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I. INTRODUCTION

This quarterly progress report describes the work performed under project agreement No. 2 of contract AT(04-3)-167 with the U. S. Atomic Energy Commission during the quarter ending December 31, 1964. Early in November, the U. S. Atomic Energy Commission requested that a proposal be submitted for a three-year neutron thermalization program. This proposal was completed and submitted to the USAEC; it supersedes the program outlined in the yearly proposal of July 1964.

During this quarter the predominant experimental effort was made on the differential scattering work which has produced some quite accurate measurements for vanadium and light water. Infinite medium spectral measurements in borated water were made as a function of boron concentration because of differences noticed between the spectra of Burkart and Reichardt⁽¹⁾ and the predictions of the H_2O scattering model. Further spectral measurements at an interface in D_2O and in a heterogeneous configuration of other moderators were held back until the feasibility studies reported herein were completed. A comparison has also been made of the spectral measurements in a uranium-water lattice with integral and S_n transport theory calculations. The intercomparison between the latter is not very satisfactory. Many more spectra have been compiled during this quarter for addition to the Spectrum Book.

A program to measure the fast and intermediate neutron leakage spectrum from a U^{235} metal ball from 1 keV upwards has been initiated. The equipment for the measurements is being assembled and the operations license application is being prepared. It is anticipated that the measurements will provide good data for comparison with theoretical calculations.

Much theoretical effort has been expended in the development of the scattering law code GASKET, which, it is hoped, will allow a more rigorous description of the effect of atomic motions on neutron scattering. The code is now partly operational and some preliminary results are presented. Further studies have also been made of coherent scattering by D_2O and of neutron scattering by polyethylene. The latter shows some interesting comparisons with the double differential measurements performed at RPI. These data together with that of Schmunk⁽²⁾ on dispersion relations of beryllium have been the only double differential experimental data of sufficient quality to be useful in guiding theoretical analyses on any of the moderators. Studies have been made of one-phonon coherent inelastic scattering by polycrystalline materials and a code has been written incorporating the formalism that has been developed. This code is not yet operational. When completed it should be of immediate

use in understanding the slow neutron scattering by beryllium. A code, HEXSCAT, has been written to compute coherent elastic scattering by hexagonal lattices. A description of the code is given in Appendix I of this report.

The following papers were presented at scientific meetings during this reporting period.

1. Transactions of the American Nuclear Society, San Francisco, November 1964, "Position - and Angular Dependent Spectrum Measurements in H_2O ," J. M. Neill, J. C. Young, and W. Brouwer.
2. "Neutron Spectrum Measurements in D_2O ," J. C. Young, J. M. Neill, and W. Brouwer.
3. "Reactivity Measurements by the Pulsed Neutron Technique," N. Corngold.
4. Transactions of the American Nuclear Society, San Francisco, November 1964, "Graphite Scattering Kernel," R. G. Bardes and J. A. Young.
5. Transactions of the American Nuclear Society, San Francisco, November 1964, "Neutron Spectra in Shields by Time of Flight," J. L. Russell, Jr.

II. ANGULAR SCATTERING MEASUREMENTS

2.1 INTRODUCTION

During this quarter considerable progress was made on the single differential scattering experiment. The experimental setup which was used included two neutron detectors whose angular position could be varied over the total angular range. Angular distribution measurements were made initially on vanadium to check the apparatus and then on light water because of the strong need for accurate differential scattering cross sections for that moderator. The refinements and checks in the apparatus will be briefly discussed in this section, although most of the experimental procedures are detailed in ref. 3. The new experimental data will also be summarized here.

2.2 TARGET PREPARATION

In order to obtain absolute cross sections directly from the angular scattering measurements, a water sample of known uniform thickness must be used. This requirement has prompted a study of sample design techniques. The specifications for the samples were 10 to 20 mils in thicknesses with good uniformity over the entire area of the collimated neutron beam and very thin walls.

The walls of the sample were made of 5-mil aluminum (1100H), stretched between two sets of heavy retaining rings. A thin aluminum spacer ring of the desired sample thickness was then coated with a film of vacuum grease to form a watertight seal and bolted between the tensioned aluminum utilizing two thin outside rings. The apparatus for stretching the aluminum walls and the finished sample are shown in Fig. 2.1. A schematic diagram of the sample design is shown in Fig. 2.2. A small hole was cut in the spacer ring to permit water filling. The sample was slowly filled with water using a hypodermic needle. The average thickness of the sample was determined by measuring the area of the sample and weighing the sample before and after it was filled with water. The thickness of the sample was further checked by performing a neutron transmission measurement at many neutron energies utilizing the angular scattering flight path. Both values were then compared with the spacer ring thickness. The results of the two independent determinations agreed to within 5 percent.

Fig. 2.1 -- Photograph of the apparatus for sample wall stretching and of the finished sample itself.

Fig. 2.2 -- Schematic diagram of the sample design

2.3 EXPERIMENTAL CORRECTIONS

The experimental corrections for the differential scattering experiment are given in Chapter X of ref. 3. It is, of course, desired to obtain the differential scattering cross section directly from the experimental data without having to renormalize the angular measurements to obtain the correct total cross section. In the past, our experiments have not been satisfactory in this respect, and it appears that most of the scattering data obtained at other laboratories have also resorted to renormalization procedures. One question has always seemed pertinent in this regard, namely: if in a differential scattering experiment one cannot integrate the directly measured data over angle and final energy to obtain the total cross section reasonably well, what assurance does one have that the shape of the "relative" cross section as a function of final energy and angle is correct. In this program, we are endeavoring to obtain absolute differential cross sections, and when the resulting integrated total cross section has been wrong we have shown subsequently that the relative shapes have also been wrong. Thus, the renormalization requirement eliminates an important integral check thereby making the data questionable. This will be discussed subsequently for the case of vanadium.

Four primary corrections must be made to the experimental data. These are: (1) the background subtraction, (2) a correction (C_f) due to the spatial variation of the intensity of the neutron beam hitting the sample, (3) an angularly dependent correction factor (C_R) arising from the distributed nature of the scatterer, and (4) a multiple scattering correction (C_m).

In these new experiments it was necessary to use a great deal of care in background subtraction. With vanadium, for example, we had to measure and subtract the counts in the Li^6 detector due to the capture γ -rays produced in the scattering sample. This had not been done in previous experiments.⁽⁴⁾ In the water experiments the γ -ray counts from the capture in hydrogen were insignificant, and a simple subtraction could usually be made after taking background data with a dummy (unfilled) thin walled container in place. However, at small scattering angles ($<30^\circ$) a new effect arose. It appeared that even though the neutron beam striking the sample was well collimated and had sharp edges, scattering in the flight path and windows tended to produce a low level fringe to this beam. This fringe intensity was down by over two orders of magnitude from the main part of the beam, but it was significant compared to the neutrons scattering from the thin sample. Thus, in order to correct the small angle data for background, we first had to subtract the random undirected neutron and

γ -background and then multiply the fringe beam count by the water sample transmission. The fringe beam counting rate can be measured by removing the water sample at each angular setting. This procedure seems to have worked very well for the water data where measurements were made to 10° scattering angle. At the 10° angle the fringe beam background counts constituted roughly 5% of the signal counts at energies around 0.01 eV but increased to nearly 50% of the signal counts at 10 eV neutron energy.

The correction factor C_f was calculated by performing a flux integration over the incident beam profile. Since the neutron beam was fairly flat, this correction factor was only 0.944. C_R was also very close to 1.0. This left C_m , the multiple scattering correction to be made to the raw data.

Procedures for calculating C_m have been made somewhat more rigorous by inclusion of the first collision description exactly in the correction.⁽³⁾ This new procedure is now included in Code MUSE I. However, correction factors using this new procedure are very nearly the same as those with the older integral P_3 transport theory approach used previously. Typical curves for the correction factor have been shown before in ref. 3, our annual summary report, and so are not repeated here. All data are now being corrected with the MUSE I correction factors. However, at this stage it is not certain how good the procedure is, and much more thought and tests need to be done before the correction can be considered standardized. As it has been pointed out before, one assumes that the scattering kernel is known in order to make this correction. However, the correction is nonnegligible, C_m varying from 1.10 to 0.60 typically. If one does not know the scattering kernel well, as is the case for water, then the correction itself may be erroneous. In the series of scattering measurements for water, two sample orientations were used with the detector set at a fixed scattering angle. After multiple scattering corrections have been performed, the same cross section should be obtained. At the lower neutron energies this usually was the case, but at 1 eV for 90° scattering results were at variance, as can be seen in Fig. 2.3. Unfortunately this difference was not studied extensively and there is no clear cut indication of the limitations of the correction procedures presently used. A study of this limitation will be undertaken shortly. Reports have been written discussing the theory of multiple scattering, and a journal article by H. C. Honeck on this matter is being prepared.

