Discus: A computer program for the calculation of multiple scattering effects in inelastic neutron scattering experiments

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DISCUSS:

A Computer Program For the Calculation
Of Multiple Scattering Effects in Inelastic
Neutron Scattering Experiments

by

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ABSTRACT

A computer program is described which enables the ratio of once-scattered to twice-
scattered neutrons detected in an inelastic neutron scattering experiment to be calculated.
The program may be used for any sample for which the scattering law is of the form
$S(q, w)$.

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Harwell

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/MWN

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1. Introduction

In any neutron scattering experiment the quantity of interest is the flux of scattered neutrons that have only been scattered once. Unfortunately the detected neutron flux contains contributions from neutrons scattered two or more times and therefore a correction has to be made for the presence of second and higher order scattered neutron fluxes.

It is easily shown that the multiple scattering correction is important. The cross-section for twice scattered neutrons is essentially a self convolution (over $Q$ and $\omega$) of the once scattered cross-section, so it is a 'smoothed out' version of the latter in both $Q$ and $\omega$ space. Where one is only interested in a $Q$ dependent cross-section and where this cross-section is already isotropic (e.g. $\delta(Q)$ for solid vanadium), obviously the multiple scattering will be approximately isotropic too and will be a relatively constant proportion of the once scattered cross-section. Where there is any sort of anisotropy in the cross-section (in $Q$ or $\omega$ space), then the 'smoothing out' effect will produce a second-order cross-section which is not a constant fraction of the first-order cross-section. Moreover, where the first order cross-section is small (compared to the average cross-section) there is the likelihood of the second scattered flux exceeding the first scattered flux. This is illustrated in Fig. 1 where the $J_1$ scattered ($J_1$ - solid lines) and $J_2$ scattered fluxes ($J_2$ - dashed lines) for an incoherently scattering, simple-diffusive liquid model is shown (the degrees refer to the neutron scattering angle). $J_1$ is strongly $Q$ and $\omega$-dependent but, as predicted, $J_2$ is much less so - being roughly 10% of the value of $J_1$ for $90^\circ$ scattering. This results in $J_2$ becoming larger than $J_1$ (for $\theta = 20^\circ$) at low energy transfers. A fuller account of the effects of multiple scattering in a diffusive system is given in 5.

These corrections may be calculated in one of two ways: by direct integration of the neutron transport equation (see for example P. Schofield in ref. 7)

$$
\phi(E, E', Q) = \int \frac{dE'}{\cos \theta} \int dQ' E' \frac{d\phi(E, E', Q')}{dQ'} x \exp (-\mu Q^2) \frac{E}{E'} \frac{E'}{Q'^2} \frac{1}{\cos \theta}
$$

$$
\left[ \int \phi(E, E', Q') \sin Q dQ \right] = \text{no. of neutrons with energies between } E \text{ and } E', \text{ crossing per sec. a surface area } dA \text{ oriented perpendicular to } \hat{Q} \text{ at } \hat{Q} \text{ while moving in a direction within } d\theta \text{ about } \hat{Q}.
$$

- 1 -
\( n_0 = \text{atomic density} \)

\[ \text{2003.5:2.52) microscopic d.d.c.} \]

or by Monte Carlo simulation technique.

Most previous calculations (ref. 1, 2, 3, 4) have been restricted to infinite plane slab samples, since it is only with such a geometry that the solution of equation 1.1 becomes tractable.

Recently, calculations involving more realistic, finite samples have been made by Bishop et al. (ref. 5) using a Monte Carlo program 'MC'. This program however includes calculation of up to tenth order scattering, which results in somewhat longer running times.

It was for this reason that a program capable of a fast calculation of the first and second order spectra was written.

This program possesses one additional feature. It is not known enough to know what proportion of the observed spectrum has been scattered once. What is generally required is the flux of once scattered neutrons that would have been observed if:

(a) there were no absorption in the sample

(b) once scattered, the neutron would emerge without further re-scattering or absorption.

and hence a hypothetical flux \( J_1 \) has been calculated with these assumptions. (Notice that \( J_1 = J_1 \) since \( J_1 \) is the flux of observed once scattered neutron). The calculation of \( J_1 \) enables the neutron scattering data to be corrected for multiple scattering, attenuation due to re-scattering, and absorption all at once. To do this one multiplies the observed flux by the ratio \( R = J_1 / (J_1 + J_2) \).

It is, of course, necessary to provide a complete set of values for the double differential neutron cross-section for all incident neutron energies. To do this the user must supply a matrix of values for the function \( S'(Q, \omega) \) defined as

\[ \frac{d^2 \sigma}{dQ \, d\omega} = \frac{Q}{2 \pi \hbar} \, S'(Q, \omega) \]

Note that the \( S'(Q, \omega) \) referred to in equation 1.2 is only identical to the dynamical structure factor \( S(Q, \omega) \) if the sample is a perfectly coherent scatterer. In general \( S'(Q, \omega) \) will be a linear combination of the coherent and incoherent dynamical structure factors.
\[ S'(Q,\omega) = \frac{1}{3} \left[ C_{cw} S(Q,\omega) + C_{iw} S_{s}(Q,\omega) \right] \]

Only values of \( S'(Q,\omega) \) for positive \( \omega \) should be supplied. Values of \( S'(Q,\omega) \) for negative \( \omega \) are calculated by the relationship 1.4.

\[ S'(Q,-\omega) = \exp \left[ \frac{-\hbar}{\beta_{0}} \right] \cdot S'(Q,\omega) \]

(b is the energy gained by the neutron at the scattering event).

The data for the double differential cross-section is supplied in a form which assumes

\[ S(Q,\omega) = S(Q,\omega) \]

and hence the program will be of use where the samples are liquids, amorphous solids or biological materials.

The program makes no attempt to provide 'models' for the function \( S'(Q,\omega) \); the user must supply the values of \( S'(Q,\omega) \) over as wide a range of \( Q \) and \( \omega \) as possible. In practice \( Q_{\max} \) should be greater than \( 2 \beta_{0} \) and preferably greater than \( 5 \beta_{0} \). In addition the user must supply an array containing values of the energy dependent scattering cross-section.

The program provides for three types of sample geometry; an infinite flat plate, a finite flat plate or a finite length cylinder. The infinite flat plate is included for comparison with other multiple scattering programs; its only virtue being the slight reduction in computer time necessary to do the calculations.

2. Theory

In a simple 'analogue' Monte Carlo simulation a neutron history is followed while neutron events are sampled in a way designed to exactly parallel nature. Because of this a great deal of computing time is wasted on neutrons which either are not scattered within the sample or which, if scattered, do not enter a detector.

In 'DISCUS' every calculation is used by forcing the neutron (where necessary) into useful trajectories, and then correcting for this by assigning a suitable statistical weight to the neutron. Further economy is effected by not only 'forcing' a neutron into a detector, but also into each energy bin of the detector. This means that the final results in adjacent energy channels are not totally uncorrelated.

The first and second order scattered neutron fluxes are calculated independently. The nomenclature is shown in Fig. 2.

