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DBLSCAT

A Computer Code for Double-scattering Corrections

by

A. K. Agrawal, S. G. Das,
and F. M. Mueller

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A Computer Code for Double-scattering Corrections

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ABSTRACT

This report describes DBLSCAT, a FORTRAN IV computer program for calculating the second-order scattering correction for double-differential slow-neutron scattering experiments in an infinite, plane-slab geometry. Included are a brief description of the theory with special cases, a discussion of numerical techniques used, input and output descriptions, sample problems, and the FORTRAN IV listing of the computer code. The program allows for both transmission- and reflection-type experiment geometries. The method used to calculate double-scattering correction is based on Vineyard's approach, except that there are no assumptions regarding the nature of the scattering cross section. Triple integrations appearing in the expression for second-order scattered-neutron current are carried out using a specified number of mesh points. Corrections due to finiteness of sample and higher-order scattering effects are not included. The code has been written with particular emphasis on efficiency and compactness. For a typical run, it takes approximately one minute of the IBM 360/75 processor time in the quasi-elastic region and about 10 sec in the inelastic region. The code uses about 85 k bytes.

I. THEORY

This report describes the theory and operating procedure for the code DBLSCAT, which computes the double-scattering correction for energy and angular differential slow-neutron scattering experiments in an infinite, plane-slab geometry. The basic method used in this code is a straightforward numerical solution of the neutron-transport equation as suggested by Vineyard.* Unlike Vineyard's method, however, this code evaluates explicitly

*G. H. Vineyard, Multiple Scattering of Neutrons, Phys. Rev. 96, 93 (1954).

the effect of inelastic scattering from a tabular input of the scattering cross section in terms of scattering law. No attempt is made to evaluate higher-order scattering corrections, because their evaluation becomes extremely time-consuming and also because the higher-order corrections are believed to be a small fraction of the second-order correction. Besides, the present formulation assumes a monoenergetic incident beam. Since in actual experiments this is hardly the case, the final double-scattering correction can then be obtained by integrating the results over incident beam spectrum. An approximate method would be to fold-in the incident neutron spectrum in final calculations, assuming, of course, that the errors caused by such an approximation are of the second order.

A. General Description

Let us consider a scattering sample, the scatters in which may or may not be uniformly distributed. Assume that a monoenergetic neutron beam of energy E_0 is incident at a direction defined by the vector $\underline{s}_0$. The nth-order scattered-neutron density is then the solution of the transport equation

$$\underline{s} \cdot \nabla P_n(E, \underline{r}, \underline{s}) + \Sigma(E) P_n(E, \underline{r}, \underline{s}) = \iint dE' \, d\Omega' \, \Sigma(E' \rightarrow E, \underline{s}' \rightarrow \underline{s}) \, P_{n-1}(E', \underline{r}, \underline{s}'),$$

$$n = 0, 1, 2, \ldots, \tag{1}$$

where $P_{-1} \equiv 0$, $P_n(E, \underline{r}, \underline{s})$ is the nth-order scattered neutrons per unit volume, of energy E within unit energy increment, which are proceeding in the direction $\underline{s}$, $\Sigma(E)$ is the macroscopic total cross section at energy E, and $\Sigma(E' \rightarrow E, \underline{s}' \rightarrow \underline{s})$ is the double-differential macroscopic cross section for scattering from energy E' to E and direction $\underline{s}'$ to $\underline{s}$. The formal solution of Eq. 1 may be written as

$$P_0(E, \underline{r}, \underline{s}) = P_0(E, \underline{r} - L\underline{s}, \underline{s}) \, \delta(E - E_0) \, \delta(\underline{s} - \underline{s}_0) \, e^{-\Sigma(E_0)L} \tag{2}$$

and

$$P_n(E, \underline{r}, \underline{s}) = \iint dE' \, d\Omega' \, \Sigma(E' \rightarrow E, \underline{s}' \rightarrow \underline{s}) \int_0^L d\xi \, e^{-\Sigma(E)\xi} P_{n-1}(E', \underline{r} - \xi\underline{s}, \underline{s}')$$

$$n = 1, 2, 3, \ldots, \tag{3}$$

where L is the distance from the point $\underline{r}$ to the surface of the sample in the direction $-\underline{s}$, as shown in Fig. 1. It is assumed that the sample is nowhere concave. The problem of calculating higher-order scattering intensities is solved by iterative procedure by combining Eqs. 2 and 3. Since the integrals involved are generally difficult to evaluate, we restrict ourselves to the infinite, plane-slab geometry only, for which the expressions for P_0 and P_n are

$$P_0(E, z, \underline{s}) = \frac{1}{2\pi} e^{-\Sigma(E) z \sec\theta_0} \delta(\cos\theta - \cos\theta_0)\, \delta(E - E_0) \tag{4}$$

and

$$P_n(E, z, \underline{s}) = \iint dE'\, d\Omega'\, \Sigma(E' \to E, \underline{s}' \to \underline{s}) \int_0^L d\xi\, e^{-\Sigma(E)\xi}$$

$$\cdot\, P_{n-1}(E', z - \xi\cos\theta, \underline{s}'), \qquad n = 1, 2, 3, \ldots, \tag{5}$$

where the system of coordinates chosen to describe the vector $\underline{s}$ is shown in Fig. 2. The chord length L is related to slab thickness t:

$$\left.\begin{aligned} L &= z \sec\theta && \text{if } \theta < \pi/2, \\ &= (z - t) \sec\theta && \text{if } \theta > \pi/2. \end{aligned}\right\} \tag{6}$$

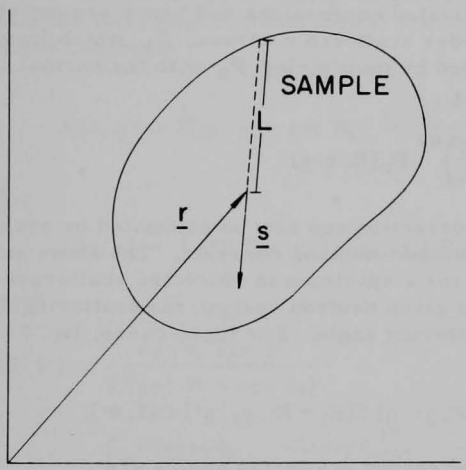

Fig. 1. Geometry of the General Case

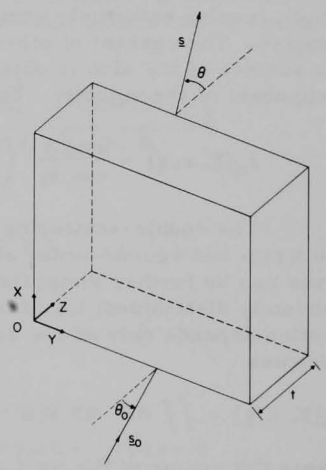

Fig. 2. Geometry of the Plane Slab

Expressions for the first- and higher-order scattered neutrons can now be obtained by iterating Eqs. 4 and 5. We note the general results for P_1 and P_2:

$$P_1(E, z, \underline{s}) = \Sigma(E_0 \to E, \underline{s}_0 \to \underline{s}) \sec\theta \cdot \frac{e^{-\Sigma_0 z \sec\theta_0} - e^{-\Sigma z \sec\theta_f(\theta)}}{\Sigma \sec\theta - \Sigma_0 \sec\theta_0} \tag{7}$$

and

$$P_2(E, z, \underline{s}) = \iint dE'\, d\Omega'\, \Sigma(E' \to E, \underline{s}' \to \underline{s})\, \Sigma(E_0 \to E', \underline{s}_0 \to \underline{s}')\, G(\theta, \theta'), \tag{8}$$

where

$$f(\theta) = 1, \quad \text{if } \theta < \pi/2,$$

$$= e^{\Sigma t \sec\theta - \Sigma_0 t \sec\theta_0}, \quad \text{if } \theta \geq \pi/2; \tag{9}$$

$$G(\theta, \theta') = \frac{\sec\theta \sec\theta'}{\Sigma' \sec\theta' - \Sigma_0 \sec\theta_0}$$

$$\cdot \left[\frac{e^{-\Sigma_0 z \sec\theta_0} - e^{-\Sigma z \sec\theta} f(\theta)}{\Sigma \sec\theta - \Sigma_0 \sec\theta_0} - \frac{e^{-\Sigma' z \sec\theta'} - e^{-\Sigma z \sec\theta} f(\theta)}{\Sigma \sec\theta - \Sigma' \sec\theta'} f(\theta') \right]; \tag{10}$$

$\Sigma \equiv \Sigma(E)$ and $f(\theta')$ is given by Eq. 9, where Σ and θ are replaced by their corresponding primed quantities. Higher-order corrections, which are small, involve extremely complicated expressions and hence are not attempted. The current of nth-order scattered neutrons, J_n, which leave the surface of the slab is obtained by multiplying P_n with the normal component of the velocity. Thus,

$$J_n(E, z, \underline{s}) = \frac{\cos\theta}{\cos\theta_0} \cdot \left(\frac{E}{E_0}\right)^{1/2} P_n(E, z, \underline{s}). \tag{11}$$

The double-scattering correction can now be estimated by evaluating the first- and second-order scattered-neutron currents. The above expressions can be further simplified for a specimen in which the scatterers are randomly distributed; i.e., for a given neutron energy, the scattering cross section depends only on the scattering angle. For these cases, Eq. 8 becomes

$$P_2(E, z, \underline{s}) = \iint dE' \, d\Omega' \, \Sigma(E' \to E, \underline{s}' \cdot \underline{s}) \, \Sigma(E_0 \to E', \underline{s}_0 \cdot \underline{s}') \, G(\theta, \theta'), \tag{12}$$

where the cosine of the first and second scattering angles are

$$\cos(\underline{s}_0 \cdot \underline{s}') = \cos\theta_0 \cos\theta' + \sin\theta_0 \sin\theta' \cos(\varphi' - \varphi_0) \tag{13}$$

and

$$\cos(\underline{s}' \cdot \underline{s}) = \cos\theta' \cos\theta + \sin\theta' \sin\theta \cos(\varphi - \varphi'), \tag{14}$$

and the vector $\underline{s}$ is specified by angles θ and φ, as shown in Fig. 2. Usually, in experimental arrangements $\underline{s}_0$, $\underline{s}$, and the normal to the sample are coplanar. In this case, $\varphi = \pi - \varphi_0$. Furthermore, we can choose our coordinate system in such a way that $\varphi_0 = 0$; then Eqs. 13 and 14 become

$$\cos(\underline{s}_0 \cdot \underline{s}') = \cos\theta_0 \cos\theta' + \sin\theta_0 \sin\theta' \cos\varphi' \tag{15}$$

and

$$\cos(\underline{s}' \cdot \underline{s}) = \cos\theta' \cos\theta - \sin\theta' \sin\theta \cos\varphi'. \tag{16}$$

The first- and second-order scattered-neutron currents can now be calculated by combining Eqs. 7, 11, and 12. Note that the calculation of J_1 is straightforward, since it is related to the scattering cross section through a "geometric factor," while in J_2, triple integration over the variables E', θ, and φ' is to be numerically performed. Several special cases are first considered before going into the details of computational schemes.