Fig. 2.3 -- Scattering of 1 eV neutrons from H_2O

2.4 EXPERIMENTAL RESULTS

2.4.1 Vanadium Scattering Experiments

It will be recalled that the neutron scattering from vanadium measured on the original experimental setup was nonisotropic by some 20 to 30%.⁽⁵⁾ Furthermore, the calculated angular distribution using the frequency distribution of Eisenhauer and Pelah⁽⁵⁾ even appeared to substantiate these initial erroneous experimental results. New measurements were performed of this angular scattering distribution at 55 energies from 0.01 eV to 10 eV. Scattering angles were 30° , 45° , 60° , 90° , 120° , 135° , 150° . After proper subtraction of all backgrounds, as mentioned in the previous section, the differential scattering cross section turned out to be very nearly the same for all energies and angles. Although final analysis of the data is not completed, a cross section variation with angle of less than 10% would appear to be the largest possible. In addition, the absolute total cross section determined from an integration of the measured differential data agreed with the best value available⁽⁶⁾ to within 10%; this gives us confidence in the whole experimental procedure.

2.4.2 Water Data

Since data accumulation rates are very rapid on the new angular distribution setup, two angles can be measured in about one hour of Linac operation. Thus data were taken for water with two scattering sample thicknesses (19 mils and 13 mils) at 55 energies from 0.005 to 10 eV, and at 29 different scattering angles. In addition, a few runs at varied sample orientations were made. Experimental data are still being reduced and compiled, but three examples of the preliminary results are shown for 1.0, 0.1 and 0.01 eV neutron energies in Figs. 2.3, 2.4, and 2.5 respectively. Experimental results gave absolute cross sections directly since by integration over angle the total cross section could be obtained. In all cases examined so far this integral check has been obtained within 10% of the best measured results available. The experimental values shown by the circles in the three figures have, however, been adjusted so that the experimental cross section on integration will give the best total cross section.⁽⁷⁾ The original Nelkin model⁽⁸⁾ was used in calculating the theoretical curves. The theory appears to be in agreement with experiment over much of the angular range but consistently gives low results at back angles. This general observation was pointed out previously.⁽⁴⁾ Only statistical experimental error is shown presently on the data points. Systematic error due to exactness of the multiple scattering procedure may constitute a comparable factor. In Fig. 2.4 are shown the results of Springer⁽⁹⁾ for single differential

Fig. 2.4 -- Scattering of 0.1 eV neutrons from H₂O

Fig. 2.5 -- Scattering of 0.01 eV neutrons from H₂O

scattering at 0.1 eV. They are in remarkably good agreement with our results except in the 120 to 140 degree region. Similarly good agreement has also been obtained with the other Springer angular distributions for H₂O at 0.022, 0.044, and 0.071 eV. Since the experimental methods and data correction procedures used by Springer are completely different from ours, it is very encouraging to obtain this agreement.

The plans for the immediate future are to complete the data reduction for H₂O and compile in report form fifty measurements of $\frac{d\sigma}{d\Omega}$ from $<.01$ eV to >5 eV. We will select an energy mesh consistent with that at which we perform theoretical calculations. Theoretical predictions will probably be given for the Nelkin model only, since the Haywood⁽¹⁰⁾ model has not yet arrived from England. When the GASKET Code^(3,7) is completed, we will be able to treat the water molecule more realistically. It is hoped then to include the rotational frequency band and to calculate more accurate angular scattering distributions than was possible with the original Nelkin procedure.

One qualitative observation which seems fairly certain from the new results is that the present Nelkin model predicts somewhat too small a cross section for high momentum transfer at all incident neutron energies. This result is not incompatible with the generally accepted fact (based on integral spectral measurements) that the Nelkin model also predicts too much energy transfer in collision since large momentum transfer can occur at large scattering angles with small energy transfer.

III. SPECTRAL STUDIES

3.1 COMPARISON OF MOSTOVOI SPECTRAL MEASUREMENTS WITH INTEGRAL AND S_n TRANSPORT THEORY CALCULATIONS

In a paper given at the second international conference on the peaceful uses of atomic energy, Mostovoi⁽¹¹⁾ presented some measurements of thermal neutron spectra in a multiplying assembly. The assembly was made up of natural uranium rods 35 mm in diameter clad in aluminum and located on a triangular pitch of 50 or 60 mm in water. The whole assembly formed a 50 cm cube. A vector flux was extracted along the axis of these fuel rods in turn from the center of the moderator and the center of the fuel rod. The flux was measured by time of flight means using a mechanical chopper. Honeck and Takahashi⁽¹²⁾ analyzed this experiment using the code THERMOS⁽¹³⁾ which is an integral transport theory method. Their calculated results were in agreement with the measured values in the fuel rods but not in the moderator. They also analyzed similar measurements made by Campbell *et. al.*⁽¹⁴⁾ and there obtained agreement in the moderator but not in the fuel. Marchuk *et. al.*⁽¹⁵⁾ have also analyzed Mostovoi's measurements using S_n and integral transport theory and also by Monte Carlo methods. They claimed to have obtained good agreement between the three methods and also with the measured values. In view of the disagreement of H-T the question arose as to whether there were fundamental differences in the numerical solutions given by the two independent approaches to the problem. Consequently an analysis has been made at General Atomic of Mostovoi's measurements in order to resolve the question. The measurements considered were those at 50 mm pitch since they have the better statistics.

The analysis made here uses standard transport methods; the Nelkin⁽⁸⁾ bound kernel is calculated by the GAKER^(13,3) code, group cross sections from the GATHER⁽¹⁶⁾ code in the B_1 approximation, and S_{16} transport theory with the GAPLSN⁽¹⁷⁾ code. P_1 scattering is considered. In making the analysis, some approximations or assumptions are made in the same manner as Honeck and Takahashi. These approximations are used in transforming the lattice to a one dimensional problem in cylindrical geometry while maintaining the same fuel to water volume ratio and in smearing the aluminum cladding of the fuel uniformly through the water moderator. Reflecting boundary conditions are assumed and gross leakage from the cell is taken as zero. The slowing down source is taken as zero in the fuel and uniform in the moderator as calculated by the DSZ⁽¹⁸⁾ code.

Figure 3.1 shows the angular fluxes calculated at the center of the fuel and the moderator in this analysis compared to Honeck and Takahashi's calculations and to Mostovoi's measurements. At first glance it appears that the new analysis gives agreement in the moderator and disagreement in the fuel (some 40% too hard), the reverse of the conclusions of Honeck and Takahashi (some 90% too soft in the moderator). The most important thing to note is the substantial disagreement between the theoretical values obtained here by S_n methods and those obtained by H-T using integral transport theory methods. This disagreement is surprising in view of the almost identical approaches made to the true geometry and in view of the agreement between these methods plus Monte Carlo calculations obtained by Marchuk. There are two small differences between the two approaches. Honeck and Takahashi neglected anisotropic scattering in the final presentation since their preliminary calculations showed it to be a small effect. We have no reason to disagree with this procedure. The outer boundary conditions used in the S_n method (perfect reflection) are not satisfactory since artificial curvature is introduced into the problem by reducing the triangular cell to an equivalent cylindrical cell. The consequence of these incorrect boundary conditions is to overestimate the disadvantage factor in tightly packed lattices such as the one studied here. However, if anything, the H-T disadvantage factor for the cell is greater than that calculated using the S_n procedure. In other words, the effect is in the wrong direction to explain the differences between our results and those of Honeck and Takahashi, though it is in the right direction to reconcile our calculations with Mostovoi's measurements.

We now compare our calculations to the measured values and comment on the comparisons made by Marchuk.⁽¹⁵⁾ Initially it must be stated that the data of Fig. 3.1 are replotted values taken from the article of H-T who in turn presented the replotted measurements taken from the article of Mostovoi.⁽¹¹⁾ Naturally this procedure detracts from the accuracy of the measurements, and in addition Mostovoi presented his data in terms of $E \phi(E)$ versus $1/\sqrt{E}$ on a linear plot. Consequently there is less accuracy at the smaller values of $E \phi(E)$ associated with the higher values of E . Unfortunately this is the region in which normalization of theory and experiment to the $1/E$ slowing down flux is usually made. It is this very fact that makes it difficult if not impossible for us to comment on the comparisons of theory and experiment made by Marchuk.⁽¹⁵⁾ His normalization of theory and experiment is not made in the $1/E$ flux region but rather at the flux peak. The linear presentation of the data disguises any discrepancies that may remain in the $1/E$ region and so we cannot ascertain on our basis how good the agreement is between the three calculational procedures that he used. In the H-T article, the possibility of malaligned collimators was raised to account for the spectral discrepancy that they observed in the water. This point has been

Fig. 3.1 -- Neutron spectra in a uranium-water lattice

investigated. In Fig. 3.2 a plot is shown of the peak thermal flux in the fuel and moderator as calculated here. The flux across the water moderator is relatively flat so that poor collimation would not affect the result significantly. In the fuel rod, however, the flux varies considerably so that the flux at the center of the fuel is not characteristic of the flux averaged over the 5.6 mm by 26 mm slotted re-entrant hole. If an appropriately weighted averaging is performed, our observed spectral discrepancy in the fuel of 40% is reduced to 28%. Furthermore, it is clear that if the collimator is slightly malpositioned, the contributions from the side of the re-entrant hole would easily account for the remaining difference. In the moderator, the small discrepancy observed is ascribed to two effects: (1) The fact that the aluminum clad is smeared through the moderator in the calculation which would harden the spectrum slightly at the outer radius, and 2) The definite error in our calculation (numerical in origin) which results in the dipping of the peak flux at the outer cell boundary as shown in Fig. 3.2.

