Open issues on scattering kernels of compound nuclear reactors

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Abstract. Scattering kernel models, define the energy change and angular distribution of a scattered neutron. In the keV and fast energy ranges these are often determined by phenomenological concepts or using fits to measurements due to lack of microscopic details and/or complicated mathematical issues with some models. Some scattering kernels neglect the temperature dependency or the resonant structure of the nuclide. Moreover, most of the double differential solutions do not sum up mathematically to the integral scattering cross section itself and are in the best case artificially adapted. This study deals with the scattering kernel of compound nuclei in energy ranges mainly up to 50 keV, for structured resonance cases. It compares the two advanced approaches as far as the physics is concerned, one of which is based on classical kinematics with a quantum correction in form of the energy dependent resonances developed by Rothenstein-Dagan (RD), and the other model by Blatt-Biedenharn (BB) resembles. Both models are based on theoretical microscopic assumptions yet differ by their physics approach. The analysis in this study leads to two new main observations. On one side the importance of inclusion of the azimuth angle, and further for a quantum mechanics approach a unique mutual spin number must be defined for the total cross-section as well as the angular distribution measurements.

1 Introduction

The activities concerning the differential scattering kernels can be in general divided in four energy ranges: (i) the solid state based scattering kernel for very low energies, (ii) the epithermal energy range including the resonant dependent scattering kernel, (iii) the intermediate energy range up to 1 MeV where resonance structure is still recognizable, and (iv) the energy range above 1 MeV where the Optical Model Potential (OMP) is introduced for the differential scattering cross section. The need to introduce a theoretical basis in the calculations compared to the use of OMP was pointed out already in [1] which recommends looking for the "physical basis for the Kalbach angular distribution systematics". Further studies [2-4] introduced the dispersive optical model approach to get a better microscopic insight into the single particle properties beyond the average approach of the central potential solution. This study, on the contrary, concentrates on an alternative approach for the intermediate energy range between 1 keV and 50 keV. This energy range is particularly interesting because it introduces, to some extent, the transition from a "classical" temperature-dependent resonance structure towards enhanced quantum-mechanical effects embedded in central potential theory mentioned above. This study presents a direct comparison, on a microscopic basis, between the classical kinematic approach with quantum corrections and the (to some extent) degenerate quantum mechanical approach. The classic approach developed by Rothenstein-Dagan (RD) [5] was introduced in a practical form for implementation in most Monte Carlo (MC) codes using the Doppler Broadening Rejection Correction (DBRC) method [6]. It was validated for resonant actinides in the epithermal range. In this study, its validity check is extended to lighter isotopes. This kernel (RD) is compared with the Blatt Biedenharn (BB) scattering kernel [8] which is based on quantum mechanics and employs Legendre polynomials where the moment $l = 0$ implies isotropic scattering.

In the next section, preliminary results for both kernels are presented for 56Fe in the vicinity of specific resonances at 27.79 keV, and 46.053 keV. These results illustrate the effects of the azimuth angle used in the classical RD approach, in comparison with the BB solution. Furthermore, the importance and need of unique quantum spin number for the (states/resonances) contributing to the differential and integral cross section evaluation, and the impact of mathematical series solutions on the accuracy of the calculated data are pointed out.

The last section introduces a new innovative BB-based approach that incorporates measurements performed in RPI, in which the integral cross section itself is for the first time reproduced via the differential cross section. This is similar to the RD model in the classical approach. This method emphasizes the importance of treating both differential and integral scattering data consistently in cases which at present are

treated in an approximate way using the central potential technique mentioned above.

2 RD and BB scattering kernel for s and p resonances for 56Fe

S wave resonances are per definition isotropic in the Centre of Mass (CM) system. However, the laboratory angular distribution is not always necessarily isotropic. For heavy nuclides with pronounced resonances like 238U, it is indeed mostly the case, but for other lighter isotopes like 56Fe, as can be seen in Fig. 1 (top panel), the angular distribution is not isotropic. The angular distributions in Fig. 1 were calculated with the SAMMY code using the BB approach. At the peak of the s wave resonance at 27.7 keV, the scattering is isotropic, but it diverges towards the dip at 24.52 keV as shown in the top panel. The bottom panel presents the scattering by the p-wave resonance at 46.053 keV. The anisotropy is mostly pronounced at the peak and diminishes at both tails of the resonance. For p-wave resonances the scattering is already anisotropic in the CM system according to Breit-Wigner resonance theory. In this energy range, the BB kernel seems to be the best available quantum mechanics-based solution. Yet, the energy of the scattered neutron is not given and must be calculated separately thereafter. Usually, this open issue is solved by using the approximation of a target at rest at 0 K in the classical approach. The RD model which assumes isotropy in CM system was extended in this study to the above mentioned keV energy range.

It is demonstrated that the dependence of the azimuth angle on the polar angle as shown in [9] cannot be neglected when a qualitative comparison is performed with the BB model. However, the RD model was developed to provide global (8 up to 16) cosine bins as this is practically used in scattering kernel tables (known also as S(α,β) tables) in MC codes. Therefore, only the qualitative trend of the angular distribution obtained with the two models is compared. Strictly speaking, the comparison deals only with a very important open issue phenomenon , namely the change of the scattered probability before and after the dip of an S resonance where in contrary to what one might expect (in particular for heavy isotopes), the distribution is not isotropic and as can be seen in Fig.1 not only that it is definitely not isotropic the probability of the forward angle distributions decreases from top to bottom and vice versa for the backward angle before and after the resonance-dip.