B. Elastic Scattering

Loss of neutron energy due to a scattering collision with the specimen is not considered. By dropping the energy suffix from P_n's and Σ's, we obtain the following expressions for the first- and second-order scattered-neutron currents:

$$J_1(z, \underline{s}) = \Sigma(\underline{s}_0 \cdot \underline{s}) \cdot \sec\theta_0 \cdot \frac{e^{-\Sigma_0 z \sec\theta_0} - e^{-\Sigma z \sec\theta} \cdot f(\theta)}{\Sigma \sec\theta - \Sigma_0 \sec\theta_0} \tag{17}$$

and

$$J_2(z, \underline{s}) = \int d\Omega' \, \Sigma(\underline{s}' \cdot \underline{s}) \, \Sigma(\underline{s}_0 \cdot \underline{s}') \, F_e(\theta, \theta'), \tag{18}$$

where

$$F_e(\theta, \theta') = \frac{\sec\theta_0 \sec\theta'}{\Sigma^2(\sec\theta' - \sec\theta_0)} \cdot \left[\frac{e^{-\Sigma z \sec\theta_0} - e^{-\Sigma z \sec\theta} f(\theta)}{\sec\theta - \sec\theta_0} - \frac{e^{-\Sigma z \sec\theta'} - e^{-\Sigma z \sec\theta} \cdot f(\theta)}{\sec\theta - \sec\theta'} \cdot f(\theta') \right], \tag{19}$$

and the energy dependence of the total macroscopic cross section is disregarded. The above result reduces to those obtained by Vineyard (see footnote on page 5) for various special cases. Vineyard's quasi-static approximation can be obtained by replacing $\Sigma(\underline{s}' \rightarrow \underline{s})$ with $N\sigma/4\pi$, which is valid if the angular differential scattering cross section is a rapidly varying function of the scattering angle. The integration over the variable θ' can be carried out analytically. Readers are referred to Vineyard's paper for the analytical results obtained for transmission experiments.

C. Transmission Experiment

We now consider the problem of calculating second-order scattered-neutron current for inelastic scattering experiments in which a detector is placed on the opposite side of the incident beam. For this experimental arrangement, the angle θ which the detector makes with the slab normal is always less than $\pi/2$. Expressions for the first- and second-order scattered-neutron currents are obtained by putting $z = t$ in Eqs. 7, 11, and 12. After rearranging terms, we get

$$J_1(E, t, \underline{s}) = \left(\frac{E}{E_0}\right)^{1/2} \Sigma(E_0 \rightarrow E, \underline{s}_0 \cdot \underline{s}) \cdot g_t(\theta) \tag{20}$$

and

$$J_2(E, t, \underline{s}) = \left(\frac{E}{E_0}\right)^{1/2} \iint dE' \, d\Omega' \, \Sigma(E' \rightarrow E, \underline{s}' \cdot \underline{s}) \, \Sigma(E_0 \rightarrow E', \underline{s}_0 \cdot \underline{s}') \, F_t(\theta, \theta'), \tag{21}$$

where

$$g_t(\theta) = \sec \theta_0 \frac{e^{-\Sigma_0 t \sec \theta_0} - e^{-\Sigma t \sec \theta}}{\Sigma \sec \theta - \Sigma_0 \sec \theta_0}, \tag{22}$$

$$F_t(\theta, \theta') = \frac{\sec \theta_0 \sec \theta'}{\Sigma' \sec \theta' - \Sigma_0 \sec \theta_0}$$

$$\cdot \left[\frac{e^{-\Sigma_0 t \sec \theta_0} - e^{-\Sigma t \sec \theta}}{\Sigma \sec \theta - \Sigma_0 \sec \theta_0} - \frac{e^{-\Sigma' t \sec \theta'} - e^{-\Sigma t \sec \theta}}{\Sigma \sec \theta - \Sigma' \sec \theta'} f(\theta') \right], \tag{23}$$

and $f(\theta')$ is defined by Eq. 9 with Σ and θ replaced by their corresponding primed quantities. The scattering angle is $|\theta - \theta_0|$. Numerical evaluation of the triple integration appearing in Eq. 21 will be considered in Section E.

D. Reflection Experiment

In the reflection experiment, the detector is placed on the same side of the scatterer as the incident beam. The angle between the scattered beam and the slab normal is therefore always greater than $\pi/2$. Expressions for J_1 and J_2 are obtained by setting $z = 0$ in Eqs. 7, 11, and 12 and specializing the results for $\theta > \pi/2$. We find

$$J_1(E, 0, \underline{s}) = \left(\frac{E}{E_0}\right)^{1/2} \Sigma(E_0 \rightarrow E, \underline{s}_0 \cdot \underline{s}) \cdot g_r(\theta) \tag{24}$$

and

$$J_2(E, 0, \underline{s}) = \left(\frac{E}{E_0}\right)^{1/2} \iint dE'\, d\Omega'\, \Sigma(E' \to E, \underline{s}' \cdot \underline{s})\, \Sigma(E_0 \to E', \underline{s}_0 \cdot \underline{s}') \cdot F_r(\theta, \theta'), \tag{25}$$

where

$$g_r(\theta) = -e^{\Sigma t \sec\theta} g_t(\theta) \tag{26}$$

and

$$F_r(\theta, \theta') = -e^{\Sigma t \sec\theta} F_t(\theta, \theta'). \tag{27}$$

The scattering angle is again $|\theta - \theta_0|$.

E. Numerical Method

The evaluation of the second-order scattered-neutron current for either the transmission or reflection experiment involves triple integration on E, θ', and φ'. The integration on φ' can be performed first, since φ' appears only through the momentum transfer variable $\varkappa$ in the expression for the double-differential cross section. The scattering cross section $\Sigma(E_0 \to E, \alpha)$ can be written in terms of another function called scattering law $S(\varkappa, \omega)$:

$$\Sigma(E_0 \to E, \alpha) = N \frac{n\sigma}{4\pi\hbar} \left(\frac{E}{E_0}\right)^{1/2} S(\varkappa, \omega), \tag{28}$$

where the momentum and energy transfer variables $\varkappa$ and ω are given by

$$\varkappa = \left(\frac{\hbar^2}{2m}\right)^{1/2} (E + E_0 - 2\sqrt{EE_0} \cos\alpha)^{1/2} \tag{29}$$

and

$$\omega = (E - E_0)/\hbar. \tag{30}$$

In these equations, m is the neutron mass, and, for molecular systems with n identical scattering atoms per molecule, N is the molecular density and σ is the bound-atom scattering cross section. The scattering law is in units of 10^{-12} sec. For monoatomic systems, n = 1 and N is the atomic density. For more complicated systems, the quantities n, σ, and $S(\varkappa, \omega)$ take their effective values. The φ'-dependent term in Eq. 21 or 25 can be written as

$$\int_0^{2\pi} d\varphi' \; \Sigma(E' \to E, \underline{s}' \cdot \underline{s}) \; \Sigma(E_0 \to E', \underline{s}_0 \cdot \underline{s}') =$$

$$\left(\frac{Nn\sigma}{4\pi\hbar}\right)^2 \left(\frac{E}{E_0}\right)^{1/2} \int_0^{2\pi} d\varphi' \; S(\varkappa_2, \omega_2) \; S(\varkappa_1, \omega_1), \tag{31}$$

where

$$\varkappa_1 = \left(\frac{\hbar^2}{2m}\right)^{1/2} [E' + E_0 - 2\sqrt{E'E_0} \cos (\underline{s}_0 \cdot \underline{s}')]^{1/2},$$

$$\varkappa_2 = \left(\frac{\hbar^2}{2m}\right)^{1/2} [E + E' - 2\sqrt{EE'} \cos (\underline{s}' \cdot \underline{s})]^{1/2},$$

$$\omega_1 = (E' - E_0)/\hbar,$$

$$\omega_2 = (E - E')/\hbar, \tag{32}$$

and $\cos (\underline{s}_0 \cdot \underline{s}')$ and $\cos (\underline{s}' \cdot \underline{s})$ are given by Eqs. 15 and 16, respectively.

The scattering law is input to the code for a number of positive ω and $\varkappa$ values. In other words, the scattering law is stored as a two-dimensional matrix $SKW_{i,j}$ for i = 1, 2, ..., IKAPA and j = 1, 2, ..., IOMEGA. For intermediate values of $\varkappa$ and ω, $S(\varkappa, \omega)$ is calculated by using the following interpolation scheme. Let $\varkappa$ and $|\omega|$ satisfy the relationships

$$\left.\begin{aligned} &\varkappa_m \le \varkappa \le \varkappa_{m+1}, \qquad m < \text{IKAPA}, \\ &\text{and} \\ &\omega_n \le |\omega| \le \omega_{n+1}, \qquad n < \text{IOMEGA}. \end{aligned}\right\} \tag{33}$$

Within $\varkappa_m$ and $\varkappa_{m+1}$, the $\varkappa$-dependence of $S(\varkappa, \omega)$ is assumed to be approximated by

$$S(\varkappa, \omega) = a(\omega)\varkappa^{b(\omega)}. \tag{34}$$

$S(\varkappa, \omega_n)$ and $S(\varkappa, \omega_{n+1})$ are calculated by using Eq. 34. We get

$$S(\varkappa, \omega_n) = SKW_{m,n} \exp[\log (SKW_{m,n}/SKW_{m+1,n}) \cdot \log (\varkappa/\varkappa_m)/\log (\varkappa_m/\varkappa_{m+1})] \tag{35}$$

and a similar equation for $S(\varkappa, \omega_{n+1})$. $S(\varkappa, |\omega|)$ is then obtained by linear interpolation. Thus,

$$S(\varkappa, |\omega|) = \frac{S(\varkappa, \omega_{n+1}) - S(\varkappa, \omega_n)}{\omega_{n+1} - \omega_n} (|\omega| - \omega_n). \tag{36}$$

For negative values of ω, the principle of detailed balance gives

$$S(\varkappa, -|\omega|) = e^{\omega/T} S(\varkappa, |\omega|). \tag{37}$$

For $\varkappa < \varkappa_1$, m in Eq. 35 is set equal to 1; for $\varkappa > \varkappa_{IKAPA}$, m is set equal to IKAPA - 1. Equation 36 then evaluates $S(\varkappa, |\omega|)$. For $|\omega| > \omega_{IOMEGA}$, $S(\varkappa, \omega)$ is set equal to zero. Since logarithms of functions are taken by the computer code, neither $\varkappa$ nor $S(\varkappa, \omega)$ should ever be set to zero in the input. This would result in a diagnostic error.