Strong conclusions on the analysis performed cannot be drawn. There is a remaining discrepancy between measurement and S_n transport theory calculations which has not been properly accounted for although several possibilities for its cause have been discussed. The integral transport theory results of Honeck and Takahashi give different results from the values calculated here. No satisfactory reason for this difference has been found and it is to be noted that generally the S_n method has given values closer to the measured neutron spectra.

3.2 FEASIBILITY STUDIES

3.2.1 H₂O - D₂O Interface

Neutron spectra at an interface between H₂O and D₂O have been calculated. The theoretical configuration envisaged a 12 in. by 6 in. by 4 in. tank containing boric acid (H₂O) solution (24 gms/liter) next to a 12 in. by 6 in. by 12 in. tank containing cadmium nitrate (D₂O) solution (25.8 gms/liter). The pulsed neutron source was located next to the tank containing H₂O. The slowing down distributions which were previously observed in these moderators and tank sizes have then been used to generate an appropriate source distribution. The purpose of this calculational study was to determine the feasibility of the proposed configuration for integral measurements under strong flux gradients as checks on the P_1 scattering for H₂O and D₂O. The scalar neutron spectra across this interface which were calculated by using the Nelkin model for both H₂O and D₂O are presented in Fig. 3.3, and show large changes of spectral shape with position. The changes on both sides are large and measurable, but the smaller positional dependence on the D₂O side should facilitate the comparison between

Fig. 3.2 -- Spatial variation of thermal flux in a uranium water lattice

Fig. 3.3 -- Calculated scalar neutron spectra across an $H_2O - D_2O$ interface

experiment and theory. The fluxes are highly anisotropic and a dependence on P_1 scattering is exhibited. The vector fluxes normal to the interface show an even greater dependence on P_1 scattering. Consequently, the proposed measurements appear to be both desirable and feasible.

3.2.2 POLYETHYLENE CELL

Measurements were made recently⁽³⁾ of the positional variation of the neutron spectrum in a mocked-up lattice cell. The mocked-up cell comprised slabs of iron and pure polyethylene, each 0.5 or 1 in. thick. In those studies, the re-entrant hole size was varied in order to determine quantitatively the perturbation of the flux caused by the hole. As far as could be determined, it was possible to use a re-entrant hole as large as 0.375 in. diameter in the case of 1 in. thick slabs without significantly distorting the neutron spectrum. The conclusions, however, were tentative due to a variety of experimental difficulties. These difficulties arose because of the poor statistics of some of the data and due to the difficulty of properly aligning the re-entrant hole and precollimator. Some of the latter difficulties were related to having to machine separately the two different materials, iron and polyethylene. Another difficulty with this first experiment was the fact that the spectral difference between the center of the iron and the polyethylene was not large enough to indicate clearly where averaging over the re-entrant hole void had occurred. Consequently, we performed a study of the feasibility of measuring neutron spectra across a cell consisting of 1 in. slabs of pure and of 1% boron loaded polyethylene. The mechanical difficulties are overcome mostly by the easier simultaneous machining of the two materials, and also the positional variation of the neutron flux is larger than before. The neutron spectra calculated here are compared in Fig. 3.4 to the spectra calculated for a cell of 1 in. polyethylene and 1 in. iron. The difference in peak flux between the cell centers increased by about 50% in the new configuration. The measurement looks feasible. Furthermore, these studies will help us in the development of techniques to measure neutron spectra within an actual fuel rod itself. An experimental assembly has therefore been constructed and spectral measurements are planned at several positions across a cell using different size re-entrant holes.

3.3 TEMPERATURE DEPENDENT SCALAR NEUTRON SPECTRA IN H₂O

Infinite medium neutron spectra in water poisoned with a $1/v$ absorber were measured previously⁽⁷⁾ as a function of moderator temperature in order to determine the importance of molecular binding at temperatures comparable to actual operating reactors. These measurements required the use of a pressure vessel containment. During this quarter, preparations have been made to reactivate this pressure vessel

Fig. 3.4 -- Calculated 0° angular neutron spectra in two cell configurations

to extend these measurements to neutron spectra in water poisoned with resonance absorbers. The poisons for this series of measurements will be gadolinium and erbium since they are of interest as burnable poisons in reactors. The resonance structure of erbium will also be useful in testing more severely the P_0 scattering of the bound hydrogen model around 0.3 to 0.4 eV than was previously possible. At present small test cylinders (3-3/4 by 1 in. diameter) are being made from the same type of stainless steel used in the pressure vessel. These cylinders will be filled with gadolinium and erbium solutions and heated to 600° F to check the corrosion resistance of the pressure vessel to these solutions at high temperature and pressures. The pressure vessel in the spectrum measurement position is depicted in Fig. 3.5. A complete description of this pressure vessel is given in ref. 7. Since the pressure vessel has not been used for some time, it is being set up in a test area for checkout at the operating temperatures and pressures. These tests will be performed with pure water.

3.4 INFINITE MEDIUM SPECTRAL MEASUREMENTS IN WATER AT DIFFERENT POISON CONCENTRATIONS

Several requests for the neutron spectrum in water as a function of the concentration of a $1/v$ absorber have prompted a series of infinite-medium neutron spectrum measurements. In addition, attempts to analyze spectral data currently published on $1/v$ poisoned water spectra have led to inconsistencies between theory and experimental art between one experiment and another. Boric acid poisoning was employed at concentrations of about 1, 2, 3, 4 and 5 barns/hydrogen atom. These measurements were made in the typical quasi-infinite medium geometry shown in Fig. 3.6. Three source monitors were utilized in an attempt to preserve the relative intensity between the spectra as one changed poison concentration. These measurements are presently being analyzed and will be reported in the next quarter.

3.5 FAST REACTOR SPECTRUM

A program is underway with the objective of measuring the leakage spectrum from a fast U^{235} metal ball reactor. The spectrum will be measured by time-of-flight methods using the General Atomic Linac to provide the intense pulsed neutron source, a 50-m evacuated drift tube, and the APFA reactor built by DASA for transient radiation studies. The range of the measurements will be from ~ 1 keV to 10 MeV. This measurement is one of the most basic to all fast reactor technology. In fact, the most studied and analyzed fast reactor spectra is that of GODIVA, which the DASA ball resembles. A point of major interest will be to examine the measured spectra to ascertain if a surplus of low kilovolt neutrons is present over that calculated. Other evidence indicates that this may possibly occur.

Fig. 3.5 -- Pressure vessel showing the zirconium scatterer and background plug drive mechanisms

Fig. 3.6 -- Experimental arrangement for infinite medium measurement in borated water

To perform this measurement the reactor must be set up in front of the flight path in the Linac experimental room. The license amendment to permit operation of the reactor in the Linac area is being prepared and will be submitted to the AEC DRL in January 1965. Some of the equipment is being borrowed from ORNL and LASL. A control room building has been completed and installation of the control console will begin shortly.

IV. THEORETICAL STUDIES

4.1 SPECTRUM BOOK

The Spectrum Book is a compilation of the best spectral measurements made at General Atomic. The purpose of this book has been described previously,⁽³⁾ but in brief it illustrates typical comparisons between present day analytical methods used in reactor analysis and clean experiments. The book has been issued to some 40 organizations, and the response from these groups during this last quarter has provided further support for its usefulness as a design aid. Since the last progress report, thirty-three additional cases have been compiled and issued. These data include spectral measurements in graphite and BeO, and in water under various poisons and geometries.

The difficulties in the normalization of experiment to theory, discussed in ref. 3, are still present and until they are resolved, the normalization will consist of a simple fit in the $1/E$ portion of the flux spectrum. We hope that ultimately the use of the code GASKET^(3,7) replacing the SUMMIT⁽¹⁹⁾ and GAKER^(13,3) codes will generate a scattering kernel that will go smoothly to the free gas limit and thereby eliminate most of the present anomalies.