1st Order: \[ J \]

The path length (l) travelled by each incident neutron (l = \( \beta_{l} \) in Fig. 2).
within the specimen is sampled according to the distribution:

\[ P(i) = \frac{\frac{\text{exp}[-\frac{2}{\xi}j]}{1 - \text{exp}[-\frac{2}{\xi}]} }{[1 - \text{exp}[-2\xi]]} \]

where \( 0 \leq i \leq D \), \( I_r(k_0) \) is the energy dependent total cross-section and \( P(i) \) is the probability (per unit length) of a distance \( i \) being chosen. For the infinite flat plate \( D \) is constant for every incident neutron. For the finite sample geometries the point at which the neutron enters the specimen is sampled (with a square distribution - the incident beam is assumed to be uniform) and in general the value of \( D \) will not be the same for each neutron.

The neutron history is then assigned a weight \( W_n \) equal to \( 1 - \text{exp}[-2\xi] \) to compensate for the truncated distribution. This distribution (eq. 2.1) is achieved by setting

\[ f = \ln[1 - \xi (1 - \text{exp}[-2\xi])] \]

where \( \xi \) is a pseudorandom number, 0\leq\xi\leq1.

Having sampled the position of the neutron's first event \( x_1 \), this is deemed to be a scattering event and \( W_n \) is multiplied by a further compensating weight \( c_1(k_0)/c_1(k_0) \).

The direction of the neutron after the scattering event is 'forced' to be that required to reach the detector and a final weight \( W_0(E) \) is added to each energy channel of the detector spectrum:

\[ W_0(E) = A_1 B_1 C_1 D_1 \]

where

\[ A_1 = 1 - \text{exp}[-2\xi k_0 D] \]

\[ B_1 = \frac{c_1(k_0)}{c_1(k_0)} \]

\[ C_1 = \frac{d^2\sigma E d\Omega}{2\pi 
\frac{I_r (k_0)}{I_r (k_0)}} \]

\[ D_1 = e^{-2\xi k_0 D} \]

e to compensate for restricting \( x_1 \) to lie within the sample

e to compensate for restricting the first event to be a scattering event

e to compensate for the neutron to be scattered at \( x_1 \) into unit solid angle about the direction \( h_1 \), with energy change \( \frac{\Delta E}{E} = \frac{\Delta E}{E} (h_1^2 - k_0^2) \)

e to compensate for assuming the neutron to have passed from \( x_1 \) to the sample boundary without another event.
\( J_n \) is calculated by the same procedure by setting \( C_0 = 0 \) and \( D_0 = 1 \).

2nd Order: \( J_2 \)

In calculating the flux of twice scattered neutrons, the procedure is similar to that of the once scattered flux except that another scattering event is included. The procedure is as follows:

1. Sample the position at which each neutron strikes the sample. (A constant in the case of the infinite plane slab).
2. Sample the first event position \( f_1 \) restricting this to be within the sample.
3. Sample a scattering event selecting \((Q_1, \omega_1)\) with a square distribution in \( Q - \omega \) space, in which \( Q \) is chosen from the continuum \( Q_{MIN} < Q < Q_{MAX} \), and \( \omega \) is chosen from the values \( \omega = I \cdot \Delta \omega \) where integer \( I \) is \( 0 < I < (2nN-1) \). From the \((Q, \omega)\) values calculate the new momentum \( k_2 \).
4. Having calculated the distance \( D_1 \), the distance along \( k_1 \) from \( f_1 \) to the sample boundary, a second scattering event position \( r_2 \) is sampled with the restriction that \( r_2 \) is within the sample.
5. The neutron is now 'forced' to scatter into the detector with a series of weights \( W_{n}(E) \) are calculated and added to each energy bin.

Thus the final weight for the twice scattered neutron flux added to the energy bin \( 'E' \) is:

\[
W_n(E) = A_2 \cdot E_2 \cdot C_2 \cdot D_2 \cdot E_2 \cdot F_2
\]

\[
A_2 = 1 - \exp \left[ -2 \cdot (k_2) D \right]
\]

to compensate for restricting \( r_2 \) to lie within the sample.

\[
B_2 = \frac{\sigma(k_2) \cdot S(Q_1, \omega_1)}{4\pi Q_1 \Delta \omega \Delta Q_1}
\]

to compensate for restricting the first event to be a scattering event, with event parameters \( Q_1, \omega_1 \).

\[
C_2 = 1 - \exp \left[ -E \cdot (k_2) D' \right]
\]

to compensate for restricting \( r_2 \) to lie within the sample.
\[ D_2 = \frac{a}{b} \left( k_2 \right) \]

\[ f_2 = \exp \left[ -3 \left( k_2 \right)^2 \right] \]

To compensate for restricting the 2nd event to be a scattering event.

To compensate for restricting the neutron to be scattered at \( R_2 \) into unit solid angle about \( \theta \) with energy change \( -\frac{E}{k_2} (k_2^2 - k_1^2) \).

To compensate for assuming the neutron to have passed from \( R_2 \) to the boundary of the sample without another event.

For both the once and twice scattered neutron calculations it should be noted that at the first scattering event a weight is calculated for every energy channel in the detector spectrum. Since adjacent energy channels are effectively 'sharing' a common neutron history, they are not statistically independent. The only result of this effect is that the errors in the final spectra for \( J_1 \), \( J_2 \) or \( J_3 \) cannot be obtained from the 'scatter' of neighbour points. The error may be obtained by repeating the program (with different random number generators) and noting the deviation of the results. An example is shown in Fig.1 (see also 3).

Some explanation should be given of the choice of a square distribution sampling for \( \langle Q, u \rangle \) at the first event point of the \( J_2 \) calculation. If the program were to sample the new energy direction values for the neutron in a strictly analogue fashion (i.e. Prob. of \( \Delta = A \langle Q, u \rangle - \langle Q, u \rangle \), \( A \) being a constant) it would mean that in liquid samples, for example, virtually all of the first scattering events would be quasi-elastic \((q.e.)\) events. This would result in very good statistics for the q.e.-q.e. double scattering processes, but poor inelastic - q.e. and very poor inelastic - inelastic statistics. By using a square distribution in the sampling of \( \langle Q, u \rangle \) the balance is restored, and a reasonably uniform accuracy is produced over the whole energy spectrum.

The weighting factor \( \sigma \langle Q, u \rangle / \sigma \langle Q, u \rangle \) in the square sampling arises from the fact that:

\[ \frac{\sigma}{\sigma \langle Q, u \rangle} = \frac{\sigma}{\sigma \langle Q, u \rangle} = \frac{\sigma}{\sigma \langle Q, u \rangle} \]

\[ = 6 \]
\[
\tilde{J}_{1}(E) = \frac{1}{N_1} \sum_{i=1}^{N_1} W_i \tilde{J}_i, \quad \tilde{J}_{2}(E) = \frac{1}{N_2} \sum_{i=1}^{N_2} W_i \tilde{J}_i
\]

(\text{where } N_1, N_2 \text{ are the number of neutron histories}).

These quantities are essentially cross sections since they represent the total number of neutrons leaving the sample surface within unit energy increment and unit solid angle (about the detector direction) per incident neutron.

It is not possible to talk in terms of an emerging neutron flux density (i.e., neutrons crossing a unit area, perpendicular to their direction, in unit time) with finite samples, since the scattered neutron beam from a finite sample will not, in general, be uniform.

4. Running the Program

3.1 Time/Space Requirements

The program has been written in FORTRAN IV and developed on the Harwell IBM 370/165 computer. All of the functions and subroutines used by the program (except for the standard FORTRAN subroutines) are given in the appendix. The program requires 120 K bytes (30 K words) of store.

