LA-UR-11-04656

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Title:	Derivation and Sampling of the Double-Differential Thermal Neutron Scattering Cross Section for Bound Incoherent Inelastic Scattering
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Intended for:	MCNP Documentation

Derivation and Sampling of the Double-Differential Thermal Neutron Scattering Cross Section for Bound Incoherent Inelastic Scattering

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August 16, 2011

1 Introduction

In the thermal energy region, translational, vibrational and other quantum effects affect the thermal neutron double-differential scattering cross sections. This makes the calculation of the bound thermal scattering cross section more complicated than the free scattering cross section. The cross section for bound isotopes depends on the material it is bound. The bound and free cross sections are the same at high energies, but vary below $< 4\ eV$. At thermal energies, scattering may result in either a gain or loss in neutron energy. In discussing the cross section, we are interested in both energy and angle varying continuously during these scattering events. Also, interference effects involving different atomic spacings between the target and neutron are ignored. Thus, in the discussion of scattering for bound isotopes at thermal energies, the focus is on incoherent inelastic scattering. This paper goes through the derivation of the double differential scattering cross section for incoherent inelastic scattering in terms of a scattering law, which contains the details of the scattering process. Then, a procedure for sampling the scattering law in Monte Carlo software is outlined.

2 Derivation

To examine the interactions of neutrons with atoms, we must first look at the relative size of each. The neutron diameter is on the order of a femtometer ($1\ \text{fm} = 10^{-15}$ m) whereas the diameter of an atom is on the order of an Angstrom ($1\ \mathring{A} = 10^{-10}$ m). Therefore, because the neutron is small by comparison, it can be regarded as a point-like particle. We then define the energy of the incident and scattered neutron [1] in non-relativistic

wave form in order to assess the interference effects that occur during the scattering process,

$$E = \frac{\vec{p}^{\,2}}{2m} = \frac{\hbar^2 |\underline{k}_i|^2}{2m} \text{ and } E' = \frac{\vec{p'}^{\,2}}{2m} = \frac{\hbar^2 |\underline{k}_f|^2}{2m}, \tag{1}$$

where $\vec{p}$ is the momentum vector, $\hbar$ is the modified Planck's constant and $\underline{k}$ is the wave vector. The wave vector is related to the wavelength, λ, by $|\underline{k}| = \frac{2\pi}{\lambda}$. In describing the neutron-nucleus interactions, we must consider a potential $V(\underline{r})$, where $\underline{r}$ represents the neutron position. To simplify the derivation, the so-called Born Approximation [2] is used which simplifies the determination of the wave function by using the fact that the scattering probability is small because of the small size of the neutron. The problem, however, is that the nuclear potential is strong and the Born Approximation is not valid here. To compensate for this, a modified potential, the Fermi Pseudopotential [3], is used. This fictitious potential can be used in place of the actual potential because, in our derivation, we are only interested in the scattering length, which depends only on the volume integral of the potential,

$$b = \frac{1}{\Lambda^2 kT} \int d^3r \; V^*(\underline{r}), \tag{2}$$

where b is the scattering length, Λ is the de Broglie wavelength, kT is the ambient temperature and $V^*(\underline{r})$ is the Fermi Pseudopotential. The de Broglie wavelength is commonly expressed as $\Lambda = \hbar\sqrt{\frac{2\pi}{mkT}}$. Substituting this definition of the de Broglie wavelength into Eq.(2) yields

$$b = \frac{m}{2\pi\hbar^2} \int d^3r \; V^*(\underline{r}). \tag{3}$$

Because the de Broglie wavelength is larger than the length scale of the neutron-nucleus interaction, it cannot resolve the structure of the bound material. To the neutron, the potential is just an impulse and the interaction can be treated as a delta function, where

$$\int d^3r \; \delta(\underline{r}) = 1. \tag{4}$$

Hence, by Eq.(4), we conclude that

$$V^*(\underline{r}) = \frac{2\pi\hbar^2}{m} \; b \; \delta(\underline{r}). \tag{5}$$

For a target with N nuclei, Eq.(5) is expressed as

$$V^*(\underline{r}) = \frac{2\pi\hbar^2}{m} \sum_{i=1}^{N} b_i \; \delta(\underline{r} - \underline{R}_i), \tag{6}$$

where $\underline{r}$ is the neutron position and $\underline{R}_i$ is the position of the i^{th} nucleus. Next, the double differential scattering cross section is defined as the number of neutrons scattered into a solid angle interval $(\Omega, \Omega + d\Omega)$ with energy transfer interval $(E, E + dE)$. In other words,

$$\sigma(E \to E', \Omega \to \Omega') = \frac{\text{flux of neutrons in the solid angle } d\Omega \text{ per unit energy}}{\text{flux of incoming neutrons}}. \quad (7)$$

For this analysis, we consider only plane wave solutions for the incident and scattered neutrons.

