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Neutron Next-Event Estimators Kinematics

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Abstract

This paper reviews the kinematics of neutron elastic and inelastic scattering with moving and stationary targets for contributions to Neutron Next-Event Estimators (NEEs). NEEs are often used for simulating the response of detectors in locations that have few random walk particles. Contributions to NEEs from collisions differ from sampling the outgoing particle state in standard random walk collisions as the location of the estimator is fixed, thus fixing the scattering angle between the incoming and outgoing directions. To calculate contributions to NEEs, the outgoing energies and probabilities of scatter toward the estimator must be calculated. This paper presents the most general case that encompasses elastic and inelastic scattering with both moving and stationary targets. The moving target case is required for elastic scattering with thermal motion due to the free gas thermal treatment approximation. The stationary target equations are presented for comparison with equations presented in canonical Monte Carlo texts.

1 Background

A few of the canonical Monte Carlo texts provide some of the equations that govern contributions to neutron next-event estimators (NEEs) due to scattering with stationary targets[1, 2]. These texts only provide the final forms of the equations and don't show the derivations. The kinematics presented in descriptive physics texts are also generally limited to stationary targets[3]. More so, there are no texts or papers that provide the equations needed for contributions to NEE due to neutron scattering on moving targets. It is likely that a memo was prepared that described neutron elastic scattering with a moving target for the implementation of contributions due to the free gas thermal treatment in the MCNP®[4] code. However, if such a memo was written, its existence is lost to history. The purpose of this paper is to document the equations describing such contributions and to show that all cases can be covered by a single set of equations.

2 Neutron Next-Event Estimators

2.1 Introduction

The Next-Event Estimator (NEE), first described by Kalos[5], is a method of calculating the particle fluence at a point in space. These estimators are called “point detectors” or just “detectors” in the MCNP®[4] software. The NEE method is useful for calculating the response to detectors located in regions that have few or no random walk particles. The same kinematics is used for creating virtual particles for the DXTRAN variance reduction method in MCNP.

The NEE calculates the response at a point for each source and collision event. At each random walk source or collision event, a pseudo-particle is created, which travels directly from the event to the NEE location. The pseudo-particle properties (energy, statistical weight) are calculated from the event. In the case of a scattering event, the pseudo-particle properties are calculated from kinematics. The equation used to calculate the response of the NEE is:

$$S(R', E'_l) = \frac{w}{2\pi(R - R')^2} h(\mu_l, E_l \rightarrow E'_l) \exp \left[- \int_R^{R'} \Sigma_t(s, E'_l) ds \right] \quad (1)$$

Where R represents the location of the event, R' is the location of the NEE, E_l is the energy of the particle in the laboratory (LAB) frame prior to the event, E'_l is the LAB frame energy of the resulting pseudo-particle calculated from kinematics for collisions, μ_l is the cosine of the pseudo-particle LAB frame scattering angle (θ), $h(\mu_l, E_l \rightarrow E'_l)$ is the probability of scattering into the cosine of the scattering angle (μ_l) for the outgoing energy E'_l , $\Sigma_t(s, E'_l)$ is the total particle cross-section at location s and energy E'_l , and w is the random walk particle's statistical weight prior to collision. In Eq. 1, the exponential represents the attenuation of the pseudo-particle between the source or collision event and the next-event estimator location. The integral of the total cross-section between the source or collision event to the NEE location is done by ray-casting through the geometry. A notional diagram of the next-event estimator is provided in Figure 1.

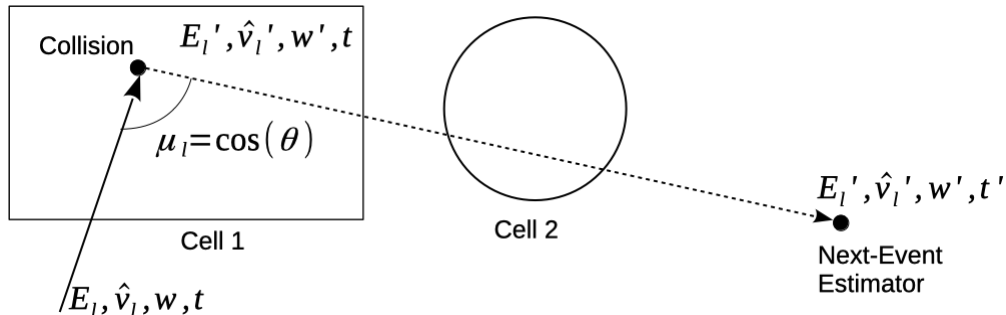


Figure 1: Notational diagram of a next-event estimator, with an incoming particle of energy E_l , unit direction $\hat{\mathbf{v}}_l$, statistical weight w , and time t . The random walk particle (solid-arrow) collides in Cell 1. At the collision point a pseudo-particle (dashed-arrow) is used to calculate the response of the NEE. The LAB frame scattering angle between the incoming particle direction ($\hat{\mathbf{v}}_l$) and the direction of the pseudo-particle ($\hat{\mathbf{v}}_l'$) toward the NEE is θ . The pseudo-particle is attenuated through Cell 1 & 2.

2.2 Notation

This document describes the kinematics using three different frames of reference: 1) In the laboratory frame of reference, denoted as the LAB frame, the particles move relative to the laboratory or fixed geometry of the simulation. 2) The center-of-mass frame of reference (or more accurately the center-of-momentum frame), denoted as the COM frame, is defined with the zero total momentum. 3) In the target-at-rest frame of reference, denoted as the TAR frame, the target has zero velocity. Many texts only consider the kinematics of systems where the target has zero velocity in the LAB frame, in such cases the LAB and TAR frames are equivalent. This case is also referred to as the stationary target case.

The notation of the particle kinematic properties used in this document is provided in Appendix A . The projectile is denoted by a lower case v and the target is denoted with an upper case V . Vectors are denoted with bold typeface (such as \mathbf{v}), a unit vector is denoted with hat notation ($\hat{\mathbf{v}}$), and a scalar is denoted with normal type (v). A l subscript denotes the LAB frame (\mathbf{v}_l), a c subscript denotes the COM frame (\mathbf{v}_c), and a t subscript denotes the TAR frame (\mathbf{v}_t). Prime notation denotes a property after collision (such as \mathbf{v}_l') in contrast to a property before collision which is denoted without a prime (\mathbf{v}_l). A is the ratio of the mass of the target to the projectile.

2.3 Quantities to Calculate from Kinematics

In order to solve the response of the NEE from Eq. 1, three primary quantities need to be calculated: 1) The outgoing neutron energy in the LAB frame, E_l' . 2) The probability of scatter toward the detector, $h(\mu_l; E_l \rightarrow E_l')$. 3) The scattering angle in the COM frame, ϕ , which is necessary for accessing nuclear data provided in the COM frame.

The LAB frame scattering angle, θ , (and thus the cosine of the LAB scattering angle, μ_l) is readily calculated from the dot products of the projectile's incoming unit vector, $\hat{\mathbf{v}}_l$, and outgoing

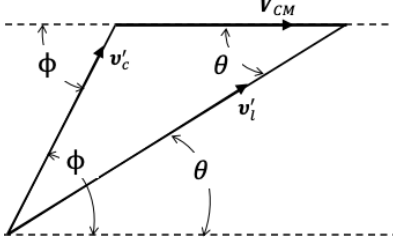


Figure 2: Relationships between the final projectile velocity vectors in the COM (\mathbf{v}'_c) and LAB (\mathbf{v}'_l) systems and velocity vector of the COM system relative to the LAB system (\mathbf{V}_{cm}).

vectors, $\hat{\mathbf{v}}'_l$:

$$\mu_l = \cos \theta = \hat{\mathbf{v}}_l \cdot \hat{\mathbf{v}}'_l \quad (2)$$

And thus the θ or μ_l can be considered to be a fundamental quantity from the collision, along with the incoming projectile energy, E_l .

If the probability of scatter is provided by the nuclear data in the LAB frame, the determination of the probability of scatter toward the NEE, $h(\mu_l, E_l \rightarrow E'_l)$, is straightforward. However, the probability of scatter as a function of angle is often provided in the COM frame and thus conversion to the LAB frame is required. The conversion of the scattering probability from COM to LAB is calculated from:

$$h(\mu_l; E_l \rightarrow E'_l) = h(\mu_c; E_c \rightarrow E'_c) \frac{\partial \mu_c}{\partial \mu_l} \quad (3)$$

where $h(\mu_c; E_c \rightarrow E'_c)$ is the COM frame nuclear data. Thus E_c , μ_c , and $\partial \mu_c / \partial \mu_l$ must be calculated from kinematics. For elastic scattering, E'_c will be calculated using conservation of energy. For inelastic scattering, E'_c will be provided by the nuclear data. The derivations of equations for E_c , E'_c , E'_l , μ_c , and $\partial \mu_c / \partial \mu_l$ will be presented in the sections that follow.

