*PHYSOR 2012 Advances in Reactor Physics Linking Research, Industry, and Education*
Knoxville, Tennessee, USA, April 15-20, 2012, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2012)

# CONVERGENCE OF LEGENDRE EXPANSION OF DOPPLER-BROADENED DOUBLE-DIFFERENTIAL ELASTIC SCATTERING CROSS SECTION

**G. Arbanas, M. E. Dunn, N. M. Larson, L. C. Leal, and M. L. Williams**
Oak Ridge National Laboratory
Oak Ridge, TN 37831-6171, USA
arbanasg@ornl.gov; dunnme@ornl.gov; larsonnm@ornl.gov; leallc@ornl.gov; williamsml@ornl.gov

**B. Becker**
Department of Mechanical, Aerospace and Nuclear Engineering
Rensselaer Polytechnic Institute NES Bldg. 1-9, 3021 Tibbits Ave.
Troy, NY 12180, USA
beckeb3@rpi.edu

**R. Dagan**
Institut für Neutronenphysik und Reaktortechnik
Forschungszentrum Karlsruhe Gmbh
Postfach 3640, 76021 Karlsruhe, Germany
dagan@inr.fzk.de

## ABSTRACT

Convergence properties of Legendre expansion of a Doppler-broadened double-differential elastic neutron scattering cross section of $^{238}$U near the 6.67 eV resonance at temperature $10^3$ K are studied. A variance of Legendre expansion from a reference Monte Carlo computation is used as a measure of convergence and is computed for as many as 15 terms in the Legendre expansion. When the outgoing energy equals the incoming energy, it is found that the Legendre expansion converges very slowly. Therefore, a supplementary method of computing many higher-order terms is suggested and employed for this special case.

*Key Words:* Doppler broadening, Legendre moments, double-differential elastic scattering, resonance

## 1. INTRODUCTION

Scattering kernels that account for Doppler broadening due to thermal motion of the target nuclei are important for accurate neutron transport computations. An analytical expression for Legendre moments of Doppler-broadened double-differential elastic neutron scattering near low-energy resonances of heavy targets was derived by Ouisloumen and Sanchez in [1], but its usage was limited to the lowest-order Legendre moment because of complicated expressions and high computational requirements needed to compute higher moments. Computation of higher-order Legendre moments was made possible by a method developed and implemented in [2] in which the first six Legendre moments were presented and checked against a reference Monte Carlo computation. The same method was used to compute the lowest 15 Legendre moments (as well as

their covariance matrix) from which a double-differential cross section (and its variance) were computed in [3].

The Monte Carlo code developed by Becker *et al.* in [4,5] was used to compute Legendre moments that were used to test those computed by a deterministic method in [2,3]. Although an excellent agreement was found between Legendre moments computed by the two methods, it was not determined how many terms in the Legendre expansion are needed to accurately compute a double-differential cross section. That is the motivation for this work.

Therefore, we investigate convergence of the Legendre expansion computed deterministically against a reference Monte Carlo computation of double-differential cross sections for incoming energy 6.5 and 6.8 eV, that is, just below and above the 6.67 eV resonance of $^{238}$U, where the effects of up- and down-scattering, respectively, are known to be significant. We also suggest a method that overcomes a slow convergence of Legendre expansion when the outgoing neutron energy equals the incoming neutron energy, an issue that was identified in [3].

## 2. FORMALISM

In this work we will study convergence properties of a Doppler-broadened double-differential elastic scattering cross section computed deterministically via a Legendre expansion:

$$\sigma_s^{TN}(E \to E', \mu_{\text{lab}}) = \sum_{n=0}^{N} (n + 1/2)\sigma_{sn}^{T}(E \to E')P_n(\mu_{\text{lab}}), \tag{1}$$

where $T$ is the temperature; $\mu_{\text{lab}} \equiv \cos\angle(\vec{v}, \vec{v}')$, $\vec{v}$ and $\vec{v}'$ are the initial and the final velocity corresponding to the initial and the final energy $E$ and $E'$ in the laboratory frame, respectively; $P_n(\mu_{\text{lab}})$ are the Legendre polynomials; and the summation stops at $N$. We will study how this Legendre expansion converges to a Monte Carlo reference computation of a double-differential cross section, as a function of $N$.

