International Conference on Mathematics, Computational Methods & Reactor Physics (M&C 2009)
Saratoga Springs, New York, May 3-7, 2009, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2009)

A NEW APPROACH TO THE USE OF GROUP SCATTERING DATA IN MONTE CARLO NEUTRON TRANSPORT

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ABSTRACT

When comparing deterministic (e.g. Sn) neutronics codes with their Monte Carlo counterparts, it is appropriate to use the same nuclear data. Whereas most of the transport data stored in group libraries can easily be adapted for Monte Carlo use, the selection of secondary particle emission angle is more problematic. Group to group angular scattering distributions are reconstructed from a limited number of Legendre coefficients, which can lead to angles of scatter for outgoing particles which have negative probabilities when an overly truncated expansion is used. This paper documents the modifications made to the existing method found in AWE's Monte Carlo codes for eliminating these negative probability regions of the scattering distribution.

Key Words: Nuclear data, Monte Carlo transport, Legendre polynomials

1. INTRODUCTION

There are two good reasons to use group nuclear data in Monte Carlo calculations: first, it allows the exploitation of modern fine group libraries in Monte Carlo based neutronics codes and second, it becomes easier to inter-compare neutron transport codes (deterministic and Monte Carlo) as each code will use the same nuclear data library.

When comparing deterministic codes with their Monte Carlo counterparts, it is necessary to adapt group data for use with Monte Carlo sampling methods. This presents problems, due to the way in which deterministic angular distribution data is reconstructed from stored Legendre coefficients and can lead to angles of scatter for outgoing particles which have negative probabilities.

The current study documents the modification of the existing AWE method to overcome these negative probabilities, so that a greater range of physical quantities of the original distribution recreated from these Legendre coefficients, is preserved.

2. THE INVESTIGATION

2.1. Background

The angular distribution of secondary neutrons emitted from a neutron-nucleus scattering event is given by;

$$\beta_{g'g}(\mu) \approx \sum_{l=0}^{L} \frac{(2l+1)}{2} \beta_{g'g}^{l} P_l(\mu) \tag{1}$$

Where;

$\beta_{g'g}$ is the distribution of outgoing neutrons scattering from group g' to g
μ is the cosine of the angle of scatter
β^l represents the lth order Legendre coefficient
and
$P_l(\mu)$ is the lth order Legendre polynomial

The probability of scatter to a specific μ value may be found by normalising (1). Due to the nature of the Legendre polynomials, regions of negative probability may be generated through the use of an overly truncated expansion. The first few Legendre polynomials are given in appendix A.

Monte Carlo codes simulate particle scattering by creating an angular distribution using the specified nuclear data (either point x y data or group data and expression (1)) and then statistically sampling this distribution in order to determine the outgoing direction of travel.

Negative probabilities lead to problems when carrying out this sampling and so a fix to this problem has previously been developed and employed in a number of AWE codes.

2.2. The Original Method

This fix involves several stages:

1) calculate the angular distribution to the desired order of approximation using (1) and the Legendre coefficients given in the available group-to-group scatter matrices
2) set any negative regions which are present to zero on the grounds that they are non-physical
3) apply the weighting function $e^{\alpha\mu}$ to each point of the distribution, where α is a constant calculated using Newton-Raphson iteration such that the average cosine of scatter or first moment of the distribution is preserved.

This method is compared below with an unmodified distribution generated using (1).

These are for a neutron scattering elastically from ^{239}Pu in the energy range 2.4-2.1 MeV and remaining in that range after the collision – so-called “within group” scatter.

