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On the Importance of a New Formula for the Double Differential Scattering Kernel

R. Dagan*
Forschungszentrum Karlsruhe Institut für Reaktorsicherheit, P.O. Box 3640, 76021 Karlsruhe Germany

The original double differential scattering kernel developed by Rothenstein and Dagan for heavy isotopes, differs from the current NJOY solution procedure. The main difference is in the exclusion of the strong scattering resonances in the latter. The scattering kernel of many materials of interest like U238 is strongly dependent on the cross section profile, mainly in the vicinity of resonances, which leads to changes in the absorption and in the Doppler-effect. Moreover, former investigations and the current one indicate that the MCNP treatment in the epithermal region is questionable as the code applies unjustified approximations.
New mathematical formalism by Rothenstein enabled the implementation of the modified kernel within the THERMR module of NJOY. The problematic of the existing kernel in NJOY is thus demonstrated and preliminary results emphasize the importance of using the new formula for the scattering kernel for nuclides with strongly energy dependent scattering cross–sections. The essential steps to improve the MCNP sampling methods are also discussed.

KEYWORDS: Double Differential Scattering, $S(a,b)$**, resonant absorption**

1. Introduction

The slowing down of neutrons is a known important part of any thermal core simulation. At the lower epithermal range, one can assume that the scattering collision between the neutron and its target is elastic as the first excited level of the light and heavy scattering isotopes is several KeV. Thereafter the common way to handle the energy change of the neutron after an elastic collision is by utilizing the so called “asymptotic” scattering kernel. The probability density in this case is independent of the out-coming neutron energy. Further it is assumed that the target-nuclei is at rest before the collision. When the thermal agitation of the target nuclei is introduced the light and heavy isotopes treatment is different mainly due to the energy dependent cross section of the fuel isotopes like U238. For the light isotopes which assume constant scattering cross section the so called $S(a,b)$ equation provides the double differential scattering kernel including the energy after scattering as well as the cosine of the scattering angle. This equation was obtained directly in a classical way by Rothenstein [1] on the basis of momentum and energy considerations. Originally, it was derived as a simplified case of a quantum mechanical treatment (M.M.R. Williams [5]) where the excited target levels are degenerated and the nuclei are reacting as an ideal gas

The NJOY [2] procedure in its THERMR module is based on light isotopes $S(a,b)$ treatment for all materials. The cumulative kernel over all angles is then normalized according to the scattering cross-section based on the BROADR module in NJOY. For heavy isotopes with pronounced resonances this is not quite accurate as “The secondary energy distribution will be still incorrect” (THERMR manual [2]).

* R. Dagan, Tel. 0049-7247-823441, FAX 0049-7247-823718,E-mail:dagan@irs.fzk.de

Ouislouman and Sanchez [6] showed that in the vicinity of resonances the asymptotic kernel predicts considerable erroneous values indicating that the moderation of neutrons is significantly different than the one commonly used. The solution of the MCNP [4] code in the resonance range is based on a statistic procedure called: "Sampling the Velocity of the Target nuclei". It is assumed that "for heavy nuclei where $s_s(rel)$ can vary rapidly, the moderating effect of scattering is small so that the consequences of the approximation (for the probability distribution) will be negligible". In light of the Ouislouman and Sanchez paper it is questionable to what extent the approximated treatment, of the neutron energy and its spatial angle after scattering, is valid.

In the next sections the double differential scattering kernel for heavy isotopes is introduced and the new mathematical formula developed by Rothenstein [3] is discussed. In his work, Rothenstein had provided the way in which NJOY can be improved making use of the developments[1] which were not available when the original models were included in NJOY. This new "Rothenstein" scattering kernel treatment is illuminated and its importance is discussed in terms of its application for the MCNP code as well as the impact on the absorption and the feedback reactivity for selected unit cell calculations.

2. The double differential scattering kernel

The solution of the $S(a,b)$ equation based on classical approach strengthened the idea of finding solution for isotopes with strong energy dependent cross sections like pronounced resonances. Consequently the underlying assumptions exclude the chemical binding effects in the mathematical considerations. Practically, the developed formalism is restricted to temperatures above the Debye temperature which is a measurement of the maximal free vibration frequency of the atom in its solid structure. The Debye temperature for oxide uranium is 500^0 K and for metallic uranium is less than 200^0 K.
Consequently, for most practical core applications the new kernel is relevant.