An expression for the $n^{\text{th}}$-order Legendre moment (in the lab frame) of an isotropic angular distribution in the center-of-mass frame taken from [1] is

$$\sigma_{sn}^{T}(E \to E') = \frac{\beta^{5/2}}{4E} e^{E/kT} \int_0^\infty t\sigma_s^{\text{tab}}(E''(t))e^{-t^2/A}\psi_n(t)\mathrm{d}t, \tag{2}$$

where $E$ and $E'$ are the incident and outgoing neutron energies in the laboratory frame, $T$ is the temperature in degrees Kelvin, $k$ is the Boltzmann constant, $\beta \equiv (A+1)/A$, $A$ is the target mass in units of neutron mass $m$, $E''(t) \equiv \beta kTt^2/A$ is an energy in the lab frame, and $\sigma_s^{\text{tab}}(E_{\text{lab}})$ is a tabulated elastic scattering cross section* at zero degrees Kelvin. The $\psi_n(t)$ is computed via Eqs. (13–26) of [2], where $\psi_n(t)$ is the $\psi_{n0}(t)$ in a generalized notation introduced in [2]. The integration variable $t$ is related to the neutron velocity $u$ in the center-of-mass frame as $t = u\sqrt{(A+1)m/(2kT)}$.

*Usually given as a function of energy in the lab frame.

## 3. RESULTS

Legendre moments $\sigma_{sn}^{T}(E \to E')$ in Eq. (2) were computed in [3] for $n = 0, ..., 14$, for incoming energies $E$ =6.5 and 6.8 eV, at $T = 10^3$ K. These Legendre moments are used here to study convergence properties of Legendre expansion in Eq. (1) for $N = 0, ..., 14$, and are plotted in Fig. 1 for completeness. It was observed by Ouisloumen and Sanchez in [1] that maxima of Legendre moments occur "at $E' = E$ due to the fact that all collisions can produce neutrons with energy $E' = E$, whereas this is not the case for any other value of $E'$". In the context of this work, an unfortunate consequence of the maxima at $E' = E$ is slow convergence of Legendre expansion at $E' = E$, as will be explained below.

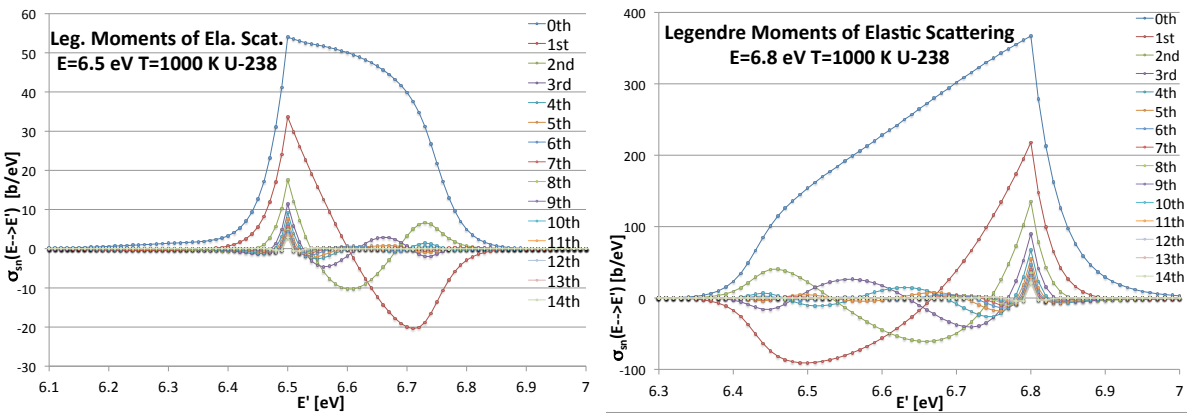


**Figure 1. Legendre moments $\sigma_{sn}^{T}(E \to E')$, $n = 0, \ \ldots, 14$ of $^{238}$U elastic neutron scattering cross section for incoming energy $E$ =6.5 eV (left) and 6.8 eV (right), at temperature $T = 10^3$ K, from [3] were used in this work.**

A Legendre expansion using these moments is to be compared with a reference Monte Carlo computation of double-differential cross section. Since the angular dependence of a reference Monte Carlo double-differential cross section is reported for 16 equal bins of $\mu$ spanning $[-1, 1]$, that is for bins $[\mu_i, \mu_{i+1}]$, where $\mu_i = 1 - (i-1)\Delta\mu$, $i = 1, ..., 16$, and $\Delta\mu = 2/16 = 0.125$, a corresponding quantity computed via Legendre expansion, which will be used below to study convergence, is

$$\sigma_s^{TN}(E \to E', i) \equiv \int_{\mu_{i+1}}^{\mu_i} \sigma_s^{TN}(E \to E', \mu) \mathrm{d}\mu, \tag{3}$$

where $\mu$ is in the lab frame, for $0 \leq N \leq 14$. The integration over d$\mu$ was performed analytically:

$$\int_{\mu_{i+1}}^{\mu_i} P_n(\mu') \mathrm{d}\mu' = \frac{1}{2n+1} [P_{n+1}(\mu) - P_{n-1}(\mu)]|_{\mu_{i+1}}^{\mu_i}. \tag{4}$$

A plot of $\sigma_s^{TN}(E \to E', i)$ for $N = 5, 10, 14$ at $T = 10^3$ K shows how it converges toward a reference Monte Carlo computation with increasing $N$: for $E = 6.5$ eV in Fig. 2 for $i = 1, ..., 8$, and in Fig. 3 for $i = 9, ..., 16$, and for $E = 6.8$ eV in Fig. 4 for $i = 1, ..., 8$, and in Fig. 5 for $i = 9, ..., 16$. The plots indicate a satisfactory convergence is reached for $N = 14$ everywhere except for $E' = E$, for which a supplementary method is suggested below.