Therefor it is highly interesting to analyse this issue with the RD model not only because it is implemented (via the DBRC model) in MC codes but also because the OMP (also employed at high energy range in MC codes) cannot handle this issue at all. In view of the above, the BB kernel as seen in Fig. 1 and the RD model were compared at two energy points, before and after the dip of the s-wave resonance (Fig. 1 top panel) and for the p resonance before and after the peak shown in the bottom panel. This type of analysis is, as mentioned above, insofar unique because the forward scattering (0°) is maximal before the dip and minimal after the dip and

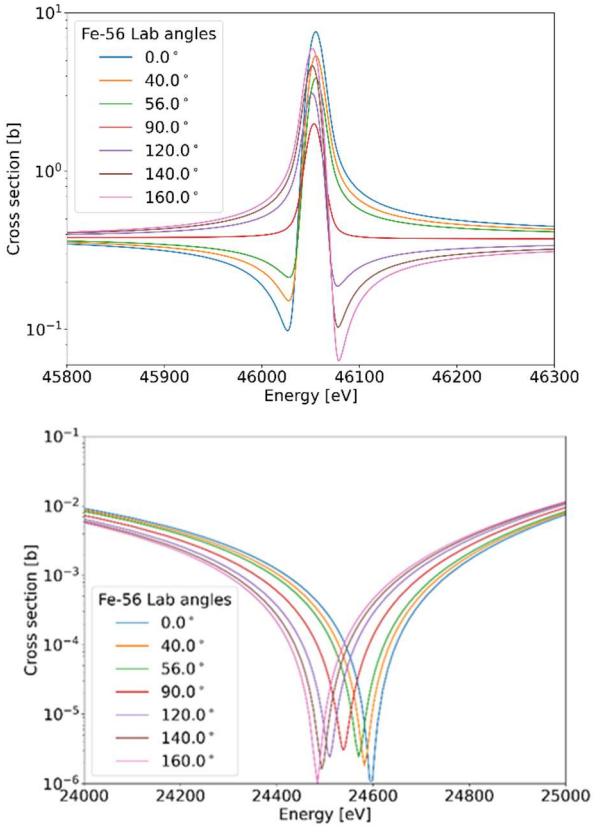

Figure 1. Top panel: Anisotropic angular distribution at seven angles at energies around the dip of the s-wave resonance of ^{56}Fe at 27.79 keV. Bottom panel: a p-wave at 46.053 keV. The strong anisotropy at the peak of the resonance converges quickly to almost isotropic scattering.

vice versa for the peak in the bottom panel. It turns out that for the s-wave resonance, the same qualitative trend occurs before and after the dip when using the complete formula (with the correct azimuth dependent angle) of the RD model. This result emphasizes the link between these two seemingly "different physics" solutions and confirms the need for dedicated high-resolution measurements for ^{56}Fe in this energy range. It should be noted that W. Rothenstein showed already in [10] that one can convert the RD formula to a Legendre polynomial, namely to the BB structure, and in doing so enabled the direct comparison -from the mathematical point of view- between quantum mechanical and classical solutions. The kernel in the notation of BB [8] is given by

$$\frac{d\sigma}{d\Omega} = \lambda\!\!\!^{-2} \sum_{L=0}^{\infty} B_L P_L(\cos\theta) \qquad (1)$$

where B_L involves quantum-mechanical based complicated factors similar to the Rothenstein [10] formalism

$$\sigma_s^T(E \to E', \mu_{lab}) = \sum_{L\geq 0} \frac{1}{2L+1} \sigma_{sL}^T(E \to E') P_L(\mu_{lab}) \qquad (2)$$

where the coefficients of the Polynomials of order L PL:

$$\sigma_{sL}^{T}(E \rightarrow E') \quad (3)$$

are classical-based and T is the temperature dependence.

Consequently, the two approaches represent the same phenomena in different ways. (solid angles vs quantum numbers).

3 Generation of integral cross section from differential ones with RD and BB models

In the keV energy range, the RD model allows one to calculate the outgoing energy and angular distribution of the emitted neutron via the correct azimuth angle and temperature dependence. From the emitted neutron spectrum one can obtain the same integral scattering Doppler broadened cross section as provided directly by the NJOY processing code. Based on the relations between the RD and BB model, an innovative idea was suggested and implemented at RPI. The BB method is used to generate resonance structured total cross sections, and the spin quantum numbers are extracted by adjustments to the BB-based angular distributions. Those specific spin quantum numbers are then introduced to generate an adaptable total cross section which is not available otherwise. Such a procedure was successfully demonstrated in [11], where ^{208}Pb total cross sections were generated above 1 MeV [11] and for the first time, the resonance parameters were defined and confirmed against dedicated measurements.

4 Conclusion

This work suggests that in the lower keV energy range, the current practice of using 0 K scattering should be replaced by the DBRC approach, which is already implemented in most Monte Carlo codes for energies up to 1 keV, thus resolving one of the open issues related to secondary neutron scattering. Moreover, we have highlighted the importance of the azimuth angles. In the case of ^{56}Fe, we have shown that the azimuth angle dependency is essential to get the correct solution that agrees with the spherical harmonic approach used in the BB model. This agreement is confirmed by the results we obtain when we apply for the first time the correct dependency of the azimuth angle in the RD model. The angular distributions agree with the BB results shown in Fig. 1 (top) for s-wave resonances. The agreement between the classical azimuth-dependent approach and the quantum mechanics-based form is the main new observation in this study, which emphasizes the need for further dedicated measurements accompanied by development of mathematically accurate resonance-structure based approaches rather than the average central potential approach, which is however needed at very high energies.

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