4.2 COHERENT SCATTERING BY D₂O

In the last annual report⁽³⁾ an account was given on the role of interference effects in neutron scattering by D₂O. It was found that integral quantities such as the total cross section and weakly space dependent neutron spectra were practically unaffected by interference because of mutual cancellation of the inner and outer effects. Differential quantities, however, were strongly modified and were quite different from the values obtained in the incoherent approximations. Using Butler's⁽²⁰⁾ generalization of Nelkin's⁽⁸⁾ water model for the intramolecular scattering and Debye's static hard sphere theory for the outer effect (both summarized in ref. 3), we calculated the integrated angular cross section $\frac{d\sigma}{d\Omega}$ and compared the values obtained with Springer's⁽⁹⁾ experimental results. The agreement obtained was surprisingly good, although experimentally the largest of the diffraction peaks was always narrower than the predicted ones. This comparison is shown in Figs. 4.1 to 4.3. The very narrow peaks found experimentally seem to corroborate the generally accepted fact that in the

Fig. 4.1 -- Scattering by D_2O at 0.04 eV incident neutron energy

Fig. 4.2 -- Scattering by D_2O at 0.07 eV incident neutron energy

Fig. 4.3 -- Scattering by D_2O at 0.1 eV incident neutron energy

liquid state the molecules are grouped in relatively large aggregates retaining to some extent the structure of the solid. Therefore, it would be interesting to calculate the coherent elastic scattering in the most extreme case, namely, a microcrystalline system having the lattice structure of heavy ice.

Other quantities showing the influence of interference scattering are the average cosine of the scattering angle, and the transport cross section. The values obtained for these quantities from the present calculations are shown in Figs. 4.4 and 4.5.

4.3 NEUTRON SCATTERING BY POLYETHYLENE

A scattering kernel for polyethylene, obtained from Lin and Koenig's⁽²¹⁾ theoretical treatment of the vibrations of infinite CH_2 chains, was described in ref. 22. The optical part of the corresponding frequency spectrum is shown in Fig. 4.6. The calculations reported in ref. 22 were performed by lumping this distributed spectrum into 4 discrete lines with the frequencies and weights of Spectrum A shown in Table 4.1.

Table 4.1

<u>Spectrum</u>	<u>Frequencies</u>	<u>Weights</u>
A	0.090	0.0775
	0.140	0.2320
	0.174	0.3095
	0.360	0.3095
	0 (translation)	0.0715
B	0.09	0.1005
	0.170	0.4930
	0.360	0.3350
	0 (translation)	0.0715
Goldman ⁽²³⁾	0.089	0.232
	0.187	0.232
	0.354	0.232
	0.533	0.232
	0 (translation)	0.072

It is interesting to compare the double differential cross section obtained from this model with the experimental data recently obtained at RPI.⁽²⁴⁾ Because of the crudeness of the lumping procedure one cannot expect a quantitative agreement with the measurements. However, qualitatively speaking, one should be able to reproduce the essential

Fig. 4.4 -- Variation of $\overline{\mu}$ for D_2O with incident neutron energy

Fig. 4.5 -- Transport cross section for D_2O as a function of neutron energy

Fig. 4.6 -- Histogram of the frequency spectrum of polyethylene

features, or structure of the double differential cross section, especially at larger scattering angles, where the recoil energy taken up by the scatterer broadens the otherwise too narrow peaks predicted by a discrete spectrum. Another way of lumping the spectrum of Fig. 4.6 is into the three lines listed under Spectrum B of Table 4.1. It is clear that a smaller number of discrete lines of the lumped spectrum will exaggerate the structure of the double differential cross section, but on the other hand it eliminates the need for using the short collision approximation at relatively low energies. This need is, of course, a consequence of the numerical limitations imposed by the code GAKER^(13, 3) used for all the computations reported here. Fig. 4.7 compares the experimental double differential cross section at $E_0 = 0.23$ eV and $\theta = 60^\circ$ with the predicted values derived from spectra A and B (the calculation with spectrum A was actually done for $\theta = 55^\circ$). The discontinuity shown by curve A is due to switching to the short collision approximation for the lowest frequency at $E_0 - E > 0.17$ eV. This is necessary because with larger energy exchanges the third line of spectrum A can be excited and the code only allows for two excited oscillators. The cross section derived from Spectrum B shows a small peak corresponding to the 0.09 eV line which is smeared out (for Spectrum A) by increasing the number of lumped oscillators to four. The experimental curve actually does not show such a peak either. Similar comments apply to Fig. 4.8 where the theoretical and experimental cross sections are plotted for the same initial energy of 0.23 eV and a scattering angle of $\theta = 90^\circ$. In this case, however, because of the broadening effect of larger recoil energy, the excitation of the 0.09 eV line is not even seen in the cross section corresponding to Spectrum B.

Figure 4.9 compares the previous curves with the cross section resulting from Goldman's frequency spectrum, ⁽²³⁾ also given in Table 4.1. It is clearly seen that the weight attributed in this spectrum to the 0.09 eV oscillator is much too large.

Another feature becoming apparent from Figs. 4.8 and 4.9 is that the free gas treatment of the acoustical (and structural) modes shifts the peaks towards lower final energies (too much recoil of the CH_2 radical).

Fig. 4.10 compares experiment and theory (Spectrum B) for an initial energy of about 0.42 eV and $\theta = 25^\circ$. Again the structure is well predicted although, as expected, the calculated peaks are too sharp excepting the zero phonon peak which for a true crystal should be infinite (the shape of the experimental curve between 0.36 and 0.44 is not known since it went out of scale at

$$\frac{2\pi}{\sigma_f} \frac{d^2\sigma}{d\Omega dE} = 7.2 \text{ eV}^{-1}$$

Fig. 4. 7 -- Comparison at $\theta = 60^\circ$ of measured and calculated double differential cross sections for CH_2 using different oscillator frequencies

Fig. 4.8 -- Comparison at $\theta = 90^\circ$ of measured and calculated double differential cross sections for CH_2 using different oscillator frequencies

Fig. 4.9 -- Comparison at $\theta = 90^\circ$ of measured and calculated double differential cross sections for CH_2 using Goldman's frequency spectrum

Fig. 4.10 -- Comparison of experimental and theoretical scattering cross sections for CH_2 at $E_0 = 0.42 \text{ eV}$ and $\theta = 25^\circ$

in the original plot of ref. 24). Figure 4.11 again compares experiment with the cross section derived from spectrum B with $E_o \sim 0.42$ eV but for a scattering angle of 60° . Here, as it is always seen for larger scattering angles (and thus larger CH_2 recoils), the predicted peaks appear somewhat shifted towards lower final energies.

It should be mentioned that in the two last plots the 0.09 eV oscillator was treated in the short collision approximation for all final energies. This contributes to the shifting of the peaks and provides a considerable broadening as can be seen from Fig. 4.12 where the calculation for $E_o = 0.42$ eV and $\theta = 60^\circ$ has been repeated but making the short collision approximation only when $E_o - E > .31$ eV.

In conclusion, we have compared measured double differential cross sections with calculations using 3 and 4 lines lumped frequency spectra derived from Lin and Koenig's theoretical work on infinite CH_2 chains. As expected from the crudeness of the treatment, the agreement is only qualitative, but the essential features of the structure are reasonably well predicted. Of course, a much better agreement would be expected were the exact distributed frequency spectrum of Fig. 4.6 to be used. This will become possible as soon as the new code GASKET, reported in ref. 3, becomes available. It is also quite possible that the experimental cross section shapes may change significantly after multiple scattering corrections are made to the data.

4.4 COHERENT SCATTERING FROM POLYCRYSTALS

In our last progress report⁽³⁾ for this project, an expression was presented for the one-phonon coherent inelastic scattering cross section for the scattering of neutrons from a polycrystalline material. The expression is

$$\frac{d^2\sigma}{dE d\Omega} = \frac{\hbar a_c^2}{2M} \sqrt{\frac{E}{E_o}} \sum_{j, \eta=\pm 1} \int_{-1}^1 d\mu_\kappa \frac{1}{\left| \frac{\partial \omega_j(\vec{\kappa}/2\pi)}{\partial \phi} \right|_{\epsilon=\eta\hbar\omega_j}} \left[1 - e^{-\epsilon/kT} \right] \frac{1}{\epsilon} \cdot$$

$$\cdot \left| \sum_k e^{i\vec{\kappa} \cdot \vec{r}^k} \vec{\kappa} \cdot \vec{C}(k) \left| \frac{\vec{\kappa}}{j} \right| \right| \quad (1)$$

Fig. 4.11 -- Comparison of experimental and theoretical scattering cross sections for CH_2 at $E_0 = 0.42 \text{ eV}$ and $\theta = 60^\circ$

Fig. 4.12 -- Calculated double differential cross sections for CH_2
 at $E_o = 0.42 \text{ eV}$ and $\theta = 60^\circ$ using the short collision
 approximation for $(E_o - E) > 0.31 \text{ eV}$

where k denotes the unit cell index, j the various branches in the dispersion relation, μ the cosine of the polar angle of $\vec{\kappa}$, and $\emptyset$ the azimuthal angle of $\vec{\kappa}$ the momentum transfer. The remainder of the notation is standard.