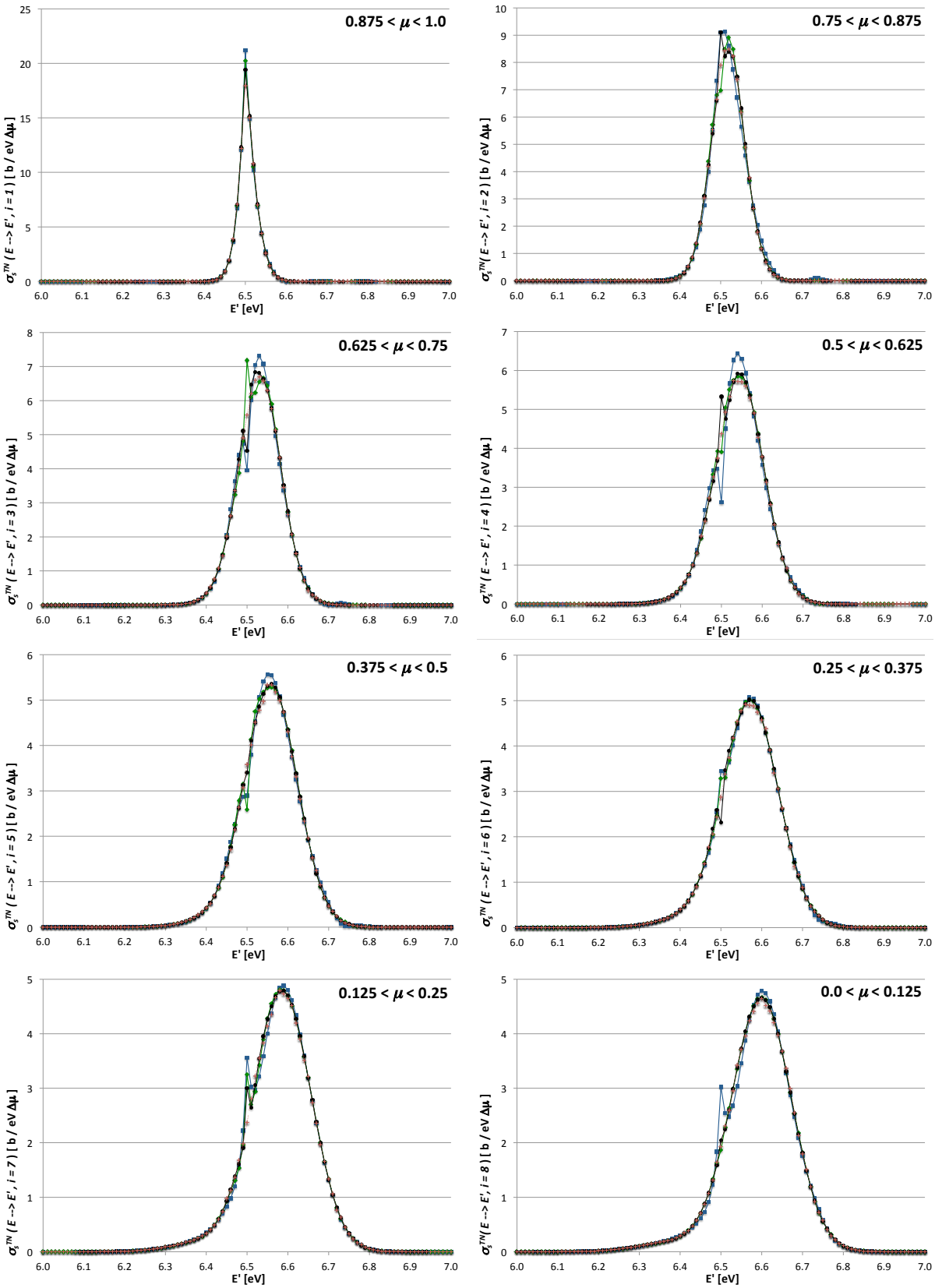


**Figure 2. Comparison of Legendre expansions for $N$ =5 (blue), 10 (green), 14 (black), and a Monte Carlo (red) computation in cosine bins $\Delta\mu = 0.125$, for $\mu > 1$ and $E = 6.5$ eV.**