Integrations are carried out in a straightforward manner using Simpson's rule with a specified number of mesh points in θ' and φ' integrations. The integration in E' is also carried out by Simpson's rule, for which the upper and lower limits, as well as the integration grid (ΔE), are supplied externally. The code is written in such a way that energy values are added (subtracted) in steps of ΔE to (from) the incident neutron energy. This method ensures correct estimates of the second-order scattered-neutron current, even in the elastic region. Our experience with this code has indicated that nine mesh points in both θ' and φ' integrations are sufficient, while many more mesh points should be used in E' integration. We recommend using ΔE (the energy mesh size) of 0.1 or 0.2 meV in the quasi-elastic region; ΔE of 0.2 or 0.4 meV should be used in inelastic region.

In cold-neutron scattering experiments, the scattered intensity and neutron energy are usually observed in time-of-flight scale. Hence, the above results for J_1 and J_2 for either transmission or reflection experiments are to be transformed to the time-of-flight scale. This is done by noting that the number of neutrons recorded within a unit time-of-flight increment should be the same as the number of neutrons recorded within a unit-energy increment. One therefore has

$$J(E)|dE| = J(f)|df|, \tag{38}$$

where f is the time of flight. Equation 38 can also be written as

$$J(f) = 2\left(\frac{2}{m}\right)^{1/2} E^{3/2} J(E). \tag{39}$$

The code can evaluate either J(E) or J(f).

II. COMPUTER PROGRAM

The DBLSCAT program calculates the first- and second-order scattered-neutron currents for either transmission- or reflection-type inelastic-neutron-scattering experiments. Both energy and time-of-flight scale can be used. The program is written so that the correction due to double scattering is evaluated for a given scattering angle and a number of scattered neutron-energy or time-of-flight values. Units of input parameters are indicated in their description. As a rule, energy is always given in milli-electron volts, and time of flight in μsec/m. The scattering law is read in units of 10^{-12} sec for a range of the momentum-transfer values $\varkappa$ (in $\mathring{A}^{-1}$) and a range of the energy-transfer variable ω (in 10^{12} sec^{-1}). Both $\varkappa$ and ω are to be specified in an ascending sequence of positive values, with ω starting from $\omega = 0$, while $\varkappa = 0$ should be avoided.

A. Description of Input

The input data required by the DBLSCAT program and the corresponding format are described below.

Input cards are numbered to simplify the description of input. These card numbers may be written in spaces 73-80 if desired, since these columns are not read here.

Except for the title card, all the input data are to be given in one of the two formats I6 or E12.5 as indicated below.

Card No.					
1000	Title card, with 1 in column one and any information in columns 2-72.				
1100	IKAPA	IOMEGA			
	I6	I6			
	IKAPA:	Number of $\varkappa$ variables. It must be ≤ 100.			
	IOMEGA:	Number of ω variables. It must be ≤ 100.			
1200	KAPA(1)	KAPA(2)	KAPA(3)	...	KAPA(IKAPA)
	E12.5	E12.5	E12.5		E12.5
	KAPA(I)	Momentum-transfer variables in ascending order in units of $\mathring{A}^{-1}$. There are as many cards of this number as needed to specify IKAPA values with six values per card. KAPA(I) should not be 0.			

Card No.					
1300	OMEGA(1)	OMEGA(2)	OMEGA(3)	...	OMEGA(IOMEGA)
	E12.5	E12.5	E12.5		E12.5

OMEGA(I): Energy-transfer variables in ascending order for positive values only, starting with $\omega = 0$ in units of 10^{12} per sec. There are as many cards of this number as needed to specify IOMEGA values with six values per card.

1400	SKW(1,1)	SKW(1,2)	SKW(1,3)	...	SKW(1,IOMEGA)
	SKW(2,1)	SKW(2,2)	SKW(2,3)	...	SKW(2,IOMEGA)
	SKW(3,1)	SKW(3,2)	SKW(3,3)		SKW(3,IOMEGA)
	SKW(IKAPA,1)	SKW(IKAPA,1)			SKW(IKAPA,IOMEGA)
	E12.5	E12.5	E12.5		E12.5

SKW(I,J): Scattering law in units of 10^{-12} sec for Ith value of $\varkappa$ and Jth value of ω. $S(\varkappa, \omega)$ for the first $\varkappa$ value and IOMEGA values of ω (starting with $\omega = 0$) are first read. This process is repeated for the second $\varkappa$ value, and so on, until $S(\varkappa, \omega)$ for all $\varkappa$ and ω values are read. There are as many cards of this number as needed to specify IKAPA×IOMEGA values with six entries per card. Note that SKW should not be input as 0 or negative number.

1500	NENRGY	NEXP	ITHETA	IPHI	IE
	I6	I6	I6	I6	I6

NENRGY: ≤ 0, if time-of-flight scale is used.

> 0, if energy scale is used.

NEXP: ≤ 0, for transmission experiment.

> 0, for reflection experiment.

ITHETA: Number of meshes in θ' integration. It must be odd and ≤ 31.

IPHI: Number of meshes in φ' integration. It must be odd and ≤ 31.

IE: Number of scattered-neutron energy values for which double-scattering calculations are to be performed. It must be ≤ 50.

Card No.

1600 FLUX NPMOLE SIGMAB A_1 A_2 A_3

E12.5 E12.5 E12.5 E12.5 E12.5 E12.5

FLUX: Incident neutron beam flux.

NPMOLE: Number of scattering atoms per molecule.

SIGMAB: Bound-atom scattering cross section, in barns.

A_1, A_2, A_3: There are constants which appear in the following expression for total macroscopic cross section: $\Sigma(E) = A_1 + A_2 E^{+A_3}$, E being in millielectron volts.

1700 THICK TEMP THETAO DENSTY TOFO

E12.5 E12.5 E12.5 E12.5 E12.5

THICK: Slab thickness, in cm.

TEMP: Sample temperature, in °K.

THETAO: Angle between incident-neutron beam and slab normal.

DENSTY: Molecular density of the specimen in 10^{24} cm^{-3}.

TOFO: Incident neutron time of flight, in μsec/m, if NENRGY ≤ 0. Incident neutron energy, in meV, if NENRGY > 0.

1800 ELOWER EUPPER THETA

E12.5 E12.5 E12.5

ELOWER: Lower limit in E' integration, in meV.

EUPPER: Upper limit in E' integration, in meV.

THETA: Angle between scattered-neutron beam and slab normal.

1900 TF(1) TF(2) TF(3) ... TF(IE)

E12.5 E12.5 E12.5 E12.5

TF(I): Scattered-neutron time of flight, in μsec/m, if NENRGY ≤ 0. Scattered-neutron energy, in meV, if NENRGY > 0. There are as many cards of this number as needed to specify IE values with six entries per card.

Card No.					
2000	DELE(1)	DELE(2)	DELE(3)	...	DELE(IE)
	E12.5	E12.5	E12.5		E12.5

DELE(I): Energy mesh size in E' integration in meV. This quantity is varied with final neutron energy so that computer time is economized. For quasi-elastic peak, it should be either 0.1 or 0.2; for inelastic region, it could be either 0.2 or 0.4. There are as many cards of this number as needed to specify IE values with six entries per card. $(E_{upper}-E_{lower})/$ DELE(I) must be ≤ 497.

B. Output Description

The output of the DBLSCAT program is self-explanatory. To begin with, the scattering law $S(\varkappa, \omega)$ is printed for a given $\varkappa$ value. Note that the units of $\varkappa$, ω, and $S(\varkappa, \omega)$ are also printed to check for consistency.

A consistency check is made between the experimental geometry and the angle θ that the scattered neutron makes with the slab normal. That is to say, θ must be less than $\pi/2$ for transmission experiments, and it must be greater than $\pi/2$ for reflection experiments. If these conditions are not satisfied, an error message is printed and calculations are terminated.

The description of the sample and other parameters are then printed. This printout is primarily for verifying the input data. Following this description, results of the computation are printed for each scattered-neutron energy. These results include J_1, J_2, (J_1+J_2) and the scattering cross section for the single scattering as well as single plus double scattering. The percentage correction is also printed in terms of $(J_1+J_2)/J_1$. The scattering angle is always given by $|\theta - \theta_0|$.

C. Sample Problems

Two sample problems are presented here. They are identical in all respects, with the following exceptions: Problem 1 is for transmission experiment in which scattered-neutron intensities are observed in units of time-of-flight scale; Problem 2 is for reflection experiment in which scattered-neutron intensities are observed in energy units. A hypothetical cold-neutron experiment with liquid argon is used, basic data for which are given in Table I.

The complete set of input data forms and printouts for the above case is shown on the pages following Table I. In the second case, the computer-printed output for the scattering law is not included, since this is the same as that for the first problem.

The computer time is determined primarily by the number of grid points used in θ', φ', and E' integrations. For the problems under discussion, we have used $N(\theta') = N(\varphi') = 9$ and $N(E') = 193$ in the elastic region and $N(E') = 97$ in the inelastic region. For $N(\theta') = N(\varphi') = 9$; each energy mesh takes about 250 msec of IBM 360/75 processor time. The total processor time used for Problems 1 and 2 was about 3 min.

