ANL-6551
Physics
(TID-4500, 18th Ed.)
AEC Research and
Development Report

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois

A PROCEDURE FOR THE EVALUATION OF NEUTRON-SCATTERING CROSS SECTION IN THE INCOHERENT APPROXIMATION

by

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September 1962

Operated by The University of Chicago
under
Contract W-31-109-eng-38

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Using some simplifying assumptions about the details of phonon-frequency distribution, we evaluated exactly the contributions of 25 phonons. By means of these contributions, the differential scattering cross section $\sigma(E \rightarrow E', \theta)$, the scattering law $S(\alpha, \beta)$, or inelastic-scattering matrices and transport cross sections for multigroup calculations may be calculated. In the evaluation of multigroup parameters use is made of an asymptotic expression when the phonon expansions fail to converge.

When the phonon-frequency distribution is considered dependent on the direction of polarization (as in graphite), then averages over all directions are obtained.

I. INTRODUCTION

The basic ideas underlying present scheme of evaluation of the inelastic neutron cross section have been explained briefly in a paper presented at a meeting of the American Nuclear Society.[1] This report is intended to complete the presentation of the procedure, which is oriented towards computer application. Thus, in addition to a brief derivation of mathematical formulae, this report includes descriptions of calculational procedures which may be used with a computing machine. Some measures taken are obviously somewhat arbitrary and have been included in this description for the sake of completeness.

Essentially, we propose to evaluate the inelastic-scattering cross section in the incoherent approximation for a simple cubic Bravais lattice. The main formula[2] does not depend on the polarization of the phonons.

The basic part of the procedure (see Chapter III) is the evaluation of repeated convolutions to obtain contributions due to 25 phonons. To avoid errors in multiple integrations, it is assumed initially that the phonon-frequency distribution $\rho(\omega)$ is such that

$$f(\omega) = \frac{\rho(\omega)}{\omega \operatorname{sh}(\omega/2kT)}$$

can be represented by a broken line with break points at integral multiples of $\Delta\omega$. (Usually $\Delta\omega$ is much smaller than kT.) Then the multiphonon contributions are determined exactly by a simple procedure [see Eqs. (16) and (17)].

Having the multiphonon contributions we can calculate differential scattering cross sections $\sigma(E \rightarrow E', \theta)$, the scattering law $S(\alpha, \beta)$, or inelastic scattering matrices and transport cross sections to be used in multigroup calculations. In all these cases it is assumed that contributions of neglected phonons decrease in a geometric progression. A correction term is added if it is smaller than 10% of the total. Otherwise, it must be considered that the expansion using only 25 phonons is unsatisfactory for the determination of $\sigma(E \rightarrow E', \theta)$ and $S(\alpha, \beta)$. Fortunately, this is unlikely for experimentally observable energy and momentum transfers.

In the evaluation of multigroup scattering matrices, integration over scattering angle θ has been performed analytically, and $\sigma(E \rightarrow E')$ is computed by use of the multiphonon expansion if it converges satisfactorily; otherwise, an asymptotic expression has been chosen to fit the region of drop-off of the inelastic cross section at high energies, $|E - E'| \approx \mu(\sqrt{E} + \sqrt{E'})^2$. It is not good for much larger energy transfers. However, the inelastic cross section in that region is very small, and thus the error is not expected to affect the subsequent flux calculations. In the instances in which the energy change is finite but the incident energy is very large, the asymptotic expansion may not be good, but in this case the multiphonon expansion still converges (provided $n_{max} \geqq 4a_2g(0)$, as seen in Appendix B). In any case, the value of this nearly elastic cross section is not expected to effect great changes in the reactor flux.

Similar asymptotic expressions have been used previously by Schofield and Hassit[2] and by Sjölander.[3] However, they have used this approach to evaluate individual multiphonon contributions. In our procedure this expansion is used for the main formula as a whole, thus saving an appreciable amount of computation.

Although in our main formula it is assumed that phonon-frequency distribution is independent of polarization, for general polycrystalline media one can consider that $\rho(\omega)$ depends upon the direction of polarization and upon the kinds of atoms of the lattice. Then the inelastic-scattering cross section can be obtained by using our main formula repeatedly for various directions and averaging the obtained results. Currently, this has been attempted for graphite only where results depend only on the angle of the momentum-transfer vector with crystalline planes in graphite.[4] Averaging over this angle is done as the last step for the first two calculations and in the evaluation of multigroup scattering matrices averaging over this angle is done immediately prior to averaging over initial energies.