The procedure for comparison with experiment is to calculate the above expression and add it to the calculations made by GASKET^(3,7) in the incoherent approximation. The one phonon incoherent ("self") scattering cross section must then be subtracted. A machine program COIN has been written to compute Eq. (1), for hexagonal lattices where the polarization vectors $\vec{C}$ are known or can be evaluated. While COIN is not debugged as yet so that preliminary results must await the next report, Fig. 4.13 does show the existing situation for beryllium that it is hoped COIN will correct. In Fig. 4.13 the curvy lines are the measurements by Schmunk⁽²⁾ and the smooth, almost straight curve is a calculation by GASKET for the same situation in the incoherent approximation. The influence of interference as clearly seen is very large, and leads to differences for small momentum transfers of almost an order of magnitude between theory and experiment. The same situation will also be true for other coherent scatterers such as BeO and graphite.

Since the quantities $\omega_j(\vec{\kappa}/2\pi)$ and $\vec{C}(k/\vec{\kappa}/2\pi)$ can be computed most cheaply for graphite, the first calculations of COIN are currently being done for this moderator. When more confidence has been gained in the use of COIN the important and more interesting case of beryllium will be studied.

The procedure used in COIN is to choose ϵ , and Ω which fixes $|\vec{\kappa}|$ and then to express κ and the unit cell vectors in terms of the reciprocal lattice and lattice vectors respectively. A search must then be made for those points in reciprocal space so that $\epsilon = \eta \omega_j(\vec{\kappa}/2\pi)$. For neutron up-scattering $\eta = -1$. The derivative is readily computed at these points and then Eq. (1) is evaluated.

While COIN will of necessity be rather complicated, if successful, it will go a long way in clearing up a situation of great importance in the scattering of slow neutrons from polycrystalline samples, and allow much more sensitive checks on the theory.

4.5 STUDY OF LIQUID DYNAMICS BY GREEN'S FUNCTION TECHNIQUES

As mentioned in the annual report for last year,⁽³⁾ a study of the Van Hove correlation function $G(r, t)$ is being made using the theory of thermodynamic Green's functions. An approximate expression for $G(r, t)$ has been obtained in closed form for the Lennard-Jones potential. Nevertheless, the expression is sufficiently complicated that a numerical

Fig. 4.13 -- Calculated and experimental scattering law for beryllium

analysis is necessary, and is currently being performed. As a check on the theory, the static pair correlation function will be evaluated and compared to experiment. It is hoped that some numerical results will be available for the next report.

4.6 GASKET: CODE STATUS AND INITIAL RESULTS

The GASKET code is designed to generate the scattering laws accurately for the various moderators taking into account the atomic motions more rigorously than was previously possible. Calculations made within the last quarter have shown that the basic methods (as described in the last annual report) used in GASKET can successfully calculate the scattering law for a variety of frequency spectra. The scattering laws for frequency spectra having a large Debye-like component and one quite different (beryllium) have been calculated successfully.

Figure 4.14 is a plot of the scattering law $S(\alpha, \beta)$ versus β for $\alpha = 2.11$ for a Debye frequency spectrum with a mass 12 scatterer at room temperature. The curve illustrates a numerical difficulty encountered when calculations are made with a distributed frequency mode only: there is not enough damping of the χ -function to provide acceptable $S(\alpha, \beta)$ values for a reasonable integration mesh. The critical points of the S -function (corresponding in energy to sharp peaks and the cutoff frequency of the frequency spectrum) are subject to oscillations. These oscillations result from attempting to integrate the product of two damped periodic functions ($\chi(t)$ becomes periodic for large t) of nearly the same frequency. The integrals must be terminated before the product $\chi(t) \cos(\epsilon t)$ has become truly insignificant in order to reduce computation time, thus causing the oscillations. The numerical problems have been removed by including a small amount of free gas (mode 1) in the χ -function causing a Gaussian damping of the large t region of $\chi(t)$.

The code has been changed to allow a more reasonable method of combining both free gas and distributed frequency spectrum χ functions. Previously,

$$\chi(t) = \chi_1(t) \chi_3(t)$$

$$= \exp \left[-\frac{p^2}{2} \frac{W_1}{M} \left(\frac{i}{4T} + Tt^2 \right) \right] \cdot \exp \left\{ \frac{p^2}{2} \frac{W_3}{M} \left[\gamma \left(t + \frac{i}{2T} \right) - \gamma(0) \right] \right\}$$

where the symbols are defined in ref 3. $\chi_3(t)$ approaches a constant (the Debye-Waller factor) after very small oscillations about the constant, and the details of these oscillations are lost by the predominant Gaussian damping of $\chi_1(t)$. The code has been changed to calculate the χ function split into two parts, χ_a and χ_b instead.

Fig. 4.14 -- Scattering law for a mass 12 scatterer with a Debye frequency spectrum at $\alpha = 2.11$

$$\begin{aligned}\chi(t) &= \chi_a(t) + \chi_b(t) \\ &= \chi_1(t) \left\{ \chi_3(t) / \exp \left[-\frac{p^2}{2} \frac{W_3}{M} \gamma(0) \right] - 1.0 \right\} \\ &\quad + \exp \left[-\frac{p^2}{2} \frac{W_3}{M} \gamma(0) \right] + \chi_1(t) \exp \left[-\frac{p^2}{2} \frac{W_3}{M} \gamma(0) \right] .\end{aligned}$$

Splitting the χ function also permits the exact calculation of the Debye-Waller factor. Previously, it was taken to be the value of the χ function at the largest value of t calculated, lumping together the non-zero contribution from the distributed frequency spectrum and the decaying contribution from the free gas χ function. Now, $\chi_b(t)$, the modified free gas part of $\chi(t)$, does not contribute to the Debye-Waller factor, which is calculated exactly and is independent of the integration mesh. Figure 4.15 indicates the increased stability produced by splitting the χ function.

$\chi_1(t)$ produces a broadened elastic line at $\beta = 0$. If W_1 is small, the line is narrow. Calculations have shown that very little free gas need be added to remove the numerical problems mentioned above. In these cases, where the free gas is added as a numerical convenience and not as part of the physical description of the scatterer, the contribution to $S(\alpha, \beta)$ from $\chi_b(t)$ can be deleted.

Figure 4.16 is a plot of $S(\alpha, \beta)e^{\beta/2}$ versus β for a room temperature Debye spectrum, with $\theta_D = .06$ eV and a mass of 9. Free gas with weight $W_1 = .001$ has been used to damp the χ function. Since the cross section depends on $S(\alpha, \beta)e^{\beta/2}$ rather than on $S(\alpha, \beta)$, the curves have been presented multiplied by $e^{\beta/2}$, displaying any large β errors more clearly than plots of $S(\alpha, \beta)$ itself. The behavior of the curves with increasing α is as expected: at low α (one phonon term contribution) a function closely related to the input frequency spectrum is reproduced. As α increases (and higher phonon terms contribute), the curve begins to show structure at $\beta > \frac{\theta_D}{T}$.

The solid line in Fig. 4.17 is the $\chi_a(t)$ used in calculating $S(\alpha = 0.25, \beta)$; the crosses indicate $\chi_a(t)$ for $\alpha = 5$, which is considerably more damped.

Figure 4.18 is a scattering law calculation using the beryllium frequency spectrum, with the addition of a small amount of free gas ($W_1 = .002$). This represents an extreme case, a frequency spectrum with several sharp spikes and with very little Debye-like behavior at low frequency. Again one sees that for low α the frequency spectrum is nearly reproduced due to the fact that only the one phonon term is dominant. In another section of this report (4.4), a curve is provided which shows

Fig. 4.15 -- Improved scattering law for a mass 12 scatterer with a Debye frequency spectrum at $\alpha = 2.11$

Fig. 4.16 -- Scattering law for a mass 9 scatterer with a Debye frequency spectrum plus some free gas

Fig. 4.17 -- χ functions used in the scattering law calculations

Fig. 4.18 -- Calculated scattering law for beryllium

that the results given by GASKET using a frequency spectrum for beryllium, developed under this project, agree fairly well with the measurements of $S(\alpha, \beta)$ by Schmunk. (2)

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APPENDIX

HEXSCAT

COHERENT ELASTIC SCATTERING OF NEUTRONS
BY HEXAGONAL LATTICES

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HEXSCAT
COHERENT ELASTIC SCATTERING OF NEUTRONS
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U.S. Atomic Energy Commission

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The HEXSCAT computer code is described herein as it existed on December 15, 1964. The code has been in continuous development for one year and in its presented form has been applied successfully by General Atomic to the kind of problems discussed later in this report. Duplication of results (or even close agreement) between problems run with the code as published and the code as it existed either before or after this time is not necessarily to be expected.