3 Kinematics for the General Case of Neutron Scattering

The most general case will be presented first. The most general case is inelastic scattering with a moving target. Although this case generally has little real application, it provides a singular set of equations that can be used for both inelastic and elastic scattering as well as for stationary and moving targets.

3.1 COM Scattering Angle

The conversion from the cosine of the LAB scattering angle, μ_l , to the cosine of the COM scattering angle, μ_c , can be found from the vector relationship between the outgoing laboratory frame velocity vector (\mathbf{v}'_l), the outgoing center-of-mass frame velocity vector (\mathbf{v}'_c), and the velocity vector of the COM frame relative to the LAB frame (\mathbf{V}_{cm}). Using the definition of the velocity of the COM frame relative to the LAB frame:

$$\mathbf{v}'_l = \mathbf{v}'_c + \mathbf{V}_{cm} \quad (4)$$

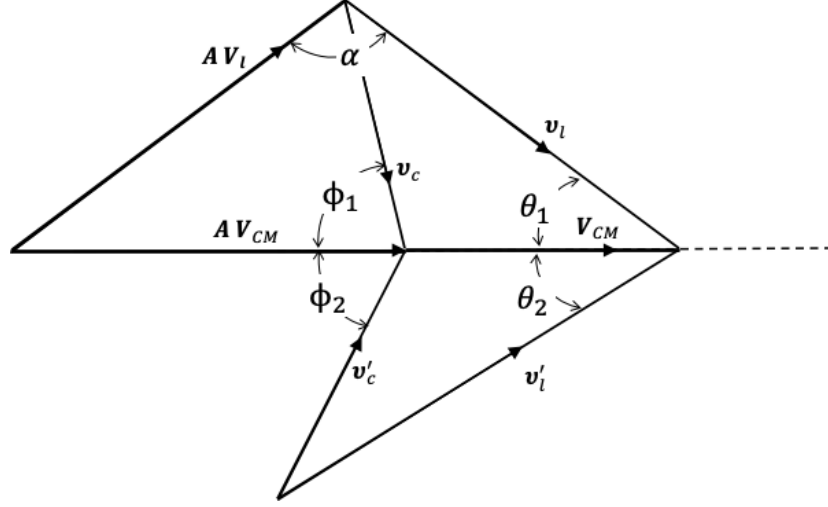


Figure 3: Relationships of the projectile and target velocity vectors (both initial and final) in the LAB and COM frames for scattering with a moving target, which has a target to projectile mass ratio of A .

This vector relationship is shown graphically in Figure 2. Translating (4) to the horizontal, which is aligned along the direction of the COM frame results in:

$$v'_l \cos \theta = v'_c \cos \phi + V_{cm} \quad (5)$$

However, Figure 2 and Eq. 5 are not useful without defining \mathbf{V}_{cm} . \mathbf{V}_{cm} is aligned in the direction of incoming particle velocity, \mathbf{v}_l , in the special case of a stationary target, but is not the general case of a moving target. A more complete diagram [6, 7], that defines \mathbf{V}_{cm} for the moving target case, is presented in Figure 3. In the moving target vector diagram, the basic diagram from Figure 2 represents the lower triangle. To denote the angles correctly, Eq. 5 must be re-written changing θ to θ_2 and ϕ to ϕ_2 :

$$v'_l \cos \theta_2 = v'_c \cos \phi_2 + V_{cm} \quad (6)$$

Or using $\mu_{l,2}$ and $\mu_{c,2}$ as shorthand for $\cos \theta_2$ and $\cos \phi_2$ respectively:

$$v'_l \mu_{l,2} = v'_c \mu_{c,2} + V_{cm} \quad (7)$$

Solving Eq. 7 for $\mu_{c,2}$, the cosine of the scattering angle between the velocity vector of COM frame relative to the LAB frame and the outgoing projectile vector in the LAB frame:

$$\mu_{c,2} = \frac{1}{v'_c} (v'_l \mu_{l,2} - V_{cm}) \quad (8)$$

From conservation of momentum $V'_{cm} = V_{cm}$ and the momentum of the COM system is equal to the sum of the momentum of the projectile and target:

$$(A + 1)\mathbf{V}'_{cm} = (A + 1)\mathbf{V}_{cm} = \frac{A\mathbf{V}_l + \mathbf{v}_l}{A + 1} \quad (9)$$

This vector relationship is depicted graphically as the entire upper triangle (above the horizontal dotted line) in Figure 3. Rearranging (9) to solve for V_{cm} and V'_{cm} :

$$\boxed{\mathbf{V}'_{cm} = \mathbf{V}_{cm} = \frac{A\mathbf{V}_l + \mathbf{v}_l}{A + 1}} \quad (10)$$

We can use Eq. 10 to define the equivalent energy (E_{cm}) of a neutron traveling at the speed of the COM frame relative to the LAB frame.

$$\boxed{E_{cm} = \frac{1}{2}(V_{cm})^2} \quad (11)$$

Substituting (11) into (8) we obtain a general solution for the cosine of the COM scattering angle:

$$\boxed{\mu_{c,2} = \frac{1}{\sqrt{E'_c}} \left[\sqrt{E'_l} \mu_{l,2} - \sqrt{E_{cm}} \right]} \quad (12)$$

Alternatively, additional expressions for E_{cm} can be obtained using the law of cosines, using the angle, α , between the initial target and projectile vectors:

$$E_{cm} = \frac{1}{2}(V_{cm})^2 = \frac{1}{2(A + 1)^2} (A^2V_l^2 + v_l^2 - 2AV_lv_l \cos \alpha) \quad (13)$$

Converting to energy and using $E_{T,l}$ to denote the energy of the target in the LAB frame:

$$\begin{aligned} E_{cm} &= \frac{1}{(A + 1)^2} \left(A^2 \frac{E_{T,l}}{A} + E_l - 2A \sqrt{\frac{E_{T,l}}{A}} \sqrt{E_l} \cos \alpha \right) \\ &= \frac{1}{(A + 1)^2} \left(AE_{T,l} + E_l - 2\sqrt{AE_{T,l}E_l} \cos \alpha \right) \end{aligned} \quad (14)$$

OR in terms of the dot product of the initial target and projectile unit vectors:

$$\begin{aligned} E_{cm} &= \frac{1}{2(A + 1)^2} \left[A^2V_l^2 + v_l^2 - 2AV_lv_l(\hat{\mathbf{V}}_l \cdot \hat{\mathbf{v}}_l) \right] \\ &= \frac{1}{(A + 1)^2} \left[AE_{T,l} + E_l - 2\sqrt{AE_{T,l}E_l}(\hat{\mathbf{V}}_l \cdot \hat{\mathbf{v}}_l) \right] \end{aligned} \quad (15)$$

3.2 The Outgoing Neutron Energy in the Laboratory Frame, E'_l

Using the lower triangle in Figure 3 and the law of cosines we can derive an expression of the outgoing neutron energy as a function of COM scattering angle, $\mu_{c,2}$ (note that the angle between

\mathbf{v}'_c and \mathbf{V}_{cm} is $\pi - \phi_2$):

$$\begin{aligned}
E'_l &= \frac{1}{2}v'_l{}^2 \\
&= \frac{1}{2} \left[v'_c{}^2 + V_{cm}{}^2 - 2v'_c V_{cm} \cos(\pi - \phi_2) \right] \\
&= \frac{1}{2} \left[v'_c{}^2 + V_{cm}{}^2 + 2v'_c V_{cm} \cos(\phi_2) \right] \\
&= \frac{1}{2} \left[v'_c{}^2 + V_{cm}{}^2 + 2v'_c V_{cm} \mu_{c,2} \right] \\
&= \frac{1}{2} \left[2E'_c + 2E_{cm} + 2\sqrt{2E'_c} \sqrt{2E_{cm}} \mu_{c,2} \right] \\
&= E'_c + E_{cm} + 2\sqrt{E'_c} \sqrt{E_{cm}} \mu_{c,2}
\end{aligned} \tag{16}$$

Substituting (12) for $\mu_{c,2}$:

$$\begin{aligned}
E'_l &= E'_c + E_{cm} + 2\sqrt{E'_c} \sqrt{E_{cm}} \left(\frac{1}{\sqrt{E'_c}} \left[\mu_{l,2} \sqrt{E'_l} - \sqrt{E_{cm}} \right] \right) \\
&= E'_c + E_{cm} + 2\sqrt{E_{cm}} \left[\mu_{l,2} \sqrt{E'_l} - \sqrt{E_{cm}} \right] \\
&= E'_c + \cancel{E_{cm}} + 2\sqrt{E_{cm}} \sqrt{E'_l} \mu_{l,2} - 2E_{cm} \\
&= E'_c + 2\sqrt{E_{cm}} \sqrt{E'_l} \mu_{l,2} - E_{cm}
\end{aligned} \tag{17}$$