The detailed derivation of the following equation (2.1) can be found in Rothenstein and Dagan [1]. The velocities vectors and angles shown in figure 1 are the basis for the kernel formulation.
The scattering kernel for isotopes with strong scattering resonances is:

$$
\begin{aligned}
& s_s^T(E \to E', \vec{\Omega}, \vec{\Omega}') = \frac{1}{2p} s_s^T(E \to E', m_0^{lab}) = \\
& \frac{1}{2p}\sqrt{\frac{A+1}{Ap}}\sqrt{\frac{\exp(E/(K_B T)}{E}}\int_0^\infty dt[t s_s^{tab}(E_r,0)\exp(-t^2/A) \\
& \times\left[H(t_+ - t)H(t - t_-)\int_{e_{\max}-t}^{t+e_{\min}} dx \exp^{-x^2} + H(t-t_+)\int_{t-e_{\min}}^{t+e_{\min}} dx \exp^{-x^2}\right] \\
& \times\frac{P(u,\hat{m}_0^{CM})}{2p}\frac{4e_{\max}e_{\min}x^2}{B_0 \sin\hat{f}} 2H(\cos\hat{f}+1)H(1-\cos\hat{f})
\end{aligned}
\qquad (2.1)
$$

where:

$$t = u\sqrt{(A+1)} \quad ; \quad x = c\sqrt{(A+1)} \quad ; e = v\sqrt{(A+1)} \quad ;$$

and:

$e_{\max}$, $e_{\min}$ are the extreme values that e can get based on the velocity diagram in figure 1.

Further: $t_{\pm} = \dfrac{(e_{\max} \pm e_{\min})}{2}$

$\dfrac{P(u, \widehat{m}_0^{CM})}{2p}$ - The probability density per unit solid angle in the Centre of Mass system.

One should note that the scattering energy dependent cross section is within the integral. If the cross section is constant the solution can be done in the laboratory system to give the $S(a, b)$ treatment of light (constant cross section) isotopes.

The basis of (2.1) is the conservation of the energy and momentum which is implicitly incooperated through 6 constraints. The Heavyside functions H express some of them.

The numerical solution of Equation 2.1 is very cumbersome for numerical solution. In particular the B_0 -term is a square root of quadric equation which requires unpractical long computational time. Rothenstein [3] succeeded to simplify Equation 2.1. For example, the quadric equation was decoupled and was reformulated as a bi-quadratic equation. This allowed for the implementation of the new modified kernel into the THERMR module of NJOY. Consequently, the angle and energy distribution of the scattered neutron can be directly assessed in the "cosine bins" manner and the comparison with the existing kernel in NJOY points out the importance of the "Rothenstein" kernel.