General Atomic has exercised due care in preparation, but does not warrant the merchantability, accuracy, and completeness of the code or of its description contained herein. The complexity of this kind of program precludes any guarantee to that effect. Therefore, any user must make his own determination of the suitability of the code for any specific use, and of the validity of the information produced by use of the code.

I. FORMULATION

The HEXSCAT code calculates the P_0 and P_1 components of the polycrystalline coherent elastic neutron scattering cross section per nucleus for a hexagonal lattice, according to the general expression given below:⁽¹⁾

$$\sigma_\ell = \frac{\sigma_{\text{coh}} \lambda^2}{2 \sqrt{3} \alpha^2 c} \sum_{\tau}^{\tau/2\pi \leq \frac{2}{\lambda}} (m_\tau / \tau) f_\ell \exp \left[-(\hbar^2 \tau^2 / 2M) \int_0^{\omega_{\text{max}}} (\rho(\omega) / \omega) \coth(\omega / kT) d\omega \right] \frac{|F|^2}{N}, \quad (1)$$

where

$$f_\ell = \begin{cases} 1 & \ell = 0 \text{ (} P_0 \text{ component)} \\ 1 - (\tau^2 \lambda^2 / 8\pi^2) & \ell = 1 \text{ (} P_1 \text{ component)}; \end{cases}$$

$\lambda = \pi \hbar \sqrt{2/mE}$; m and M are neutron and scatterer masses, respectively; $(\tau/2\pi)^2 = (4/3 \alpha^2) (\ell_1^2 + \ell_2^2 + \ell_1 \ell_2) + \ell_3^2 / c^2$; N is the number of atoms per unit cell; σ_{coh} is the coherent scattering cross section; m_τ is the number of reciprocal lattice vectors τ of equal magnitude produced by different combinations of the integers ℓ_1, ℓ_2, ℓ_3 ; $|F|^2$ is the form factor appropriate to the crystal; and α and c are the magnitudes of the lattice vectors, corresponding to the basis shown in the sketch below.

The sum $\sum_{\tau} m_\tau \dots$ is a sum over all possible values of τ obtained by varying ℓ_1, ℓ_2, ℓ_3 over the negative and positive integers and zero, and satisfying the condition, $\tau/2\pi \leq 2/\lambda$. This sum can be written in the form

$$\sigma_\ell = \sum_{\ell_1=-\infty}^{\infty} \sum_{\ell_2=-\infty}^{\infty} \sum_{\ell_3=-\infty}^{\infty} g(\ell_1, \ell_2, \ell_3) \quad (2)$$

where Σ' refers to the restriction

$$\tau/2\pi \leq 2/\lambda. \quad (3)$$

This sum can be replaced by one over zero and the positive integers with finite limits by the following arguments:

All the limits may be reduced from a range of $(-\infty, \infty)$ to $(0, \infty)$ by grouping all those $g(l_1, l_2, l_3)$ corresponding to the same absolute values of l_1, l_2, l_3 . To determine $l_1^{\max}$, the upper limit of l_1 , we first note that $l_3 = 0$ gives the largest l_1 . $l_1^{\max}$ occurs for $l_2 < 0$, when the cross term $l_1 l_2$ (in the expression for τ) subtracts from $l_1^2 + l_2^2$. Then τ is parabolic in l_2 , with a minimum at $|l_2| = l_1/2$, or

$$\begin{aligned}\phi &= (\tau^{\max}/2\pi)^2 = (4/3\alpha^2) (l_1^2 + l_2^2 - l_1 |l_2|) \\ &= (4/3\alpha^2) (l_1^2 + l_1^2/4 - l_1^2/2)\end{aligned}$$

Hence, $l_1^{\max} = \alpha \sqrt{\phi}$.

For a given l_1 , $l_2^{\max}$ is determined from the above expression, giving $l_2^{\max}(l_1) = (1/2) [l_1 + \sqrt{3(\alpha^2 \phi - l_1^2)}]$. Given l_1 and l_2 , $l_3^{\max}$ is then

$$l_3^{\max}(l_1, l_2) = c \sqrt{\phi - (4/3\alpha^2) (l_1^2 + l_2^2 - l_1 l_2)}.$$

Since $g(l_1, l_2, l_3) = g(l_2, l_1, l_3)$, the lower limit of l_2 can be taken as l_1 , with g multiplied by a weight of $M_1 = 2$ when $l_1 \neq l_2$ and $M_1 = 1$ when $l_1 = l_2$. The sign permutations of l_1, l_2, l_3 which need to be calculated can be reduced from 8 to 2 by considering the symmetry properties of $(\tau/2\pi)^2$ and $|F|^2$ under sign changes.

Form factors $|F|^2$ are symmetric in l_1, l_2 for hexagonal crystals. In general, for any crystal,

$$|F|^2 = \left| \sum_{j=1}^N e^{2\pi i \lambda_j} \right|^2 = N + 2 \sum_{m>n}^N \cos 2\pi (\lambda_m - \lambda_n),$$

where N is the number of atoms per cell. For graphite, the λ 's are given by $\lambda_1 = 0$, $\lambda_2 = (-l_1 + l_2)/3$, $\lambda_3 = -(2/3)l_1 - (1/3)l_2 + (1/2)l_3$,

$\lambda_4 = -(1/3)\ell_1 + (1/3)\ell_2 + (1/2)\ell_3$. This may be simplified to

$$|F|^2 = \begin{cases} 6 + 10 \cos [2\pi(\ell_1 - \ell_2)/3] & \ell_3 \text{ even} \\ 4 \sin^2 [\pi(\ell_1 - \ell_2)/3] & \ell_3 \text{ odd} . \end{cases}$$

For beryllium,

$$|F|^2 = 2 + 2 \cos [\pi(2\ell_1 - 2\ell_2 + 3\ell_3)/3] .$$

Since both τ and $|F|^2$ are unchanged for $\ell_3 \rightarrow -\ell_3$, the 8 sign combinations may be grouped

$$(i) \begin{cases} (+\ell_1, +\ell_2, \pm\ell_3) \\ (-\ell_1, -\ell_2, \pm\ell_3) \end{cases} \quad (ii) \begin{cases} (+\ell_1, -\ell_2, \pm\ell_3) \\ (-\ell_1, +\ell_2, \pm\ell_3) , \end{cases}$$

leaving 4 sets, each weighted by $M_3 = 2$ ($\ell_3 \neq 0$) or $M_3 = 1$ ($\ell_3 = 0$). Next, the cases in (i) are equivalent to each other, as are those in (ii), so that only one of each need be calculated, weighted by $M_2 = 2$ when $\ell_1 \neq 0$, $\ell_2 \neq 0$ (since then the set ℓ_1, ℓ_2 gives two distinct τ -vectors), $M_2 = 1$ when ℓ_1 or $\ell_2 = 0$ but not both (since then ℓ_1, ℓ_2 gives only one distinct τ -vector), and $M_2 = 1/2$ when $\ell_1 = \ell_2 = 0$ (since in this case all four combinations reduce to the same one). In summary the weighting factors are as follows:

$$M(\ell_1, \ell_2, \ell_3) = M_1 M_3 M_2$$

$$M_1 = \begin{cases} 2 & \ell_1 \neq \ell_2 \\ 1 & \ell_1 = \ell_2 \end{cases}$$

$$M_3 = \begin{cases} 2 & \ell_3 \neq 0 \\ 1 & \ell_3 = 0 \end{cases}$$

$$M_2 = \begin{cases} 2 & \ell_1 \neq 0, \ell_2 \neq 0 \\ 1 & \ell_1 \text{ or } \ell_2 = 0, \text{ but not both} \\ 1/2 & \ell_1 = \ell_2 = 0 . \end{cases}$$

The final form of the sum used in the code is then

$$\sum_{\tau} g(\ell_1, \ell_2, \ell_3) \rightarrow \alpha \sqrt{\phi} \sum_{\ell_1=0}^{\max(\ell_1)} \sum_{\ell_2=\ell_1}^{\max(\ell_1, \ell_2)} \sum_{\ell_3=0}^{\max(\ell_1, \ell_2)} M(\ell_1, \ell_2, \ell_3) [g(\ell_1, \ell_2, \ell_3) + g(\ell_1, -\ell_2, \ell_3)] . \quad (4)$$

II. CODE

HEXSCAT (written in FORTRAN IV for the IBM 7044) evaluates eq. (4) and averages the cross sections over energy groups. The averaging is necessary since the coherent elastic cross section exhibits a good deal of structure within a typical low energy group. The code takes as input a set of energy group boundaries, a cutoff energy E_c , and the number of points per group for averaging below and above E_c , NAVX and NAV, respectively. When the upper group energy is less than E_c , the code determines subgroup energy boundaries within the group by evaluating τ throughout the group, finding every change of magnitude of τ within the group, and using the energies corresponding to these changes as the subgroup boundaries. Each subgroup contains NAVX evenly spaced points. If the upper group boundary energy is greater than E_c , NAV evenly spaced points are added within the group.