Rearranging in the form of a quadratic:

$$E'_l - 2\sqrt{E_{cm}} \sqrt{E'_l} \mu_{l,2} - E'_c + E_{cm} = 0 \tag{18}$$

Now we can solve for $\sqrt{E'_l}$ with the standard quadratic formula (or a more accurate version as one may alternatively choose [8]):

$$\begin{aligned}
\sqrt{E'_{l,2}} &= \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \quad \text{where:} \\
a &= 1 \\
b &= -2\sqrt{E_{cm}} \mu_{l,2} \\
c &= -E'_c + E_{cm}
\end{aligned} \tag{19}$$

Thus

$$\begin{aligned}
\sqrt{E'_{l,2}} &= \frac{1}{2} \left[2\sqrt{E_{cm}} \mu_{l,2} \pm \sqrt{(2\sqrt{E_{cm}} \mu_{l,2})^2 - 4(-E'_c + E_{cm})} \right] \\
&= \sqrt{E_{cm}} \mu_{l,2} \pm \sqrt{E_{cm} \mu_{l,2}^2 + E'_c - E_{cm}} \\
&= \sqrt{E_{cm}} \left[\mu_{l,2} \pm \sqrt{(\mu_{l,2}^2 - 1) + \frac{E'_c}{E_{cm}}} \right]
\end{aligned} \tag{20}$$

Squaring both sides:

$$\boxed{E'_{l,2} = E_{cm} \left[\mu_{l,2} \pm \sqrt{(\mu_{l,2}^2 - 1) + \frac{E'_c}{E_{cm}}} \right]^2} \tag{21}$$

We can simplify Eq. 21 by representing the discriminate with D^2 and the square root of the discriminate as D :

$$D = \sqrt{(\mu_{l,2}^2 - 1) + \frac{E'_c}{E_{cm}}} \quad (22)$$

Now:

$$E'_{l,2} = E_{cm} [\mu_{l,2} \pm D]^2 \quad (23)$$

3.3 The COM Scattering Angle

We need the COM scattering angle, μ_c (not just $\mu_{c,2}$), in order to look up the scattering probabilities from either tabular or functional data. Using the moving target vector diagram, Figure 3, and applying the law of cosines we can develop an expression for μ_c ($\cos \phi$) by calculating the magnitude of the vector (\mathbf{c}) between the starting points of \mathbf{v}_l and \mathbf{v}'_l .

$$\begin{aligned} c^2 &= v_l^2 + v'_l{}^2 - 2v_l v'_l \cos \theta \\ &= v_l^2 + v'_l{}^2 - 2v_l v'_l \mu_l \end{aligned} \quad (24)$$

And similiar application of the law of cosines for the vector between the starting points of \mathbf{v}_c and \mathbf{v}'_c .

$$\begin{aligned} c^2 &= v_c^2 + v'_c{}^2 - 2v_c v'_c \cos \phi \\ &= v_c^2 + v'_c{}^2 - 2v_c v'_c \mu_c \end{aligned} \quad (25)$$

And combining

$$v_l^2 + v'_l{}^2 - 2v_l v'_l \mu_l = v_c^2 + v'_c{}^2 - 2v_c v'_c \mu_c \quad (26)$$

Then converting to energy:

$$E_l + E'_l - 2\sqrt{E_l}\sqrt{E'_l}\mu_l = E_c + E'_c - 2\sqrt{E_c}\sqrt{E'_c}\mu_c \quad (27)$$

Eq. 27 can be arranged to solve for μ_c :

$$-2\sqrt{E_c}\sqrt{E'_c}\mu_c = E_l + E'_l - 2\sqrt{E_l}\sqrt{E'_l}\mu_l - E_c - E'_c \quad (28)$$

$$\mu_c = \frac{1}{2\sqrt{E_c}\sqrt{E'_c}} \left(E_c + E'_c + 2\sqrt{E_l}\sqrt{E'_l}\mu_l - E_l - E'_l \right) \quad (29)$$

All terms, except for one, on the left side of the equation are known. The incoming projectile energy in the laboratory frame, E_l , is known from the pre-collision particle state. The outgoing laboratory frame energy, E'_l , is given by Eq. 23. The outgoing energy in the center-of-mass frame, E'_c , is given from the nuclear data for inelastic scattering or from conservation of energy for elastic scattering. The remaining unknown term is the incoming projectile energy in the COM frame, E_c .

3.4 The Incoming Projectile Energy in the COM frame, E_c

An expression for the incoming projectile energy in the COM frame, E_c , can be obtained from defining a relationship between \mathbf{v}_c and \mathbf{v}_l , similar to Eq. 4:

$$\mathbf{v}_l = \mathbf{v}_c + \mathbf{V}_{cm} \quad (30)$$

Rearranging to solve for \mathbf{v}_c and substituting the equation for \mathbf{V}_{cm} from Eq. 10:

$$\begin{aligned} \mathbf{v}_c &= \mathbf{v}_l - \mathbf{V}_{cm} \\ &= \mathbf{v}_l - \frac{A\mathbf{V}_l + \mathbf{v}_l}{A+1} \\ &= \frac{1}{A+1} (\mathbf{v}_l[A+1] - A\mathbf{V}_l - \mathbf{v}_l) \\ &= \frac{A}{A+1} (\mathbf{v}_l - \mathbf{V}_l) \end{aligned} \quad (31)$$

Defining the TAR frame as the frame of reference with respect to the target, the initial velocity of the projectile in the TAR frame is:

$$\mathbf{v}_t = \mathbf{v}_l - \mathbf{V}_l \quad (32)$$

Then the energy of the projectile in the TAR frame, E_t , is:

$$E_t = \frac{1}{2}v_t^2 = \frac{1}{2}|\mathbf{v}_l - \mathbf{V}_l|^2 \quad (33)$$

Thus we can define E_c for scattering with a moving target in terms of E_t . From Eqs. 31 and 33 :

$$\begin{aligned} E_c &= \frac{1}{2}v_c^2 \\ &= \frac{1}{2} \frac{A^2}{(A+1)^2} |\mathbf{v}_l - \mathbf{V}_l|^2 \\ &= \frac{1}{2} \frac{A^2}{(A+1)^2} v_t^2 \end{aligned} \quad (34)$$

$$\boxed{E_c = \frac{A^2}{(A+1)^2} E_t} \quad (35)$$

Now Eq. 29 can be cast to:

$$\mu_c = \frac{A+1}{2A\sqrt{E_t}\sqrt{E'_c}} \left(\frac{A^2}{(A+1)^2} E_t + E'_c + 2\sqrt{E_l}\sqrt{E'_l}\mu_l - E_l - E'_l \right) \quad (36)$$

In the case of a stationary target $E_t = E_l$ thus:

$$\begin{aligned}
\mu_c &= \frac{A+1}{2A\sqrt{E_l}\sqrt{E'_c}} \left(\frac{A^2}{(A+1)^2} E_l + E'_c + 2\sqrt{E_l}\sqrt{E'_l}\mu_l - E_l - E'_l \right) \\
&= \frac{1}{2} \frac{A+1}{A} \left[\frac{A^2}{(A+1)^2} \frac{\sqrt{E_l}}{\sqrt{E'_c}} + \frac{\sqrt{E'_c}}{\sqrt{E_l}} + 2\frac{\sqrt{E'_l}}{\sqrt{E'_c}}\mu_l - \frac{\sqrt{E_l}}{\sqrt{E'_c}} - \frac{\sqrt{E'_l}}{\sqrt{E_l}} \frac{\sqrt{E'_l}}{\sqrt{E'_c}} \right] \\
&= \frac{1}{2} \frac{A+1}{A} \left[\left(\frac{A^2}{(A+1)^2} - 1 \right) \frac{\sqrt{E_l}}{\sqrt{E'_c}} + \frac{\sqrt{E'_c}}{\sqrt{E_l}} + 2\frac{\sqrt{E'_l}}{\sqrt{E'_c}}\mu_l - \frac{\sqrt{E'_l}}{\sqrt{E_l}} \frac{\sqrt{E'_l}}{\sqrt{E'_c}} \right] \\
&= \frac{1}{2} \frac{A+1}{A} \frac{\sqrt{E'_c}/\sqrt{E'_l}}{\sqrt{E'_c}/\sqrt{E'_l}} \left[\left(\frac{A^2}{(A+1)^2} - 1 \right) \frac{\sqrt{E_l}}{\sqrt{E'_c}} + \frac{\sqrt{E'_c}}{\sqrt{E_l}} + 2\frac{\sqrt{E'_l}}{\sqrt{E'_c}}\mu_l - \frac{\sqrt{E'_l}}{\sqrt{E_l}} \frac{\sqrt{E'_l}}{\sqrt{E'_c}} \right] \\
&= \frac{1}{2} \frac{A+1}{A} \frac{\sqrt{E'_l}}{\sqrt{E'_c}} \left[\left(\frac{A^2}{(A+1)^2} - 1 \right) \frac{\sqrt{E_l}}{\sqrt{E'_l}} + \frac{E'_c}{\sqrt{E_l E'_l}} + 2\mu_l - \frac{\sqrt{E'_l}}{\sqrt{E_l}} \right] \\
&= \frac{1}{2} \frac{A+1}{A} \left[\left(\frac{A^2}{(A+1)^2} - 1 \right) \frac{\sqrt{E_l}}{\sqrt{E'_c}} + \frac{\sqrt{E'_c}}{\sqrt{E_l}} + 2\mu_l \frac{\sqrt{E'_l}}{\sqrt{E'_c}} - \frac{E'_l}{\sqrt{E'_c}\sqrt{E_l}} \right]
\end{aligned} \tag{37}$$

3.5 The Outgoing Neutron Energy in the COM Frame, E'_c

For inelastic scattering, the outgoing neutron energy in the COM frame is provided by the nuclear data in accordance with the Q value relationship given in Eq. 89 . In the case of elastic scattering, the outgoing neutron energy is obtained from conservation of energy. Further discussion on obtaining E'_c is found in later sections on inelastic and elastic scattering.

