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# Modelling a Resonance Dependent Angular Distribution via DBRC in Monte Carlo Codes

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The development of a new energy dependent double differential resonance scattering kernel by Rothenstein & Dagan, Annals of Nuclear Energy (1998) was shown to have a significant impact on core calculations as far as their criticality, Doppler Effect and the nuclide inventory is concerned. Thereafter, it was of great interest to experimentally validate this scattering kernel in addition to analytically proving its consistency with the integral Doppler broadened cross section, which was achieved by integrating the new kernel over all angles and all scattered energies. This study deals with the unique experiment suggested by Y. Danon at the Gaerttner Linear Accelerator Laboratory at Rensselaer Polytechnic Institute (RPI). The main advantage of this facility is the ability to move the neutron production source off axis relative to the detector beam line. It was, therefore, possible to position the sample, from which the neutron were scattered, on the same axis as the detector. In this way it was possible to directly measure the angular distribution of scattered neutron from heavy nuclides with pronounced resonances. In this study the previous results obtained for $^{238}$U were extended to $^{232}$Th. Improvements were made to the new resonance scattering kernel by development of a stochastic formalism known as DBRC (Doppler Broadened Rejection Correction) which was implemented by Becker *et al.* in several Monte Carlo codes. Based on the good agreement between this DBRC model and the measurements presented in this paper, it was shown that the standard asymptotic back angle scattering used previously in Monte Carlo codes differs by almost 80% for highly scattering resonances. Moreover, the scattering angle measurements and the ability to simulate it accurately by means of stochastic methods emphasized the deficiencies of the current methods which use only transmission and capture measurements.

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## I. INTRODUCTION

The importance of energy dependent cross sections is well known in the field of nuclear physics. For the last several decades, nuclear cross sections have been measured and evaluated as accurately as possible in order to produce resonance parameters. The final evaluation of those resonance parameters is mostly based upon transmission and capture experiments. The resonance parameters are at 0 K and a Doppler Broadening procedure is applied to generate cross sections at room temperature.

The development of the energy dependent double differential scattering kernel by Rothenstein & Dagan [1] corrected an inconsistency in the Doppler Broadening algorithm within the Boltzmann transport solvers. The introduction of the Doppler correction, via probability tables also known as S($\alpha$,$\beta$) tables [2], for heavy nuclei within Monte Carlo codes showed quantitatively that the impact of the new kernel on core criticality and the Doppler Effect is significant [3,4]. The above mentioned developments and evaluation assumed that the resonance parameters themselves are independent of the scattering kernel model.

A measurement, suggested by Y. Danon [5] was performed to experimentally validate the new resonance kernel and its Doppler Broadening angular distribution of the scattered neutron. In parallel to Danon's experiment, a new stochastic resonance kernel -equivalent

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to the S($\alpha$,$\beta$) tables - was generated and implemented within Monte Carlo codes (Becker *et al.* [4]). The stochastic kernel enabled very fast evaluations of different resonances for different isotopes and in particular different angles of scattering.

In this study we present the results of the latest measurements performed at the RPI facility for $^{232}$Th resonances. Based on the good agreement with the new stochastic kernel, we extended the simulation to other nuclides with pronounced scattering resonances for all probable scattering angles. The fact that for several main resonances all the back scattering angles, used so far in neutronic codes, are strongly affected is discussed. Moreover, the impact of the RPI experiment on the method to determine the resonance parameters themselves is highlighted. Finally, the role of solid state effects on the resonance parameters is discussed in view of the current experiment.

## II. ANALYTICAL AND STOCHASTIC RESONANCE SCATTERING KERNEL

The evolution of the scattering kernel process from the very basic hard sphere two body kinematics through the inclusion of the temperature and finally the resonance effects was extensively discussed [6,7]. The full analytical double differential ideal gas based scattering kernel developed by Rothenstein and Dagan [1] allowed for the determination of the angular distribution as a function of the resonances and the relevant temperature within the scattering kernel formula. Equation (1) is taken from [1] where all the variables are defined. The formalism of Eq. (1) was further developed [8] into a form which suited the THERMR module in NJOY [9] and enabled the preparation of an input for MCNP [10] in form of S($\alpha$,$\beta$) probability tables for heavy nuclei [2].