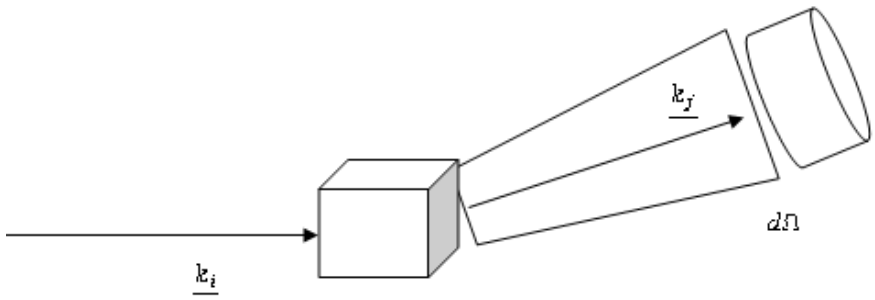

Figure 1: Wave vector pre- and post-collision

The momentum transfer is expressed by

$$\hbar\kappa = \hbar\underline{k}_i - \hbar\underline{k}_f, \quad (8)$$

and the energy transfer is expressed by

$$\hbar\omega = \frac{\hbar^2}{2m}(\underline{k}_i^2 - \underline{k}_f^2). \quad (9)$$

Considering scatter from an initial state $\lambda_i\underline{k}_i$ to a final state $\lambda_f\underline{k}_f$, the double differential scattering cross section of Eq.(7) is expressed as

$$\sigma(E \to E', \Omega \to \Omega') = \frac{P_{\underline{k}_i\lambda_i \to \underline{k}_f\lambda_f}}{\phi_0 \; d\Omega}, \quad (10)$$

where $P_{\underline{k}_i\lambda_i \to \underline{k}_f\lambda_f}$ is the transition probability from the initial state to the final state and ϕ_0 is the incoming flux. The incoming flux is a ratio of the neutron velocity through a volume. From Fig.1, we consider a cubic target with volume V_{cube} [4]. Then, the incoming flux is expressed as

$$\phi_0 = \frac{\hbar\underline{k}_i}{V_{\text{cube}}m}. \quad (11)$$

The transition probability is found using Fermi's Golden Rule, which determines the transition rate from one energy eigenstate of a quantum system into a continuum of energy eigenstates. Without the details of Fermi's Golden Rule, the transition probability is expressed as

$$P_{\underline{k}_i\lambda_i\rightarrow\underline{k}_f\lambda_f} = \frac{2\pi}{\hbar}\left|\left\langle \underline{k}_f\lambda_f\left|V^*\right|\underline{k}_i\lambda_i\right\rangle\right|^2 \rho_{\underline{k}_f}(E)\ \delta(\hbar\omega + E_{\lambda_i} - E_{\lambda_f}), \tag{12}$$

In Eq.(12), $\rho_{\underline{k}_f}(E)$ represents the density of final quantum states. It is the number of final states with momentum $\underline{k}_f$ within $d\Omega$ per unit energy range. The number of final neutron states with momentum $\underline{k}_f$ within $d\Omega$ with energy between E' and $E' + dE'$ is given by $\rho_{\underline{k}_f}(E)dE'$. It is the ratio of the number of wavevector points within the unit cell volume,

$$\rho_{\underline{k}_f}(E)dE' = \frac{\underline{k}_f^2\ d\underline{k}_f\ d\Omega}{(2\pi)^3}V_{\text{cube}}. \tag{13}$$

Using Eq.(1), the derivative of E' with respect to $\underline{k}_f$ is determined,

$$dE' = \frac{\hbar^2\underline{k}_f}{m}\ d\underline{k}_f. \tag{14}$$

Substituting Eq.(14) into Eq.(13) and simplifying yields

$$\rho_{\underline{k}_f}(E) = \frac{V_{\text{cube}}}{(2\pi)^3}\frac{m\underline{k}_f}{\hbar^2}d\Omega. \tag{15}$$