3.6 Limits on the Range of Validity

An obvious limit is the outgoing particle energy in the COM frame, E'_c , must be positive. For elastic scattering this is always true. For inelastic scattering this ensures that the minimum energy for the threshold reaction is satisfied.

In order to prevent out-going energies with an imaginary solution from Eq. 21, D^2 must be greater than or equal to zero.

$$\boxed{D^2 \geq 0} \tag{38}$$

Thus from Eq. 22 for D :

$$\begin{aligned}
\mu_{l,2}^2 - 1 + \frac{E'_c}{E_{cm}} &\geq 0 \\
\mu_{l,2}^2 &\geq 1 - \frac{E'_c}{E_{cm}}
\end{aligned} \tag{39}$$

$$\boxed{|\mu_{l,2}| \geq \sqrt{1 - \frac{E'_c}{E_{cm}}}} \tag{40}$$

So any NEE location's that have cosine scattering angles such that Eq. 40 is not met will have a zero contribution from the scatter event.

Another restriction is that the outgoing projectile speed (or square root of the energy) must be positive. So from Eq. 20:

$$\mu_{l,2} \pm \sqrt{(\mu_{l,2}^2 - 1) + \frac{E'_c}{E_{cm}}} > 0 \quad (41)$$

Then the lower root (root with the $-$ sign) only exists when the scattering angle is positive and when:

$$\begin{aligned} \mu_{l,2} - \sqrt{(\mu_{l,2}^2 - 1) + \frac{E'_c}{E_{cm}}} > 0 \\ \mu_{l,2}^2 > (\mu_{l,2}^2 - 1) + \frac{E'_c}{E_{cm}} \\ 1 > \frac{E'_c}{E_{cm}} \end{aligned} \quad (42)$$

Lower root (root with $-$ sign) exists when: $\mu_{l,2} > 0$ AND $E_{cm} > E'_c$

(43)

And the upper root (root with the $+$ sign) only exists when:

$$\mu_{l,2} + \sqrt{(\mu_{l,2}^2 - 1) + \frac{E'_c}{E_{cm}}} > 0 \quad (44)$$

This is true for all positive angles but places a limit on negative angles. Evaluating for negative angles:

$$\begin{aligned} \mu_{l,2} + \sqrt{(\mu_{l,2}^2 - 1) + \frac{E'_c}{E_{cm}}} > 0 \\ \sqrt{(\mu_{l,2}^2 - 1) + \frac{E'_c}{E_{cm}}} > |\mu_{l,2}| \quad \text{if } \mu_{l,2} \leq 0 \\ (\mu_{l,2}^2 - 1) + \frac{E'_c}{E_{cm}} > \mu_{l,2}^2 \quad \text{if } \mu_{l,2} \leq 0 \\ \frac{E'_c}{E_{cm}} > 1 \quad \text{if } \mu_{l,2} \leq 0 \\ E'_c > E_{cm} \quad \text{if } \mu_{l,2} \leq 0 \end{aligned} \quad (45)$$

Upper root (root with $+$ sign) exists when: $\mu_{l,2} > 0$ OR $(\mu_{l,2} < 0$ AND $E'_c > E_{cm})$

(46)

These limits can be summarized as:

1. If $|\mu_{l,2}| < \sqrt{1 - E'_c/E_{cm}}$ or $E'_c \leq 0$, no roots are valid.
2. If $E'_c > E_{cm}$, only the root with the $+$ sign is valid.
3. If $E'_c < E_{cm}$ and $\mu_{l,2} > 0$, both roots are valid.

3.7 Calculating the Probability of Scatter in the Laboratory Frame

The final quantity that we need is the probability of scattering into the LAB scattering angle θ . To convert probabilities given in the COM frame of reference to the LAB frame of reference we have to take the derivate of $\cos \phi$, or μ_c , with respect to the LAB scattering angle $\cos \theta$, or μ_l . With $h(\mu_l; E)_{lab}$ and $h(\mu_c; E)_{cm}$ representing the scattering probabilities in the LAB and COM frames of reference respectively:

$$\begin{aligned} h(\mu_l; E)_{lab} \partial \mu_l &= h(\mu_c; E)_{cm} \partial \mu_c \\ h(\mu_l; E)_{lab} &= h(\mu_c; E)_{cm} \frac{\partial \mu_c}{\partial \mu_l} \end{aligned} \quad (47)$$

To get an expression for the COM cosine scattering angle, μ_c , from the LAB cosine scattering angle (μ_l), the final COM energy (E'_c), and the COM frame energy (E_{cm}), we insert (23) into (12):

$$\begin{aligned} \mu_{c,2} &= \frac{1}{\sqrt{E'_c}} \left[\mu_{l,2} \sqrt{E'_l} - \sqrt{E_{cm}} \right] \\ &= \frac{1}{\sqrt{E'_c}} \left[\mu_{l,2} \sqrt{E_{cm}} \left[\mu_{l,2} \pm \sqrt{(\mu_{l,2}^2 - 1) + \frac{E'_c}{E_{cm}}} \right] - \sqrt{E_{cm}} \right] \\ &= \frac{\sqrt{E_{cm}}}{\sqrt{E'_c}} \left[\mu_{l,2} \left[\mu_{l,2} \pm \sqrt{(\mu_{l,2}^2 - 1) + \frac{E'_c}{E_{cm}}} \right] - 1 \right] \\ &= \frac{\sqrt{E_{cm}}}{\sqrt{E'_c}} \left[\mu_{l,2}^2 - 1 \pm \mu_{l,2} \sqrt{(\mu_{l,2}^2 - 1) + \frac{E'_c}{E_{cm}}} \right] \end{aligned} \quad (48)$$

The derivative of (48):

$$\begin{aligned} \frac{\partial \mu_c}{\partial \mu_l} &= \frac{\partial}{\partial \mu_l} \left[\frac{\sqrt{E_{cm}}}{\sqrt{E'_c}} \left(\mu_{l,2}^2 - 1 \pm \mu_{l,2} \sqrt{(\mu_{l,2}^2 - 1) + \frac{E'_c}{E_{cm}}} \right) \right] \\ &= \frac{\sqrt{E_{cm}}}{\sqrt{E'_c}} \left(2\mu_{l,2} \pm \left[\sqrt{(\mu_{l,2}^2 - 1) + \frac{E'_c}{E_{cm}}} + \mu_{l,2} \frac{1}{2} \frac{2\mu_{l,2}}{\sqrt{(\mu_{l,2}^2 - 1) + \frac{E'_c}{E_{cm}}}} \right] \right) \\ &= \frac{\sqrt{E_{cm}}}{\sqrt{E'_c}} \left(2\mu_{l,2} \pm \left[\sqrt{(\mu_{l,2}^2 - 1) + \frac{E'_c}{E_{cm}}} + \frac{\mu_{l,2}^2}{\sqrt{(\mu_{l,2}^2 - 1) + \frac{E'_c}{E_{cm}}}} \right] \right) \end{aligned} \quad (49)$$

Substituting in D for the square root of the discriminate from (22):

$$\begin{aligned} \frac{\partial \mu_c}{\partial \mu_l} &= \frac{\sqrt{E_{cm}}}{\sqrt{E'_c}} \left(2\mu_{l,2} \pm \left[D + \frac{\mu_{l,2}^2}{D} \right] \right) \\ &= \frac{\sqrt{E_{cm}}}{\sqrt{E'_c}} \frac{1}{D} (2D\mu_{l,2} \pm [D^2 + \mu_{l,2}^2]) \end{aligned} \quad (50)$$