II. INITIAL CALCULATION OF SEVERAL PARAMETERS

For simple cubic Bravais lattice the differential scattering cross section in the incoherent approximation can be written[2,4] as

$$\sigma(E \to E', \theta) = (\sigma_b/8\pi^2)(E'/E)^{1/2} \int_{-\infty}^{\infty} dt \exp\{-it(E - E') + \mu\gamma[g(t) - g(0)]\} \quad , \qquad (1)$$

where E and E' are initial and final energy of the neutron; θ is the angle of scattering; σ_b is the cross section for a bound atom; μ is the ratio of neutron mass and the mass of the atom; γ is proportional to the square of momentum transfer:

$$\gamma = E + E' - 2\cos\theta \sqrt{EE'} \quad ;$$

and g(t) is a Fourier transform:

$$g(t) = \int_{-\infty}^{\infty} \frac{d\omega}{\omega} \frac{\rho(\omega)}{\exp(\omega/kT) - 1} e^{-i\omega t} \quad .$$

Here $\rho(\omega)$ is assumed to be an even function of ω. It is proportional to the number of modes of vibration of energy ω, and it is normalized to unity, that is,

$$\int_0^{\infty} \rho(\omega)\, d\omega = 1 \quad .$$

Further, k is the Boltzmann constant, T the absolute temperature, and $[\exp(\omega/kT) - 1]^{-1}$ is the average occupation number for a phonon of frequency ω.

Operation with complex quantities in g(t) can be avoided by shifting the path of integration. Substituting T = t' + (i/2kT), rearranging terms, and omitting primes, we can rewrite Eq. (1) as

$$\sigma(E \to E', \theta) = (\sigma_b/8\pi^2)(E'/E)^{1/2} \exp\{[(E - E')/2kT] - \mu\gamma g(0)\} \int_{-\infty}^{\infty} dt \exp\{-it(E - E') + \mu\gamma G(t)\} \quad , \qquad (2)$$

where G(t) is the even function defined by

$$G(t) = \int_0^{\infty} f(\omega) \cos \omega t \, d\omega \quad , \qquad (3)$$

$$g(0) = G(i/2kT) = \int_0^{\infty} f(\omega)\, ch(\omega/2kT)\, d\omega \quad , \qquad (4)$$

and

$$f(\omega) = \frac{\rho(\omega)}{\omega \mathrm{sh}(\omega/2kT)} \quad .$$

In the present formulation of the problem, $\rho(\omega)$ will be given in unnormalized form at equidistant points:

$$\rho_u(j\Delta\omega) = \rho_j \quad \text{for} \quad 1 \leq j \leq m-1 \quad .$$

It will be assumed that

$$\rho_u(0) = 0 \text{ and } \rho_u(j\Delta\omega) = 0 \quad \text{for} \quad j \geq m \quad .$$

Then we can compute

$$f_u(j\Delta\omega) = f_j = \frac{\rho_j}{j\Delta\omega\, \mathrm{sh}(j\Delta\omega/2kT)} \quad , \text{for} \quad 1 \leq j \leq m-1 \quad , \tag{5}$$

assuming f_0 as given. If ρ is approximately parabolic for $\omega \leq \Delta\omega$,

$$f_0 \approx \rho_1 \frac{2kT}{(\Delta\omega)^2} \quad .$$

If we assume now that f_u has values given by Eq. (5) for integral multiples of $\Delta\omega$ and is linear in between, we can compute easily the normalization factor N, g(0), and G(t). With this assumption, f_u is really a weighted sum of shifted rooflike functions:

$$f_u = \sum f_j\, c^{(1)}(\omega - j\Delta\omega) \quad ,$$

where $c^{(1)}(\omega)$ is a broken-line function equal to one for $\omega = 0$ and vanishing for all other integral multiples of $\Delta\omega$. G(t) is then

$$\begin{aligned} G(t) &= \int_0^\infty f(\omega) \cos\omega t\, d\omega \\ &= \frac{2\Delta\omega}{N} \frac{1 - \cos\Delta\omega t}{(\Delta\omega t)^2} \left[\frac{1}{2} f_0 + \sum_{j=1}^{m-1} f_j \cos j\Delta\omega t \right] \quad , \end{aligned} \tag{6}$$

since

$$\int_{-\infty}^{\infty} d\omega\, c^{(1)}(\omega) \cos\omega t = 2 \int_0^{\Delta\omega} d\omega \left(1 - \frac{\omega}{\Delta\omega}\right) \cos\omega t = 2\, \frac{1 - \cos\Delta\omega t}{(\Delta\omega t)^2} \quad .$$