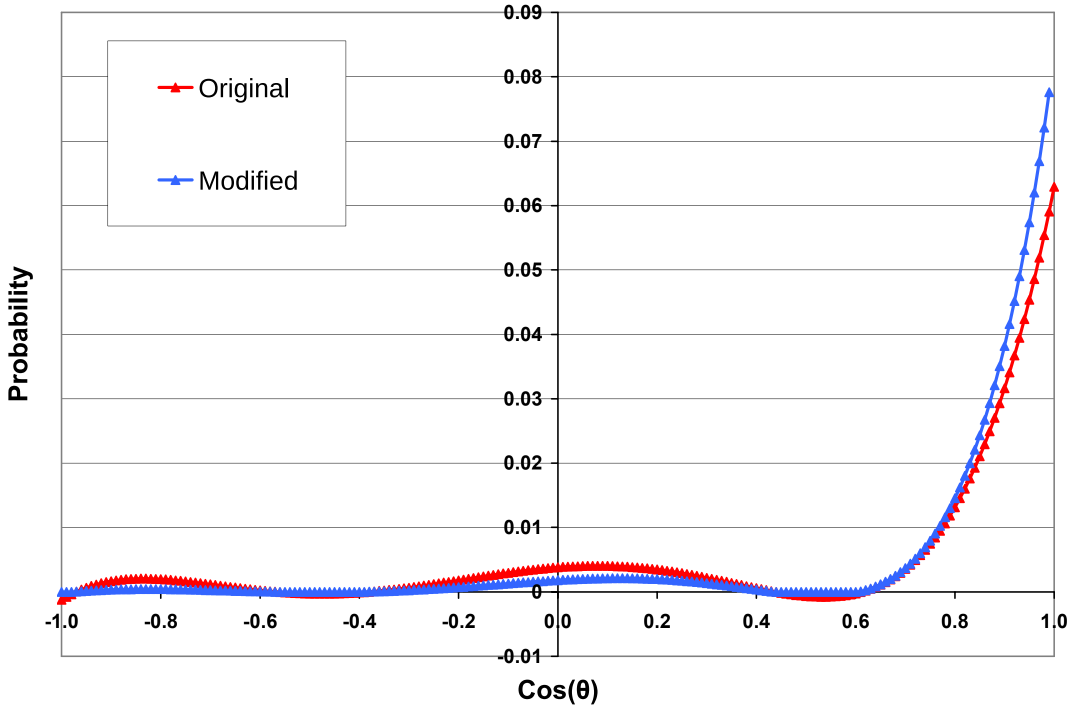

Figure 1. a comparison between the functions β(μ) and β*(μ)e$^{\alpha\mu}$
(β*(μ) is the original distribution with the negative regions set to zero)

2.3. A New Method

To increase the confidence in using group data in Monte Carlo calculations, the previous method for eliminating negative regions was modified in this study to also preserve the second moment of the distribution and therefore the variance. This was achieved by modifying the exponential weighting function so that the new distribution is given by;

$$\beta^*(\mu)e^{\alpha\mu+\gamma\mu^2} \tag{2}$$

where, γ is a second constant introduced to help preserve a second physical quantity.

α and γ are found in this case by computationally scanning an adaptive search grid of α, γ and m(α, γ) values, where m(α, γ) is a minimisation function, given in appendix B, designed to equal zero when both the original mean and variance are preserved.

Shown below is a comparison of the new distribution against the original for the same ^{239}Pu case used previously.