The highest root is:

$$\begin{aligned}\frac{\partial\mu_c}{\partial\mu_l} &= \frac{\sqrt{E_{cm}}}{\sqrt{E'_c}} \frac{1}{D} (2D\mu_{l,2} + D^2 + \mu_{l,2}^2) \\ &= \frac{\sqrt{E_{cm}}}{\sqrt{E'_c}} \frac{1}{D} (D + \mu_{l,2})^2\end{aligned}\tag{51}$$

The lowest root is:

$$\begin{aligned}\frac{\partial\mu_c}{\partial\mu_l} &= \frac{\sqrt{E_{cm}}}{\sqrt{E'_c}} \frac{1}{D} (2D\mu_{l,2} - D^2 - \mu_{l,2}^2) \\ &= -\frac{\sqrt{E_{cm}}}{\sqrt{E'_c}} \frac{1}{D} (D^2 - 2D\mu_{l,2} + \mu_{l,2}^2) \\ &= -\frac{\sqrt{E_{cm}}}{\sqrt{E'_c}} \frac{1}{D} (D - \mu_{l,2})^2\end{aligned}\tag{52}$$

We only need the absolute value of $\frac{\partial\mu_c}{\partial\mu_l}$ so both roots can be written in a single expression as:

$$\boxed{\frac{\partial\mu_c}{\partial\mu_l} = \frac{\sqrt{E_{cm}}}{\sqrt{E'_c}} \frac{1}{D} (D \pm \mu_{l,2})^2}\tag{53}$$

From Eq. 23, $E'_{l1,2} = E_{cm}(\mu_{l,2} \pm D)^2$ then:

$$(D \pm \mu_{l,2})^2 = \frac{E'_l}{E_{cm}}\tag{54}$$

So $\partial\mu_c/\partial\mu_l$ can be written in terms of outgoing neutron energy:

$$\begin{aligned}\frac{\partial\mu_c}{\partial\mu_l} &= \frac{\sqrt{E_{cm}}}{\sqrt{E'_c}} \frac{1}{D} \frac{E'_l}{E_{cm}} \\ &= \frac{E'_l}{\sqrt{E_{cm}}\sqrt{E'_c}} \frac{1}{D}\end{aligned}$$

$$\boxed{\frac{\partial\mu_c}{\partial\mu_l} = E'_l \frac{1}{\sqrt{E'_c E_{cm} D^2}}}\tag{55}$$

4 Stationary Target Kinematics

In the case of a stationary target, several expressions can be simplified. E_{cm} from Eq. 11 becomes:

$$\text{Stationary Target: } E_{cm} = \frac{E_l}{(A+1)^2}\tag{56}$$

The TAR frame energy, E_t , from Eq. 33 becomes:

$$\text{Stationary Target: } E_t = E_l \quad (57)$$

And the expression for the scattering angle in the COM frame from Eq. 12 and noting $\mu_{c,2} = \mu_c$ and $\mu_{l,2} = \mu_l$ for a stationary target:

$$\text{Stationary Target: } \mu_c = \frac{1}{\sqrt{E'_c}} \left[\sqrt{E'_l} \mu_l - \frac{\sqrt{E_l}}{A+1} \right] \quad (58)$$

Which is Eq. 5.10 of Carter and Cashwell[2].

To calculate the outgoing neutron energy solutions, $E'_{l1,2}$, for a stationary target we replace E_{cm} from Eq. 56 into Eq. 21 and replace $\mu_{l,2}$ with μ_l :

$$\text{Stationary Target: } E'_{l1,2} = \frac{E_l}{(A+1)^2} \left[\mu_l \pm \sqrt{(\mu_l^2 - 1) + (A+1)^2 \frac{E'_c}{E_l}} \right]^2 \quad (59)$$

This matches Eq. 5.14 of Carter and Cashwell for scattering with a stationary target. Now D from Eq. 22 becomes:

$$\text{Stationary Target: } D = \sqrt{(\mu_l^2 - 1) + (A+1)^2 \frac{E'_c}{E_l}} \quad (60)$$

For a stationary target $E_t = E_l$ so E_c , from Eq. 35, becomes:

$$E_c = \frac{A^2}{(A+1)^2} E_l \quad (61)$$

5 Inelastic Scattering

5.1 Inelastic Scattering with a Moving Target

For inelastic scattering the outgoing neutron energy, E'_c , is provided by the nuclear data. However, conversion of the incoming projectile energy from the LAB frame to the COM frame (in which the data is usually provided) is usually done assuming a stationary target. Q-value relationships for the moving target case, provided in Appendix B, show that the incoming particle energy must simply be transformed into the TAR frame in order to determine the outgoing neutron energy, E'_c , from the provided nuclear data. The energy of the projectile in the TAR frame, E_t , is provided by Eq. 33.

For inelastic scattering with a moving target the equations governing the NEE response are the most general case, E_{cm} from Eq. 11, E_c from Eq. 34, $\mu_{c,2}$ from Eq. 12, E'_l from Eq. 23, D from Eq. 22, μ_c from Eq. 29, and $\partial\mu_c/\partial\mu_l$ from Eq. 55.

5.2 Inelastic Scattering with a Stationary Target

For a stationary target $E_t = E_l$. Thus, nuclear data lookup using E_l to obtain E'_c is straightforward.

For inelastic scattering with a stationary target the equations governing the NEE response are modified by the stationary target equations, E_{cm} from Eq. 56, E_c from Eq. 61, $\mu_{c,2}$ from Eq. 58, E'_l from Eq. 23 or Eq. 59, D from Eq. 60, μ_c from Eq. 29, and $\partial\mu_c/\partial\mu_l$ from Eq. 55.

5.2.1 Limits

To find the limits for inelastic scattering with a stationary target we evaluate Eq. 38 by substitution E_{cm} for a stationary target from Eq. 56:

$$\begin{aligned}\mu_{l,2}^2 &> 1 - \frac{E'_c}{E_{cm}} \\ &> 1 - (A+1)^2 \frac{E'_c}{E_l}\end{aligned}\tag{62}$$

Finding the limit where the lower root exists by evaluating Eq. 43 by substitution E_{cm} for a stationary target from Eq. 56:

$$\begin{aligned}E_{cm} &> E'_c \\ E_l &> (A+1)^2 E'_c\end{aligned}\tag{63}$$

Substituting Eq. 89 for E'_c from the definition of Q-Value and substituting E_l for E_t for a stationary target:

$$\begin{aligned}E_l &> (A+1)^2 \left[Q \left(\frac{A}{A+1} \right) + E_l \left(\frac{A}{1+A} \right)^2 \right] \\ E_l &> QA(A+1) + E_l A^2 \\ E_l(1-A^2) &> QA(A+1) \\ E_l(A^2-1) &< -QA(A+1) \\ E_l &< -QA \frac{A+1}{A^2-1} \\ E_l &< -QA \frac{A+1}{(A+1)(A-1)} \\ E_l &< -Q \frac{A}{A-1}\end{aligned}\tag{64}$$

This is the upper limit of *Case 3* of Eq. 5.14 of Carter and Cashwell.

6 Elastic Scattering

6.1 Elastic Scattering with a Moving Target

From conservation of energy for elastic scattering (both with a moving and stationary targets) the outgoing projectile energy in the COM frame is equal to the incoming projectile energy.

$$E'_c = E_c\tag{65}$$

The LAB frame cosine scattering angle, $\mu_{c,2}$, which is defined in Eq. 12, can be simplified for elastic scattering by substituting E_c for E'_c from in Eq. 35:

$$\begin{aligned} \text{Elastic Moving Target: } \mu_{c,2} &= \frac{1}{\sqrt{\frac{A^2}{(A+1)^2} E_t}} \left[\sqrt{E'_l} \mu_{l,2} - \sqrt{E_{cm}} \right] \\ &= \frac{A+1}{A} \frac{1}{\sqrt{E_t}} \left[\sqrt{E'_l} \mu_{l,2} - \sqrt{E_{cm}} \right] \end{aligned} \quad (66)$$

And the LAB frame outgoing projectile energy for elastic scattering with a moving target follows from Eq. 21 by substituting E_c for E'_c and the substituting Eq. 35 for E_c :

$$\begin{aligned} \text{Elastic Moving Target: } E'_{l,2} &= E_{cm} \left[\mu_{l,2} \pm \sqrt{(\mu_{l,2}^2 - 1) + \frac{E_c}{E_{cm}}} \right]^2 \\ &= E_{cm} \left[\mu_{l,2} \pm \sqrt{(\mu_{l,2}^2 - 1) + \frac{A^2}{(A+1)^2} \frac{E_t}{E_{cm}}} \right]^2 \end{aligned} \quad (67)$$

Evaluating the limit on the scattering angle by substituting E_c for elastic scattering from Eq. 35 into Eq. 38:

$$\begin{aligned} \mu_{l,2}^2 - 1 + \frac{E'_c}{E_{cm}} &> 0 \\ \mu_{l,2}^2 - 1 + \frac{A^2}{(A+1)^2} \frac{E_t}{E_{cm}} &> 0 \end{aligned} \quad (68)$$