TABLE I. Data Used in Sample Problems 1 and 2

Specimen:	Liquid argon
Temperature:	85°K
Liquid density:	1.42 g/cm^3
Slab thickness:	0.1 cm
Atomic density:	$0.0213877 \times 10^{24}/\text{cm}^3$
Total cross section:	$\sigma(E) = 1.0 + 2.30735 \times E^{-0.584963}$ barns, where E is in meV
Macroscopic cross section:	$\Sigma(E) = 0.0213877 \times 10^{24}/\text{cm}^3 \times \sigma(E)$ $= 0.0213877 + 0.0493489\ E^{-0.584963}\ \text{cm}^{-1}$
Scattering model:	Simple diffusion
Self-diffusion coefficient:	$1.88 \times 10^{-5}\ \text{cm}^2/\text{sec}$
Incident neutron energy:	1036.0 μsec/m or 4.87 meV
Scattered neutron energy:	800.0, 1036.0, and 1100.0 μsec/m or 8.17, 4.87, and 4.32 meV

COMPUTER INPUT DATA FORM

COST CODE _____

PROGRAM DBLSCAT **PROBLEM** ARGON at 85 K **ORIGINATOR** A. K. AGRAWAL **DATE** 2/10/71 **PAGE** 1 **OF** 2

1	2	3	4	5	6	7	8
1 2 3 4 5 6 7 8 9	0 1 2 3 4 5 6 7 8 9	0 1 2 3 4 5 6 7 8 9	0 1 2 3 4 5 6 7 8 9	0 1 2 3 4 5 6 7 8 9	0 1 2 3 4 5 6 7 8 9	0 1 2 3 4 5 6 7 8 9	0
1 *	DBLSCAT * SAMPLE PROBLEM 1* -1	TRANSMISSION EXPT. -TIME OF FLIGHT	1000				
10	12		1100				
0.1	0.5	1.0	1.5	2.0	3.0		1200
4.0	5.0	6.0	7.0				1200
0.0	0.5	1.0	2.0	5.0	10.0		1300
20.0	30.0	40.0	50.0	60.0	70.0		1300
3.183	10E-01	2.375	8.2E-03	5.973	3.04E-04	1.45	1400
1.496	0.E-06	6.649	1.4E-07	3.740	1.44E-07	6.93E-07	1400
13.183	10E-01	15.037	2.2E-02	9.01E-02	3.696	7.5E-03	1400
3.739	70E-05	1.6622	2.8E-05	9.350	3.5E-06	7.1E-06	1400
3.183	10E-01	1.3666	2.6E-01	5.037	2.3E-02	9.0E-02	1400
1.495	35E-04	6.6477	7.5E-05	3.739	7.0E-05	2.3993	5.1E-05	1.6622	2.8E-05	2.271E-05	1400
3.183	10E-01	2.0100	6.7E-01	9.462	0.6E-02	3.044	2.0E-02	5.293	2.0E-03	1.348	7.8E-03	1400
3.336	2.6E-04	1.495	3.5E-04	8.413	0.9E-05	5.384	8.9E-05	3.739	7.0E-05	2.747	6.2E-05	1400
3.183	10E-01	2.388	9.1E-01	1.366	2.6E-01	5.037	2.3E-02	9.295	1.6E-03	2.375	8.2E-03	1400
5.973	0.0E-04	2.657	4.4E-04	1.495	3.5E-04	9.571	8.8E-05	6.647	7.5E-05	2.815	6.1E-05	1400
3.183	10E-01	2.773	3.3E-01	2.000	6.7E-01	9.462	0.6E-02	2.017	7.6E-02	5.293	2.0E-03	1400
1.340	7.8E-03	5.973	0.0E-04	3.362	5.7E-04	2.115	2.8E-04	1.495	3.5E-04	1.098	7.6E-04	1400
3.183	10E-01	2.938	8.5E-01	2.388	9.1E-01	1.366	2.6E-01	3.418	5.8E-02	9.295	1.6E-03	1400
2.375	8.2E-03	1.060	3.2E-03	5.973	0.0E-04	3.825	3.0E-04	2.657	4.4E-04	1.952	8.3E-04	1400
1 2 3 4 5 6 7 8 9	0 1 2 3 4 5 6 7 8 9	0 1 2 3 4 5 6 7 8 9	0 1 2 3 4 5 6 7 8 9	0 1 2 3 4 5 6 7 8 9	0 1 2 3 4 5 6 7 8 9	0 1 2 3 4 5 6 7 8 9	0
1	2	3	4	5	6	7	8

COMPUTER INPUT DATA FORM

COST CODE _____

PROGRAM DBLSCAT **PROBLEM** ARGON at 85 K **ORIGINATOR** A. K. AGRAWAL **DATE** 2/10/71 **PAGE** 2 **OF** 2

1	2	3	4	5	6	7	8
3.1830E-01	3.0222E-01	2.6244E-01	1.7199E-01	5.0327E-02	1.4289E-02	1400	
3.6996E-03	1.6513E-03	9.8222E-04	5.9730E-04	4.1550E-04	3.0500E-04	1400	
3.1830E-01	3.0699E-01	2.7775E-01	2.0000E-00	6.7810E-02	2.0017E-02	1400	
5.2996E-03	2.3756E-03	1.3400E-03	9.5194E-04	5.9730E-04	4.3900E-04	1400	
3.1830E-01	3.0999E-01	2.8701E-01	2.2191E-01	8.5708E-02	2.6840E-02	1400	
7.1655E-03	3.2250E-03	1.8222E-03	1.1683E-03	8.1240E-04	5.9730E-04	1400	
-1	-1	9	9	3		1500	
1.0	1.0	.0622	2.1388E-02	4.9340E-02	-0.5840	9603	1600
0.1	8501.0	1000.0	2.1388E-02	10360.0			1700
2.0	3010.0	4000.0					1800
8000.0	10360.0	11000.0					1900
0.2	0.1	0.1					2000
1	2	3	4	5	6	7	8

DBLSCAT *SAMPLE PROBLEM 1* - TRANSMISSION EXPT. - TIME OF FLIGHT

LISTING OF SCATTERING LAW BEING USED IN DBLSCAT CODE

KAPA= 0.100 ANGSTROMS

OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC
0.0	3.18310E-01	5.00000E-01	2.37582E-03	1.00000E 00	5.97300E-04	2.00000E 00	1.49535E-04
5.00000E 00	2.39351E-05	1.00000E 01	5.98410E-06	2.00000E 01	1.49600E-06	3.00000E 01	6.64900E-07
4.00000E 01	3.74014E-07	5.00000E 01	2.39369E-07	6.00000E 01	1.66228E-07	7.00000E 01	1.22127E-07

KAPA= 0.500 ANGSTROMS

OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC
0.0	3.18310E-01	5.00000E-01	5.03722E-02	1.00000E 00	1.42890E-02	2.00000E 00	3.69675E-03
5.00000E 00	5.97300E-04	1.00000E 01	1.49535E-04	2.00000E 01	3.73970E-05	3.00000E 01	1.66228E-05
4.00000E 01	9.35035E-06	5.00000E 01	5.98422E-06	6.00000E 01	4.15571E-06	7.00000E 01	3.05318E-06

KAPA= 1.000 ANGSTROMS

OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC
0.0	3.18310E-01	5.00000E-01	1.36626E-01	1.00000E 00	5.03723E-02	2.00000E 00	1.42890E-02
5.00000E 00	2.37582E-03	1.00000E 01	5.97300E-04	2.00000E 01	1.49535E-04	3.00000E 01	6.64775E-05
4.00000E 01	3.73970E-05	5.00000E 01	2.39351E-05	6.00000E 01	1.66228E-05	7.00000E 01	1.22127E-05

KAPA= 1.500 ANGSTROMS

OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC
0.0	3.18310E-01	5.00000E-01	2.00067E-01	1.00000E 00	9.46206E-02	2.00000E 00	3.04420E-02
5.00000E 00	5.29620E-03	1.00000E 01	1.34078E-03	2.00000E 01	3.33626E-04	3.00000E 01	1.49535E-04
4.00000E 01	8.41309E-05	5.00000E 01	5.38489E-05	6.00000E 01	3.73970E-05	7.00000E 01	2.74762E-05

KAPA= 2.000 ANGSTROMS

OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC
0.0	3.18310E-01	5.00000E-01	2.38891E-01	1.00000E 00	1.36626E-01	2.00000E 00	5.03723E-02
5.00000E 00	9.29516E-03	1.00000E 01	2.37582E-03	2.00000E 01	5.97300E-04	3.00000E 01	2.65744E-04
4.00000E 01	1.49535E-04	5.00000E 01	9.57188E-05	6.00000E 01	6.64775E-05	7.00000E 01	2.81561E-05

KAPA= 3.000 ANGSTROMS

OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC
0.0	3.18310E-01	5.00000E-01	2.77333E-01	1.00000E 00	2.00067E-01	2.00000E 00	9.46206E-02
5.00000E 00	2.01776E-02	1.00000E 01	5.29620E-03	2.00000E 01	1.34078E-03	3.00000E 01	5.97300E-04
4.00000E 01	3.36257E-04	5.00000E 01	2.15286E-04	6.00000E 01	1.49535E-04	7.00000E 01	1.09876E-04

KAPA= 4.000 ANGSTROMS

OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC
0.0	3.18310E-01	5.00000E-01	2.93885E-01	1.00000E 00	2.38891E-01	2.00000E 00	1.36626E-01
5.00000E 00	3.41858E-02	1.00000E 01	9.29516E-03	2.00000E 01	2.37582E-03	3.00000E 01	1.06032E-03
4.00000E 01	5.97300E-04	5.00000E 01	3.82530E-04	6.00000E 01	2.65744E-04	7.00000E 01	1.95283E-04

KAPA= 5.000 ANGSTROMS

OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC
0.0	3.18310E-01	5.00000E-01	3.02234E-01	1.00000E 00	2.62466E-01	2.00000E 00	1.71961E-01
5.00000E 00	5.03723E-02	1.00000E 01	1.42890E-02	2.00000E 01	3.69670E-03	3.00000E 01	1.65365E-03
4.00000E 01	9.32297E-04	5.00000E 01	5.97300E-04	6.00000E 01	4.15029E-04	7.00000E 01	3.05025E-04