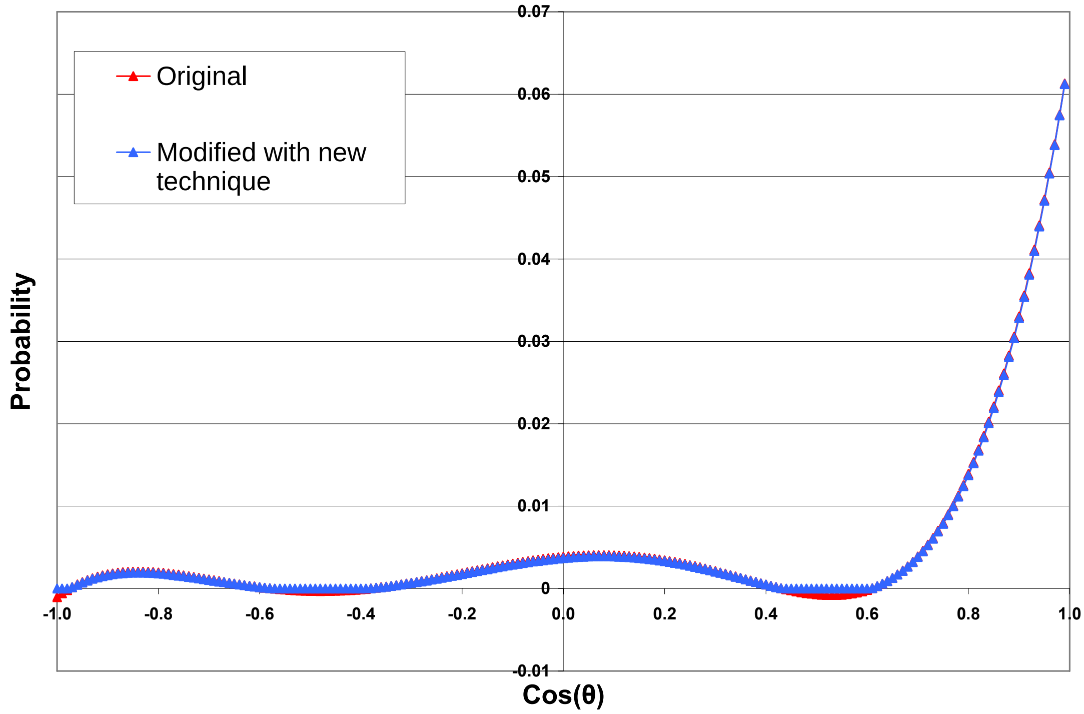

Figure 2. A comparison of β(μ) and β*(μ)e$^{\alpha\mu+\gamma\mu\text{^}2}$

2.4. An Alternative Method

This method however, relies upon setting the negative regions present to zero, but these negative regions may change depending upon the order of the expansion used. A second method which also preserved both the mean and variance was therefore developed to avoid this procedure of explicitly setting negative regions to zero.

The majority of angular distributions for neutron scatter are forward peaked, i.e. they increase steeply as they approach $\mu = 1$ and so the alternative method was designed to cater primarily for these well defined forward peaks.

This method involves the following stages

1) Calculate the original distribution using expression (1) as standard
2) Calculate the mean value of μ, where the mean value is given by:

$$\mu_{avge} = \int_{-1}^{+1} \beta(\mu)\mu d\mu \quad (3)$$

3) Set every value of the distribution for $\mu < \mu_{avge}$ equal to the same value, so that the total area of the distribution remains the same as the original's, i.e.

$$\beta(\mu) = \frac{\int_{-1}^{\mu_{avge}} \beta(\mu) d\mu}{\int_{-1}^{\mu_{avge}} \mu d\mu} \qquad \text{for } \mu < \mu_{avge} \qquad (4)$$

4) Apply a smoothing function in the region about μ_{avge}

5) Apply the weighting function $e^{\alpha\mu+\gamma\mu^2}$ after computing α and γ using an adaptive grid search as done for the previous method.

The results generated using this method (referred to from now on as 'Option B'; with the previous method now 'Option A') are compared to those of the previous method below, in figures 3 and 4, for the case of a 14 MeV neutron scattering elastically from Pu^{239} and remaining within the same energy group.

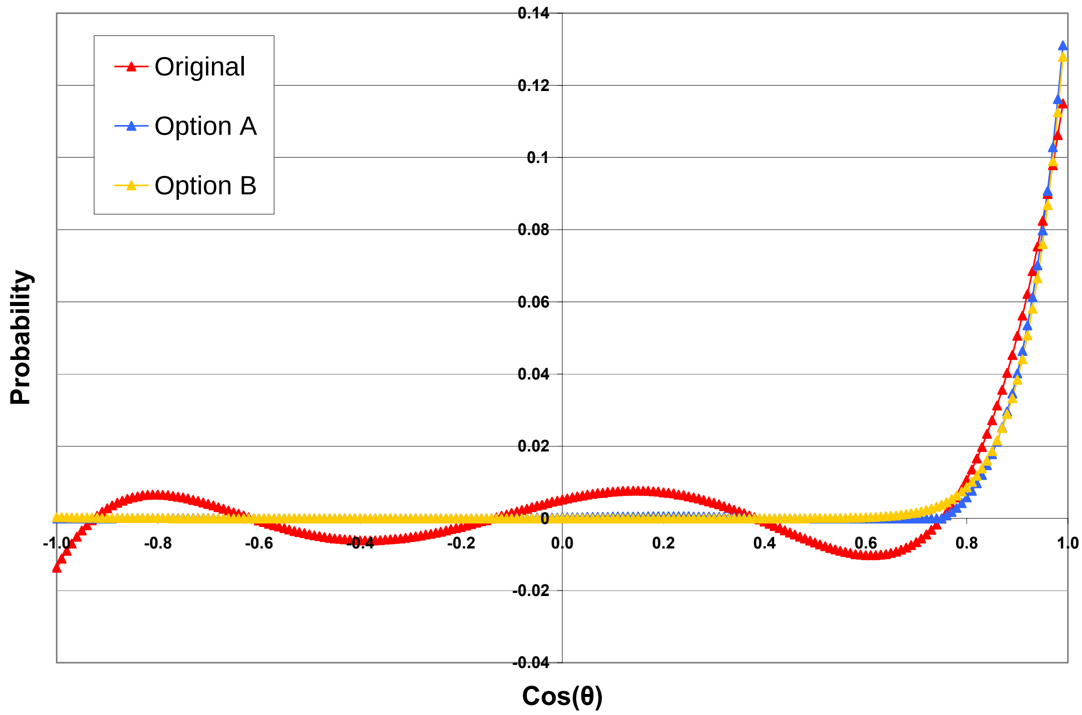

Figure 3. A comparison with both Options A and B.