The running times depend on the size of the energy spectrum, number of detectors, etc. In general, it is more efficient to run with a large number of scattering angles since some of the computation is common to all and is completed at the beginning of the program. The times taken for some typical calculations on the Harwell IBM 370/165 are shown in Table 1. It will be seen that the time taken is approximately 0.42 sec per energy bin per 1000 neutron histories.

- 7 -
<table>
<thead>
<tr>
<th>Time (sec)</th>
<th>No. of Scattering Angles</th>
<th>No. of Energy Bins</th>
<th>NQ</th>
<th>NW</th>
<th>NRUN1</th>
<th>NRUN2</th>
</tr>
</thead>
<tbody>
<tr>
<td>128</td>
<td>4</td>
<td>75</td>
<td>9</td>
<td>40</td>
<td>200</td>
<td>1000</td>
</tr>
<tr>
<td>158</td>
<td>5</td>
<td>75</td>
<td>9</td>
<td>40</td>
<td>200</td>
<td>1000</td>
</tr>
<tr>
<td>111</td>
<td>2</td>
<td>126</td>
<td>17</td>
<td>100</td>
<td>200</td>
<td>1000</td>
</tr>
<tr>
<td>60</td>
<td>1</td>
<td>126</td>
<td>17</td>
<td>100</td>
<td>200</td>
<td>1000</td>
</tr>
</tbody>
</table>

### 3.2 Data Specifications

This section defines the input variable names and explains the format in which they are read. A subsequent section will deal with them in more detail.

**COLUMN (inclusive)**

**VARIABLE**

**CARD 1** (2044)

<table>
<thead>
<tr>
<th>Column</th>
<th>Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 - 10</td>
<td>TITLE</td>
</tr>
</tbody>
</table>

A title supplied by the user to identify the run.

**CARD 2** (4110)

<table>
<thead>
<tr>
<th>Column</th>
<th>Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 - 10</td>
<td>NRUN1</td>
</tr>
<tr>
<td>11 - 20</td>
<td>NRUN2</td>
</tr>
</tbody>
</table>

The number of once-scattered neutron histories to be followed.

The number of twice-scattered neutron histories to be followed.

**CARD 3** (3,6,5,3)

<table>
<thead>
<tr>
<th>Column</th>
<th>Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 - 10</td>
<td>THICK</td>
</tr>
<tr>
<td>11 - 20</td>
<td>WIDTH</td>
</tr>
<tr>
<td>21 - 30</td>
<td>HEIGHT</td>
</tr>
</tbody>
</table>

The thickness of the sample. THICK is irrelevant for cylindrical geometry.

The width or diameter of the sample (if IGEOM = 2 or 3 respectively).

The height of the sample. (If IGEOM = 2 or 3).

All dimensions in cm.
<table>
<thead>
<tr>
<th>CARD 4</th>
<th>(310)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1  -  10</td>
<td></td>
</tr>
<tr>
<td>11  -  20</td>
<td></td>
</tr>
<tr>
<td>21  -  30</td>
<td></td>
</tr>
<tr>
<td>31  -  40</td>
<td></td>
</tr>
</tbody>
</table>

**The sample geometry indicator.**

- 1 for infinite flat plate sample.
- 2 for finite flat plate sample.
- 3 for finite cylindrical sample.

**The mask option indicator.**

- 0 for no mask.
- 1 for mask present.

(see 3.3 for full details.)

<table>
<thead>
<tr>
<th>CARD 5</th>
<th>(4F10.3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1  -  10</td>
<td></td>
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<tr>
<td>11  -  20</td>
<td></td>
</tr>
<tr>
<td>21  -  30</td>
<td></td>
</tr>
<tr>
<td>31  -  40</td>
<td></td>
</tr>
</tbody>
</table>

**The number of detectors.**

- Value of N det. inv.

**Temperature of the sample (in °K).**

**Atomic density of the sample (in atoms/A^2).**

**Absorption cross-section at the incident neutron momentum (in barns).**

**Bound atom cross-section (in barns).**

<table>
<thead>
<tr>
<th>CARD 6</th>
<th>(4F10.3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1  -  10</td>
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</tr>
<tr>
<td>11  -  20</td>
<td></td>
</tr>
<tr>
<td>21  -  30</td>
<td></td>
</tr>
<tr>
<td>31  -  40</td>
<td></td>
</tr>
</tbody>
</table>

**The direction cosine of the incident neutron beam.**

**The value of the incident neutron momentum (in \(10^{-1}\)).**

<table>
<thead>
<tr>
<th>CARD 7</th>
<th>(3I5,5I2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1  -  5</td>
<td></td>
</tr>
<tr>
<td>6  -  10</td>
<td></td>
</tr>
<tr>
<td>11  -  15</td>
<td></td>
</tr>
<tr>
<td>16  -  20</td>
<td></td>
</tr>
<tr>
<td>21  -  25</td>
<td></td>
</tr>
<tr>
<td>26  -  30</td>
<td></td>
</tr>
</tbody>
</table>

**The number of points on the Q axis of the (Q,\(\omega\)) mesh. (NQ < 40).**

**The number of points on the \(\mathbf{w}\) axis of the (Q,\(\omega\)) mesh. ( NW < 150).**

**The number of points in the SIGMA(N2) array (N2 < 200).**

**Interval between points on the \(\mathbf{Q}\) axis of the (Q,\(\omega\)) mesh (in \(10^{-1}\)).**

**Interval between points on the \(\mathbf{w}\) axis of the (Q,\(\omega\)) mesh (in mev).**

**The minimum value of Q on the (Q,\(\omega\)) mesh (in A^(-1)).**

- 9 -
On cards B, B, ..., L (L = B + NQ/8) are the NQ values of SIGSS in barns.

SIGSS(I) is the scattering cross-section

\[ \sigma_s^r(k) = \frac{\sigma_0}{(0^+)^2} \int \frac{d^2q}{(2\pi)^2} \left| S(q) \right|^2 \]

for a neutron with momentum \( k \) in [0, Q].

On cards 1+1, 1+2, ..., there follow the values of \( S^r(Q,\omega) \) at the mesh points defined by \( DQ, DN, NW, QMIN \). \( S^r(Q,\omega) \) values are in units of \( meV^{-1} \).