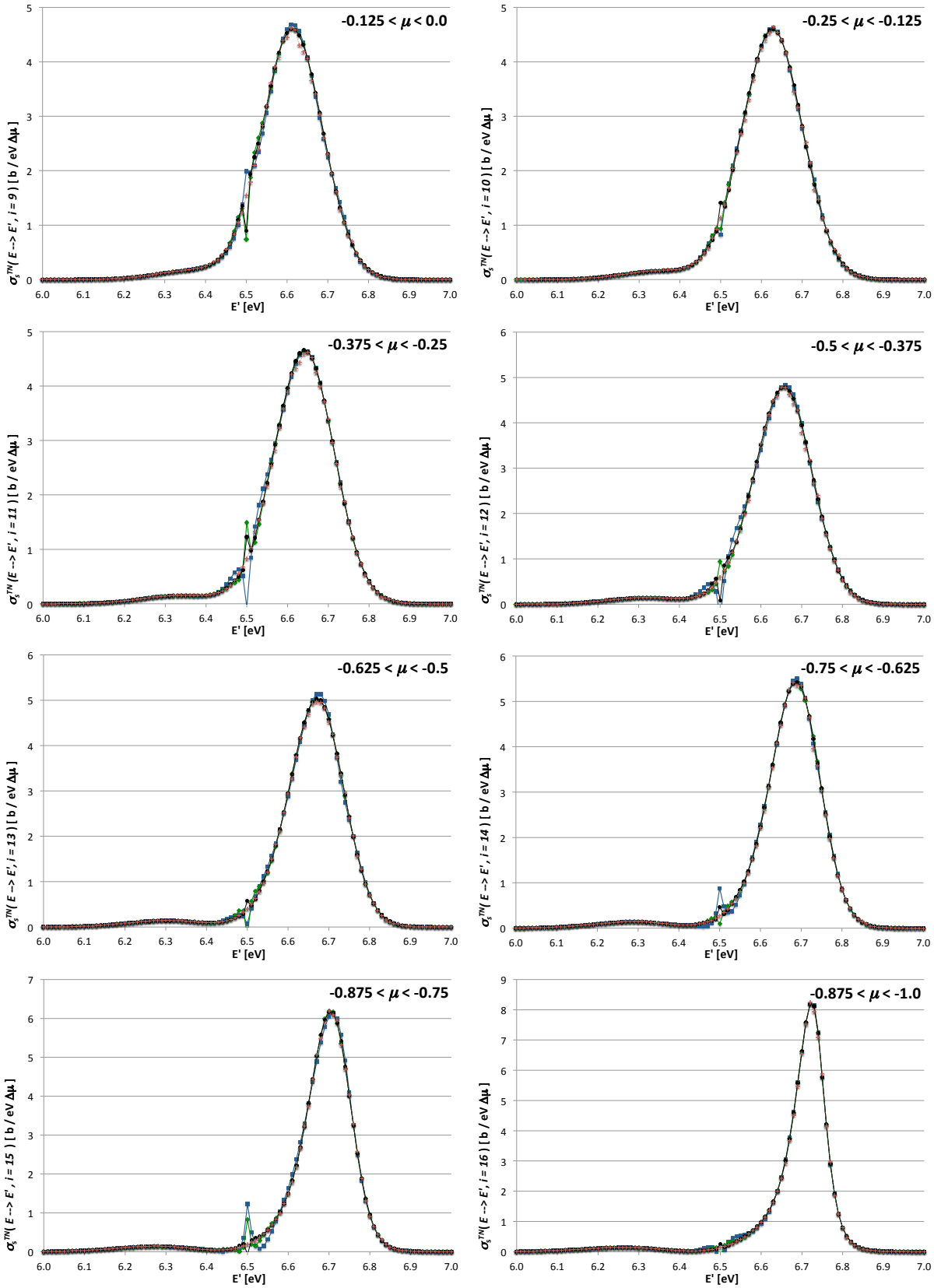


**Figure 3. Comparison of Legendre expansions for $N$ =5 (blue), 10 (green), 14 (black), and a Monte Carlo (red) computation in cosine bins $\Delta\mu = 0.125$, for $\mu < 1$ and $E = 6.5$ eV.**