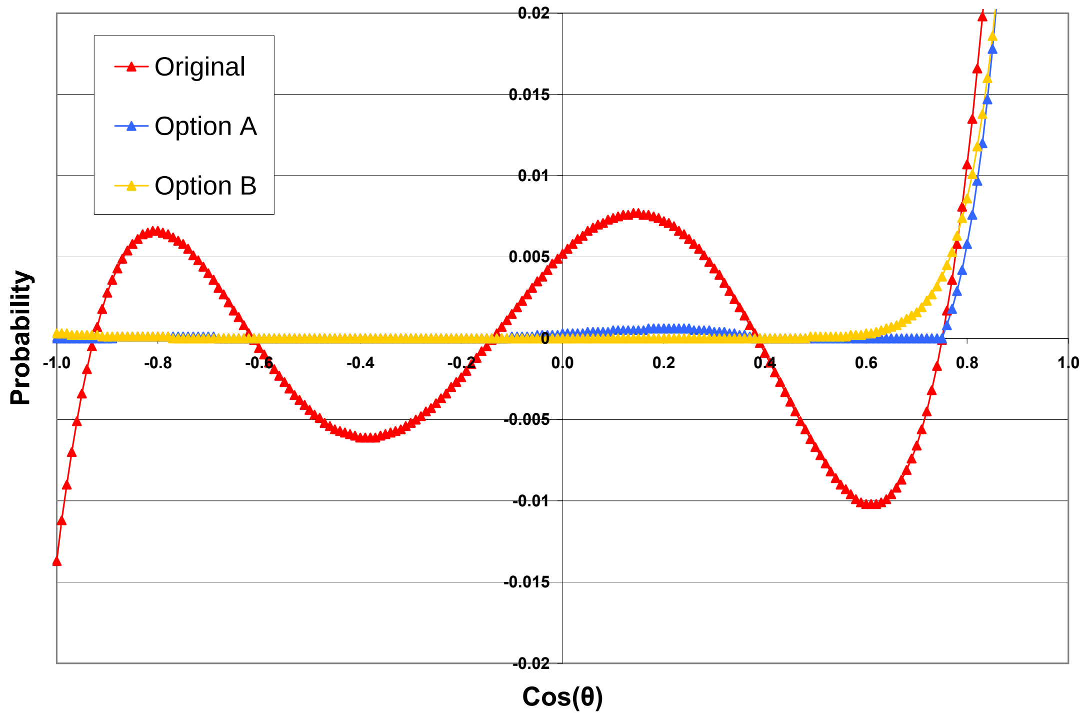

Figure 4. A close-up of the Cos(θ) axis shows the smoother nature of option B compared to option A.

3. BENCHMARK STUDIES

3.1 Benchmark results

AWE's Monte Carlo neutron transport code ROULETTE was modified to include both of the new scattering techniques, so that their effect upon the results of calculations could be investigated.

A range of systems were then studied and the results with both options A & B were consistent with one another and similar to the original fix-up method.

Results are shown below in Tables I to III for a set of simple source-detector problems. The counts recorded in two shielded detectors after 100 ns, from a central high energy fission neutron source, are compared for each method. Each system contains a different shielding material between the source and detectors. An L=4 order Legendre expansion was used in each case.