$$\begin{aligned}
&\sigma_s^T\left(E \to E', \vec{\Omega} \to \vec{\Omega}'\right) = \frac{1}{2\pi}\sigma_s^T\left(E \to E', \mu_0^{lab}\right) \\
&= \frac{1}{2\pi v}\left(\frac{A+1}{A}\right)^4\left(\frac{A}{\pi}\right)^{3/2}\int 2\pi u^2 du \int d\mu_u \int c^2 dc \\
&\int (u')^2 du' \int d\mu_{u'} \int \frac{2}{\sin\varphi} d\cos\varphi \frac{\delta(u'-u)}{(u')^2} \\
&\exp\left[v^2 - (A+1)\left(\frac{u^2}{A} + c^2\right)\right] \qquad (1) \\
&\frac{1}{uvc}\delta\left[\mu_u - \frac{(v^2 - c^2 - u^2)}{2uc}\right] \\
&\frac{1}{2u'cK_BT}\delta\left[\mu_{u'} - \frac{(v')^2 - (u')^2 - c^2}{2u'c}\right] \\
&\frac{4vv'c^2}{B_0'}\delta(\cos\varphi - \cos\hat{\varphi})u\sigma_s(E_r)\frac{P(u,\mu_0^{CM})}{2\pi}
\end{aligned}$$

In this study we use the stochastic form developed by Becker*et al.* [4] which is physically identical to the analytical form of Eq. (1). However the delta functions, which define the restriction of the allowed combinations of the free gas temperature dependent target velocities and the angle of interaction between this target nucleus and the neutron, are replaced by the rejection technique, often used in a stochastic algorithm. In addition the new Doppler Broadened rejection correction (DBRC [4]) formalism is applied. Equation (2) describes the essence of this new stochastic formalism for the scattering probability *P(V,$\mu$)* of a neutron with a target nuclei $V$ and a collision angle $\mu$ as was introduced within different Monte Carlo codes (MCNP5 [10], *etc.*).

$$\begin{aligned}
&P(V,\mu) = C'\left\{\frac{\sigma_s(v_r,0)}{\sigma_s^{\max}(v_\xi,0)}\right\}\left\{\frac{v_r}{v+V}\right\} \\
&\left\{\frac{(2\beta^4)V^3e^{-\beta^2V^2} + (\beta v\sqrt{\pi}/2)(4\beta^3/\sqrt{\pi})V^2e^{-\beta^2V^2}}{1+\beta v\sqrt{\pi}/2}\right\}
\end{aligned} \qquad (2)$$

The meaning of the variables can be found in [4]. Actually they are the same as they appear in MCNP manual [10] with the exception that the first term in brackets $\sigma_s(v_r,0)/\sigma_s^{max}(v_\xi,0)$ appears explicitly in form of an additional restriction on the random sampling of the target nuclei $V$ and the collision angle $\mu$, which is the last term in Eq. (2). Equations (1) – (2) are equivalent in their physical meaning. However, the embedded stochastic approach is more practical as far as its accuracy and simplicity are concerned. In particular, it enabled the simulation of many resonances in reasonable time.

## III. THE ANGULAR DISTRIBUTION EXPERIMENT AT RPI

The experimental facility at RPI consists of accelerated electrons impinging on a tantalum target which generates neutrons with an evaporation spectrum having a mean energy of about 1 MeV. The use of Tantalum as a target enables the flexibility of entering the target room and easily handling the tantalum neutron source. In particular one can move the tantalum target off axis with respect to the beam line leading to the detector. This advantage was used by Y. Danon [5] to design an angular distribution measurement which is shown schematically in Fig. 1.

The neutrons hit the $^{232}$Th sample and are scattered with different probabilities in all angular directions. Nevertheless, only those which are scattered in the direction of the beam line will reach the detector. In the case of the current experiment, as shown schematically in Fig. 1, only the neutrons which are backscattered at 140.8$^{\circ}$ reach the detector. It should be mentioned that for thick samples neutrons can be scattered more than one time before leaving the sample at a specific angle. This might affect the counting rates of the detector at the specific angle it is set to. This phenomenon is known as the multiple scattering effect.