In Eq.(12), the delta function ensures that energy is conserved during the scattering process. Substituting Eq. (15) into Eq. (12) and then substituting this result along with Eq. (11) into Eq.(10) yields

$$\sigma(E\rightarrow E', \Omega\rightarrow\Omega') = V_{\text{cube}}^2\left(\frac{m}{2\pi\hbar^2}\right)^2\frac{\underline{k}_f}{\underline{k}_i}\left|\left\langle \underline{k}_f\lambda_f\left|V^*\right|\underline{k}_i\lambda_i\right\rangle\right|^2. \tag{16}$$

Next, the matrix element in Eq. (16) is rewritten in integral form,

$$\left\langle \underline{k}_f\lambda_f\left|V^*\right|\underline{k}_i\lambda_i\right\rangle = \int \psi^*_{\underline{k}_f}\ \phi^*_{\lambda_f}\ V^*\ \psi_{\underline{k}_i}\ \phi_{\lambda_i}\ d^3r\ d^{3N}R, \tag{17}$$

In Eq. (17), $d^{3N}R = d^3R_1\ d^3R_2\cdots d^3R_N$. The neutron wavefunctions, $\psi_{\underline{k}_f}$ and $\psi_{\underline{k}_i}$ are expressed as

$$\psi_{\underline{k}_f} = \frac{1}{\sqrt{V_{\text{cube}}}}e^{i\underline{k}_f\cdot\underline{r}} \text{ and } \psi_{\underline{k}_i} = \frac{1}{\sqrt{V_{\text{cube}}}}e^{i\underline{k}_i\cdot\underline{r}}. \tag{18}$$

Substituting Eq. (18) into Eq. (17) yields

$$\left\langle \underline{k}_f \lambda_f \left| V^* \right| \underline{k}_i \lambda_i \right\rangle = \frac{1}{V_{\text{cube}}} \left\langle \lambda_f \left| V^* \right| \lambda_i \right\rangle e^{i\underline{\kappa}\cdot\underline{r}}, \tag{19}$$

where κ is defined by Eq. (8). Substituting Eq. (19) into Eq. (16) and simplifying yields

$$\sigma(E \to E', \Omega \to \Omega') = \frac{\underline{k}_f}{\underline{k}_i} \left| \sum_{i=1}^{N} b_i \left\langle \lambda_f \left| \int_{-\infty}^{\infty} \delta(\underline{r} - \underline{R}_i) e^{i\underline{\kappa}\cdot\underline{r}} \, d\underline{r} \right| \lambda_i \right\rangle \right|^2 \delta(\hbar\omega + E_{\lambda_i} - E_{\lambda_f}). \tag{20}$$

This equation can be simplified further by taking the Fourier Transform of the delta function,

$$\int_{-\infty}^{\infty} \sum_{i=1}^{N} \delta(\underline{r} - \underline{R}_i) e^{i\underline{\kappa}\cdot\underline{r}} \, d\underline{r} = \sum_{i=1}^{N} e^{i\underline{\kappa}\cdot\underline{R}_i}. \tag{21}$$

Substituting Eq. (21) into Eq. (20) yields

$$\sigma(E \to E', \Omega \to \Omega') = \frac{\underline{k}_f}{\underline{k}_i} \left| \left\langle \lambda_f \left| \sum_{i=1}^{N} b_i \, e^{i\underline{\kappa}\cdot\underline{R}_i} \right| \lambda_i \right\rangle \right|^2 \delta(\hbar\omega + E_{\lambda_i} - E_{\lambda_f}). \tag{22}$$

In Eq.(22), consideration must be given to the fact that there is a range of initial states that can be used with weight p_λ. Also, averages of nuclear spin and orientation must be considered. Hence, Eq.(22) is rewritten as

$$\sigma(E \to E', \Omega \to \Omega') = \overline{\frac{\underline{k}_f}{\underline{k}_i} \sum_{\lambda_i} p_{\lambda_i} \left| \left\langle \lambda_f \left| \sum_{i=1}^{N} b_i \, e^{i\underline{\kappa}\cdot\underline{R}_i} \right| \lambda_i \right\rangle \right|^2 \delta(\hbar\omega + E_{\lambda_i} - E_{\lambda_f})}. \tag{23}$$