Table I. Number of boundary crossings into each detector for each scattering method for the case of iron shielding slabs +/- 1 standard deviation / 1×10^{20}

	Original	Option A	Option B
Detector 1	8.868 +/- 0.094	8.806 +/- 0.070	8.621 +/- 0.106
Detector 2	8.814 +/- 0.135	8.830 +/- 0.106	8.710 +/- 0.090

Table II. Number of boundary crossings into each detector for each scattering method for the case of polythene shielding slabs +/- 1 standard deviation / 1x10^{20}

	Original	Option A	Option B
Detector 1	8.784 +/- 0.097	8.945 +/- 0.082	8.947 +/- 0.122
Detector 2	8.716 +/- 0.122	8.785 +/- 0.121	8.859 +/- 0.108

Table III. Number of boundary crossings into each detector for each scattering method for the case of water shielding slabs +/- 1 standard deviation / 1x10^{20}

	Original	Option A	Option B
Detector 1	8.854 +/- 0.110	8.804 +/- 0.138	8.992 +/- 0.119
Detector 2	8.789 +/- 0.082	9.093 +/- 0.137	8.989 +/- 0.121

Figure 5, below, shows the geometry of the systems studied, as well as the tracks of the first 50 neutrons emitted by the source, when the original fix-up method is used in the code. As can be seen, ROULETTE employs cylindrical axial symmetry.

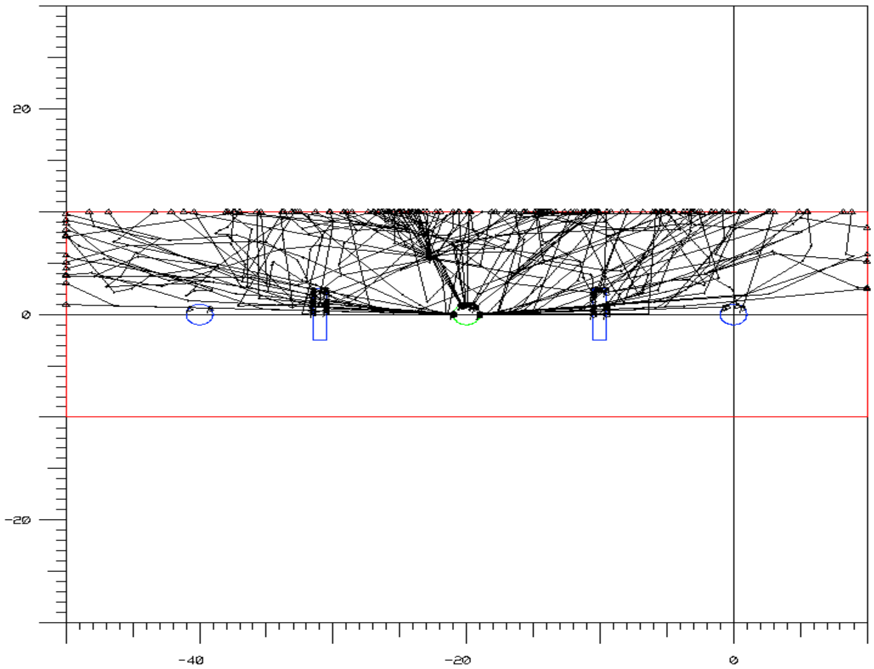

Figure 5. The problem geometry and the first 50 neutron tracks when the original fix-up method is used with plastic shielding slabs

The systems described above consist of a central neutron source and two detector spheres of Deuterium, shielded from the source by slabs of material which differ for each system.

3.2. Which is preferable?

With the results of neutronics calculations with each method being equivalent, it was necessary to investigate which technique best represented the original scattering distribution, i.e. before decomposition into a finite number of Legendre coefficients.

To address this, arbitrary scattering distributions were selected and Legendre coefficients then extracted from these using the following expression, valid as the Legendre polynomials are orthogonal to one another:

$$\beta_l(E'\to E) = \frac{2l+1}{2}\int_{-1}^{+1} f(\mu, E'\to E) P_l(\mu) d\mu \qquad (5)$$

Where f(μ,E'→E) is a differential scattering cross section.

A Legendre expansion to L=5 order was plotted for each and then options A & B applied and the results obtained from these compared against the original distribution and the Legendre expansion.

The results showed that the option A results closely mirrored those of the Legendre expansion at μ > 0.75, whilst option B was a closer match to the plot of the original scattering distribution in the same forward scatter region, in the cases studied, as demonstrated in figure 6 below.