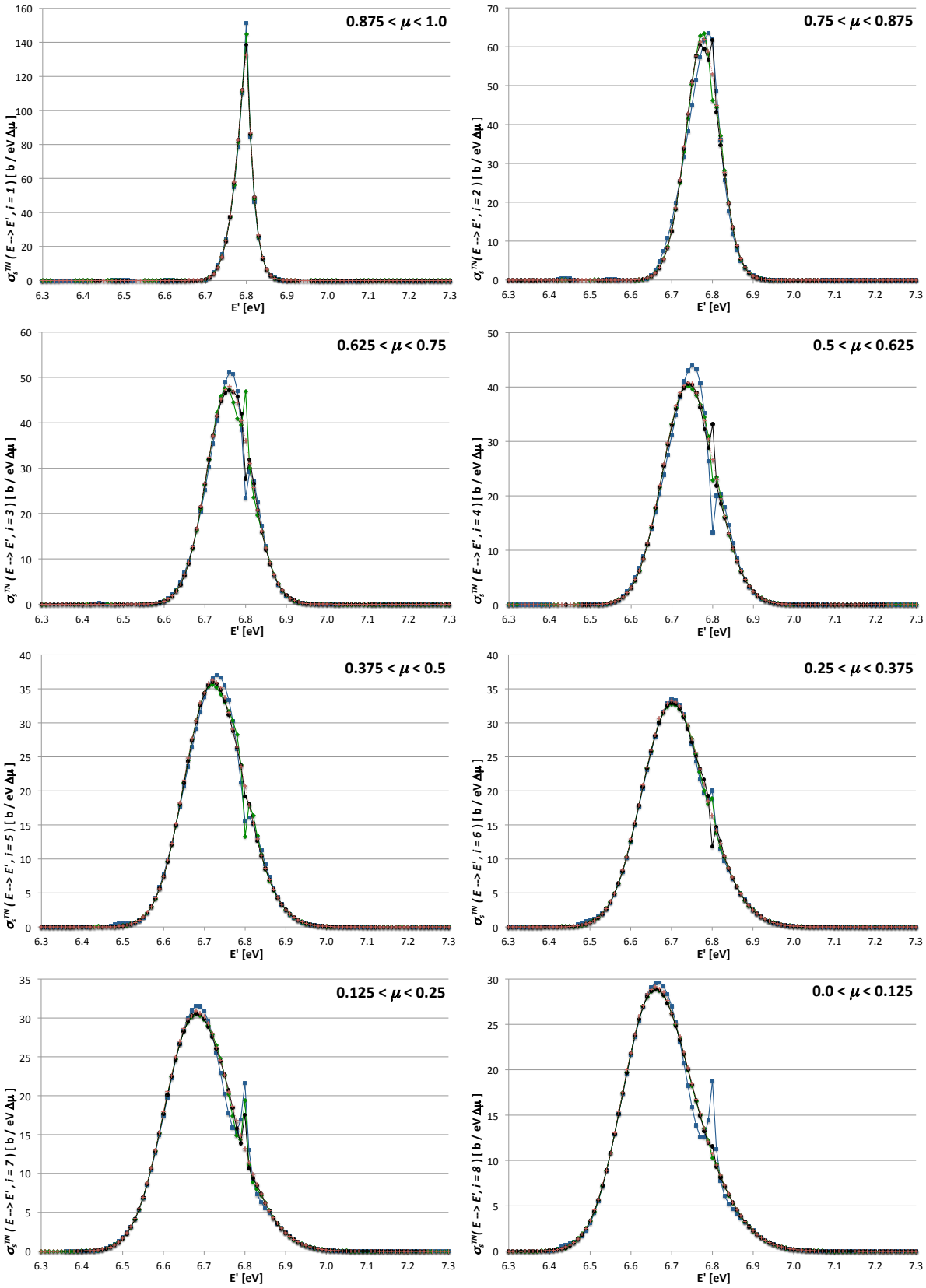


**Figure 4. Comparison of Legendre expansions for $N$ =5 (blue), 10 (green), 14 (black), and a Monte Carlo (red) computation in cosine bins $\Delta\mu = 0.125$, for $\mu > 1$ and $E = 6.8$ eV.**