Next, the delta function is expressed in integral form,

$$\delta(\hbar\omega + E_{\lambda_i} - E_{\lambda_f}) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \; \exp\left(-it \frac{\hbar\omega + E_{\lambda_i} - E_{\lambda_f}}{\hbar} \right). \tag{24}$$

Substituting Eq.(24) into Eq.(23), suppressing the average bar and rearranging yields

$$\sigma(E \to E', \Omega \to \Omega') = \frac{\underline{k}_f}{\underline{k}_i} \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \; e^{-i\omega t} \sum_{\lambda_i \lambda_f} p_{\lambda_i} C_1 \; C_2, \tag{25}$$

where

$$C_1 = \left\langle \lambda_f \left| e^{it\frac{E\lambda_f}{\hbar}} \sum_{i'=1}^{N} b_{i'} \; e^{i\underline{\kappa}\cdot\underline{R}'_i} e^{-it\frac{E_{\lambda_i}}{\hbar}} \right| \lambda_i \right\rangle, \tag{26}$$

$$C_2 = \left\langle \lambda_i \left| \sum_{i=1}^{N} b_{i^*} \; e^{-i\underline{\kappa}\cdot\underline{R}_i} \right| \lambda_f \right\rangle. \tag{27}$$

The completeness relation states

$$\sum_{\lambda} |\lambda\rangle\langle\lambda| = 1 \tag{28}$$

Using this in Eq.(25) yields

$$\sigma(E \to E', \Omega \to \Omega') = \frac{\underline{k}_f}{\underline{k}_i} \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \; e^{-i\omega t} \sum_{i,i'} b_{i^*} b_{i'} \left\langle e^{-i\underline{\kappa}\cdot\underline{R}_i} e^{i\underline{\kappa}\cdot\underline{R}_{i'}} \right\rangle. \tag{29}$$

In Eq.(29), the following relations apply:

$$\overline{b_{i^*} b_{i'}} = \left|\bar{b}\right|^2 + \delta_{i,i'} \left(\overline{|b|^2} - \left|\bar{b}\right|^2 \right), \tag{30}$$

$$b_{\text{coh}} = \bar{b}, \tag{31}$$

$$b_{\text{inc}} = \sqrt{\overline{|b|^2} - |\bar{b}|^2}, \tag{32}$$

$$\sigma = 4\pi b^2. \tag{33}$$

Substituting Eqs.(30) through (33) into Eq.(29) yields

$$\sigma(E \to E', \Omega \to \Omega') = \frac{\underline{k}_f}{\underline{k}_i} \frac{1}{2\pi\hbar} \left[\frac{\sigma_{\text{coh}}}{4\pi} + \delta_{i,i'} \frac{\sigma_{\text{inc}}}{4\pi} \right] \sum_{i,i'} \int_{-\infty}^{\infty} dt \; e^{-i\omega t} \left\langle e^{-i\underline{\kappa}\cdot\underline{R}_i} e^{i\underline{\kappa}\cdot\underline{R}_{i'}} \right\rangle. \tag{34}$$

By Eq.(1), the wave vector is related to energy by

$$\frac{\underline{k}_f}{\underline{k}_i} = \sqrt{\frac{E'}{E}}, \tag{35}$$

where E is the initial energy and E' is the scattered energy. Because interference effects are insignificant in inelastic scattering, we ignore the coherent term. Applying this and Eq.(35) to Eq.(34) yields

$$\sigma(E \to E', \Omega \to \Omega') = \frac{\sigma_{\text{inc}}}{4\pi\hbar}\sqrt{\frac{E'}{E}}\frac{1}{2\pi}\int_{-\infty}^{\infty} dt\ e^{-i\omega t}\left\langle e^{-i\underline{\kappa}\cdot\underline{R}_i}e^{i\underline{\kappa}\cdot\underline{R}_{i'}}\right\rangle. \tag{36}$$