KAPA= 6.000 ANGSTROMS

OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC
0.0	3.18310E-01	5.00000E-01	3.06971E-01	1.00000E 00	2.77333E-01	2.00000E 00	2.00067E-01
5.00000E 00	6.78142E-02	1.00000E 01	2.01776E-02	2.00000E 01	5.29619E-03	3.00000E 01	2.37582E-03
4.00000E 01	1.34078E-03	5.00000E 01	8.59402E-04	6.00000E 01	5.97300E-04	7.00000E 01	4.39051E-04

KAPA= 7.000 ANGSTROMS

OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC	OMEGA 10(12)/SEC	S(K,W) 10(-12) SEC
0.0	3.18310E-01	5.00000E-01	3.09900E-01	1.00000E 00	2.87140E-01	2.00000E 00	2.21940E-01
5.00000E 00	8.57088E-02	1.00000E 01	2.68493E-02	2.00000E 01	7.16565E-03	3.00000E 01	3.22507E-03
4.00000E 01	1.82218E-03	5.00000E 01	1.16860E-03	6.00000E 01	8.12441E-04	7.00000E 01	5.97300E-04

```
*DBLSCAT* *SAMPLE PROBLEM 1* - TRANSMISSION EXPT. - TIME OF FLIGHT

                    THICK= 1.00000E-01 CM
                     TEMP= 8.50000E 01 K
                   THETAO= 1.00000E 01 DEG
        MOLECULAR DENSITY= 2.13877E-02 X10(24)/CM(3)
                     FLUX= 1.00000E 00
NO.OF SCATTERERS PER MOLECULE= 1.00000E 00
    BOUND ATOM CROSS SECTION= 6.20000E-01BARNS
                 SIGMA(E)= 2.13877E-02 +  4.93489E-02 *E**(-5.84930E-01)
                   ELOWER= 2.00000E 00 MEV
                   EUPPER= 4.00000E 01 MEV
            NO.OF MESHES USED IN THETA INTEGRATION=     9
            NO.OF MESHES USED IN PHI   INTEGRATION=     9

 TIME OF FLIGHT SCALE IS USED.
 TRANSMISSION EXPERIMENT GEOMETRY IS USED.
```

```
*DBLSCAT* *SAMPLE PROBLEM 1* - TRANSMISSION EXPT. - TIME OF FLIGHT

 TIME OF FLIGHT SCALE IS USED

 TRANSMISSION EXPERIMENT GEOMETRY IS USED.

 INCIDENT TIME OF FLIGHT= 1.03600E 03 MICROSEC/METER
                     EO= 4.87340E 00 MEV
                  THETA= 4.00000E 01 DEG
       SCATTERING ANGLE= 3.00000E 01 DEG
```

T OF F MICROSEC/M	E MEV	NO.OF ENERGY MESHES	J1	J2	(J1+J2)	SIGMA1 BARNS/MICROSEC/METER	SIGMA12	(J1+J2)/J1
8.00000E 02	8.17281E 00	97	1.34342E-08	7.67675E-09	2.11110E-08	4.79786E-06	7.53951E-06	1.57143E 00
1.03600E 03	4.87340E 00	193	4.85225E-07	9.24505E-09	4.94470E-07	2.24486E-04	2.28763E-04	1.01905E 00
1.10000E 03	4.32281E 00	193	4.51888E-08	5.48519E-09	5.06740E-08	2.21998E-05	2.48945E-05	1.12138E 00

COMPUTER INPUT DATA FORM

COST CODE _____

PROGRAM DBLSCAT **PROBLEM** ARGON at 85 K **ORIGINATOR** A. K. AGRAWAL **DATE** 2/10/71 **PAGE** 1 **OF** 1

1	2	3	4	5	6	7	8
1	*DBLSCAT *SAMPLE PROBLEM	2* -REFLECTION EXPT.		-ENERGY SCALE			1000
	(CAR DS 110 TO 140	OF THE SAMPLE PROB	LEM NO. 1	DESCRIBING S(K,W))			
	1	1	9	9	3		1500
1.0		1.0		0.62		2.138 77E-02	4.934 89E-02 -0.584 963	1600
0.1		85.0		10.0		2.138 77E-02	4.87	1700
2.0		30.0		120.				1800
8.17		4.87		4.32				1900
0.2		0.1		0.1				2000

```
*DBLSCAT* *SAMPLE PROBLEM 2* - REFLECTION EXPERIMENT- ENERGY SCALE

                    THICK= 1.00000E-01 CM
                     TEMP= 8.50000E 01 K
                   THETAO= 1.00000E 01 DEG
        MOLECULAR DENSITY= 2.13877E-02 X10(24)/CM(3)
                     FLUX= 1.00000E 00
NO.OF SCATTERERS PER MOLECULE= 1.00000E 00
    BOUND ATOM CROSS SECTION= 6.20000E-01BARNS
                 SIGMA(E)= 2.13877E-02 +  4.93489E-02 *E**(-5.84930E-01)
                  ELOWER= 2.00000E 00 MEV
                  EUPPER= 4.00000E 01 MEV
            NO.OF MESHES USED IN THETA INTEGRATION=     9
            NO.OF MESHES USED IN PHI   INTEGRATION=     9

 ENERGY SCALE IS USED.
 REFLECTION EXPERIMENT GEOMETRY IS USED.
```

```
*DBLSCAT* *SAMPLE PROBLEM 2* - REFLECTION EXPERIMENT- ENERGY SCALE

 ENERGY SCALE IS USED.

 REFLECTION EXPERIMENT GEOMETRY IS USED.
            EO= 4.87000E 00 MEV
         THETA= 1.20000E 02 DEG
 SCATTERING ANGLE= 1.10000E 02DEG
```

E MEV	NO.OF ENERGY MESHES	J1	J2	(J1+J2)	SIGMA1 BARNS/MEV	SIGMA12 BARNS/MEV	(J1+J2)/J1
8.17000E 00	97	-5.10316E-06	-3.57040E-07	-5.46020E-06	1.82446E-03	1.93211E-03	1.06996E 00
4.87000E 00	193	-5.15028E-05	-9.42090E-07	-5.24449E-05	2.38610E-02	2.42975E-02	1.01829E 00
4.32000E 00	193	-2.47638E-05	-6.61946E-07	-2.54258E-05	1.21833E-02	1.25090E-02	1.02673E 00