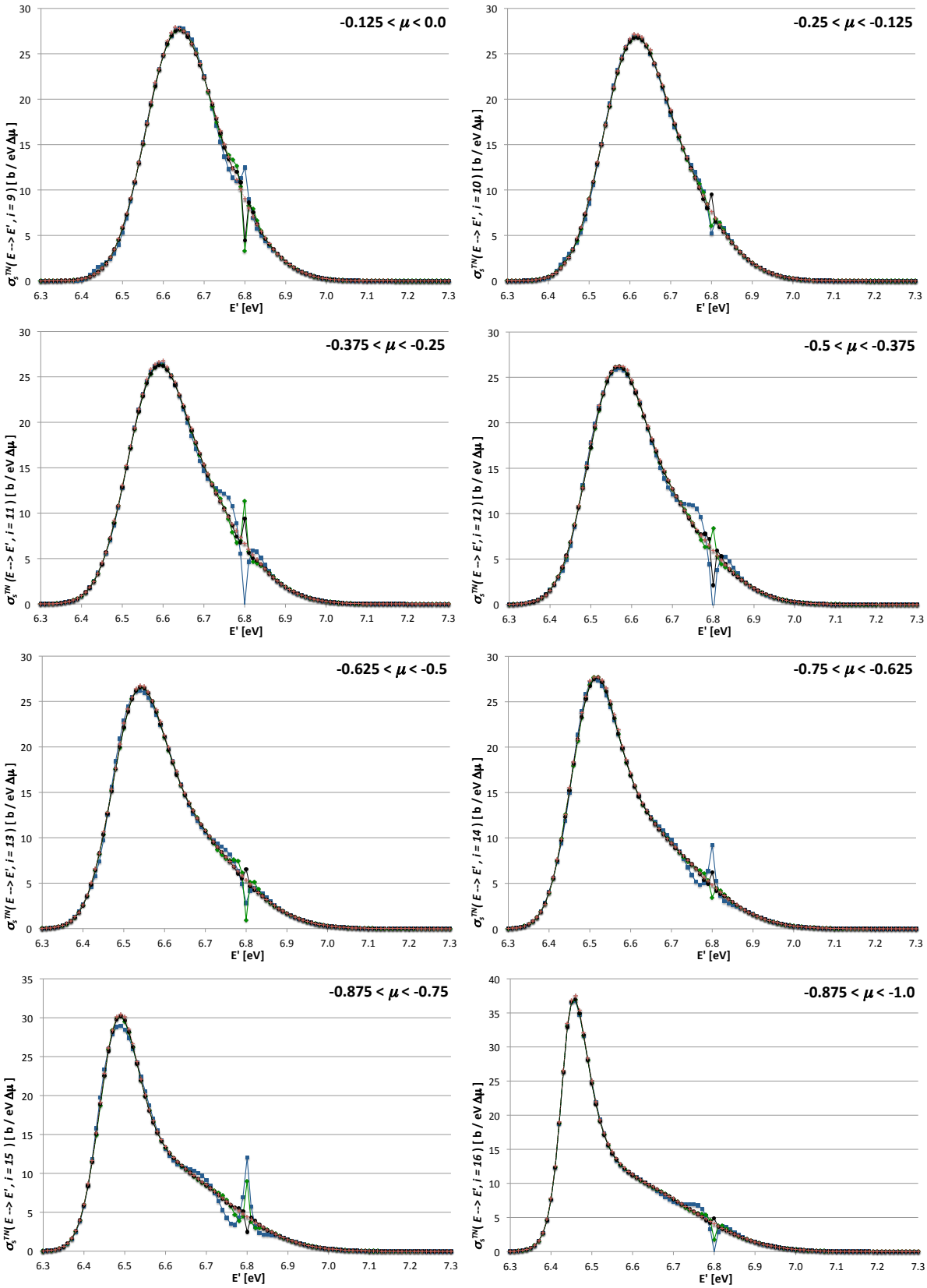


**Figure 5. Comparison of Legendre expansions for $N$ =5 (blue), 10 (green), 14 (black), and a Monte Carlo (red) computation in cosine bins $\Delta\mu = 0.125$, for $\mu < 1$ and $E = 6.8$ eV.**

A square-root of variance between Legendre expansion and the reference Monte Carlo computation is used as a measure of convergence:

$$\sqrt{\mathrm{var}(N)} \equiv \frac{\{\int \mathrm{d}E' \sum_{i=1}^{16} [\sigma_s^{TN}(E \to E', i) - \sigma_s^{T(\mathrm{MC})}(E \to E', i)]^2\}^{1/2}}{\sigma_s^{T(\mathrm{MC})}(E)}, \tag{5}$$

where a reference Monte Carlo total elastic scattering cross section $\sigma_s^{T(\mathrm{MC})}(E) = \int \mathrm{d}E' \sum_{i=1}^{16} \sigma_s^{T(\mathrm{MC})}(E \to E', i)$ normalizes the expression. A square-root of relative variance was computed for $0 \leq N \leq 14$ at incoming energies $E$ =6.5 and 6.8 eV in Fig. 6. For $N > 10$ it starts to decrease relatively slowly, mainly because of a very slow convergence near $E' \approx E$, where many higher order terms in the Legendre expansion are needed to achieve further decrease. This motivated the method developed below.