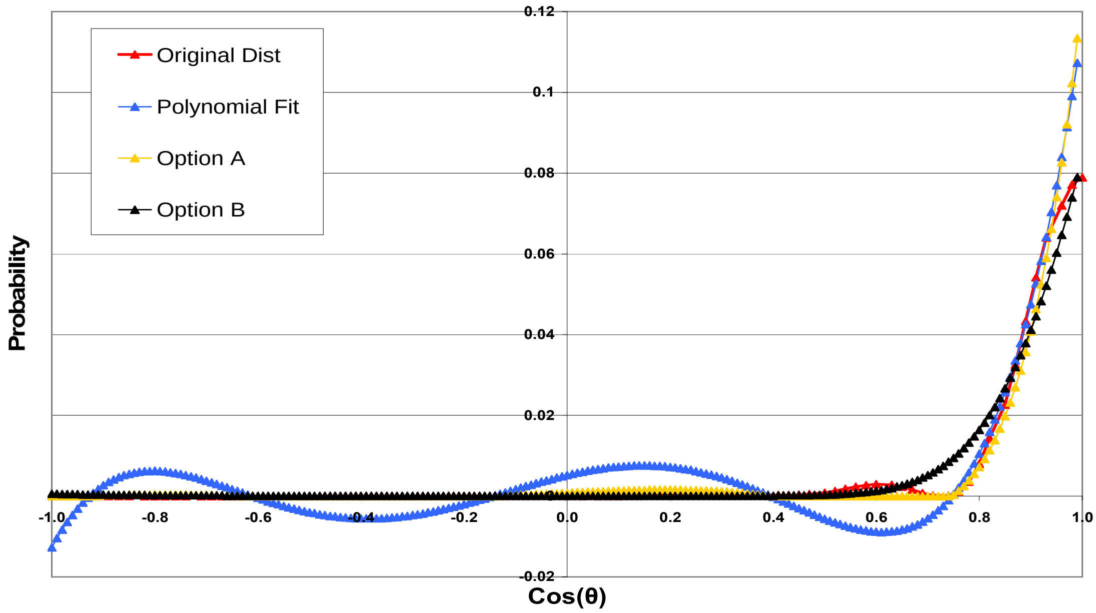

Figure 6. A comparison of the original distribution, the Legendre expansion and options A and B, for a 14MeV neutron scattered elastically from Pu239

The matter of which is preferable remains subjective; as although we would ideally wish to approximate the original scattering distribution as closely as possible; for the purposes of a Monte Carlo versus deterministic comparison we would still wish to match the Legendre expansion.

4. PRESERVING THE THIRD MOMENT

A short study was made into the practicality and necessity of preserving the third moment of the distribution. This was achieved by modifying both the minimization and weighting functions to include a third constant, ε.

ε was found via a 3 dimensional search grid in the same manner as α and γ, but due to this extra dimension, calculation times for computing each parameter were high and it was also seen that through the process of preserving the zeroth, first and second moments, the third was itself already preserved to a suitable accuracy in most cases.

5. CONCLUSIONS

In summary, two new methods for utilising group nuclear data in Monte Carlo codes have been developed. Both methods overcome the drawback of regions of negative probability of scatter and have the advantage of preserving the mean and variance of the original scattering distribution.

ACKNOWLEDGMENTS

The author wishes to acknowledge the original work undertaken in this area by Bruce Thom, also of AWE.

APPENDIX A

The first few Legendre terms are given below;

$$P_0(\mu) = 1$$
$$P_1(\mu) = \mu$$
$$P_2(\mu) = \tfrac{1}{2}(3\mu^2 - 1)$$
$$P_3(\mu) = \tfrac{1}{2}(5\mu^3 - 3\mu)$$
$$P_4(\mu) = \tfrac{1}{8}(35\mu^4 - 30\mu^2 + \mu)$$
$$P_5(\mu) = \tfrac{1}{8}(63\mu^5 - 70\mu^3 + 15\mu)$$

APPENDIX B

i) The minimisation function used to compute α and γ to preserve both mean and variance is given below;

$$f(\alpha,\gamma) = \left(\overline{\mu} - \frac{\int_{-1}^{+1} \beta^* e^{\alpha\mu+\gamma\mu^2} \mu d\mu}{\int_{-1}^{+1} \beta^* e^{\alpha\mu+\gamma\mu^2} d\mu} \right)^2 - \left(\sigma^2 - \frac{\left(\int_{-1}^{+1} \beta^* e^{\alpha\mu+\gamma\mu^2} \mu^2 d\mu - \left(\int_{-1}^{+1} \beta^* e^{\alpha\mu+\gamma\mu^2} \mu d\mu \right)^2 \right)}{\int_{-1}^{+1} \beta^* e^{\alpha\mu+\gamma\mu^2} d\mu} \right)^2$$