Finding the limit where the lower root exists by evaluating Eq. 43 with the substitution of E'_c for elastic scattering from Eq. 35:

$$\begin{aligned} E_{cm} &> E'_c \\ E_{cm} &> \frac{A^2}{(A+1)^2} E_t \end{aligned} \quad (69)$$

$$\text{Lower root exists when: } \mu_{l,2} > 0 \quad \text{AND} \quad E_t < E_{cm} \frac{(A+1)^2}{A^2} \quad (70)$$

6.2 Elastic Scattering with a Stationary Target

The COM cosine scattering angle defined in Eq. 66 can be simplified using E_{cm} (Eq. 56), E_t (Eq. 57), and $\mu_{c,2} = \mu_c$ for a stationary target:

$$\begin{aligned} \text{Elastic Stationary Target: } \mu_c &= \frac{A+1}{A} \frac{1}{\sqrt{E_l}} \left[\sqrt{E'_l} \mu_l - \frac{1}{A+1} \sqrt{E_l} \right] \\ &= \frac{1}{A} \left[\frac{\sqrt{E'_l}}{\sqrt{E_l}} (A+1) \mu_l - 1 \right] \end{aligned} \quad (71)$$

And again substituting E_{cm} (Eq. 56), E_t (Eq. 57), and $\mu_{l,2} = \mu_l$ for a stationary target into the equation for the outgoing projectile energy in the LAB frame(Eq. 67):

$$\begin{aligned} \text{Elastic Stationary Target: } E'_{l1,2} &= \frac{E_l}{(A+1)^2} \left[\mu_l \pm \sqrt{(\mu_l^2 - 1) + \frac{A^2}{(A+1)^2} (A+1)^2 \frac{E_l}{E_t}} \right]^2 \\ &= \frac{E_l}{(A+1)^2} \left[\mu_l \pm \sqrt{(\mu_l^2 - 1) + A^2} \right]^2 \end{aligned} \quad (72)$$

This matches the expected result for elastic scattering with a stationary target from Eq. 3.14 of Lux and Koblinger.

Evaluating the laboratory angle scattering limit described by Eq. 68 by substitution of E_{cm} (Eq. 56), E_t (Eq. 57), and using $\mu_l = \mu_{l,2}$ for a stationary target:

$$\begin{aligned} \mu_l^2 - 1 + \frac{A^2}{(A+1)^2} \frac{E_t}{E_{cm}} &> 0 \\ \mu_l^2 - 1 + \frac{A^2}{(A+1)^2} \frac{E_l}{E_t} (A+1)^2 &> 0 \\ \mu_l^2 - 1 + A^2 &> 0 \end{aligned} \quad (73)$$

This implies that all angles are possible for elastic scattering on stationary targets for all isotopes except for hydrogen. For hydrogen only positive scattering angles ($\mu_l > 0$) are possible.

Likewise evaluating Eq. 70 by substitution of E_{cm} (Eq. 56) and E_t (Eq. 57) for a stationary target, defines the physical limit of the lower root of Eq. 72:

$$\begin{aligned} E_t &< E_{cm} \frac{(A+1)^2}{A^2} \\ E_l &< \frac{E_l}{(A+1)^2} \frac{(A+1)^2}{A^2} \\ 1 &< \frac{1}{A^2} \end{aligned}$$

$$\text{Lower root exists when: } \mu_l > 0 \quad \text{AND} \quad A^2 < 1 \quad (74)$$

This implies that the lower root of Eq. 72 does not exist except for cases where the projectile mass exceeds the target mass, which is not generally applicable to neutron elastic scattering. The neutron is slightly heavier than the proton (0.14%) but they are normally considered to have equivalent masses for neutron transport applications.

6.3 Elastic Scattering with Stationary Hydrogen

Hydrogen is usually considered a special case for elastic scattering. Substituting of $A = 1$ for hydrogen in the equation for the outgoing projectile energy in the LAB frame (Eq. 72) and noting

that only the positive root can exist:

$$\begin{aligned}
\text{Elastic Stationary Hydrogen Target: } E'_l &= \frac{E_l}{(1+1)^2} \left[\mu_l + \sqrt{(\mu_l^2 - 1) + 1^2} \right]^2 \\
&= \frac{E_l}{4} [2\mu_l]^2 \\
&= E_l \mu_l^2
\end{aligned} \tag{75}$$

The COM cosine scattering angle defined in Eq. 71 can be simplified using Eq. 75 for E'_l/E_l and substituting $A = 1$ for hydrogen:

$$\begin{aligned}
\text{Elastic Stationary Hydrogen Target: } \mu_c &= \frac{1}{1} \left[\frac{\sqrt{E'_l}}{\sqrt{E_l}} (1+1)\mu_l - 1 \right] \\
&= 2\sqrt{\mu_l^2} \mu_l - 1 \\
&= 2\mu_l^2 - 1
\end{aligned} \tag{76}$$

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References

- [1] I. Lux and L. Koblinger. *Monte Carlo Particle Transport Methods: Neutron and Photon Calculations*. CRC Press, 1991. DOI: 10.1201/9781351074834.
- [2] L L Carter and E D Cashwell. *Particle-transport simulation with the Monte Carlo method*. ERDA Technical Information Center, Jan. 1975. ISBN: 0-87079-021-8. DOI: 10.2172/4167844. URL: https://mcnp.lanl.gov/pdf_files/1a-carter-cashwell.pdf.
- [3] Esam M.A. Hussein. “CHAPTER TWO - COLLISION KINEMATICS”. In: *Radiation Mechanics*. Ed. by Esam M.A. Hussein. Oxford: Elsevier Science Ltd, 2007, pp. 67–151. ISBN: 978-0-08-045053-7. DOI: <https://doi.org/10.1016/B978-008045053-7/50003-3>. URL: <https://www.sciencedirect.com/science/article/pii/B9780080450537500033>.
- [4] T Goorley et al. “Initial MCNP6 release overview”. In: *Nuclear Technology* 180.3 (2012), pp. 298–315. DOI: 10.13182/NT11-135.
- [5] M.H. Kalos. “On the Estimation of Flux at a Point by Monte Carlo”. In: *Nucl. Sci. Eng.* 16 (1963), p. 111.
- [6] B. R. Wienke. “Anisotropic Elastic Scattering and Moving Media”. In: *Nuclear Science and Engineering* 52.4 (1973), pp. 482–484. DOI: 10.13182/NSE73-A23316.
- [7] G. Lansing Blackshaw and Raymond L. Murray. “Scattering Functions for Low-Energy Neutron Collisions in a Maxwellian Monatomic Gas”. In: *Nuclear Science and Engineering* 27.3 (1967), pp. 520–532. DOI: 10.13182/NSE86-A17617. eprint: <https://doi.org/10.13182/NSE86-A17617>. URL: <https://doi.org/10.13182/NSE86-A17617>.
- [8] William H. Press et al. *Numerical Recipes in C*. ISBN 0-521-43108-5. Cambridge: Cambridge University Press, 1992, pp. 183–184. URL: <http://numerical.recipes/C210>.
- [9] T. Adams et al. ““Monte Carlo Application ToolKit (MCATK)””. In: *Annals of Nuclear Energy* 82 (2015), pp. 41–47. URL: <http://www.sciencedirect.com/science/article/pii/S0306454914004472>.

Appendix A Kinematic Notation

m is the mass of the projectile particle.

M is the mass of the target particle.

A is the ratio of the target mass to projectile mass = M/m .

\mathbf{v}_l is the initial particle velocity in the laboratory frame.

v_l is the initial particle speed in the laboratory frame = $|\mathbf{v}_l|$.

$\hat{\mathbf{v}}_l$ is the initial particle velocity unit-vector in the laboratory frame = \mathbf{v}_l/v_l .

E_l is the initial particle energy in the laboratory frame = $mv_l^2/2$.

\mathbf{v}_c is the initial particle velocity in the center-of-mass frame.

v_c is the initial particle speed in the center-of-mass frame = $|\mathbf{v}_c|$.

$\hat{\mathbf{v}}_c$ is the initial particle velocity unit-vector in the center-of-mass frame = \mathbf{v}_c/v_c .

E_c is the initial particle energy in the center-of-mass frame = $mv_c^2/2$.

\mathbf{v}_t is the initial particle velocity in the target-at-rest frame = $\mathbf{v}_l - \mathbf{V}_l$.

v_t is the initial particle speed in the target-at-rest frame = $|\mathbf{v}_t|$.

$\hat{\mathbf{v}}_t$ is the initial particle velocity unit-vector in the target-at-rest frame = \mathbf{v}_t/v_t .

E_t is the initial particle energy in the target-at-rest frame = $mv_t^2/2$.

