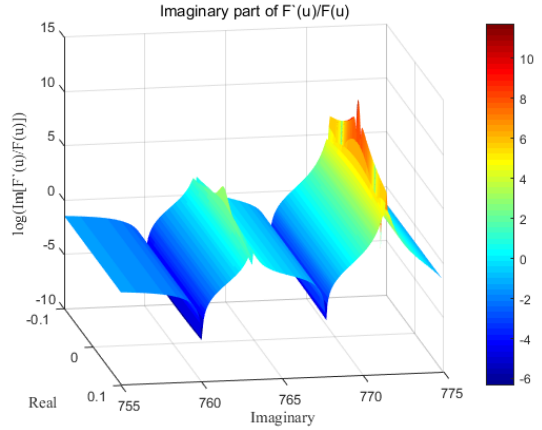

Fig. 4. Imaginary part of $F'(u)/F(u)$ for Ni-60 p-wave resonances.

As illustrated in Figs. 1 and 2, many roots of $F(u)$ for p-wave resonances of Ni-60 are clustered in the vicinity of $0.0+771j$. The logarithmic derivatives of $F(u)$ used in the Newton-Raphson iteration are shown in Figs. 3 and 4. Due to numerical instability issue, the roots (poles) cannot be converged even though the quad precision is applied. Figs. 5 and 6 show the pole movement during the first 100 iterations, respectively.

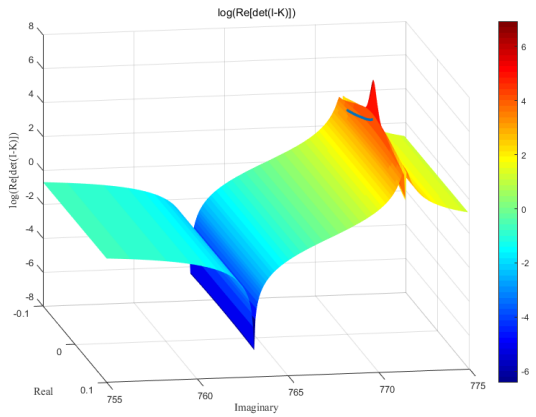

Fig.5. Movement of non-s-wave-like poles (real part) for Ni-60.

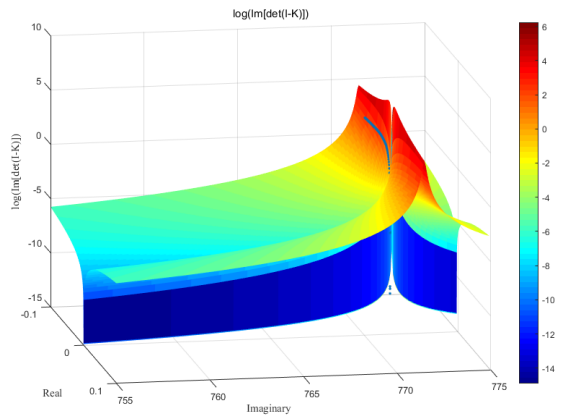

Fig.6. Movement of non-s-wave-like poles (imaginary part) for Ni-60.

It can be seen that, both real and imaginary parts of these root moves weirdly and abnormally on the surface of $\det(I-K)$. Since so many poles are gathered together, there is a very large gradient at these initial guesses. As the number of iterations increase, these steps of Newton-Raphson method change slowly as to be concealed by numerical truncation error.

2. Preliminary Solution

To avoid the numerical instability issue, a great deal of time is spent and the effort includes several aspects in the following.

Simultaneous Iteration

There should exist error accumulation issue in the root elimination process during the traditional Newton-Raphson iteration, especially in the case that number of poles being more than 900 [6]. Thus, a simultaneous solution can be taken, which principle is to update all the roots in each step of iteration by assuming that all the roots come to be converged except the current one.