Next, a relation between $\left\langle e^{-i\underline{\kappa}\cdot\underline{R}_i}e^{i\underline{\kappa}\cdot\underline{R}_{i'}}\right\rangle$ and a self-correlation function is determined,

$$\left\langle e^{-i\underline{\kappa}\cdot\underline{R}_i}e^{i\underline{\kappa}\cdot\underline{R}_{i'}}\right\rangle = e^{i\underline{\kappa}\cdot\underline{r}}G\left(\underline{r},t\right), \tag{37}$$

where $G\left(\underline{r},t\right)$ is the probability that, given a nucleus at the origin at time zero, the same nucleus will be in $d\underline{r}$ about $\underline{r}$ at time t. Substituting Eq.(37) into Eq.(36) yields

$$\sigma(E \to E', \Omega \to \Omega') = \frac{\sigma_{\text{inc}}}{4\pi\hbar}\sqrt{\frac{E'}{E}}\frac{1}{2\pi}\int_{-\infty}^{\infty} dt\ e^{i(\underline{\kappa}\cdot\underline{r}-\omega t)}G\left(\underline{r},t\right). \tag{38}$$

Next, we simplify Eq.(38) by using Fourier Transforms. This is done by defining the intermediate scattering function [5] $\chi(\underline{\kappa},t)$, which is the spatial Fourier Transform of $G(\underline{r},t)$, and the dynamic structure factor $S(\underline{\kappa},\omega)$, which is the time Fourier Transform of $G(\underline{r},t)$,

$$\chi(\kappa,t) = \int d\underline{r}\ e^{i\underline{\kappa}\cdot\underline{r}}G(\underline{r},t), \tag{39}$$

$$S(\underline{\kappa},\omega) = \frac{1}{2\pi}\int dt\ e^{-i\omega t}\chi(\underline{\kappa},t). \tag{40}$$

Substituting Eqs.(39) and (40) into Eq.(38) yields

$$\sigma(E \to E', \Omega \to \Omega') = \frac{\sigma_{\text{inc}}}{4\pi\hbar}\sqrt{\frac{E'}{E}}S(\underline{\kappa},\omega). \tag{41}$$

Next, we examine further the structure factor $S(\underline{\kappa},\omega)$ by applying the detailed balance relation to Eq.(41). Detailed balance always holds in a close and isolated system. The detailed balance relation is

$$\phi(E)\sigma(E \to E', \Omega \to \Omega') = \phi(E')\sigma(E' \to E, -\Omega' \to -\Omega), \tag{42}$$

where the flux, $\phi(E)$, is the Maxwellian flux,

$$\phi(E) = \frac{E}{(kT)^2} \exp\left(-\frac{E}{kT}\right). \tag{43}$$

Substituting Eq.(41) and (43) into Eq.(42) yields

$$\frac{E}{(kT)^2} \exp\left(-\frac{E}{kT}\right) \frac{\sigma_{\text{inc}}}{4\pi\hbar} \sqrt{\frac{E'}{E}} S(\underline{\kappa}, \omega) = \frac{E'}{(kT)^2} \exp\left(-\frac{E'}{kT}\right) \frac{\sigma_{\text{inc}}}{4\pi\hbar} \sqrt{\frac{E}{E'}} S(-\underline{\kappa}, -\omega). \tag{44}$$

Simplifying Eq.(44) yields

$$\exp\left(\frac{E' - E}{2kT}\right) S(\underline{\kappa}, \omega) = \exp\left(\frac{E - E'}{2kT}\right) S(-\underline{\kappa}, -\omega). \tag{45}$$

We can define a dimensionless parameter that describes the energy transfer, β,

$$\beta = \frac{E - E'}{kT}. \tag{46}$$

Substituting Eq.(46) into Eq.(45) yields

$$S(\underline{\kappa}, \omega) = e^{\beta} S(-\underline{\kappa}, -\omega). \tag{47}$$

One notices that $S(\underline{\kappa}, \omega)$ is an even function of e^{β}. Likewise, we can define a dimensionless parameter, α, that describes the momentum transfer,

$$\alpha = \frac{E + E' - 2\mu\sqrt{EE'}}{AkT}. \tag{48}$$

Next, a change of variables is performed between $S(\underline{\kappa}, \omega)$ and $S(\alpha, \beta)$, keeping an exponential term for symmetry,

$$S(\underline{\kappa}, \omega) = \exp\left(-\frac{\beta}{2}\right) \left|\frac{d\beta}{d\omega}\right| S(\alpha, \beta). \tag{49}$$