\mathbf{v}'_l is the final particle velocity in the laboratory frame.

v'_l is the final particle speed in the laboratory frame = $|\mathbf{v}'_l|$.

$\hat{\mathbf{v}}'_l$ is the final particle velocity unit-vector in the laboratory frame = \mathbf{v}'_l/v'_l .

E'_l is the final particle energy in the laboratory frame = $mv'^2_l/2$.

\mathbf{v}'_c is the final particle velocity in the center-of-mass frame.

v'_c is the final particle speed in the center-of-mass frame = $|\mathbf{v}'_c|$.

$\hat{\mathbf{v}}'_c$ is the final particle velocity unit-vector in the center-of-mass frame = \mathbf{v}'_c/v'_c .

E'_c is the final particle energy in the center-of-mass frame = $mv'^2_c/2$.

\mathbf{V}_l is the initial target velocity in the laboratory frame.

V_l is the initial target speed in the laboratory frame = $|\mathbf{V}_l|$.

$\hat{\mathbf{V}}_l$ is the initial target velocity unit-vector in the laboratory frame = \mathbf{V}_l/V_l .

\mathbf{V}_c is the initial target velocity in the center-of-mass frame.

V_c is the initial target speed in the center-of-mass frame = $|\mathbf{V}_c|$.

$\hat{\mathbf{V}}_c$ is the initial target velocity unit-vector in the center-of-mass frame = \mathbf{V}_c/V_c .

\mathbf{V}'_l is the final target velocity in the laboratory frame.

V'_l is the final target speed in the laboratory frame = $|\mathbf{V}'_l|$.

$\hat{\mathbf{V}}'_l$ is the final target velocity unit-vector in the laboratory frame = \mathbf{V}'_l/V'_l .

\mathbf{V}'_c is the final target velocity in the center-of-mass frame.

V'_c is the final target speed in the center-of-mass frame = $|\mathbf{V}'_c|$.

$\hat{\mathbf{V}}'_c$ is the final target velocity unit-vector in the center-of-mass frame = \mathbf{V}'_c/V'_c .

\mathbf{V}_{cm} is the initial center-of-mass frame velocity of the relative to the laboratory frame
= $(\mathbf{v}_l + A\mathbf{V}_l)/(1 + A)$.

V_{cm} is the initial center-of-mass frame speed of the relative to the laboratory frame.

$\hat{\mathbf{V}}_{cm}$ is the initial center-of-mass frame unit-vector of the relative to the laboratory frame.

\mathbf{V}'_{cm} is the final center-of-mass frame velocity of the relative to the laboratory frame = \mathbf{V}_{cm} .

θ is the particle's final scattering angle in the laboratory frame.

μ_l is the cosine of the particle's final scattering angle in the laboratory frame = $\cos \theta$.

ϕ is the particle's final scattering angle in the center-of-mass frame.

μ_c is the cosine of the particle's final scattering angle in the center-of-mass frame = $\cos \phi$.

$\pi - \phi$ is the target's final scattering angle in the center of mass frame.

Velocity Relations

$$\mathbf{V}_{cm} = \mathbf{v}_l - \mathbf{v}_c ; \quad \mathbf{V}_{cm} = \mathbf{V}_l - \mathbf{V}_c$$

$$\mathbf{V}_{cm} = \mathbf{v}'_l - \mathbf{v}'_c ; \quad \mathbf{V}_{cm} = \mathbf{V}'_l - \mathbf{V}'_c$$

$$\mathbf{V}_{cm} = \mathbf{v}_l - \mathbf{v}_c = \mathbf{V}_l - \mathbf{V}_c = \mathbf{v}'_l - \mathbf{v}'_c = \mathbf{V}'_l - \mathbf{V}'_c$$

$$\mathbf{v}_t = \mathbf{v}_l - \mathbf{V}_l = \mathbf{v}_c - \mathbf{V}_c$$

Appendix B Q-Value Relationships for Moving Targets

As Q-value expressions are generally derived using a stationary target, we need to re-visit the Q-value equations to see if the energy of the projectile can simply be transformed into the target-at-rest (TAR) frame.

To express the Q-value we express the reaction with the following notation:



Where the incident projectile is denoted as “a”, the target nucleus is denoted as “A”, the compound nucleus is denoted as “C”, the emitted particle is “b”, and the residual nucleus is denoted as “B”.

We can express the Q value as the difference between the entrance channel energy (ϵ_a) and exit channel energy (ϵ_b):

$$Q = \epsilon_b - \epsilon_a \quad (78)$$

The entrance channel energy is the kinetic energy of the incident projectile and the target particle in the center-of-mass frame

$$\epsilon_a = E_{a,c} + E_{A,c} \quad (79)$$

We can replace the energies with the speed of the incident particle in the center-of-mass frame, v_c , and the velocity of the target nucleus in the center-of-mass frame, V_c .

$$\epsilon_a = \frac{1}{2}v_c^2 + \frac{1}{2}AV_c^2 \quad (80)$$

Defining the velocity of the COM system with respect to the LAB frame from the total momentum of the center-of-mass system:

$$\begin{aligned} \mathbf{V}_{cm}(1 + A) &= A\mathbf{V}_l + \mathbf{v}_l \\ \mathbf{V}_{cm} &= \frac{A\mathbf{V}_l + \mathbf{v}_l}{1 + A} \end{aligned} \quad (81)$$

Using $\mathbf{v}_c = \mathbf{v}_l - \mathbf{V}_{cm}$ and $\mathbf{V}_c = \mathbf{V}_l - \mathbf{V}_{cm}$ and replacing the velocity in the center-of-mass frame

in (80):

$$\begin{aligned}
\epsilon_a &= \frac{1}{2}|\mathbf{v}_l - V_{cm}|^2 + \frac{1}{2}A|\mathbf{V}_l - V_{cm}|^2 \\
&= \frac{1}{2} \left(\left| \mathbf{v}_l - \frac{A\mathbf{V}_l + \mathbf{v}_l}{1+A} \right|^2 + \frac{1}{2}A \left(\left| \mathbf{V}_l - \frac{A\mathbf{V}_l + \mathbf{v}_l}{1+A} \right|^2 \right) \right) \\
&= \frac{1}{2(A+1)^2} |\mathbf{v}_l(A+1) - (A\mathbf{V}_l + \mathbf{v}_l)|^2 + \frac{1}{2(A+1)^2} A |\mathbf{V}_l(A+1) - (A\mathbf{V}_l + \mathbf{v}_l)|^2 \\
&= \frac{1}{2(A+1)^2} |\mathbf{v}_l A - A\mathbf{V}_l|^2 + \frac{1}{2(A+1)^2} A |\mathbf{V}_l - \mathbf{v}_l|^2 \\
&= \frac{A^2}{2(A+1)^2} |\mathbf{v}_l - \mathbf{V}_l|^2 + \frac{A}{2(A+1)^2} |\mathbf{V}_l - \mathbf{v}_l|^2 \\
&= \frac{A}{2(A+1)^2} (A|\mathbf{v}_l - \mathbf{V}_l|^2 + |\mathbf{V}_l - \mathbf{v}_l|^2) \\
&= \frac{A}{2(A+1)^2} |\mathbf{v}_l - \mathbf{V}_l|^2 (A+1) \\
&= \frac{A}{2(A+1)} |\mathbf{v}_l - \mathbf{V}_l|^2
\end{aligned} \tag{82}$$

And using the TAR frame projectile energy from Eq. 33, the entrance channel energy, ϵ_a , becomes:

$$\boxed{\epsilon_a = E_t \frac{A}{A+1}} \tag{83}$$

This provides some comfort for the use of the fluid-frame energy in place of the laboratory-frame energy as we would for a stationary target, as the entrance channel energy for the target-at-rest (TAR) case is

$$\epsilon_{a,TAR} = E_t \frac{A}{A+1} \tag{84}$$

Likewise defining the exit channel energy:

$$\begin{aligned}
\epsilon_b &= E_{b,cm} + E_{B,cm} \\
\epsilon_b &= \frac{1}{2}v_c'^2 + \frac{1}{2}AV_c'^2
\end{aligned} \tag{85}$$

By definition the momentum of the center-of-mass system is zero:

$$\mathbf{v}'_c = A\mathbf{V}'_c \tag{86}$$

$$\begin{aligned}
\epsilon_b &= \frac{1}{2}v_c'^2 + \frac{1}{2}A \frac{v_c'^2}{A^2} \\
\epsilon_b &= E'_c \left(1 + \frac{1}{A}\right) \\
A\epsilon_b &= E'_c (A+1) \\
\epsilon_b &= E'_c \frac{(A+1)}{A}
\end{aligned}$$

$$\boxed{\epsilon_b = E'_c \frac{A+1}{A}} \quad (87)$$

Substitution (83) and (87) into the expression for Q :

$$\begin{aligned} Q &= \epsilon_b - \epsilon_a \\ Q &= E'_c \frac{A+1}{A} - E_t \frac{A}{1+A} \end{aligned} \quad (88)$$