Table I. Result of Converged Poles

# of p-wave resonances	# of poles	Original	Simultaneous
2	8	6	6
5	20	12	18
10	40	22	32
199	796	400	589

Restart Capability

R. Hwang increased the flexibility of WHOPPER code by using restart capability to improve the initial guesses. This strategy can be accomplished to divide the large number of resonances into several group, more or less 100 resonances in each group. Suppose that all the poles in certain group are converged after some iterations, these poles should be updated as the initial guesses for all group of poles. This method is naturally working when using simultaneous iteration techniques.

Table II. Result of Numbers of Iterations to Converge

p-wave resonances index	Poles index	w/o restart	w/ restart
1	1	7	1
1	2	29	1
1	3	64	201
1	4	7	1
2	5	7	1
2	6	15	1
2	7	24	1
2	8	7	1
3	9	5	1
3	10	62	1
3	11	34	1
3	12	6	1
4	13	5	1
4	14	201	201
4	15	61	1
4	16	6	1
5	17	5	1
5	18	21	1
5	19	22	1
5	20	5	1
total	--	593	420

Cancel Shift Factor Approximation

R. Hwang has been examined the impact of shift factor for the higher angular momentum resonances. It is stated that the converting formalism are constructed on the assumption that shift factor is set to be zero. That is to say, all of resonances are s-wave. Therefore, a very weak dependence exists between multi-poles of p-wave resonances and their resonance parameters in Reich-Moore.

$$F(u)=\det(I-K)\times q_l(u)\times\prod_{\lambda}^{N}\left(E_\lambda-u^2+\Delta_\lambda^{(l)}(u)-i\frac{\Gamma_{\lambda\gamma}}{2}\right)=0 \quad (14)$$

$$(I-K)_{cc'}=\delta_{cc'}-\frac{i}{2}\sum_{\lambda}\frac{\Gamma_{\lambda c}^{1/2}\Gamma_{\lambda c'}^{1/2}}{E_\lambda-E+\Delta_\lambda^{(l)}(E)-\frac{i}{2}\Gamma_{\lambda\gamma}} \quad (15)$$

$$\Delta_\lambda^{(l)}=\frac{S_l(|E_\lambda|)-S_l(u)}{2P_l(|E_\lambda|)}\Gamma_{\lambda n} \quad (16)$$

As shown from Eq.(14), $\Delta_\lambda^{(l)}(u)$ is the shift factor, which is caused by the interference of so many poles in the same spin group in physics. However, this shift factor is approximated in R. Hwang's derivation for the conversion of multi-poles and corresponding residues from R-Matrix resonance parameters. Therefore, to take into consideration of shift factor for higher angular momentum, the logarithmic derivatives of $F(u)$ used in the Newton-Raphson iteration should be re-derived completely with shift factors.

Arbitrary Precision

An arbitrary precision computation package ARPREC is developed by David H, Bailey, which is written in C++ for highly performing arithmetic with an arbitrarily high level of numeric precision [11]. This pack should be of use in solving multi-poles conversion with clustered roots of its polynomial.

Table III. Result of converged poles for Ni-60

# of p-wave resonances	Total # of poles	Original	Optimized
2	8	6	8
3	12	8	10
5	20	12	19
10	40	22	35
15	60	32	47
20	80	42	61
199	796	400	609

To show the current status of convergence for multi-poles converting from Reich-Moore resonance parameters, Table I shows the converged poles number improved by simultaneous technique application in Newton-Raphson iteration for Ni-60.

Table II lists the comparison of number of iterations, which is needed to make these poles converged with restart capability or not.

Table III tabulates the convergence results with all these optimized preliminary solution for the multi-poles conversion with comparison of original results just using Newton-Raphson iteration.

IV. CONCLUSION

The paper presents Multi-Poles converting methods from R-Matrix based resonance parameters, which has been applied and developed in UNIST in-house Multi-Poles conversion code. Although most of important isotopes in reactor engineering can be converted successfully, numerical instability issue occurs in calculation of the non s-wave poles for higher angular momentum states. Implementation of simultaneous root finding method, restart capability, shift factor approximation cancelation along with arbitrary precision, allows to achieve the convergence of more poles for the higher orbital angular momenta was achieved.

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