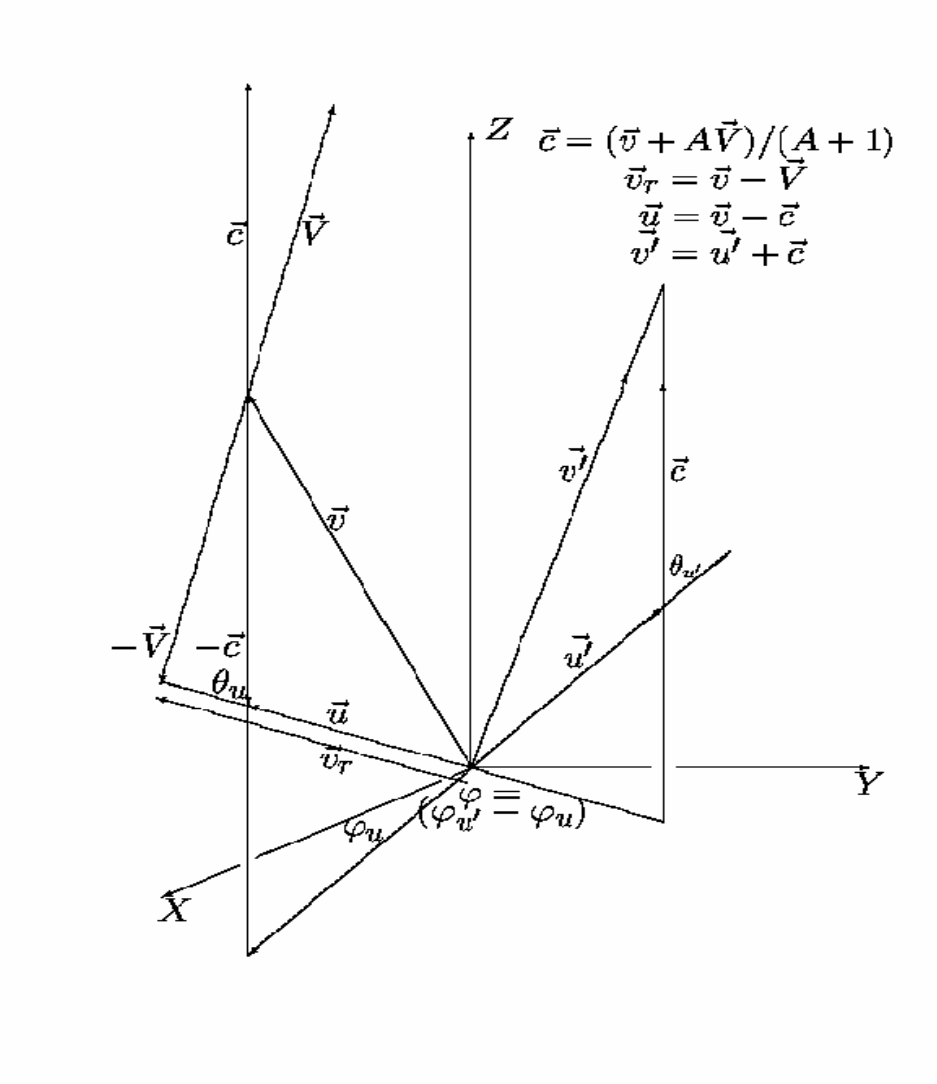

Fig. 1: Definition of Velocities and angles after and before the neutron scattering.

3. Representative results of the new kernel

The results of the double differential scattering kernel are divided into two parts. First the integrated (isotropic) kernel is introduced in a unit cell calculation and the absorption rate as well as the Doppler-effect dependency on the scattered neutron energy distribution (including up scattering) is quantitatively evaluated. Next the influence of including the scattered angle distribution as was done within the new kernel in NJOY is analysed.

The isotropic kernel (basically the one developed originally by Ouisloumen and Sanchez [6]) was inserted into the OZMA code [7]. This code calculates the reaction rates very accurately for one dimensional unit cells. Two types of cells are presented. The first unit cell is based on the Tellier [8] benchmark which dealt directly with resonant absorption in a pure U238 oxide unit cell without fissionable materials. The second cell is a more practical one dealing with the TRIGA fuel with relevancy to the ongoing TRADE [9] project. The latter unit cell differs from the first one in the U235 and also in the zirconium hydride (ZrH) within the fuel. In both cases the new kernel including its up-scattering is considered only for the U238 treatment. Employing the new kernel solely for the U238 is justified as the up-scattering is pronounced mainly in the vicinity of the resonances with considerably high scattering resonance (Γ_n) width. In table I the absorption fraction per 1 neutron entering the 3.3 KeV (far away from having influence on the relevant 100 eV region) is presented for the two unit cells:

Table 1: Absorption fraction per 1 neutron entering the 3.3 KeV for Tellier and TRIGA unit cells with and without up-scattering.

Temperature (K)	Without up-scattering	Without up-scattering	With up-scattering	With up-scattering
	Tellier	TRIGA	Tellier	TRIGA
300	0.205508	0.043672	0.206683	0.043722
600	0.214834	0.048806	0.216733	0.048984
900	0.222281	0.052425	0.225076	0.052740
1200	0.228722	0.055232	0.232428	0.055661

Table 1 presents two cases. In the Tellier benchmark, there is no fissile material and no hydrogen in the fuel. The absorption the epithermal region and in particular the resonant absorption between 6 and 120 eV is well pronounced. In the TRIGA case the existing fissile material generates excessive neutrons and the Hydrogen tends to increase the escape probability from the resonant zone. Thus fractional absorption is significantly reduced. The Doppler-effect was measured between 300 K and 1200 K. Form table 1 one can show that the Doppler-effect is more important for the TRIGA case as it causes an increase of about 26% in the absorption in comparison to about 11% in the Tellier case. Yet, the absolute value is for the Tellier benchmark clearly higher. In addition the up-scattering effect is as expected much more pronounced in the Tellier case (~11%) compared to the TRIGA case (~3.5%). These two cells could be regarded as extreme cases. In general, one can expect that the value of the absorption and Doppler effect will lie for other used fuel types between those values.