Subroutines for the evaluation of $|F|^2/N$ for graphite and beryllium have been written. They are listed, along with the main program and an interpolation routine in the appendix.

A description of the card input follows:

<u>Card</u>	<u>Format</u>	<u>Variable Name</u>	
1	13A6, A2	(HOL(I), I=1, 14)	Comment card
2	6E10. 4	SCOH	σ_{coh} (barns)
		A	α (cm) magnitude of base plane lattice vector-see sketch.
		c	c (cm) magnitude of lattice vector out of base plane-see sketch.
		AMSC	M = scatterer mass (neutron mass units)
		WAL2	$\alpha_2 = (1/M) \int_0^{\omega_{\text{max}}} \frac{f(\omega)}{\omega^2} \coth\left(\frac{\omega}{kT}\right) d\omega \text{ from}$ SUMMIT output. (2)
		EXACT	E_c = cutoff energy described above (eV)
3	4I5	NES	Number of energy group <u>boundaries</u>
		NAV	described above
		NAVX	described above
		IP	With IP > 0, the point values of the cross section calculated within each group are printed.
4	7E10. 4	(E(I), I = 1, NES)	Group boundary energies (eV).

The group averaged P_0 and P_1 cross sections are punched on cards in a IP5E12. 5 format, suitable for input to the GATHER II library program. (3)

III. RESULTS

Figure 1 compares the calculated and measured values of $\sigma_{\text{coh}}^{\text{Be}}(E)$ reported in Amaldi⁽¹⁾ with the code results. Since these results only include elastic scattering they start deviating from experiment when the inelastic scattering becomes significant.

Fig. 1 -- Coherent elastic cross section of beryllium

REFERENCES

1. Amaldi, E., Handbuch der Physik, Neutrons and Related Gamma Ray Problems, Vol. XXXVIII/2, Berlin, Gottingen, Heidelberg: Springer-Verlag, 1959.
2. Bell, J., SUMMIT Code, General Atomic report GA-2492 (1962).
3. Smith, C. V. and H. A. Vieweg, GGC-II, General Atomic report GA-4436 (1963).

APPENDIX A

FORTRAN-IV LISTING

```

* $IBFTC HXSCAT LIST,DECK,REF
C   COHERENT ELASTIC SCATTERING IN HEXAGONAL CRYSTALS
    DIMENSION E(1000),ALAM(1000),SIGZ(1000),SIG1(1000),SIGMAZ(300),
1  SIGMA1 (300),EIN(300),HOL(14)
    TAU(Q000FL,Q001FL,Q002FL)=(T5*(Q000FL**2+Q001FL**2+Q000FL*Q001FL)+
1  Q002FL**2/CSQ)*TWOPI
    PI=3.1415927
    PI4S=(4.0*PI)**2
    TWOPI=(2.0*PI)**2
    T3=PI/3.0
    T4=1.0/(8.0*PI**2)
    HBAR=1.05444 E-27
1  READ (5,2)HOL,SCOH,A,C,      AMSC, WAL2,EXACT,NES,NAV,NXAV,IP,
1  (EIN(I),I=1,NES)
2  FORMAT(13A6,A2/6E10.4/4I5/(7E10.4))
    CL1=1.732051*A/2.
    ASQ=A**2
    WINT=WAL2*0.658173E-15*AMSC
    AMNE=1.67474E-24
    AMBE=AMSC*1.65983E-24
    ECON=(8.*AMNE/HBAR)*(1.60207E-12/HBAR)
    T1=SQRT(2.0/AMNE)*PI*HBAR
    T2=HBAR/(2.0*AMBE)
    T5=4.0/(3.0*A**2)
    CSQ=C**2
    DIP=SCOH/(2.0*A**2*C*1.732051)
    DO 400 IOE=2,NES
    IF(EIN(IOE).GT.EXACT) GO TO 401
    TMAX=EIN(IOE)*ECON
    TMIN=EIN(IOE-1)*ECON
    NF=NXAV+2
    E(1)=EIN(IOE)
403 CALL INEXT(TMAX,TAUN,TWOPI,T5,1./CSQ,CL1,ASQ,C)
    IF(TAUN.LT.TMIN) GO TO 402
    E(NF)=(TAUN/ECON)*1.0000001
    NF=NF+NXAV+1
    TMAX=TAUN
    GO TO 403
402 E(NF)=EIN(IOE-1)
    NXAV1=NXAV+1
    DO 404 INE=1,NF,NXAV1
    INEM=INE+NXAV1
    DELE=(E(INEM)-E(INE))/FLOAT(NXAV1)
    DO 404 J=1,NXAV
    JJ=INE+J
404 E(JJ)=E(JJ-1)+DELE
    N=NF
    GO TO 405
401 E(1)=EIN(IOE)
    NAV1=NAV+1

```

```

E(NAV1+1)=EIN(IOE-1)
DELE=(EIN(IOE)-EIN(IOE-1))/FLOAT(NAV1)
DO 406 J=2,NAV1
406 E(J)=E(J-1)-DELE
N=NAV+2
405 CONTINUE
DO 40 I=1,N
ALAM(I)=T1/SQRT(E(I)*1.60207E-12)
AL2=ALAM(I)**2
C2P=AL2*T4
D1=D1P*AL2
ULIM=(4.0/AL2)*TWOPIS
SUMPZ=0.0
SUMP1=0.0
PHI=ULIM/TWOPIS
L1M=A*SQRT(PHI)
L1S=0
DO 100 L1=L1S,L1M
FL1=L1
L2M=INT(0.5*(FL1+SQRT(3.*(ASQ*PHI-FL1**2))))
DO 101 L2=L1,L2M
FL2=L2
X=PHI-T5*(FL1**2+FL2**2-FL1*FL2)
L3M=0
IF(X.GT.0.)L3M=C*SQRT(X)
DO 102 L3=L1S,L3M
FL3=L3
WM=2.
IF(L1.EQ.L2) WM=1.
W3=2.
IF(L3.EQ.0) W3=1.
W2=2.
IF(L1.EQ.0.OR.L2.EQ.0) W2=1.
IF(L1.EQ.0.AND.L2.EQ.0) W2=0.5
W=WM*W3*W2
TSQP=TAU(FL1,FL2,FL3)
IF(TSQP.LE.0.0.OR.TSQP.GT.ULIM) GO TO 103
TAUP=SQRT(TSQP)
SUM=EXP(-TSQP*T2*WINT)*FORM(FL1,FL2,FL3)*W/TAUP
SUMPZ=SUMPZ+SUM
SUMP1=SUMP1+SUM*(1.-TSQP*C2P)
103 TSQM=TAU(FL1,-FL2,FL3)
IF(TSQM.LE.0.0.OR.TSQM.GT.ULIM) GO TO 102
TAUM=SQRT(TSQM)
SUM=EXP(-TSQM*T2*WINT)*FORM(FL1,-FL2,FL3)*W/TAUM
SUMPZ=SUMPZ+SUM
SUMP1=SUMP1+SUM*(1.-TSQM*C2P)
IF(L3M.EQ.0) GO TO 101
02 CONTINUE
01 CONTINUE