APPENDIX

FORTRAN Program Listing

```
      REAL *4 KAPA,NPMOLE                                               MAIN0010
CC*********************************************************************MAIN0020
CC        THIS PROGRAM CALCULATES ONCE AND TWICE SCATTERED NEUTRON      MAIN0030
CC        CURRENT. FOR BOTH TRANSMISSION AND REFLECTION TYPE EXPTS.     MAIN0040
CC*********************************************************************MAIN0050
      DIMENSION TITLE(18),TF(50),DELE(50),E(50),P1(50),P2(50),P12(50),  MAIN0060
     1SIGM1(50),SIGM12(50),RATIO(50)                                    MAIN0070
      COMMON /SUB/FLUX,C1  ,THICK,A1,A2,A3,DENSTY,NEXP                  MAIN0080
      COMMON /SUC/EO,COTO,SITO,COT,SIT,COTT,COTP(31),SITP(31),COPHI(31),MAIN0090
     1ITHETA,IPHI,ELOWER,EUPPER                                         MAIN0100
      COMMON /SET/KAPA(100),OMEGA(100),SKW(100,100),IKAPA,IOMEGA,TEMP   MAIN0110
      DATA CONST/5.2306E+6/,DTOR/0.017453/,PI/3.141593/,C2/8.74488E-04/ MAIN0120
CC*********************************************************************MAIN0130
CC                                                                      MAIN0140
CC        KAPA      IS THE MOMENTUM TRANSFER VARIABLE IN ANGSTROM(-1),  MAIN0150
CC        IKAPA     IS THE NUMBER OF KAPA VARIABLES,                    MAIN0160
CC        OMEGA     IS THE ENERGY TRANSFER VARIABLE IN 10(12) SEC(-1),  MAIN0170
CC        IOMEGA    IS THE NUMBER OF OMEGA VARZABLES.                   MAIN0180
CC        SKW       IS THE SCATTERING LAW IN 10(-12) SEC,               MAIN0190
CC                  IKAPA*IOMEGA ENTRIES.                               MAIN0200
CC        NENRGY    IS LESS THAN OR EQUAL TO 0 IF TIME OF FLIGHT SCALE  MAIN0210
CC                  IS USED.                                            MAIN0220
CC                  IF NENRGY IS GREATER THAN 0, ENERGY SCALE IS USED,  MAIN0230
CC        NEXP      IS LESS THAN OR EQUAL TO 0 FOR TRANSMISSION EXPTS,  MAIN0240
CC                  IS GREATER THAN 0 FOR REFLECTION EXPTS.             MAIN0250
CC        ITHETA    IS THE NUMBER OF MESH POINTS TO BE USED IN THETA    MAIN0260
CC                  PRIME INTEGRATION.                                  MAIN0270
CC                  IT MUST BE AN ODD NUMBER.                           MAIN0280
CC        IPHI      IS THE NUMBER OF MESH POINTS TO BE USED IN PHI      MAIN0290
CC                  PRIME INTEGRATION.                                  MAIN0300
CC                  IT MUST BE AN ODD NUMBER.                           MAIN0310
CC        IE        IS THE NUMBER OF SCATTERED NEUTRON ENERGY VALUES.   MAIN0320
CC        FLUX      IS THE INCIDENT BEAM FLUX.                          MAIN0330
CC        NPMOLE    NO. OF SCATTERERS PER MOLECULE.                     MAIN0340
CC        SIGMAB    BOUND ATOM SCATTERING CROSS SECTION IN BARNS.       MAIN0350
CC        A1,A2,A3  ARE PARAMETERS OF TOTAL MACROSCOPIC CROSS SECTION.  MAIN0360
CC                  SIGMA(E)=A1+A2*E**(+A3) WHERE E IS IN MILLIVOLTS.   MAIN0370
CC                  A1 IS IN CM(-1).                                    MAIN0380
CC        THICK     IS THE SAMPLE SLAB THICKNESS IN CM.                 MAIN0390
CC        TEMP      IS THE SAMPLE TEMPRATURE IN K.                      MAIN0400
CC        THETAO    IS THE ANGLE MADE BY THE INCIDENT BEAM WITH SLAB    MAIN0410
CC                  NORMAL.                                             MAIN0420
CC                  IT IS IN DEGREES.                                   MAIN0430
CC        DENSTY    IS THE MOLECULAR DENSITY.                           MAIN0440
CC        TOFO      IS INCIDENT TIME OF FLIGHT IF NENRGY IS LESS THAN   MAIN0450
CC                  OR EQUAL TO ZERO.                                   MAIN0460
CC                  IT IS INCIDENT NEUTRON ENERGY IF NENRGY IS GREATER  MAIN0470
CC                  THAN ZERO.                                          MAIN0480
CC        ELOWER AND EUPPER ARE LOWER AND UPPER ENERGY VALUES IN ENERGY MAIN0490
CC                  INTEGRATION.                                        MAIN0500
CC                  THESE ARE IN MILLIELECTRON VOLTS.                   MAIN0510
CC        THETA     IS THE ANGLE BETWEEN OUTGOING NEUTRON BEAM AND      MAIN0520
CC                  SLAB NORMAL.                                        MAIN0530
CC                  IT IS IN DEGREES.                                   MAIN0540
CC        SCTANG    IS THE SCATTERING ANGLE.                            MAIN0550
CC                  IT IS IN DEGREES.                                   MAIN0560
CC        IE        IS THE NUMBER OF FINAL NEUTRON ENERGY VALUES.       MAIN0570
CC        TF        ARE THE TIME OF FLIGHT OF OUTGOING NEUTROM IF NENRGYMAIN0580
CC                  IS LESS THAN OR EQUAL TO 0.                         MAIN0590
CC                  ARE THE ENRGY OF OUTGOING NEUTRON IF NENRGY         MAIN0600
CC                  IS GREATER THAN 0.                                  MAIN0610
CC                  IF TF ARE ENERGY, THEY MUST BE IN MEV.              MAIN0620
CC        DELE      IS THE ENERGY MESH SIZE IN E PRIME INTEGRATION.     MAIN0630
CC                  IT CAN BE VARRIED WITH TF.                          MAIN0640
CC                                                                      MAIN0650
CC*********************************************************************MAIN0660
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      READ  (5,7000)     (TITLE(I),I=1,18)                                MAIN0670
      READ  (5,7005)     IKAPA,IOMEGA                                     MAIN0680
      READ  (5,7010)     (KAPA(I),I=1,IKAPA)                              MAIN0690
      READ  (5,7010)     (OMEGA(I),I=1,IOMEGA)                            MAIN0700
      READ  (5,7010)     ((SKW(I,J),J=1,IOMEGA),I=1,IKAPA)                MAIN0710
CC                                                                        MAIN0720
CC    LISTING OF S(K,W) FUNCTION                                          MAIN0730
CC                                                                        MAIN0740
      WRITE (6,8000)     (TITLE(J),J=1,18)                                MAIN0750
      DO 100             I=1,IKAPA                                        MAIN0760
      WRITE (6,8005)     KAPA(I)                                          MAIN0770
      WRITE (6,8010)     (OMEGA(J),SKW(I,J),J=1,IOMEGA)                   MAIN0780
  100 CONTINUE                                                            MAIN0790
      READ  (5,7005)     NENRGY,NEXP,ITHETA,IPHI,IE                       MAIN0800
      READ  (5,7010)     FLUX,NPMOLE,SIGMAB,A1,A2,A3                      MAIN0810
      READ  (5,7010)     THICK,TEMP,THETAO,DENSTY,TOFO                    MAIN0820
      READ  (5,7010)     ELOWER,EUPPER,THETA                              MAIN0830
      READ  (5,7010)     (TF(I),I=1,IE)                                   MAIN0840
      READ  (5,7010)     (DELE(I),I=1,IE)                                 MAIN0850
CC                                                                        MAIN0860
CC    EDITING OF INPUT DATA                                               MAIN0870
CC                                                                        MAIN0880
      IF (NEXP .LE. 0 .AND. THETA .GE. 90.0) GO TO 110                    MAIN0890
      IF (NEXP .GE. 1 .AND. THETA .LE. 90.0) GO TO 115                    MAIN0900
      GO TO 125                                                           MAIN0910
  110 WRITE (6,8015)                                                      MAIN0920
      GO TO 120                                                           MAIN0930
  115 WRITE (6,8020)                                                      MAIN0940
  120 GO TO 155                                                           MAIN0950
  125 WRITE (6,8025)     (TITLE(J),J=1,18),THICK,TEMP,THETAO,DENSTY,FLUX,MAIN0960
     1                   NPMOLE,SIGMAB,A1,A2,A3,ELOWER,EUPPER,ITHETA,IPHIMAIN0970
      IF (NENRGY .LE. 0) WRITE (6,8030)                                   MAIN0980
      IF (NENRGY .GT. 0) WRITE (6,8035)                                   MAIN0990
      IF (NEXP .LE. 0)   WRITE (6,8040)                                   MAIN1000
      IF (NEXP .GT. 0)   WRITE (6,8045)                                   MAIN1010
      C1=DENSTY*NPMOLE*SIGMAB/(4.*PI*1.0544/1.602)                        MAIN1015
      COTO=COS(DTOR*THETAO)                                               MAIN1020
      SITO=SIN(DTOR*THETAO)                                               MAIN1030
      COT=COS(DTOR*THETA)                                                 MAIN1040
      SIT=SIN(DTOR*THETA)                                                 MAIN1050
      SCTANG=ABS(THETA-THETAO)                                            MAIN1060
      COTT=COS(DTOR*SCTANG)                                               MAIN1070
      DTHETA=PI/(ITHETA-1)                                                MAIN1080
      DO 130             I=1,ITHETA                                       MAIN1090
      X1=(I-1)*DTHETA                                                     MAIN1100
      COTP(I)=COS(X1)                                                     MAIN1110
  130 SITP(I)=SIN(X1)                                                     MAIN1120
      DPHI=PI/(IPHI-1)                                                    MAIN1130
      DO 135 I=1,IPHI                                                     MAIN1140
  135 COPHI(I)=COS((I-1)*DPHI)                                            MAIN1150
      IF (NENRGY .GT. 0) GO TO 145                                        MAIN1160
      EO=CONST/TOFO/TOFO                                                  MAIN1170
      DO 140             I=1,IE                                           MAIN1180
      E(I)=CONST/TF(I)/TF(I)                                              MAIN1190
      CALL JONE(PO1,E(I))                                                 MAIN1200
      CALL JTWO(PO2,E(I),DELE(I))                                         MAIN1210
      X2=E(I)*SQRT(E(I))*C2                                               MAIN1220
      P1(I)=PO1*X2                                                        MAIN1230
      P2(I)=PO2*X2                                                        MAIN1240
      P12(I)=P1(I)+P2(I)                                                  MAIN1250
      SIGM1(I)=CROSS(P1(I),E(I))                                          MAIN1260
      SIGM12(I)=CROSS(P12(I),E(I))                                        MAIN1270
  140 RATIO(I)=P12(I)/P1(I)                                               MAIN1280
      WRITE (6,8050)     (TITLE(J),J=1,18)                                MAIN1290
      IF (NEXP .LE. 0)   WRITE (6,8040)                                   MAIN1300
      IF (NEXP .GT. 0)   WRITE (6,8045)                                   MAIN1310
      WRITE (6,8055)     TOFO,EO,THETA,SCTANG                             MAIN1320
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      WRITE (6,8060)  (TF(I),E(I),DELE(I),P1(I),P2(I),P12(I),SIGM1(I),SIMAIN1330
     1                GM12(I),RATIO(I),I=1,IE)                          MAIN1340
      GO TO 155                                                         MAIN1350
  145 EO=TOFO                                                           MAIN1360
      DO 150 I=1,IE                                                     MAIN1370