By changing the sample position to the right side of the Ta target it is possible to obtain in the RPI facility

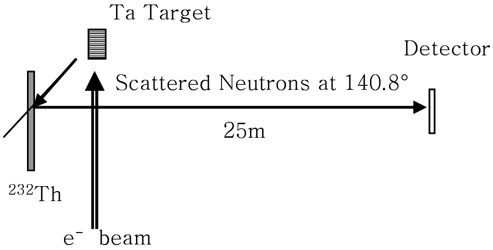

Fig. 1. Sketch of the experimental geometry. The Ta target is off axis with respect to the beam channel line to the detector, and the neutron detector is ~25 m away from the scattering sample.

one forward scattering angle of about 45°. In view of the given isotopes and their measured resonances, it is possible to insert a moderator layer between the source and the sample. In this way more neutrons are slowed down to the resonance energy range and the intensity of the neutrons impinging on the $^{232}$Th sample is preferentially increased by factor of ~3 which increases the count rate and thus shortens the experiment time. The penalty on the accuracy of the scattering angle -due to the fact that the source (moderator) is no longer a point source- is small.

Finally an improvement of the accuracy is achieved by special monitoring system to account for variations in the neutron beam intensity.

## IV. THORIUM BACKSCATTERING SIMULATION AND COMPARISON TO THE EXPERIMENTAL RESULTS

Based on the experimental configuration outlined in the previous section, the counting rates of neutrons scattered from a $^{232}$Th sample at the back scattered angle 140.8° were measured. In particular, the measurement concentrated on the resonance at 69.2 eV. This resonance has a pronounced scattering width ($\Gamma_n \approx 44$ meV) compared to the radiation width ($\Gamma_\gamma \approx 22$ meV). Therefore, it is expected that for this resonance the importance of the double differential energy dependent scattering kernel (introduced in Section I) will be evident. Moreover, this experiment for $^{232}$Th should confirm previous results obtained for $^{238}$U [5] that validated the new scattering kernel. If the experimental results confirm the new kernel which uses a Maxwellian distribution for the target nuclei, then the solid state effects, which are believed to be meaningful for the scattering process, appears to be negligible at 300 K.

In Figs. 2 – 3 the measurements results for a thin (0.1524 cm) and a thick (0.3048 cm) $^{232}$Th sample are presented in the vicinity of the 69.2 eV resonance.

The counting rate differences between the current model used in Monte Carlo codes like MCNP and the modified MCNP code with the DBRC algorithm are clearly noticeable at the 68 eV range, just below the 69.2 eV resonance peak. The experimental results are in full agreement to the DBRC model for the thin sample (Fig. 2) not only at the peak points but, more important, also in the width of the counting rate plot around the peak at 68.2 eV. It should be mentioned that the calculations were normalized to the experimental data in the energy region above 70 eV where both models give the same count rate.

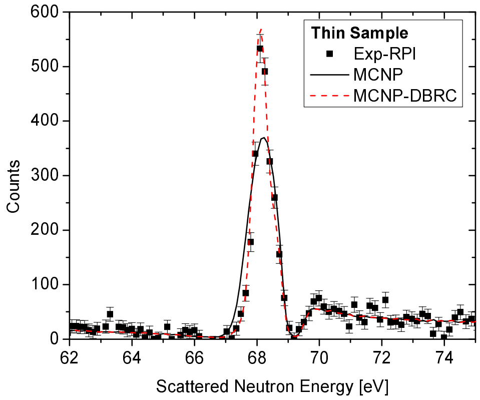

Fig. 2. (Color online) Comparison of the measured neutron counts to standard and DBRC MCNP models at the vicinity of the 69.2 eV resonance of $^{232}$Th for sample thickness of 0.1524 cm.

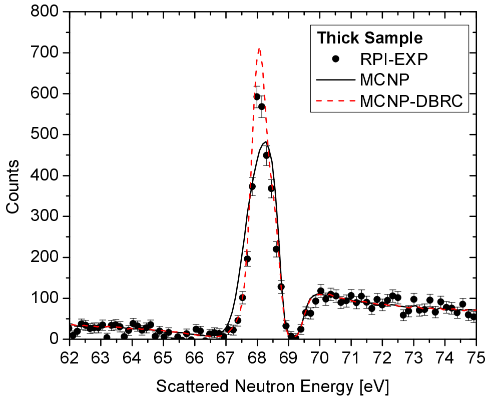

Fig. 3. (Color online) Comparison of the measured neutron counts to standard and DBRC MCNP models at the vicinity of the 69.2 eV resonance of $^{232}$Th for a sample thickness of 0.3048 cm.