To solve Eq.(49), we note that β and ω are related by

$$\beta = \frac{\hbar\omega}{kT}. \tag{50}$$

Thus,

$$\left|\frac{d\beta}{d\omega}\right| = \frac{\hbar}{kT}. \tag{51}$$

Substituting Eq.(51) into Eq.(49) yields

$$S(\underline{\kappa},\omega) = \frac{\hbar}{kT}\exp\left(-\frac{\beta}{2}\right)S(\alpha,\beta). \tag{52}$$

Substituting Eq.(52) into Eq.(41) yields the double-differential thermal scattering cross section in terms of the scattering law, $S(\alpha,\beta)$,

$$\sigma(E\to E',\Omega\to\Omega') = \frac{\sigma_{\text{inc}}}{4\pi kT}\sqrt{\frac{E'}{E}}\exp\left(-\frac{\beta}{2}\right)S(\alpha,\beta). \tag{53}$$

Expressing the angle in terms of μ in Eq.(53) is done by integrating over the azimuthal angle, 2π,

$$\boxed{\sigma(E\to E',\mu) = \frac{\sigma_{\text{inc}}}{2kT}\sqrt{\frac{E'}{E}}\exp\left(-\frac{\beta}{2}\right)S(\alpha,\beta)}. \tag{54}$$

3 Sampling the Scattering Law

Unlike sampling for the free gas, where a rejection scheme is implemented because of the presence of relative speed, the sampling for $S(\alpha,\beta)$ is more direct because α and β can be directly determined. The following procedure [6,7] is likely the method used in pre-processing codes such as NJOY to determine distribution functions for energy and angle. To sample in terms of the variables α and β, the first step is to convert the double-differential thermal scattering cross section from E, E' and μ to α and β. This is done using a transformation matrix,

$$\underline{\underline{B}} = \begin{bmatrix} \frac{d\alpha}{dE} & \frac{d\alpha}{d\mu} \\ \frac{d\beta}{dE} & \frac{d\beta}{d\mu} \end{bmatrix}. \tag{55}$$

The change of variables is of the form

$$\sigma(E\to E',\mu) = \sigma(\alpha,\beta)\ \det(\underline{\underline{B}}), \tag{56}$$

where $\det(\underline{\underline{B}})$ is the determinant of the transformation matrix $\underline{\underline{B}}$. Using Eqs.(46) and (48), we know

$$\frac{d\alpha}{dE} = \frac{1-\mu\sqrt{\frac{E'}{E}}}{AkT} \text{ and } \frac{d\alpha}{d\mu} = \frac{-2\sqrt{EE'}}{AkT}, \tag{57}$$

$$\frac{d\beta}{dE} = \frac{1}{kT} \text{ and } \frac{d\beta}{d\mu} = 0. \tag{58}$$

Substituting Eqs.(57) and (58) into Eq.(55) and taking the determinant yields

$$\det(\underline{\underline{B}}) = \frac{2\sqrt{EE'}}{A(kT)^2}. \tag{59}$$

Substituting Eq.(59) into Eq.(56) and solving for $\sigma(\alpha, \beta)$ yields

$$\sigma(\alpha, \beta) = \frac{A(kT)^2}{2\sqrt{EE'}}\ \sigma(E \to E', \mu). \tag{60}$$

Substituting Eq.(54) into Eq.(60) yields

$$\sigma(\alpha, \beta) = C \exp\left(-\frac{\beta}{2}\right) S(\alpha, \beta), \tag{61}$$

where

$$C = \frac{AkT}{4E}\sigma_{\text{inc}} = const. \tag{62}$$

To get the scattering cross section as a function of incident energy, E, an integration over Eq.(61) is performed,

$$\sigma_s(E) = \int_{\beta_-}^{\beta_+}\int_{\alpha_-}^{\alpha_+} d\alpha\ d\beta\ \sigma(\alpha, \beta). \tag{63}$$

The scattered neutron energy equal to zero, $E' = 0$, corresponds to the maximum value of β and the minimum value is when the incident and scattered neutron energies are equal. Thus,

$$\beta_+ = \frac{E}{kT}, \tag{64}$$

$$\beta_- = 0. \tag{65}$$

Likewise, the maximum momentum transfer occurs for reverse scattering (when $\mu = -1$) and the minimum momentum transfer occurs for forward scattering (when $\mu = 1$). Applying this to Eq.(48) yields