      E(I)=TF(I)                                                        MAIN1380
      CALL JONE(PO1,E(I))                                               MAIN1390
      CALL JTWO(PO2,E(I),DELE(I))                                       MAIN1400
      P1(I)=PO1                                                         MAIN1410
      P2(I)=PO2                                                         MAIN1420
      P12(I)=P1(I)+P2(I)                                                MAIN1430
      SIGM1(I)=CROSS(P1(I),E(I))                                        MAIN1440
      SIGM12(I)=CROSS(P12(I),E(I))                                      MAIN1450
  150 RATIO(I)=P12(I)/P1(I)                                             MAIN1460
      WRITE (6,8065)     (TITLE(J),J=1,18)                              MAIN1470
      IF (NEXP .LE. 0)  WRITE (6,8040)                                  MAIN1480
      IF (NEXP .GT. 0)  WRITE (6,8045)                                  MAIN1490
      WRITE (6,8070)     EO,THETA,SCTANG                                MAIN1500
      WRITE (6,8075)  (E(I),DELE(I),P1(I),P2(I),P12(I),SIGM1(I),SIGM12(IMAIN1510
     1                ),RATIO(I),I=1,IE)                                MAIN1520
  155 STOP                                                              MAIN1530
 7000 FORMAT(18A4)                                                      MAIN1540
 7005 FORMAT(12I6)                                                      MAIN1550
 7010 FORMAT(6E12.5)                                                    MAIN1560
 8000 FORMAT(1H1,18A4//5X,'LISTING OF SCATTERING LAW BEING USED IN DBLSCMAIN1570
     AAT CODE'//)                                                       MAIN1580
 8005 FORMAT(1H0,7X,'KAPA=',F7.3,' ANGSTROMS'//4(7X,'OMEGA',9X,'S(K,W)',MAIN1590
     A3X)/4(4X,'10(12)/SEC',5X,'10(-12) SEC')/)                         MAIN1600
 8010 FORMAT(8(3X,1PE12.5))                                             MAIN1610
 8015 FORMAT(1H1,//5X,'*** ERROR MESSAGE ***'//5X,'SCATTERED BEAM ANGLE MAIN1620
     ATHETA MUST BE LESS THAN 90 DEGREES FOR TRANSMISSION EXPT.')       MAIN1630
 8020 FORMAT(1H1,//5X,'*** ERROR MESSAGE ***'//5X,'SCATTERED BEAM ANGLE MAIN1640
     ATHETA MUST BE GREATER THAN 90 DEGREES FOR REFLECTION EXPT.')      MAIN1650
 8025 FORMAT(1H1,18A4///29X,'THICK=',1PE12.5,' CM'//                    MAIN1660
     A                30X,'TEMP=',1PE12.5,' K'//                        MAIN1670
     B                28X,'THETAO=',1PE12.5,' DEG'//                    MAIN1680
     C                17X,'MOLECULAR DENSITY=',1PE12.5,' X10(24)/CM(3)MAIN1690
     D              '//30X,'FLUX=',1PE12.5//                            MAIN1700
     E                5X,'NO.OF SCATTERERS PER MOLECULE=',1PE12.5//   MAIN1710
     1                10X,'BOUND ATOM CROSS SECTION=',1PE12.5,'BARNS'/MAIN1720
     F               /26X,'SIGMA(E)=',1PE12.5,' + ',1PE12.5,           MAIN1730
     G                ' *E**(',1PE12.5,')'//                           MAIN1740
     H                28X,'ELOWER=',1PE12.5,' MEV'//                   MAIN1750
     I                28X,'EUPPER=',1PE12.5,' MEV'//                   MAIN1760
     J               20X,'NO.OF MESHES USED IN THETA INTEGRATION=',I6/MAIN1770
     K      /20X,'NO.OF MESHES USED IN PHI   INTEGRATION=',I6//)       MAIN1780
 8030 FORMAT(1H ,5X,' TIME OF FLIGHT SCALE IS USED.'/)                  MAIN1790
 8035 FORMAT(1H ,5X,' ENERGY SCALE IS USED.'/)                          MAIN1800
 8040 FORMAT(1H ,5X,' TRANSMISSION EXPERIMENT GEOMETRY IS USED.')       MAIN1810
 8045 FORMAT(1H ,5X,' REFLECTION EXPERIMENT GEOMETRY IS USED.')         MAIN1820
 8050 FORMAT(1H1,18A4///7X,'TIME OF FLIGHT SCALE IS USED'//)            MAIN1830
 8055 FORMAT(//7X,'INCIDENT TIME OF FLIGHT=',1PE12.5,' MICROSEC/METER'//MAIN1840
     A28X,'EO=',1PE12.5,' MEV'//25X,'THETA=',1PE12.5,' DEG'//14X,'SCATTEMAIN1850
     BRING ANGLE=',1PE12.5,' DEG'//5X,' T OF F',10X,'E',6X,'ENERGY',6X,'MAIN1860
     CJ1',12X,'J2',10X,'(J1+J2)',7X,'SIGMA1',8X,'SIGMA12',5X,'(J1+J2)/J1MAIN1870
     D'/30X,'MESH '/3X,'MICROSEC/M',8X,'MEV',6X,'SIZE  ',45X,'BARNS/MICRMAIN1880
     EOSEC/METER'//)                                                    MAIN1890
 8060 FORMAT(1P2E14.5,0PF6.2,1P6E14.5)                                  MAIN1900
 8065 FORMAT(1H1,18A4///6X,'ENERGY SCALE IS USED.'////)                 MAIN1910
 8070 FORMAT(/20X,'EO=',1PE12.5,' MEV'//17X,'THETA=',1PE12.5,' DEG'//   MAIN1920
     A6X,'SCATTERING ANGLE=',1PE12.5,'DEG'//7X,'E',7X,'ENERGY',6X,'J1',1MAIN1930
     B2X,'J2',10X,'(J1+J2)',7X,'SIGMA1',8X,'SIGMA12',5X,'(J1+J2)/J1'/   MAIN1940
     C16X,'MESH  '/6X,'MEV',7X,'SIZE  ',44X,'BARNS/MEV',5X,'BARNS/MEV'//MAIN1950
     D)                                                                 MAIN1960
 8075 FORMAT (1PE14.5,0PF6.2,1P6E14.5)                                  MAIN1970
      END                                                               MAIN1980
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      FUNCTION CROSS (CURENT,E)                                         CROS010
CC*********************************************************************CROS020
CC        THIS PROGRAM EVALUATES CROSS SECTION FROM CURRENT             CROS030
CC*********************************************************************CROS040
CC                                                                      CROS050
      COMMON /SUB/FLUX,CONS,THICK,A1,A2,A3,DENSTY,NEXP                  CROS060
      COMMON /SUC/EO,COTO,SITO,COT,SIT,COTT,COTP(31),SITP(31),COPHI(31), CROS070
     1ITHETA,IPHI,ELOWER,EUPPER                                         CROS080
      SGM(Y)=A1+A2*EXP(+A3*ALOG(Y))                                     CROS090
      SIGMAO=SGM(EO)/COTO                                               CROS100
      SIGMA1=SGM(E)/COT                                                 CROS110
      X=SIGMA1-SIGMAO                                                   CROS120
      IF (X.EQ.0.0) DN=1./THICK                                         CROS130
      IF (X.NE.0.0) DN=X/(EXP(-SIGMAO*THICK)-EXP(-SIGMA1*THICK))        CROS140
      CROSS=CURENT*COTO*DN*SQRT(EO/E)/DENSTY                            CROS150
      IF (NEXP .GE. 1) CROSS=CROSS*(-EXP(-SIGMA1*THICK))                CROS160
      RETURN                                                            CROS170
      END


      SUBROUTINE JONE(PO1,ENE)                                          JONE010
CC*********************************************************************JONE020
CC        THIS PROGRAM CALCULATES THE FIRST SCATTERED NEUTRON CURRENT FOR JONE030
CC        BOTH TRANSMISSION AND REFLECTION EXPERIMENTS.                 JONE040
CC*********************************************************************JONE050
      COMMON /SUB/FLUX,CONS,THICK,A1,A2,A3,DENSTY,NEXP                  JONE060
      COMMON /SUC/EO,COTO,SITO,COT,SIT,COTT,COTP(31),SITP(31),COPHI(31), JONE070
     1ITHETA,IPHI,ELOWER,EUPPER                                         JONE080
          SGM(Y)      =A1+A2*EXP(+A3*ALOG(Y))                           JONE090
          CKAPA       =0.6945*SQRT(ENE+EO-2.0*SQRT(ENE*EO)*COTT)        JONE100
          OMEGA       =(ENE-EO)*1.5184                                  JONE110
          SIGMAO      =SGM(EO)/COTO                                     JONE120
          SIGMA1      =SGM(ENE)/COT                                     JONE130
          X           =SIGMA1-SIGMAO                                    JONE140
      IF (X .EQ. 0.0) DN=THICK                                          JONE150
      IF (X .NE. 0.0) DN=(EXP(-SIGMAO*THICK)-EXP(-SIGMA1*THICK))/X      JONE160
          PO1         =FLUX*CONS/COTO *DN*ENE/EO*SKP(CKAPA,OMEGA)       JONE170
      IF (NEXP .GE. 1) PO1=PO1*(-EXP(SIGMA1*THICK))                     JONE180
      RETURN                                                            JONE190
      END                                                               JONE200


      SUBROUTINE JTWO(PO2,E,DELE)                                       JTWO010
CC*********************************************************************JTWO020
CC        THIS PROGRAM CALCULATES SECOND SCATTERED NEUTRON CURRENT FOR  JTWO030
CC        BOTH TRANSMISSION AND REFLECTION EXPERIMENTS.                 JTWO035
CC*********************************************************************JTWO040
      COMMON /SUB/FLUX,CONS,THICK,A1,A2,A3,DENSTY,NEXP                  JTWO050
      COMMON /SUC/EO,COTO,SITO,COT,SIT,COTT,COTP(31),SITP(31),COPHI(31), JTWO060
     1ITHETA,IPHI,ELOWER,EUPPER                                         JTWO070
      COMMON EX                                                         JTWO080
      EX=E                                                              JTWO090
      DELEA         =DELE/4.                                            JTWO100
      IF (E.GE.EO) GO TO 110                                            JTWO110
      RESULT        =SIMP(ELOWER,E-DELE,DELE)+SIMP(EO+DELE,EUPPER,DELE) JTWO120
      IF (E.GT.EO-2.*DELE) GO TO 100                                    JTWO130
      RESULT        =RESULT+SIMP(E-DELE,E+DELE,DELEA)                   JTWO140
     1                     +SIMP(E+DELE,EO-DELE,DELE)                   JTWO150
     2                     +SIMP(EO-DELE,EO+DELE,DELEA)                 JTWO160
      GO TO 140                                                         JTWO170
100   RESULT        =RESULT+SIMP(E-DELE,E,DELEA)                        JTWO180
     1                     +SIMP(E,EO,DELEA)                            JTWO190
     2                     +SIMP(EO,EO+DELE,DELEA)                      JTWO200
      GO TO 140                                                         JTWO210
110   IF (E.GT.EO) GO TO 120                                            JTWO220
      RESULT        =SIMP(ELOWER,EO-DELE,DELE)+SIMP(EO-DELE,EO+DELE,DELEA JTWO230
     1                )+SIMP(EO+DELE,EUPPER,DELE)                       JTWO240
      GO TO 140                                                         JTWO250
120   RESULT        =SIMP(ELOWER,EO-DELE,DELE)+SIMP(E+DELE,EUPPER,DELE) JTWO260
      IF (E.LT.EO+2.*DELE) GO TO 130                                    JTWO270
      RESULT        =RESULT+SIMP(EO-DELE,EO+DELE,DELEA)                 JTWO280
     1                     +SIMP(EO+DELE,E-DELE,DELE)                   JTWO290
     2                     +SIMP(E-DELE,E+DELE,DELEA)                   JTWO300
      GO TO 140                                                         JTWO310
130   RESULT        =RESULT+SIMP(EO-DELE,EO,DELEA)                      JTWO320
     1                     +SIMP(EO,E,DELEA)                            JTWO330
     2                     +SIMP(E,E+DELE,DELEA)                        JTWO340
140   PO2           =RESULT*CONS*CONS*FLUX*E/EO                         JTWO350
      RETURN                                                            JTWO360
      END                                                               JTWO370
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      FUNCTION      SIMP(EL,EU,DELE)                                    SIMP010
CC*********************************************************************** SIMP020
CC        IT CALCULATES INTEGRAL FROM EL TO EU WITH MESH SIZE DELE      SIMP030
CC        SIMPSON'S RULE OF INTEGRATION IS USED.                        SIMP040