They are read in by the statements:

\[
\begin{align*}
DQ & = 2\pi, DN \\
S & \text{ READ}(S,\omega) \text{ of } I(1, J), I = 1, NQ \\
\text{NQ} & \text{ FORMAT } (6G10.3)
\end{align*}
\]

Hence the values of \( S(Q,\omega) \) are arranged as follows:

\[
\begin{align*}
S(1,1) & \quad S(2,1) & \quad S(3,1) & \quad \cdots & \quad S(6,1) \\
S(1,2) & \quad \cdots & \quad \cdots & \quad \cdots & \quad S(2,1) \\
S(1,3) & \quad \cdots & \quad \cdots & \quad \cdots & \quad S(3,1) \\
& \quad \cdots & \quad \cdots & \quad \cdots & \quad \cdots \\
& \quad \cdots & \quad \cdots & \quad \cdots & \quad S(NQ,1) \\
S(1,4) & \quad S(2,1) & \quad \cdots & \quad \cdots & \quad S(4,1) \\
& \quad \cdots & \quad \cdots & \quad \cdots & \quad \cdots \\
& \quad \cdots & \quad \cdots & \quad \cdots & \quad S(NQ,2) \\
& \quad \cdots & \quad \cdots & \quad \cdots & \quad \cdots \\
& \quad \cdots & \quad \cdots & \quad \cdots & \quad S(NQ,NQ)
\end{align*}
\]

The values of \( Q \) and \( \omega \) corresponding to the element \( I(1, J) \) are given by:

\[
\begin{align*}
Q & = (I-1)^* DQ + QMIN \\
\omega & = (J-1)^* DN
\end{align*}
\]

Thus the scattering law is defined over a rectangle in \((Q,\omega)\) space having edges \( QMIN, (QMIN-I)*DQ + QMIN \), \( (NW-I)*DN \). Notice that values of \( S^r(Q,\omega) \) are only provided for \( -NQ \leq \omega \leq 0 \) (see introduction).
The values of $S'(Q,0)$ stored in the array S should be set to the average value of $S'(Q,0)$ over a small region of $(Q,0)$ space from $(Q - 0.05, 0)$ to $(Q + 0.05, 0)$ and $(0 - 0.05, 0)$ to $(0 + 0.05, 0)$. Since $S'(Q,0)$ is a smoothly varying function it is usually a reasonable approximation to set it equal to the value of $S'(Q,0)$ at the centre of the region. Near the origin of $(Q,0)$ space however ($Q = 0, \omega = 0$) the scattering law will become sharply peaked, and it is then necessary to estimate the average value over the small region.

**ORDER N1 N2 N3...**

<table>
<thead>
<tr>
<th>N1</th>
<th>N2</th>
<th>N3</th>
<th>...</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>...</td>
</tr>
</tbody>
</table>

- **DXX** The direction cosines of the detectors.
- **DKY** one set of three on each card.
- **DKZ**

### 3.3 Notes on the Data Variables

**NRUN**

A value of 200 is found to produce extremely reliable values for $J_1$, $J_2$.

**NRUN2**

The accuracy of $J_2$ obviously depends on the number of histories followed. Some idea of the accuracy of $J_2$ may be obtained by running the program several times using a different sequence of random numbers for each run. This has been done for the sample whose data is shown in the Appendix (for which NRUN = 200, NRUN2 = 1000) and the results are shown in Fig.3. For this particular case the average error on $J_2$ is $(J_1 + J_2)$, which is the real quantity of interest, is $\pm 10^3$.

This non-systematic error may be reduced (by a ratio $\frac{1000}{100}$) by increasing NRUN2 - although this is limited by the time required for the program.

**THICK**

All of these parameters are connected with the geometry of the experiment and will therefore be considered together.

**WIDTH**

The co-ordinate system in which everything is described is defined by the sample (and not the incident beam).

**HEIGHT**

**NOTE**

**MASK**

**VXX**

**VXY**

**VXZ**

**DKY**

**DKZ**

**ICSM**

In the case of the flat plate samples (both finite and infinite) the x axis is defined to be perpendicular to the...
face of the sample bathed by the incident neutron beam (see
Fig.4). Hence two of the sample faces are defined by the
equations:
\[ x = 0 \]
\[ x = \text{THICK} \]
In the case of the finite flat plate the other two axes are
assumed to be perpendicular to the other faces of the plate,
so that the remaining surfaces of the sample are defined by
the equations:
\[ y = \text{WIDE}/2 \]
\[ y = -\text{WIDE}/2 \]
\[ z = \text{HEIGHT}/2 \]
\[ z = -\text{HEIGHT}/2 \]
For the infinite flat plate the choice of the other two axes
is arbitrary, and will be made to facilitate the calculation
of \( \text{VWX},...\text{VWZ} \) etc..

In the case of cylindrical sample geometry the \( z \) axis is
defined to be the axis of the cylinder (Fig.4). Hence the
surfaces of the cylindrical sample are defined by the equations:
\[ x^2 + y^2 = \left(\frac{\text{WIDE}}{2}\right)^2 \]
\[ z = \text{HEIGHT}/2 \]
\[ z = -\text{HEIGHT}/2 \]
The direction of the incident neutron beam is defined in
relation to these axes by means of the direction cosines,
\( \text{VWX}, \text{VWY}, \text{VWZ} \).
For flat plate samples, neutrons are considered to be incident
on all or the face \( x=0 \) (and only that face); hence for these
samples
\[ \text{VWX} > 0 \] (if \( \text{EGROM} = 1,2 \)).
Apart from this constraint the choice of incident direction
is free.
For cylindrical sample geometry the incident beam is defined
to lie in the \( z-x \) plane. In this case

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Also, the neutron beam is assumed to be all of the curved surface for which \( x < 0 \), and only this surface. Incident neutron directions parallel to the cylindrical axis are not permitted. This gives rise to the constraint:

\[
\text{VX} > 0 \quad (\text{if} \quad \text{IGRAM} = 3)
\]

The directions of the detectors with respect to the sample are defined by the direction cosines \( DX, DY, DZ \). These are completely unrestricted.

There is a 'mask' option available with the finite flat plate sample. If MASK is set equal to zero then all neutrons emerging from the sample in the direction of the detector, from whatever face, are 'detected'. If MASK is set = 1, then only those neutrons emerging from a face perpendicular to the \( x \)-axis are recorded.

Fig. 5 shows the sample and detector positions used in the example listed in the Appendix. The flat plate sample lies in the \( y-z \) plane. The neutron beam is incident on the sample at 45°. With detectors at 20°, 40°, 60°, 90° to the incident beam the direction cosines would be as follows:

\[
\begin{align*}
\text{VX} = 0.7071 & \quad \text{VY} = 0.7071 & \quad \text{VZ} = 0.0 \\
\text{DX} & & \text{DY} & & \text{DZ} \\
20° & 0.9063 & 0.4226 & 0.0 \\
40° & 0.8962 & 0.4072 & 0.0 \\
60° & 0.8669 & -0.2588 & 0.0 \\
90° & 0.7071 & -0.7071 & 0.0
\end{align*}
\]

The double differential cross-section is provided by the user in the form of the scattering law surface \( S'(Q,\omega) \). The definition of \( S'(Q,\omega) \) is given in equation 1.2. Only values of \( S' \) for positive \( \omega \) (\( \omega \) = neutron energy gain) need be supplied by the user. Two important considerations are, for what area of the \( Q,\omega \) space should values of \( S' \) be provided, and what mesh size \( (Q,\Delta Q) \) should be used?

The program does not extrapolate the \( S(Q,\omega) \) surface beyond...
the area set by the user (viz. $Q_{\text{min}} < Q < (Q_{\text{max}} + Q_{\text{min}})$, $-200 \text{m} < \omega < 200 \text{m}$). If a scattering event is considered which has values of $Q$, $\omega$ outside the range provided, then the event is ignored and will not contribute to the final spectrum. (More succinctly: $g' = 0$ unless defined otherwise).

It is recommended therefore that in order to include back-scattered neutrons with a reasonable energy transfer:

$$\sqrt{(Q_{\text{max}} - Q_{\text{min}})^2 + (Q_{\text{max}} + Q_{\text{min}})^2} > 3k_0$$

where $k_0$ is the incident wave vector. The value of the lower limit of $Q$, $Q_{\text{min}}$, depends on the form of the scattering law. For incoherent scatterers the total scattering is roughly $Q$ independent, and the low $Q$ region is as important as any other. For such samples $Q_{\text{min}}$ would be set to $0$.