$$\alpha_+ = \frac{\sqrt{E} + \sqrt{E'}}{AkT}, \tag{66}$$

$$\alpha_- = \frac{\sqrt{E} - \sqrt{E'}}{AkT}. \tag{67}$$

In the sampling procedure, $\sigma(\alpha,\beta)$ is divided by the total scattering cross section at the initial energy. Doing this and rewriting yields

$$\frac{\sigma(\alpha,\beta)}{\sigma_s(E)} = \left[\frac{\int_{\alpha_-}^{\alpha_+} d\alpha\ \sigma(\alpha,\beta)}{\sigma_s(E)}\right] \cdot \left[\frac{\sigma(\alpha,\beta)}{\int_{\alpha_-}^{\alpha_+} d\alpha\ \sigma(\alpha,\beta)}\right], \tag{68}$$

where

$$\left[\frac{\int_{\alpha_-}^{\alpha_+} d\alpha\ \sigma(\alpha,\beta)}{\sigma_s(E)}\right] = M(\beta\ |E), \tag{69}$$

$$\left[\frac{\sigma(\alpha,\beta)}{\int_{\alpha_-}^{\alpha_+} d\alpha\ \sigma(\alpha,\beta)}\right] = C(\alpha\ |\ \beta, E). \tag{70}$$

In Eqs.(69) and (70), $M(\beta\ |E)$ is the probability that a downscatter will result in an energy change of less than β and $C(\alpha\ |\ \beta, E)$ is the probability that a downscatter will result in a momentum-squared change of less than α. In sampling, the integral of the distributions (69) and (70) are determined and set to random numbers, ζ and ξ,

$$\hat{M}(\beta\ |E) = \int_0^{\beta} d\beta\ M(\beta\ |E) = \zeta, \tag{71}$$

$$\hat{C}(\alpha\ |\ \beta, E) = \int_{\alpha_-}^{\alpha_+} d\alpha\ C(\alpha\ |\ \beta, E) = \xi. \tag{72}$$

The problem in storing these pdfs is that $\hat{C}(\alpha\ |\ \beta, E)$ is a three-dimensional matrix. To simplify this, a function is defined,

$$F(\alpha,\beta) = \int_0^{\alpha} d\alpha \ \exp\left(-\frac{\beta}{2}\right) \ S(\alpha,\beta). \tag{73}$$

Using Eq.(73), Eqs. (71) and (72) are rewritten,

$$\hat{M}(\beta\ |E) = \frac{\int_0^{\beta} d\beta \ [F(\alpha_+,\beta) - F(\alpha_-,\beta)]}{\int_0^{E/kT} d\beta \ [F(\alpha_+,\beta) - F(\alpha_-,\beta)]}, \tag{74}$$

$$\hat{C}(\alpha \mid \beta, E) = \frac{F(\alpha,\beta) - F(\alpha_-,\beta)}{F(\alpha_+,\beta) - F(\alpha_-,\beta)}. \tag{75}$$

Since Eq.(75) is a three-dimensional matrix, we choose not to store it. Instead, we store $F(\alpha,\beta)$, a two-dimensional matrix, and solve for α from

$$F(\alpha,\beta) = \xi F(\alpha_+,\beta) + (1-\xi)F(\alpha_-,\beta). \tag{76}$$

So, E is given and β is determined from $\hat{M}(\beta\ |E)$. Then, α is determined from $F(\alpha,\beta)$. The same procedure is done for upscattering by redefining β as a positive quantity using detailed balance, i.e.,

$$S(-\alpha,-\beta) = S(\alpha,\beta). \tag{77}$$

To summarize, β is found by storing $\hat{M}(\beta\ |E)$ for both upscattering and downscattering and then α is found by storing $F(\alpha,\beta)$. All three matrices are two-dimensional.

4 Summary

In the thermal energy range, quantum effects are significant to the scattering physics, which complicates the cross-section derivation. The derivation of the double-differential thermal scattering cross section for bound incoherent inelastic scattering is a function of many quantum effects. An approximation to the wavefunction was made by defining an alternate potential, which did not change the scattering problem. Also, a symmetric form of the scattering law was used for the double-differential cross section through detailed balance.

The sampling method outlined (proposed by Kady in 1966) is an effective way to determine discrete exiting energies and angles from the initial energy. By defining an alternate

function, $F(\alpha, \beta)$, fewer data are stored in the sampling while preserving the details of initial energy, angle and exiting energy. A procedure similar to this is what is used in pre-processing codes for the creation of cross-section data.

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