CC*********************************************************************** SIMP050
         DE          =DELE                                              SIMP060
         N           =(EU-EL)/DE+1                                      SIMP070
      IF (N.EQ.1)  N=2                                                  SIMP080
      IF (MOD(N,2).EQ.0) N=N+1                                          SIMP090
         DE          =(EU-EL)/(N-1)                                     SIMP100
         SIMP        =THETA(EL)-THETA(EU)                               SIMP110
      DO 100         I=2,N,2                                            SIMP120
         E           =EL+(I-1)*DE                                       SIMP130
100      SIMP        =SIMP+4.0*THETA(E)+2.*THETA(E+DE)                  SIMP140
         SIMP        =SIMP*DE/3.                                        SIMP150
      RETURN                                                            SIMP160
      END                                                               SIMP170

      FUNCTION      THETA(EP)                                           THET010
CC*********************************************************************** THET020
CC        THIS PROGRAM EVALUATES THETA PRIME INTEGRATION.               THET030
CC*********************************************************************** THET040
      COMMON /SUC/EO,COTO,SITO,COT,SIT,COTT,COTP(31),SITP(31),COPHI(31), THET050
     1ITHETA,IPHI,ELOWER,EUPPER                                         THET060
      COMMON E                                                          THET070
      DATA PI/3.141593/                                                 THET080
         ITHETB      =ITHETA-1                                          THET090
         THETA       =0.                                                THET100
      DO 100         I=2,ITHETB,2                                       THET110
100      THETA       =THETA+4.*SITP(I)*PHII(EP,COTP(I),SITP(I),E)*      THET120
     1               VALU(I,EP,E)+2.*SITP(I+1)*PHII(EP,COTP(I+1),       THET130
     2               SITP(I+1),E)*VALU(I+1,EP,E)                        THET140
         THETA       =THETA*PI/ITHETB/3.                                THET150
      RETURN                                                            THET160
      END                                                               THET170

      FUNCTION VALU(NTP,E1,E)                                           VALU010
CC*********************************************************************** VALU020
CC        THIS PROGRAM CALCULATES ANGLE DEPENDENT TERM IN P2            VALU030
CC*********************************************************************** VALU040
      COMMON /SUB/FLUX,CONS,THICK,A1,A2,A3,DENSTY,NEXP                  VALU050
      COMMON /SUC/EO,COTO,SITO,COT,SIT,COTT,COTP(31),SITP(31),COPHI(31), VALU060
     1ITHETA,IPHI,ELOWER,EUPPER                                         VALU070
      EQUIVALENCE (THICK,T)                                             VALU080
         SGM(Y)      =A1+A2*EXP(+A3*ALOG(Y))                            VALU090
         SIGO        =SGM(EO)/COTO                                      VALU100
         SIG         =SGM(E )/COT                                       VALU110
         X1          =SIG-SIGO                                          VALU120
      IF (ABS(COTP(NTP)) .LE.0.001) GO TO 10                            VALU130
         SIG1        =SGM(E1)/COTP(NTP)                                 VALU140
         X2          =SIG-SIG1                                          VALU150
         X3          =SIG1-SIGO                                         VALU160
         FTETA1      =1.0                                               VALU170
      IF (COTP(NTP) .LT. 0.0) FTETA1=EXP(+X3*T)                         VALU180
      IF (X1 .EQ. 0.0 .AND. X2 .EQ. 0.0)          GO TO 20              VALU190
      IF (X1 .EQ. 0.0 )        GO TO 30                                 VALU200
      IF (X2 .EQ. 0.0 )        GO TO 40                                 VALU210
      IF (X3 .EQ. 0.0 )        GO TO 50                                 VALU220
         VALU        =            ((EXP(-SIGO*T)-EXP(-SIG*T))/X1        VALU230
     A                -(EXP(-SIG1*T)-EXP(-SIG*T))*FTETA1/X2)           VALU240
     B                /COTO/COTP(NTP)/X3                               VALU250
      GO TO 100                                                         VALU260
10    IF (X1 .EQ. 0.0 )        VALU        =    T/SGM(E1)/COTO          VALU270
         VALU        =            (EXP(-SIGO*T)-EXP(-SIG*T))/X1        VALU280
     A                /COTO/SGM(E1)                                    VALU290
      GO TO 100                                                         VALU300
20       VALU        =0.0                                               VALU310
      GO TO 100                                                         VALU320
30       VALU        =            (T-(EXP(-SIG1*T)-EXP(-SIG*T))*FTETA1/X2) VALU330
     A                /COTO/COTP(NTP)/X3                               VALU340
      GO TO 100                                                         VALU350
40       VALU        =            ((EXP(-SIGO*T)-EXP(-SIG*T))/X1-T*FTETA1) VALU360
     A                /COTO/COTP(NTP)/X3                               VALU370
      GO TO 100                                                         VALU380
 50       VALU        =T/X1/COTO/COTP(NTP)                              VALU390
  100 IF (NEXP .GE.1) VALU=VALU*(-EXP(SIG*T))                           VALU400
      RETURN                                                            VALU410
      END                                                               VALU420
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      FUNCTION PHII(E1,COT1,SIT1,E)                                     PHII010
C*********************************************************************** PHII020
C     THIS PROGRAM EVALUATES PHI PRIME INTEGRATION.                     PHII030
C*********************************************************************** PHII040
                                                                        PHII050
      DIMENSION CK(2,31)                                                PHII060
      COMMON /SUB/FLUX,CONS,THICK,A1,A2,A3,DENSTY,NEXP                  PHII070
      COMMON /SUC/EO,COTO,SITO,COT,SIT,COTT,COTP(31),SITP(31),COPHI(31), PHII080
     1THETA,IPHI,ELOWER,EUPPER                                          PHII090
      DATA C1/1.5184/,C2/0.69453/,PI/3.141593/                          PHII100
      OM1=C1*(E1-EO)                                                    PHII110
      OM2=C1*(E-E1)                                                     PHII120
      R1=E1+EO                                                          PHII130
      R2=E+E1                                                           PHII140
      B1=2.*SQRT(E1*EO)                                                 PHII150
      B2=2.*SQRT(E*E1)                                                  PHII160
      IPHIA=IPHI-1                                                      PHII170
C        CALCULATION OF KAPA VALUES.                                    PHII180
      DO 100 I=1,IPHI                                                   PHII190
      CK(1,I)=C2*SQRT(R1-B1*(COTO*COT1+SITO*SIT1*COPHI(I)))             PHII200
 100  CK(2,I)=C2*SQRT(R2-B2*(COT1*COT-SIT1*SIT*COPHI(I)))               PHII210
      PHII=SKP(CK(1,1),OM1)*SKP(CK(2,1),OM2)                            PHII220
     A       -SKP(CK(1,IPHI),OM1)*SKP(CK(2,IPHI),OM2)                   PHII230
      DO 200 I=2,IPHIA,2                                                PHII240
 200  PHII=PHII+4.*SKP(CK(1,I),OM1)*SKP(CK(2,I),OM2)                    PHII250
     A          + 2.*SKP(CK(1,I+1),OM1)*SKP(CK(2,I+1),OM2)              PHII260
      PHII=PHII*PI/IPHIA/3.*2.                                          PHII270
      RETURN                                                            PHII280
      END


      FUNCTION SKP(CK,OMA)                                              SKP0010
C*********************************************************************** SKP0020
C     THIS PROGRAM INTERPOLATES S(K,W) FROM TABULAR INPUT DATA.         SKP0030
C*********************************************************************** SKP0040
      REAL *4KAPA                                                       SKP0050
      COMMON /SET/KAPA(100),OMEGA(100),SKW(100,100),IKAPA,IOMEGA,TEMP   SKP0060
         FUN(A1,A2,A3,A4)          =ALOG(ABS(A1/A2) )/ALOG(A3/A4)       SKP0070
         OM          =OMA                                               SKP0080
      IF (OMA.LT.0.0) OM=ABS(OMA)                                       SKP0090
      IF (CK.LT. KAPA(1)) GO TO 80                                      SKP0100
      IF (CK.GT. KAPA(IKAPA)) GO TO 70                                  SKP0110
         I           =1                                                 SKP0120
   10 IF ( KAPA(I).LE.CK.AND.CK.LE. KAPA(I+1)) GO TO 20                 SKP0130
         I           =I+1                                               SKP0140
      GO TO 10                                                          SKP0150
   20    IK          =I                                                 SKP0160
   30 IF (OM.GT.OMEGA(IOMEGA)) GO TO 60                                 SKP0170
         J           =1                                                 SKP0180
   40 IF (OMEGA(J).LE.OM.AND.OM.LE.OMEGA(J+1)) GO TO 50                 SKP0190
         J           =J+1                                               SKP0200
      GO TO 40                                                          SKP0210
   50    IW          =J                                                 SKP0220
      GO TO 90                                                          SKP0230
   60    SKP         =0.0                                               SKP0240
      RETURN                                                            SKP0250
   70    IK          =IKAPA-1                                           SKP0260
      GO TO 30                                                          SKP0270
   80    IK          =1                                                 SKP0280
      GO TO 30                                                          SKP0290
   90    I           =IK                                                SKP0300
         J           =IW                                                SKP0310
         SKOJ        =SKW(I,J)*EXP(FUN(SKW(I,J),SKW(I+1,J), KAPA(I),    SKP0320
     A                 KAPA(I+1))*ALOG(CK/ KAPA(I)))                    SKP0330
         SKOJ1       =SKW(I,J+1)*EXP(FUN(SKW(I,J+1),SKW(I+1,J+1), KAPA(I), SKP0340
     A                 KAPA(I+1))*ALOG(CK/ KAPA(I+1)))                  SKP0350
         SKP         =SKOJ1-(SKOJ1-SKOJ)/(OMEGA(J+1)-OMEGA(J))*         SKP0360
     A                 (OMEGA(J+1)-OM)                                  SKP0370
      IF (OMA.LT.0.0) SKP=SKP*EXP(OM/TEMP*7.6383)                       SKP0380
      IF (SKP.LT.0.0) SKP=0.                                            SKP0390
      RETURN                                                            SKP0400
      END                                                               SKP0410
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