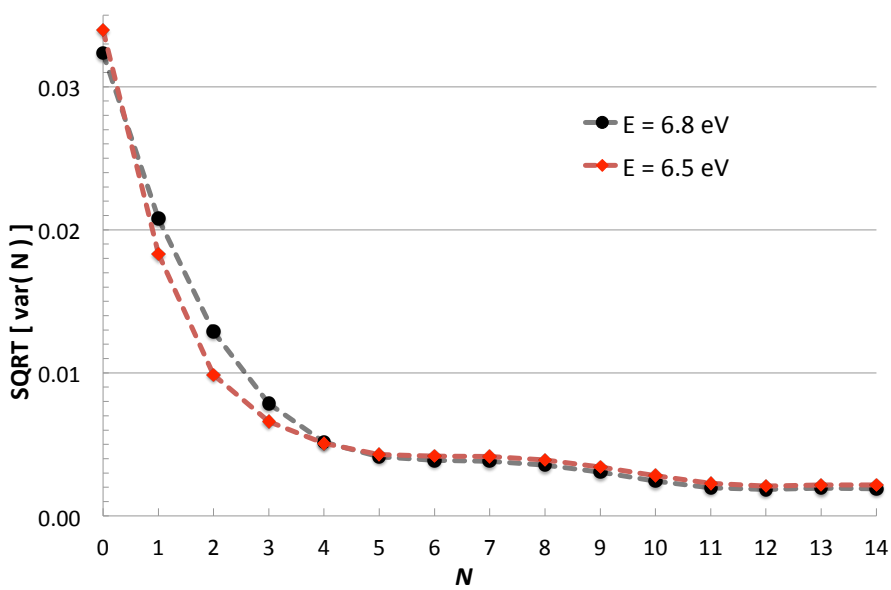


**Figure 6. The quantity in Eq. (5) decreases as the number of terms in the Legendre expansion, $N$, increases. Incoming energy $E$ =6.5 and 6.8 eV at temperature $T = 10^3$ K.**

A new method is suggested for accurate computation of higher-order contributions to the double-differential cross section for $E' = E$. This method takes advantage of a numerical finding that, for $E' = E$, a product of $(n + 1/2)\sigma_{sn}^T(E \to E)$ appearing in the Legendre expansion converges to a constant value for $n \geq 5$, as can be seen in Fig. 7. Therefore, for higher-order terms, the approximately constant product was factored out of the Legendre expansion:

$$\sigma_s^{TN'}(E \to E, \mu_{\mathrm{lab}}) = \sigma_s^{TN}(E \to E, \mu_{\mathrm{lab}}) + (N + 1/2)\sigma_{sN}^T(E \to E) \sum_{n>N}^{N'} P_n(\mu_{\mathrm{lab}}), \tag{6}$$

enabling a computation of many higher-order terms, that is for $N' \gg N$, by using the $(N =)14$ computed Legendre moments. A double-differential cross section computed using this method for $E' = E$ in Fig. 8 reveals that as many as 50 terms may be needed for Legendre expansion to converge to the Monte Carlo reference computation.

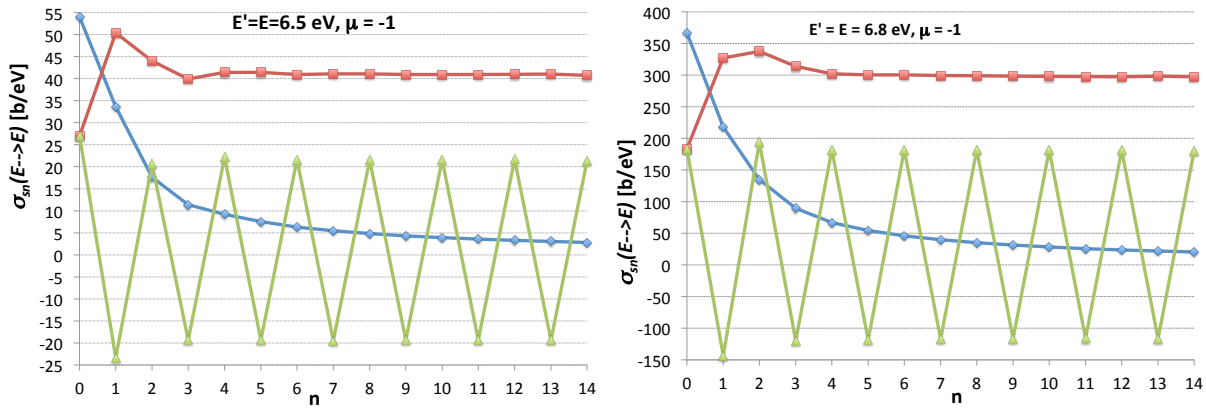


**Figure 7. The 15 Legendre moments $\sigma_{sn}^T(E \to E)$ (blue), products $(n+1/2)\sigma_{sn}^T(E \to E)$ (red), and cumulative Legendre expansions $\sum(n+1/2)\sigma_{sn}^T(E \to E)P_n(\mu = -1)$ (green) for $E = 6.5$ eV (left) and $E = 6.8$ eV (right). The observation that a product $(n + 1/2)\sigma_{sn}^T(E \to E)$ approaches a constant value for $n > 5$ was used in the derivation of Eq. (6). ($T = 10^3$ K)**