The implementation of the full double differential kernel including the cosine of the scattered angle is not yet possible in the same manner as for the isotropic kernel shown above. Nevertheless the crucial first step was done in the extension of the THERMR module. Figure 2 and 3 show the equi-probable “cosine bins” of the scattering kernel at 300^0K. Figure 2 uses

the existing kernel in NJOY and figure 3 the new one. Figure 4 and 5 are at 1000^0 K. One should look on "vertical lines" in those graphs. This means at a certain out-scattered energy E' the equal probable cosine angles lie on the cut points of a virtual vertical line (starting at E') with each of the 8 (cosine bins) lines plotted in the graph.

From those figures the difference between the two kernels can be well seen. At 300^0 K the new kernel tends to enhance the backwards scattering at the neutron energy before scattering while at certain lower energy the forwards scattering is more pronounced. By comparison with the 1000^0 K one can assess qualitatively the impact of the Doppler-effect. Comparing the 300^0 K and 1000^0 K in the original kernel one can see that the forward scattering is reduced and the energy band probability of the scattered neutron is wider. The same phenomenon occurs also using the new kernel. Nevertheless in the lower energy well below the inlet energy, the tendency of forwards scattering is more pronounced by growing temperature.

4. Proposed MCNP procedure for heavy isotopes at the resonant region

The MCNP routine COLIDN deals with the scattering kernel of heavy isotopes in the epithermal region and in particular in the vicinity of the resonances. The approach is different from the one used within NJOY. The approximations in MCNP which were mentioned before leads to the asymptotic kernel with very narrow energy range which in return means (according to Figure 2-5) that the certain scattering cosine angles in the probability wings are excluded. Furthermore the COLIDN routine uses the Rejection Technique (Ross [10]). Generally speaking this technique is "equivalent" to the delta function velocity constraints, which appears in the deterministic approach. Rothenstein [11] replaced the assumption that "the variation of $s_s(v_{rel})$ with target velocity can be ignored" (MCNP [4] CHAPTER 2) by an additional rejection process in order to take into account the essence of the modified kernel. Yet the reliability of such a statistical procedure tends to be biased exactly in the vicinity of resonances where the new kernel has its most pronounced effect.

Contrarily to the "sampling of the target velocity " solution statistical process, the $S(a,b)$ technique in MCNP is well validated. Therefore, the new presented kernel should be reformulated in a "$S(a,b)$ like" table suited for MCNP. Thus an unbiased sampling procedure is ascertained to replace the current approximated MCNP solution method.

5. Conclusions

The success of introducing the full double differential scattering kernel within THERMR elucidates the current incomplete approach of NJOY and MCNP as well. The importance of the new formula is twofold. On the practical level the quantified value of the absorption rates and the Doppler-effect were shown to be not negligible for the cumulative (isotropic) kernel. Moreover the scattered angular distribution is quite different from the one that is so far used in NJOY due to the inclusion of the energy dependent scattering cross section. This might have significant impact for heterogeneous designs which are currently being investigated. On the theoretical level the current solution of MCNP appears to be insufficient as a reference method for deterministic transport methods, especially in the epithermal region with pronounced resonances. The attempts to improve the COLIDN routine (within MCNP) by additional rejection technique were not statistically justified. Using the $S(a,b)$ "like" tables, based on the new formula, for heavy nuclides will ensure the correctness of the MCNP approach. It should be pointed out that the new kernel excludes the quantum mechanical effects and therefore only if the temperatures are not below the Debye temperature the new formula is applicable.