For coherent scatterers $S(Q)$ decreases for small $Q$ and in some instances it may be reasonable to ignore the contribution for $Q < 0.5k_0$ say. Naturally the energy range should be large enough to include all of the inelastic processes in which the user is interested. Similarly the mesh size $\Delta Q$ should be chosen so that any peaks in the energy spectrum (e.g. the quasi-elastic peak or a collective mode) have a reasonably defined shape. (This is not always possible for all $Q$, since $S(Q, \omega)\propto Q^2$ tends to a delta function as $Q \rightarrow 0$.)

The mesh size $\Delta Q$ is also important. Values of $S(Q, \omega)$ are obtained for continuously varying $Q$ along lines of constant $\omega$ by a log-quadratic interpolation. For a given $Q$ (for which $S(Q, \omega)$ is required) the three nearest mesh points with the same $\omega$ value will be called $Q^-, Q^0, Q^+$ where $Q^- < Q < Q^+$. The equation $AQ^2 + BQ + C$ which passes through the points $\ln[S(Q, \omega)^0], \ln[S(Q^-, \omega)^0], \ln[S(Q^+, \omega)^0]$ is thus found and

$$S(Q, \omega) = \exp[AP^2 + BP + C]$$

$\Delta Q$ should be small enough to justify this interpolation. Particular care should be taken where dispersing modes are present. These are not well represented by the constant $\omega$...
interpolation employed unless a small DQ is used.

An array, SIGSE(N2), of values for \( C_s(k) \) must be provided
such that

\[
\text{SIGSE}(k) = C_s(k) \quad \text{(in barns)}
\]

where \( k = 10^8 \)Q \quad \text{(in } 1^{-1})

The value of N2 is determined as follows:

During the program values of \( C_s(k) \) are interpolated (using
the method described in A1) in the array SIGSE(N2). If

\[ k < DQ \] \quad C_s = \text{SIGSE(1)}.

If \( k > 10^8 \)Q, \( C_s \) is set equal to SIGSE(N2). Thus the value

of N2 should be large enough so that either: a) all the

values of \( C_s(k) \) for \( k > 10^8 \)Q are equal to \( C_s \) (N2=DQ), or

b) \( 10^8 \)Q \( \times k_{\text{mas}} \) where \( k_{\text{mas}} \) is the highest neutron momentum

considered and is equal to:

\[
k_{\text{mas}}^2 = k_0^2 + \frac{2E}{\hbar} (\text{D.E.W})
\]

4. Correcting for Multiple Scattering

4.1 The Program Output

A specimen output from SIGSE is shown in the Appendix. The first section
simply prints out the data supplied by the user. The results for each detector
are headed DETECTOR i which is followed by the direction cosines of the detector
and the angle (in degrees) subtending the detector direction and the incident
beam.

The main quantities of interest are in the six parallel columns underneath.
These, as a function of a linear energy scale (in meV), the quantities

\( J_1, J_2, J_1J_2, J_1/J_1, J_2/J_2, J_2/J_1J_2 \) for that particular scattering angle.

The momentum transfer (in \( 1^{-1} \)) is also provided. The ratio \( J_1/J_2 \) will be
referred to as \( R(0,E) \), \( J_1/J_2 \) as \( R(Q,E) \) and \( J_2/J_1 \) as \( J_2(0,E) \).

4.2 Multiple Scattering Corrections

The multiple scattering correction may be applied in several ways (Ref.1).
The ratios \( R(Q,E), R(Q,E) \) calculated by this program may be used to correct
the observed data by the 'factor method'. Which of these two ratios is used
depends upon what is required, and what data corrections have already been
applied. (Jobs(0,E) is the observed spectrum).
If the observed flux of once scattered neutrons \( J_1(0,E)_{\text{obs}} \) is required from the total recorded flux then:

\[
J_1(0,E)_{\text{obs}} = J_{\text{obs}}(0,E)X(0,E) \tag{4.1}
\]

If \( J' \) (see § 1 for definition) is required from \( J_{\text{obs}}(0,E) \) then:

\[
J'(0,E) = J_{\text{obs}}(0,E)X'(0,E) \tag{4.2}
\]

If \( J' \) is required and \( J_{\text{obs}}(0,E) \) has already been corrected for absorption and re-scattering attenuation \( J_{\text{obs}}(0,E)_{\text{corr}} \), say, then:

\[
J'(0,E) = J_{\text{obs}}(0,E)_{\text{corr}}X'(0,E) \tag{4.3}
\]

4.5 Comparison with Experiment

Instead of correcting the observed neutron spectra before comparison with theory, it is in many ways preferable to compare the observed spectra with calculated spectra which include the higher order scattered fluxes. The values of \( J_1(0,E) \) calculated by the program enable this to be done.

In the factor method of correcting for multiple scattering effects the actual units of \( J_1 \) and \( J_2 \) are immaterial since the quantity of interest is \( J_1(J_1 + J_2) \), the ratio by which the observed intensity must be multiplied to obtain the 'observed' once scattered flux.

If, however, theory and experiment are compared by using a theoretically calculated \( Q'(Q,\phi) \) array as the input to DISCUS and then comparing the output of DISCUS, \( J_1(0,E) \) with the observed neutron spectrum, then the units of \( J_1(0,E) \) are important.

\( J_1(0,E) \) and \( J_2(0,E) \) have been calculated with the following assumptions. If any of them are invalid (2 and 3 certainly will be) the observed spectra must be corrected before comparison is possible.

Assumptions:

1. That the detector 'seen' all of the sample. (i.e. Any neutron leaving the sample within unit solid angle about the direction of the detector is detected).
2. That all the detectors have unit solid angles of acceptance.
3. That there is constant detector efficiency over the entire energy range.

To calculate the number of neutrons recorded in an actual experiment we must use the following expression:

\[
N_1(0,E) = N_{\text{inc}}J_1(0,E)P(0,1)S(0)M(0,E) \tag{4.4}
\]

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where

- $N_{1}(0, E)$ is the number of neutrons (scattered once or twice) recorded in the $E$ energy channel of the $0$ detector.
- $N_{	ext{inc}}$ is the number of neutrons incident on the sample.
- $F(0, E)$ is the detector efficiency at energy $E$ of the $0$ detector.
- $2 \Theta(0)$ is the angle of acceptance of the $0$ detector (in radians).
- $\Delta E(0, E)$ is the energy channel width (in mev) at energy $E$ of the $0$ detector.

In the case of the infinite flat plate sample we can talk in terms of an emerging neutron flux density, since it is uniform. In this case the scattered neutron flux density ($F_{1}(0, E)$ or $F_{2}(0, E)$) is given by

$$F_{1}(0, E) = F_{0}(0, E) \frac{\Delta E(0, E)}{2 \Theta(0)}$$

where $F_{0}$ is the incident flux density (i.e., the number of neutrons crossing unit area, perpendicular to $k_{0}$ within unit time).

Since the incident neutron energy and direction distributions have both been assumed to be delta functions, the effects due to the finite resolution of the instrument have not been included in equation 4.2. To correct for this effect the functions $R(0, E)$ or $J_{2}(0, E)$ should be convoluted with the known instrumental resolution function. This is, of course, making the implicit assumption that the resolution function for $J_{2}$ is the same as that for $J_{1}$; a reasonable assumption when the extra time spent in the sample by multiply scattered neutrons is small.