The simulation with the DBRC model for the thick sample as shown in Fig. 3 is generally also in good agreement with the experimental results. Nevertheless the peak values are not as well fitted as in the case of the thin sample. There could be several explanations for this phenomenon beyond those concerned directly to the experimental conditions and resolution which where to some extent different than the thin sample measurement. In particular, for a thick sample one might expect that the multiple scattering effects are more pronounced for such measurements or that maybe for $^{232}$Th the solid

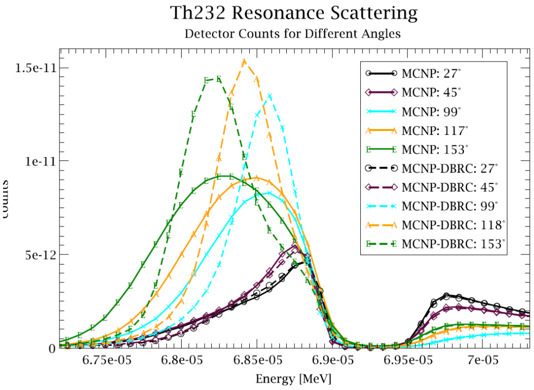

Fig. 4. (Color online) Simulation of detector counts for neutrons scattered at different angles about the 69.2 eV res. of $^{232}$Th. The counts units are normalised to one simulated source neutron.

state effects are not completely negligible.

The good agreement between the measured and the calculated counting rates at the detector allowed confidence in other analysis, namely the scattering shape at additional angles. Therefore, the above simulation at 140.8° was repeated for all different feasible scattering angles (Fig. 4).

The scattering probability at each angle was calculated twice. The first calculation was carried out with the current resonance independent scattering kernel procedure, known also as the asymptotic kernel and in a second run the DBRC model was adapted to the scattering process. A series of angles were tested from 27° deg up to 180° deg at an interval of 9°. The dashed lines are the results of the DBRC model and the full lines represent the use of the standard scattering model.

For all backwards scattering the differences of the counting rate between the current MCNP model and the confirmed DBRC model are evident and reach for some angles up to 80%. Those results emphasize that the experiment is not sensitive to changes in the scattering angle around the nominal angle of 140.8° and thus to the addition of a moderator. The differences between the two models for the forward scattering angles are small in comparison to the backwards scattering angles simulation. This type of backward scattering evaluation was repeated for selected resonances of different nuclides such as $^{240}$Pu, $^{186}$W, $^{176}$Hf, and $^{197}$Au. In most nuclei where the neutron width was dominant the same pattern of Fig. 4 was observed, in particular for the back scattering a large difference between the two above mentioned scattering models was observed. Consequently, more experiments (possibly at other than room temperature) are necessary, in particular to find out if the new scattering kernel can explain some differences between measurements and the current scattering model, which were attributed so far to solid state effects.

## V. CONCLUSIONS

A new measurement was performed to study the impact of the energy dependent scattering kernel effect on the angular distribution of scattered neutrons. The reconfirmation of the new model using the DBRC algorithm emphasizes the fact that scattering kernel can be handled based upon a Maxwellian distribution of the target nuclei. For the determination of resonance parameters it is suggested to study the effect of resonance scattering in resonance parameter analysis codes. In particular for dedicated programs like REFIT [11] or SAMMY [12] which take into account multiple scattering effects for resonance parameter determination it is evident that the inclusion of the DBRC algorithm is mandatory (due to its accuracy and relative simple installation possibility) together with the confirmation on the basis of the RPI experiments. Further the use of higher Legendre moments based on the standard constant cross section model appears to be very questionable in view of the large differences between this asymptotic (0 K) model and the experimental results. Consequently, the use of isotropic scattering for deterministic calculations is at this stage a better approach as the higher moments for heavy isotopes with pronounced resonances introduce a large deficiency of the physical description of the scattering process as they are based on the 0 K asymptotic scattering kernel.

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