```

```

100 CONTINUE
    SIGZ(I)=SUMPZ*D1
    SIG1(I)=SUMP1*D1
40 CONTINUE
    K=IOE-1
    IF(IP.NE.0)WRITE (6,10)K,SCOH,A,C,AMSC,
1      WAL2,(I,E(I),ALAM(I),SIGZ(I), SIG1(I),I=1,
2N)
10 FORMAT(1H1///15X,38HHEXAGONAL COHERENT ELASTIC SCATTERING
X20H POINT DATA, GROUP I2///5X
111HSIGMA(COH)=1PE12.5,5X,2HA=E12.5,5X,2HC=E12.5,5X,
2      15HSCATTERER MASS=E12.5/
35X,20HDEBYE-WALLER FACTOR=E12.5///16X,1HE,8X,6HLAMBDA,7X,
47HSIGMA 0,7X,7HSIGMA 1/((I6,1P4E14.6))
    IF(EIN(IOE).GT.EXACT) GO TO 412
    FN1=NXAV1
    NXAV2=NXAV+2
    SZ=0.
    S1=0.
    DE=(E(1)-E(NXAV2))/FN1
    DO 411 I=2,NXAV2
    SZ=SZ+(SIGZ(I-1)+SIGZ(I))*0.5
411 S1=S1+(SIG1(I-1)+SIG1(I))*0.5
    SZ=SZ*DE
    S1=S1*DE
    IL=N -NXAV
    II=NXAV2+1
    IF(II.GE.N) GO TO 504
    DO 414 I=II,IL,NXAV1
    IPN=I+NXAV
    DE=(E(I-1)-E(IPN))/FN1
    INTERP=MINO(3,NXAV1)
    SIGZ(I-1)=TERP(E(I),SIGZ(I),NXAV1,E(I-1),INTERP)
    SIG1(I-1)=TERP(E(I),SIG1(I),NXAV1,E(I-1),INTERP)
    IM=I-1
    IF(IP.LT.0)WRITE(6,502)IM,E(IM),SIGZ(IM),SIG1(IM)
502 FORMAT(///3H I=I3,4H E=1PE12.4,6H S 0=E12.4,6H S 1=E12.4)
    DO 414 J=I,IPN
    SZ=SZ+DE*0.5*(SIGZ(J)+SIGZ(J-1))
414 S1=S1+DE*0.5*(SIG1(J)+SIG1(J-1))
504 DEIN=EIN(IOE)-EIN(IOE-1)
    SIGMAZ(IOE)=SZ/DEIN
    SIGMA1(IOE)=S1/DEIN
    GO TO 400
412 SIGMAZ(IOE)=0.
    SIGMA1(IOE)=0.
    FN=N
    DO 413 I=1,N
    SIGMAZ(IOE)=SIGMAZ(IOE)+SIGZ(I)/FN
413 SIGMA1(IOE)=SIGMA1(IOE)+SIG1(I)/FN

```



```

400 IF(IP.LT.0) WRITE(6,503)SIGMAZ(10E),SIGMA1(10E)
503 FORMAT(//14HGROUP AVERAGED, 6H S 0=1PE12.4,6H S 1=E12.4)
      PUNCH 9,(SIGMAZ(I),I=2,NES)
      PUNCH 9,(SIGMA1(I),I=2,NES)
  9 FORMAT(1P5E12.5)
      WRITE(6,501)HOL,SCOH,A,C,      AMSC,WAL2,EXACT,NXAV,NAV,(I,EIN(I),
      1SIGMAZ(I),SIGMA1(I),I=2,NES)
501 FORMAT(1H1///15X38HHEXAGONAL COHERENT ELASTIC SCATTERING //
X30X,13A6,A2//
15X11HSIGMA(COH)=1PE12.5,5X2HA=E12.5,5X2HC=E12.5,
2      5X15HSCATTERER MASS=E12.5/5X20HDEBYE-WALLER FACTOR=E12.5/5X
325HALL PEAKS FOUND FOR E.LT. E12.5,34H RANGES BETWEEN PEAKS DIVIDE
4D INTO 13,10H INTERVALS/5X34HHIGHER ENERGY RANGES DIVIDED INTO 13,
510H INTERVALS///16X1HE,7X7HSIGMA 0,7X7HSIGMA 1//((I6, 3E14.6))
      GO TO 1
      END

```

```

$IBFTC TNEXT LIST,REF
SUBROUTINE TNEXT(TMAX,TAU,C1,C2,C3,CL1,ASQ,C)
TF(X,Y,Z)=C1*(C2*(X**2+Y**2+X*Y)+C3*Z**2)
TAU=0.
L1M=SQRT(ASQ*TMAX)
L1S=0
DO 3 L1=L1S,L1M
FL1=L1
L2M=0.5*(FL1+SQRT(3.*(ASQ*TMAX-FL1**2)))
DO 2 L2=L1 ,L2M
FL2=L2
X=TMAX-C2*(FL1**2+FL2**2-FL1*FL2)
L3M=0
IF(X.GT.0.)L3M=C*SQRT(X)
DO 1 L3=L1S,L3M
FL3=L3
TA=TF(FL1,FL2,FL3)
IF(TA.GT.TAU.AND.TA.LT.TMAX)TAU=TA
IF(L3M.EQ.0) GO TO 2
1 CONTINUE
2 CONTINUE
3 CONTINUE
RETURN
END

```

```
LIBRARY FORM: LIST, REF  
FUNCTION FORM(A1,A2,A3)  
C BE FORM FACTOR  
FORM=(1.+COS((2.*A1+4.*A2+3.*A3)*1.0471976))  
RETURN  
END
```

\$IBFTC FORM

FUNCTION FORM (A1,A2,A3)

GRAPHITE FORM FACTOR

I3=ABS(A3)+0.01

J3=FLOAT(I3)/2.

IF(J3*2.EQ.I3) GO TO 1

A3 ODD

FORM =(SIN((A1-A2)*1.0471976))**2

GO TO 2

A3 EVEN

1 FORM =(6.+10.*COS((A1-A2)*2.0943951))/4.

2 RETURN

END

\$IBFTC FORM LIST,REF

FUNCTION FORM(A1,A2,A3)

BEO FORM FACTOR

FORM=(1.+COS((2.*A1+4.*A2+3.*A3)*1.0471976))

FORM=FORM*(7.54+4.24+11.31*COS(2.356195*A3))

RETURN

END

\$IBFTC TERP LIST,DECK,REF
FUNCTION TERP(X,Y,NL,ARG,IL)

```

C-----
C THIS FUNCTION DOES LAGRANGIAN INTERPOLATION OR
C EXTRAPOLATION OF ILTH ORDER ON X AND Y FOR ARG
C WHEN THE TABLES ARE EITHER INCREASING OR DECREASING
C-----
C X          X ARRAY, INDEPENDENT VARIABLE
C Y          Y ARRAY, DEPENDENT VARIABLE
C NL         NUMBER OF ENTRIES IN TABLES OF X AND Y
C ARG        INDEPENDENT VARIABLE VALUE
C IL         ORDER OF INTERPOLATION
C-----
C DIMENSION X(2),Y(2)
C DIMENSION X(2),Y(2)
C-----
C IF(NL-IL)97,98,99
C NOT ENOUGH ENTRIES IN TABLES FOR THIS ORDER INTERPOLATION
97 IL=NL
98 L=1
GO TO 112
99 CONTINUE
IL2=IL/2
IADD=MOD(IL,2)
C CHECK IF TABLES IN INCREASING OR DECREASING SEQUENCE
C IF(X(1)-X(NL))100,100,101
C INCREASING SEQUENCE
100 ILOW=IL2+1
IHI=NL-IL2-IADD
IUSEL=1
IUSEH=NL-IL+1
IBEG=ILOW+1
IEND=IHI-1
LAST=IEND-IL2+1
IADD=0
GO TO 102
C DECREASING SEQUENCE
101 ILOW=NL-IL2
IHI=IL2+IADD+1
IUSEL=NL-IL+1
IUSEH=1
IBEG=IHI+1
IEND=ILOW-1
LAST=2
IADD=1-IADD
C CHECKS IF ARG IS SMALLER THAN TABLE VALUES
102 IF(ARG-X(ILOW))103,104,105
C SMALLER THAN SMALLEST TABLE VALUE
103 L=IUSEL
GO TO 112

```

104 TERP=Y(ILOW)
GO TO 117
C CHECKS IF ARG IS GREATER THAN TABLE VALUES
105 IF(X(IHI)-ARG)106,107,108
C ARG GREATER THAN TABLE VALUE
106 L=IUSEH
GO TO 112
107 TERP=Y(IHI)
GO TO 117
C SEARCHES X ARRAY TO BRACKET ARG
108 DO 109 N=IBEG,IEND
IF(IUSEL-1)1080,1080,1081
1080 M=N
GO TO 1082
1081 M=NL-N+1
1082 IF(X(M)-ARG)109,110,111
109 CONTINUE
L=LAST
GO TO 112
C EQUALS ARGUMENT, RETURN OK
110 TERP=Y(M)
GO TO 117
C EUREKA
111 L=M-IL2+IADD
112 CONTINUE
C INTERPOLATION SECTION
SUM=0.0
DO 115 I=1,IL
P=1.0
PK=1.0
IN=L+I-1
DO 114 IP=1,IL
IF(IP-I)113,114,113
113 INP=L+IP-1
P=P*(ARG-X(INP))
PK=PK*(X(IN)-X(INP))
114 CONTINUE
SUM=SUM+P*Y(IN)/PK
115 CONTINUE
TERP=SUM
117 RETURN
END