5. The Effects of Multiple Scattering on the Measurement of Quasi-elastic Widths in Incoherent Systems.

There have been many discussions of the effects of multiple scattering (MS) in particular systems (see for example ref. 2, 3, 4), but there seem to have been no calculations of the quantitative effects on the quasi-elastic peak widths measured for incoherent systems. Since such measurements are finding increasing application it was thought useful to quantify the errors produced by MS.

Calculations were made for the following model of $S(Q, \omega)$

$$S(Q, \omega) = \frac{p Q^{2}}{Q^{2} + (2 \pi)^{2}}$$

where

$$p = 2.9 \times 10^{-5} \text{ cm}^{-1}$$
and the remaining angle parameters are those shown in the specimen output in A3.

Fig. 1 shows the result for such a system. The sample, which scatters 12% of the incident beam, is inclined to the beam (h = 45°) at an angle of 45°. The solid lines represent the recorded fluxes of neutrons which have undergone a single scattering event, and the dashed lines twice-scattered neutrons. The angles shown on Fig. 1 are the angles between the incident beam and the detectors. The most important feature is that the second order spectra are virtually independent of scattering angle, and this feature is also found if the incident wavelength is changed to 6Å.

The correction factor \( J_1/(J_1 + J_2) \) for this model is shown in Fig. 7. At the elastic scattering point of the spectrum the corrections are small; ranging from about 5% to 10% (at 90°). As one goes further into the inelastic region, however, the corrections become much more severe. At a scattering angle of 90° the second order flux levels out at 70% of the total intensity, but at lower angles this figure rises to 90% and above.

It is interesting to consider the effect of sample thickness on the ratio \( J_2/J_1 \). Fig. 6 shows \( J_2/J_1 \) plotted as a function of sample thickness for several different neutron energies (+, 5.12 meV (elastic scattering): 5, 5.57 meV: O, 6.02 meV) and scattering angles. The remarkable result is, that for the two cases considered, they all exhibit the same thickness dependence:

\[
R^2 = \left[ \frac{t}{t_1} \right]^{0.7}
\]

where \( t \) is the thickness and \( R \) is the ratio \( J_2/J_1 \). This means that if you reduce the sample thickness by 50%, the ratio \( J_2/J_1 \) is lowered by about 40%.

Since, over the quasi-elastic region at least, the second order flux from a 1% scatterer appears to be approximately 10% of the first order scattering at 90°, this fact may be used in conjunction with equation 5.1 to give a rough idea of the multiple scattering correction to be encountered without use of a computer.

The size of the error produced by MS in measurements of quasi-elastic widths was obtained by simply plotting the quasi-elastic spectrum for \( J_1 \) and \( J_1 + J_2 \) and measuring their half-widths. The complications caused by deconvolution were ignored. The results of this procedure for \( \theta = 40°, 60° \) and 90° detectors are shown in Fig. 9. The spectra of \( J_1 + J_2 \) are always broader than those of \( J_1 \), and the differences are about 3%, 4% and 6% respectively. Since the higher Q values are usually given higher weights (because the deconvolution error is smaller) the error in determining a diffusion constant, for example,
will be closer to the 68% value. Drawing the 'best' straight lines through the points in Figs 8 gave the values

\[ D_1 = 1.3 \times 10^{-5} \text{ cm}^2 \text{s}^{-1} \] (for \( J_1 \))

\[ D_{1+2} = 2.6 \times 10^{-5} \text{ cm}^2 \text{s}^{-1} \] (for \( J_1 + J_2 \))

This must be regarded as a low estimate for the error since the highest order multiple scattering effects have been neglected.

The conclusion is that multiple scattering effects are relatively small over the quasi-elastic region, but very important in the inelastic region. The effects of multiple scattering on measured quasi-elastic widths are also small, the order of 6%, and are probably smaller than the errors introduced by deconvolution. It, however, measurements with errors less than \( \pm 10\% \) are required then the effects of multiple scattering must certainly be considered.

References

5. H. Kallin; Nucl. Inst. and Methods 201, 263 (1972).
A1: Program Structure and Subroutines

A flow diagram showing the main steps in the program is given in Fig. 6. It is hoped that this, together with the program listing and a glossary of symbols, will provide an adequate guide to its structure. The numbers beside the boxes in the flow diagram refer to the line numbers in the program.

There are four subroutines supplied with the DISCUS program. In order that a user may modify them for his own requirements their roles are specified below.

**SUBROUTINE DIST (UX, UY, UZ)**

*Given:* UX, UY, UZ (arguments)

X, Y, Z, THEK, Y, Z, IKOM, IFAIL (COMMON)

*Calculates:* The distance DL (in cm.) from a point X, Y, Z to the surface of the sample along a line with direction cosines UX, UY, UZ. Information about the type and size of the sample is contained in the parameters IKOM, THICK, Y, Z. For infinite plane slab samples the parameter IFAIL should be set = 1 if the neutron emerges from a face not perpendicular to the X-axis; otherwise it should be set = 0.

**SUBROUTINE NEW**

*Given:* XINC, YM, SIGS(N2), DENS, SIGA, DQ, N2 (COMMON)

*Calculates:* The values of:

\[ \text{SIGA}_1 = \text{SIGA}_2(k) \]

\[ \text{SIGA}_1 = \text{SIGA}_2(k) \]

and MFP (the value of the mean free path of a neutron with momentum k) for an supplied value of the neutron momentum YM.

SIGS1 is calculated by interpolating between the values of SIGS supplied by the user in SIGS(N2). The method of interpolation is as follows:

If the values of SIGS(i) are at values of the neutron momentum k(i) then the three nearest array members such that \( k(i) < k < k(i+1) < k(i+2) \) are found. The value of \( \ln(\text{SIGS}(i)) \) is then deemed to lie on the quadratic curve, \( \text{Ak}^2 + \text{Bk} + \text{C} \) which passes through the points \( \ln(\text{SIGS}(i)), \ln(\text{SIGS}(i+1)), \ln(\text{SIGS}(i+2)) \). If \( k < k(i) \) then \( \text{SIGS}_1 = \text{SIGS}(i) \), if \( k > k(i) \) then \( \text{SIGS}_1 = \text{SIGS}(i) \). Having found \( \text{SIGS}_1 \), \( \text{SIGA}_1 \) is calculated from

\[ \text{SIGA}_1 = \text{SIGA}_1 \]
and \( B_{WFE} \) is simply \( ( DENS \cdot SIGT )^{-1} \). (Note: Since \( \ln( SIGS(i) ) \) is repeatedly required in the subroutine, the values of \( SIGS(i) \) are converted and stored as their logarithms immediately after having been read in MAIN.)

**SUBROUTINE SINT**

**Given:** \( IN, Q, QMIN, QNO, S(QNO, NW) \) (COMMON)

**Calculates:** A value of \( S(Q, \omega) \) (FORTRAN variable \( SQW \)) for \( Q = \text{FORTRAN 'Q'}, \omega = (QNO - 1) \cdot \text{DIW} \). This is done by interpolating between points at constant \( \omega = (QNO - 1) \cdot \text{DIW} \) on the \((S(QNO, NW)) \) array. It uses the same log-quadratic interpolation method as NEW. In this case the three nearest mesh points fitted by a quadratic equation are \((Q0, \text{DIW}), (Q1, \text{DIW}), (Q2, \text{DIW})\), where \( 100 < Q < 101 < 102 \). If \( Q \geq \text{DIW} \) are beyond the bounds of the array \( SQW = 0 \). As for SIGS the values of \((S(QNO, NW)) \) are stored as their logarithms after being read in MAIN.