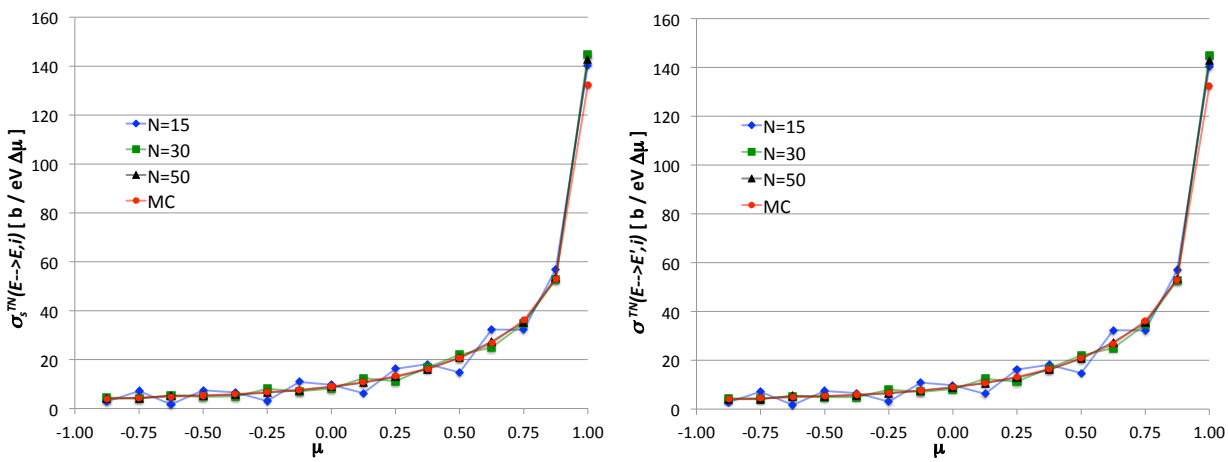


**Figure 8. Plot of Legendre expansion in Eq. (6) for $E' = E$ =6.5 eV (left) and 6.8 eV (right) using $N$ =15 (blue), 30 (green), and 50 (black) terms. Convergence to a reference Monte Carlo computation is achieved for N=50 everywhere except for the first bin $0.875 < \mu < 1.0$.**

## 4. CONCLUSIONS

We investigate convergence properties of Legendre expansion of a Doppler-broadened double-differential elastic scattering cross section by including as many as 15 terms in the Legendre expansion. A variance of Legendre expansion from a reference Monte Carlo computation of a double-differential cross section is used as a measure of convergence. A satisfactory convergence is achieved using the first 15 terms, except when the outgoing energy approximately equals the incoming energy, that is $E' \approx E$. A supplementary method for $E' = E$ was used to compute many higher-order terms in the Legendre expansion. This method reveals

that as many as 50 terms may be needed to accurately compute a double-differential cross section for $E' = E$.

## ACKNOWLEDGEMENTS

This manuscript has been authored by UT-Battelle, LLC, under contract DE-AC05-00OR22725 with the US Department of Energy.

## REFERENCES

[1] M. Ouisloumen, R. Sanchez, *Nucl. Sci. Eng.* **107**, pp. 189–200 (1991).

[2] G. Arbanas, B. Becker, R. Dagan, M.E. Dunn, N.M. Larson, L.C. Leal, M.L. Williams, *Proc. International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (MC 2011)*, May 8–12, 2011, Rio de Janeiro, Brazil, ISBN 978-85-63688-00-2, LAS/American Nuclear Society, (2011). [CD-ROM]

[3] G. Arbanas, B. Becker, R. Dagan, M.E. Dunn, N.M. Larson, L.C. Leal, and M.L. Williams, "Covariance Matrix of a Double-Differential Doppler-Broadened Elastic Scattering Cross Section," *Proceedings of The Second Workshop on Neutron Cross Section Covariances*, Vienna University of Technology, Atominstitut, September 14–16, 2011, EPJ Web of Conferences.

[4] B. Becker, R. Dagan, G. Lohnert, *Ann. Nucl. Energy* **36**, pp. 470–474 (2009).

[5] B. Becker, *On the Influence of the Resonance Scattering Treatment in Monte Carlo Codes on High Temperature Reactor Characteristics*, Doctor of Engineering Thesis, Universität Stuttgart, Stuttgart, Germany (2010).