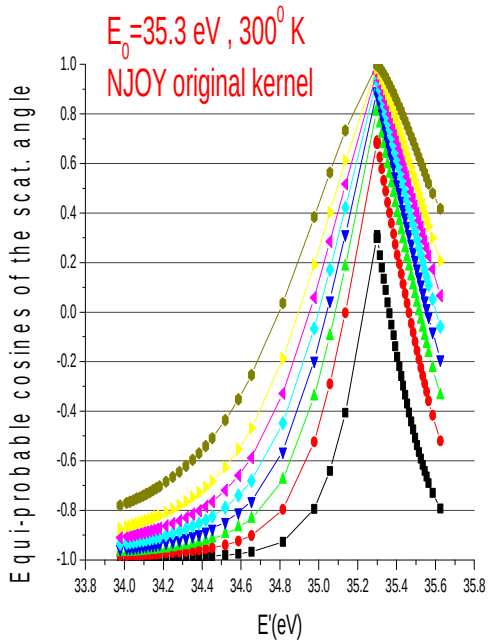

Fig. 2: Differential scattering cosine bins based on the original NJOY kernel at 300^0 K

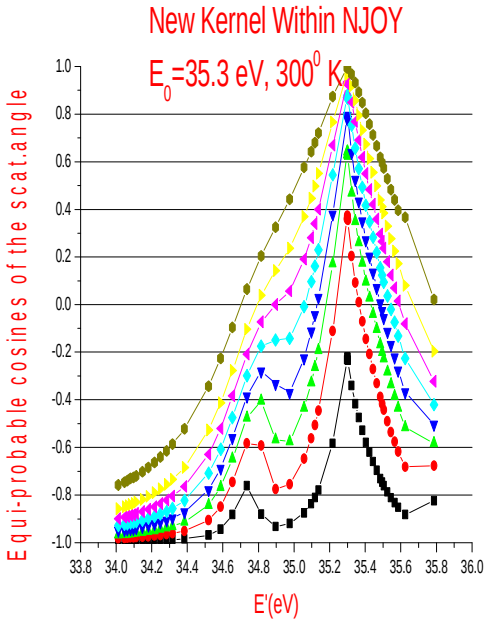

Fig. 3: Differential scattering cosine bins based on the new inserted formula in NJOY at 300^0 K

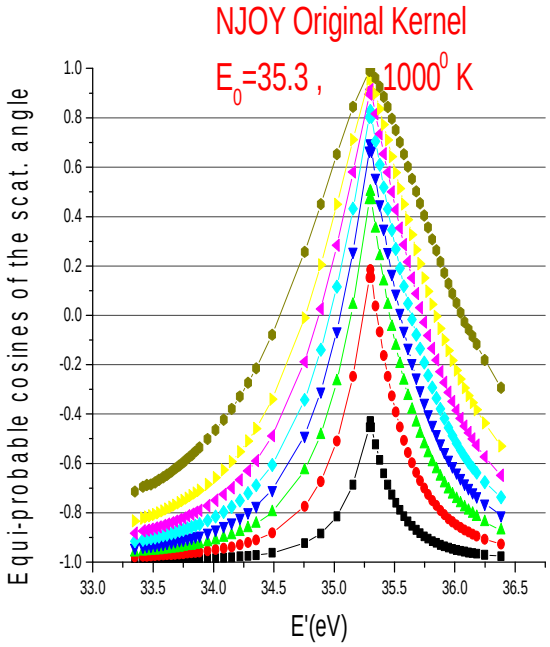

Fig. 4: Differential scattering cosine bins based on the original NJOY kernel at 1000^0 K

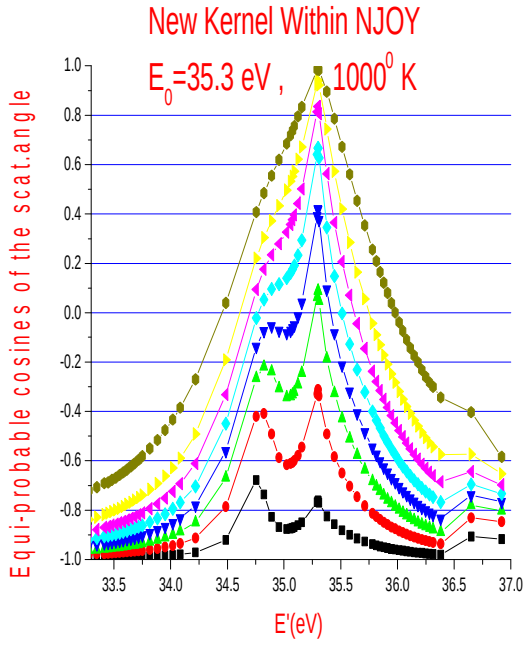

Fig. 5: Differential scattering cosine bins based on the new inserted formula in NJOY at 300^0 K

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