**SUBROUTINE ROE**

**Given:** \( MPR, REL, SIGR, YY, ZZ, THICK, IQN, WXX, WXY, WZZ, DENS \) (COMMON)

**Calculates:** \( X, Y, Z, R \)

\( X, Y, Z \) are the co-ordinates of the first event point \( P0 \). This is obtained in two stages. First a point of incidence on the specimen is sampled (for the infinite flat plate this is kept constant at \( X, Y, Z = 0 \)). Next the distance from this point of impact to emergence (in \( P1 \)) is calculated. A point along this line is then sampled for the first event point and its co-ordinates \( X, Y, Z \) calculated. The distance the neutron travels \((\xi)\) is obtained from,

\[
\xi = -MPR \ln [1 - e^{-REL \cdot DENS \cdot SIGT}] 
\]

where \( \xi \) is a pseudorandom normal with a square distribution between 0 and 1.

The weighting factor \( R \) is also passed back to MAIN.

\[
R = \frac{1 - e^{-REL \cdot SIGT}}{SIGT} 
\]

In addition to these four subroutines the user must supply the following subroutines which are required in connection with the generation of the pseudorandom number sequence.

These are all standard Harwell Subroutine Library Programs (ref.8).
REAL FUNCTION FAD1AS (I)

The function value returned by FAD1AS is a real pseudorandom number in the
range (0.0 – 1.0) if I is positive or zero; or in the range (-1.00 – 1.00)
if I is negative.

SUBROUTINE FACIDS (MAX, VALUE)

This subroutine will set VALUE to a pseudorandom integer in the interval
(1 – MAX) inclusive. Max should always be positive otherwise there will
be a bias towards zero.

SUBROUTINE FACIDS (I,J)

Restarts the value of the generator words used in FAD1AS or FAD1BS according
to the input values of I,J. J must always be odd if one uses the Harwell
subroutine library programs.

SUBROUTINE FACICS (I,J)

Passes back the current contents of the generator words via the variables
I,J.

The above four subroutines are used to calculate the random numbers used in the
sampling procedures.

If the user wishes to substitute his own random number generating routines he will
require the following information:

1) A pair of numbers JRAND, MRAND are read at the beginning of the program
and these may be used to initialise a random number generator at a
particular point.

To do this the program calls the subroutine:

CALL FACIDS (JRAND, MRAND).

2) When random numbers are required during the course of the program,
the function FAC1AS(I) or the subroutine FAC1BS(M,N) are called.

3) At the end of the program the subroutine FACICS is called:

CALL FACICS (JRAND, MRAND)

This outputs the current contents of the two generator numbers via
JRAND and MRAND. The values of JRAND, MRAND are then written out.
Hence if the values written at the end of one program are used as
starting parameters in the next the sequence of random numbers will
continue. If the same values of JRAND and MRAND are used at the
beginning of two program runs where all other input parameters are
identical then the program (using Harwell Subroutine Library Sub-
programs) will produce identical outputs. If, however, a different
pair of JRAND, MRAND numbers are used then a different sequence of
random numbers will be used during the program. The resulting dif-
ference in the output will give some indication of the accuracy of
the program.
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<th>Use</th>
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<td>DENS</td>
<td>Atomic density (in nuclei, $\text{Å}^{-2}$)</td>
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<tr>
<td>D8</td>
<td>DQ</td>
<td>Distance from current position to sample boundary (in cm).</td>
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<td>IGEEM</td>
<td>Unit of increment along Q axis used in S(Q,W) array in $\text{Å}^{-1}$.</td>
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<td>IIW</td>
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<td>INW</td>
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<td>INW1</td>
<td>Set $i=1$ if outgoing neutron passes through side of sample, ($= 0$ otherwise).</td>
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<td>Dimension of SGEES ($0 &lt; 200$).</td>
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<td>Q</td>
<td>A value of the momentum transfer ($\text{Å}^{-1}$).</td>
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<td>D7</td>
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<td>An array of values for S(Q,W).</td>
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<td>D7</td>
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<td>The thickness of flat plate samples (in cm).</td>
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<td>VKINC</td>
<td>Value of incident neutron momentum ($\text{Å}^{-1}$).</td>
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<tr>
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<td>Current value of neutron momentum ($\text{Å}^{-1}$).</td>
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<td>VX</td>
<td>Direction cosine of incident neutron beam.</td>
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<tr>
<td>D7</td>
<td>VY</td>
<td>Direction cosine of incident neutron beam.</td>
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<tr>
<td>D7</td>
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<td>Direction cosine of incident neutron beam.</td>
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<td>D7</td>
<td>VMFP</td>
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<td>ZHGT</td>
<td>HEIGHT/2.0</td>
</tr>
<tr>
<td>Code</td>
<td>Symbol</td>
<td>Use</td>
</tr>
<tr>
<td>------</td>
<td>--------</td>
<td>-----</td>
</tr>
<tr>
<td>AN</td>
<td>Cosine of angle between old and new trajectories.</td>
<td></td>
</tr>
<tr>
<td>D1</td>
<td>Value of once scattered neutron spectrum.</td>
<td></td>
</tr>
<tr>
<td>D2</td>
<td>Value of twice scattered neutron spectrum.</td>
<td></td>
</tr>
<tr>
<td>D4</td>
<td>Value of J* spectrum.</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>Direction cosine of the detector.</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>Unit of increment along the w axis.</td>
<td></td>
</tr>
<tr>
<td>FI</td>
<td>An angle, chosen at random between 0 and 2π, used in the calculation of the new neutron momentum.</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>The height (in cm.) of a flat plate or cylindrical sample.</td>
<td></td>
</tr>
<tr>
<td>HOGT</td>
<td>V/εp γ (in (meV)^{-1}).</td>
<td></td>
</tr>
<tr>
<td>IEL</td>
<td>The detector currently being considered.</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>Integer used to initiate the random number generator.</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>Integer used to describe sample mask facility.</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>Integer used to initiate the random number generator.</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>The number of neutron detectors.</td>
<td></td>
</tr>
<tr>
<td>NE</td>
<td>1 during the once-scattered neutron spectrum calculation.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2 during the twice-scattered neutron spectrum calculation.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3 during the J* calculation.</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>Current total of neutron histories calculated.</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>Number of neutron histories to be used in the calculation of J*, J*.</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>Number of neutron histories to be used in the calculation of J*.</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>Dimension of the array S(q,ω) = (NW &lt; 150).</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>A value of Q^2, where Q is the total momentum transferred to the neutron.</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>The minimum value of Q for which S(q,ω) data is provided.</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>The maximum value of Q for which S(q,ω) data is provided.</td>
<td></td>
</tr>
</tbody>
</table>

= 25 =
Code  Symbol  Use

Components of total momentum transfer.

** µ**  SIGA  Bond atom cross-section (in barns).

. σ  SIGS  Scattering cross-section (σ = W/MEC).