Solving for E'_c :

$$E'_c \frac{A+1}{A} = Q + E_t \left(\frac{A}{1+A} \right)$$

$$\boxed{E'_c = Q \left(\frac{A}{A+1} \right) + E_t \left(\frac{A}{1+A} \right)^2} \quad (89)$$

Appendix C Python for NEE Contributions due to Neutron Scattering

```
1 import math
2 import numpy as np
3
4 def square( value ):
5     return value*value
6
7 def squareMagnitude( vector ):
8     return np.sum( np.power(vector, 2 ) )
9
10 def normalize( vector ):
11     return np.divide( vector, math.sqrt( squareMagnitude(vector) ) )
12
13 def neutronMolarMass():
14     return 1.00866491597
15
16 # neutron rest mass energy in MeV from ( http://physics.nist.gov/cgi-bin/cuu/Value?
17 # mnc2mev ) in Units [MeV]. Standard Uncertainty = 0.000 023 MeV
18 neutron_rest_mass_MeV = 939.565346 # [MeV]
19
20 # speed of light in a vaccume from ( http://physics.nist.gov/cgi-bin/cuu/Value?c )
21 # Units [cm/shake]. Exact, according to NIST
22 speed_of_light = 299.7924580 # [cm/shake]
23
24 # Returns the velocity of a neutron in cm/shake from neutron's energy in [MeV]
25 # neutron_speed_from_energy_const = speed_of_light * std::sqrt( 2.0 /
26 # neutron_rest_mass_MeV ) ; // [MeV]
27
28 def speed( E, mass):
29     # Returns the velocity in cm/shake from neutron's energy in [MeV]
30     # assumes neutron to proton mass ratio is 1.0
31     return speed_of_light * math.sqrt( 2.0 * E / (mass*neutron_rest_mass_MeV) );
32
33 def energy( speed ):
34     if isinstance( speed, np.ndarray):
35         return 0.5*neutron_rest_mass_MeV * squareMagnitude(speed/speed_of_light)
36     else:
37         return 0.5*neutron_rest_mass_MeV * square(speed/speed_of_light)
38
39 def V_projectile(E_projectile):
40     return np.array( [ speed(E_projectile,1.0), 0.0, 0.0] )
41
42 def V_target(E_target, mu_target, mass):
43     V_speed = speed(E_target, mass)
44     return np.array( [ V_speed*mu_target, V_speed*math.sqrt(1-square(mu_target)) ,
45         0.0] )
46
47 def energy_target( speed, mass ):
48     return 0.5*neutron_rest_mass_MeV*mass * square(speed/speed_of_light)
49
50 def V_cm(E_l, E_target, mu_target, mass):
51     v = V_projectile( E_l )
52     V = V_target(E_target, mu_target, mass)
53     P = np.multiply(V, mass)
54     return np.add(P,v)/(mass+1.0)
```

```

52 def e_t_min(Q_value, M):
53     return -Q_value*(M+1.0)/M
54
55 def e_cm(E_l, E_target, mu_target, mass):
56     return energy( V_cm(E_l, E_target, mu_target, mass) )
57
58 def e_t(E_l, E_target, mu_target, mass):
59     v = V_projectile( E_l )
60     V = V_target(E_target, mu_target, mass)
61     V_diff = np.subtract(v,V)
62     return energy( V_diff )
63
64 def e_l_from_e_t(E_t, E_target, mu_target, mass):
65     V_speed = speed(E_target, mass)
66     V_x = V_speed*mu_target
67     V_y = V_speed*math.sqrt(1-square(mu_target))
68     E_y = energy( V_y )
69     E = E_t - E_y
70
71     V_diff_speed = speed(E, 1.0)
72     return energy( V_diff_speed + V_x )
73
74 def e_c_prime(E_t, Q_value, M):
75     return square(M/(M+1.0))*E_t + Q_value*M/(M+1.0)
76
77 def e_t_max(E_l, E_target, mu_target, Q_value, M):
78     energy_cm = e_cm(E_l, E_target, mu_target, M)
79     return (energy_cm - Q_value*M/(M+1.0)) / square(M/(M+1.0))
80
81 def mu_lab_2(E_l, E_target, mu_target, mu_lab, mass):
82     unit_V_cm = normalize( V_cm(E_l, E_target, mu_target, mass) )
83     unit_v_prime = np.array( [ mu_lab, math.sqrt(1.0-square(mu_lab)) , 0.0] )
84     return np.dot( unit_v_prime, unit_V_cm)
85
86 def min_scattering_angle(E_l, E_target, mu_target, Q_value, A_value ):
87     energy_TAR = e_t(E_l, E_target, mu_target, A_value)
88     energy_cm = e_cm(E_l, E_target, mu_target, A_value)
89     energy_c_prime = e_c_prime(energy_TAR, Q_value, A_value)
90     ratio = energy_c_prime / energy_cm
91     if ratio > 1.0:
92         return 1.0
93     return math.sqrt(1 - energy_c_prime / energy_cm)
94
95 def D2(E_l, E_target, mu_target, mu_lab, Q_value, A_value ):
96     energy_TAR = e_t(E_l, E_target, mu_target, A_value)
97     if e_t_min( Q_value, A_value) > energy_TAR:
98         return [0.0, 0.0]
99
100     energy_cm = e_cm(E_l, E_target, mu_target, A_value)
101     energy_c_prime = e_c_prime(energy_TAR, Q_value, A_value)
102     mu_LAB_2 = mu_lab_2(E_l, E_target, mu_target, mu_lab, A_value)
103     mu_LAB_2_squared = square( mu_LAB_2 )
104     return (mu_LAB_2_squared - 1.0) + energy_c_prime / energy_cm
105
106 def energy_and_probability_pos(E_l, E_target, mu_target, mu_lab, Q_value, A_value )
107 :
108     energy_TAR = e_t(E_l, E_target, mu_target, A_value)
109     if e_t_min( Q_value, A_value) > energy_TAR:
110         #print( "returning because e_t_min > energy_TAR" )

```

```

110     return [0.0, 0.0]
111
112     energy_cm = e_cm(E_l, E_target, mu_target, A_value)
113     energy_c_prime = e_c_prime(energy_TAR, Q_value, A_value)
114     mu_LAB_2 = mu_lab_2(E_l, E_target, mu_target, mu_lab, A_value)
115     mu_lab_2_squared = square( mu_LAB_2 )
116     Dsquared = (mu_lab_2_squared - 1.0) + energy_c_prime / energy_cm
117
118     if Dsquared <= 0.0:
119         #print( "returning because Dsquared < 0.0, E_l=", E_l, " energy_c_prime=",
120             energy_c_prime, " energy_TAR=", energy_TAR )
121         return [0.0, 0.0]
122
123     if mu_LAB_2 < 0.0 and energy_c_prime <= energy_cm:
124         #print( "returning because mu_LAB_2 < 0.0 and energy_c_prime <= energy_cm"
125             )
126         return [0.0, 0.0]
127
128     energy = energy_cm*square( mu_LAB_2 + math.sqrt( Dsquared ) )
129     prob = energy / math.sqrt( energy_c_prime * Dsquared * energy_cm )
130     return [ energy, prob]
131
132 def energy_and_probability_neg(E_l, E_target, mu_target, mu_lab, Q_value, A_value )
133 :
134     energy_TAR = e_t(E_l, E_target, mu_target, A_value)
135     if e_t_min( Q_value, A_value) > energy_TAR:
136         #print( "returning because e_t_min > energy_TAR" )
137         return [0.0, 0.0]
138
139     energy_cm = e_cm(E_l, E_target, mu_target, A_value)
140     energy_c_prime = e_c_prime(energy_TAR, Q_value, A_value)
141     mu_LAB_2 = mu_lab_2(E_l, E_target, mu_target, mu_lab, A_value)
142     mu_lab_2_squared = square( mu_LAB_2 )
143     Dsquared = (mu_LAB_2_squared - 1.0) + energy_c_prime / energy_cm
144
145     if Dsquared <= 0.0:
146         #print( "returning because Dsquared < 0.0, E_l=", E_l, " energy_c_prime=",
147             energy_c_prime, " energy_TAR=", energy_TAR )
148         return [0.0, 0.0]
149
150     if mu_LAB_2 < 0.0:
151         #print( "returning because mu_LAB_2 < 0.0" )
152         return [0.0, 0.0]
153
154     if energy_cm < energy_c_prime:
155         #print( "energy_cm < energy_c_prime" )
156         return [0.0, 0.0]
157
158     energy = energy_cm*square( mu_LAB_2 - math.sqrt( Dsquared ) )
159     prob = energy / math.sqrt( energy_c_prime * Dsquared * energy_cm )
160     return [ energy, prob]

```