. θ  TEMP  Temperature of sample (in °C).

. θ  TM  New value of a neutron momentum after a scattering event.

. UXX  UXY  UXZ  Current direction cosines of the neutron.

. V  V  A path length chosen from a correct distribution (in cm).

. W  W  ω, the energy gained by the neutron (in meV).

. WMAX  WMAX  = (18 - 1)ω + WINC.

. WEIGHT  WEIGHT  The final statistical weight of the neutron.

. WIDTH  WIDTH  The width (or diameter) of the sample (in cm).

. WINC  WINC  The energy (in meV) of the incident neutron.

Main Arrays

TOT (300,3)  The three calculated neutron spectra are stored in this array.

SUBROUTINE DIST

. DLX  DLX  Distance to sample face perpendicular to (x) axis where applicable.

. DLY  DLY  Distance to sample face parallel to (y) axis where applicable.

. DLZ  DLZ  Distance to cylindrical face.

COOHS

* = remains unchanged throughout the program.

D = read in as data.
FUNCTION IV LEVEL 50  MAIN  DATE 7/4/67  15/6/52  PAGE 0004

0117  VL = -(VPW+SLC1(1.0 - FAPAS1))

0117  VV = VVWV+SIG1

0117  X = X + VLMUK

0117  VV + VLMUK

0117  Z = Z + VLMUK

0159  VMK = VMK

0179  CALL DES1XK,(K1,3,6K2)

0177  IF(NNMAK#WALL>4) GO TO 1000

0176  IF(NNMAK#WALL<5) URL = 0.0

014  4007 CONTINUE

C  WE NEW LCOV WITH POSITIVE ENERGY TRANSFERS

0140  UO = 900011111A1

0141  W = LEN-11001

0142  VMK = VMK

0113  CALL NWL

0144  UX = VMKUX - VMKUX

0145  CUU = VMKU - VMKU

0146  OZ = VMKU - VMKU

0147  Z = SLTRIPUX + (0.0*0) + Q22Q21

0148  IF(L1G1<AMAX) GO TO 9003

0149  CALL SIMT

0149  A = (RXP2 - LEN) 11111A1

0149  B = (R1111 - LEN) 11111A1

0149  C = (R11111111) 11111A1

0149  TOTENMAK = TOTENMAK

0149  TOTENMAK = TOTENMAK + WEIGHT

0149  9002 CONTINUE

C  WE NEW LCOV WITH NEGATIVE ENERGY TRANSFERS

0149  IF(WALL#1) GO TO 9002

0149  UC 90201111111

0149  W = LEN-11111

0149  VMK = VMK

0149  IF(KK3#1111111111) 1111111111

0149  IF(KK3#1111111111) 1111111111

0149  9007 VMK = VMK

0149  CALL NWL

0149  UX = VMKUX - VMKUX

0149  CUU = VMKU - VMKU

0149  OZ = VMKU - VMKU

0149  Z = SLTRIPUX + (0.0*0) + Q22Q21

0149  IF(L1G1<AMAX) GO TO 9003

0149  CALL SIMT

0149  A = (RXP2 - LEN) 11111A1

0149  B = (R1111 - LEN) 11111A1

0149  C = (R11111111) 11111A1

0149  TOTENMAK = TOTENMAK

0149  TOTENMAK = TOTENMAK + WEIGHT

0149  9002 CONTINUE
CALL SINT
0,400  NODYS
   WEIGHT = 0.000025CM**4*SIGI*10**12CM**2*GPH/1000
0,11  WEIGHT = WEIGHT*SIGI**10**12CM**2*GPH/1000
0,12  VAP = VAP*(1.0-1.0)
0,13  VAP = VAP*(1.0-1.0)
0,14  VAP = VAP*(1.0-1.0)
0,15  VAP = VAP*(1.0-1.0)
0,16  VAP = VAP*(1.0-1.0)
0,17  VAP = VAP*(1.0-1.0)
0,18  VAP = VAP*(1.0-1.0)
0,19  VAP = VAP*(1.0-1.0)
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0,21  VAP = VAP*(1.0-1.0)
0,22  VAP = VAP*(1.0-1.0)
0,23  VAP = VAP*(1.0-1.0)
0,24  VAP = VAP*(1.0-1.0)
0,25  VAP = VAP*(1.0-1.0)
0,26  VAP = VAP*(1.0-1.0)
0,27  VAP = VAP*(1.0-1.0)
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0,29  VAP = VAP*(1.0-1.0)
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0,31  VAP = VAP*(1.0-1.0)
0,32  VAP = VAP*(1.0-1.0)
0,33  VAP = VAP*(1.0-1.0)
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0,40  VAP = VAP*(1.0-1.0)
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0,42  VAP = VAP*(1.0-1.0)
0,43  VAP = VAP*(1.0-1.0)
0,44  VAP = VAP*(1.0-1.0)
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0,53  VAP = VAP*(1.0-1.0)
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0,94  VAP = VAP*(1.0-1.0)
0,95  VAP = VAP*(1.0-1.0)
0,96  VAP = VAP*(1.0-1.0)
0,97  VAP = VAP*(1.0-1.0)
0,98  VAP = VAP*(1.0-1.0)
0,99  VAP = VAP*(1.0-1.0)
1.00  VAP = VAP*(1.0-1.0)
THE NEXT SECTION DEALS WITH FINITE SLAB SAMPLES
C INFINITE FLAT PLATE SAMPLES

DO 1000 VL = -(VMAX-VMIN)+1,1+VMAX+VMIN
DO 1000 JR = 0,100000,1000
DO 1000 JY = 0,100000,1000
DO 1000 JZ = 0,100000,1000

C FINITE FLAT PLATE SAMPLES

DO 1000 X = 0,100000,1000
DO 1000 Y = 0,100000,1000
DO 1000 Z = 0,100000,1000

C CYLINDRICAL SAMPLES

DO 1000 X = 0,100000,1000
DO 1000 R = 0,100000,1000
DO 1000 Z = 0,100000,1000
<table>
<thead>
<tr>
<th>ENERGY (V)</th>
<th>IONIC</th>
<th>TWICE</th>
<th>TOTAL</th>
<th>J1/J1(J1+J2)</th>
<th>J1</th>
<th>R*</th>
</tr>
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<td>1.57</td>
<td>1.87</td>
<td>0.3074-10</td>
<td>0.0571-10</td>
<td>0.0382-10</td>
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<td>1.50</td>
<td>0.4306-10</td>
<td>0.2211-10</td>
<td>0.4518-10</td>
<td>0.7675</td>
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<tr>
<td>ENERGY (eV)</td>
<td>DCL</td>
<td>DNE</td>
<td>TNE</td>
<td>TOTAL</td>
<td>SJ1/SJ2/SJ3</td>
<td>SJ1</td>
</tr>
<tr>
<td>------------</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
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AERE - R 7662 Fig. 1
First and second order scattered neutron fluxes as a function of neutron energy.
AERE - R 7682  Fig. 2
Nomenclature used in the program theory.
AERE - R 7682  Fig. 4
Sample geometry.
AERE - R 7682 Fig. 6

Flow diagram of program.
AERE - R 7682  Fig. 8
The thickness dependence of the correction factor.
The change in expected width due to multiple scattering.

FWHM derived from:

+ 1, spectra

- J, spectra

FWHM (meV)