Replacing t in Eq. (6) by $i/2kT$, we obtain

$$g(0) = \frac{1}{N} \int_0^\infty f_u(\omega) \operatorname{ch} \frac{\omega}{2kT} d\omega$$

$$= \frac{2\Delta\omega}{N} \left(\frac{2kT}{\Delta\omega}\right)^2 \left(\operatorname{ch} \frac{\Delta\omega}{2kT} - 1\right) \left[\frac{1}{2} f_0 + \sum_{j=1}^{m-1} f_j \operatorname{ch} j \frac{\Delta\omega}{2kT}\right] \quad . \quad (7)$$

Then, differentiating both sides of Eq. (7) with respect to $1/2kT$, we obtain the normalization factor N:

$$\int_0^\infty f_u(\omega)\ \omega \operatorname{sh} \frac{\omega}{2kT} d\omega = \int_0^\infty \rho_u(\omega)\, d\omega = N = 2\Delta\omega \left(\frac{2kT}{\Delta\omega}\right)^2 \left(\operatorname{ch} \frac{\Delta\omega}{2kT} - 1\right) \left[\sum_{j=1}^{m-1} \rho_j\right]$$

$$+ 2(\Delta\omega)^2 \left(\frac{2kT}{\Delta\omega}\right)^2 \left[\operatorname{sh} \frac{\Delta\omega}{2kT} - 2\left(\frac{2kT}{\Delta\omega}\right) \left(\operatorname{ch} \frac{\Delta\omega}{2kT} - 1\right)\right]$$

$$\times \left[\frac{1}{2} f_0 + \sum_{j=1}^{m-1} f_j \operatorname{ch} j \frac{\Delta\omega}{2kT}\right] \quad . \quad (8)$$

Thus, after having found f_j from Eq. (5), N from Eq. (8), and g(0) from Eq. (7), we are ready to "normalize" $f(\omega)$:

$$f_j^{(1)} = \frac{\Delta\omega}{2N} f_j \quad (9)$$

and to proceed with multiphonon expansion.

Since asymptotic expansion may be used in further calculations simultaneously with evaluation of Eqs. (5), (7), and (8), we compute also two other constants needed in Chapter V, Section C. These are the derivatives of G(t) evaluated at $t = -i/2kT$. Taking Eq. (7) and differentiating it twice with respect to $1/2kT$, we obtain

$$a_2 = \int d\omega\, \rho(\omega) \left(\coth \frac{\omega}{2kT}\right) \omega$$

$$= \frac{2\Delta\omega^3}{N} \left(\frac{2kT}{\Delta\omega}\right)^2 \left(ch \frac{\Delta\omega}{2kT} - 1\right) \left[\sum_{j=1}^{m-1} j^2 f_j \; chj \frac{\Delta\omega}{2kT}\right]$$

$$+ 2 \frac{2\Delta\omega^2}{N} \left(\frac{2kT}{\Delta\omega}\right)^2 \left[sh \frac{\Delta\omega}{2kT} - 2 \left(\frac{2kT}{\Delta\omega}\right) \left(ch \frac{\Delta\omega}{2kT} - 1\right)\right] \left[\sum_{j=1}^{m-1} \rho_j\right]$$

$$+ \frac{2\Delta\omega^3}{N} \left(\frac{2kT}{\Delta\omega}\right)^2 \left[ch \frac{\Delta\omega}{2kT} - 4\left(\frac{2kT}{\Delta\omega}\right) sh \frac{\Delta\omega}{2kT} + 6\left(\frac{2kT}{\Delta\omega}\right)^2 \left(ch \frac{\Delta\omega}{2kT} - 1\right)\right]$$

$$\times \left[\frac{1}{2} f_0 + \sum_{j=1}^{m-1} f_j \; chj \frac{\Delta\omega}{2kT}\right] \quad . \qquad (10)$$

Differentiating once again, we have:

$$a_3 = \int d\omega\, \rho(\omega)\, \omega^2$$

$$= \frac{2\Delta\omega^3}{N} \left(\frac{2kT}{\Delta\omega}\right)^2 \left(ch \frac{\Delta\omega}{2kT} - 1\right) \left[\sum_{j=1}^{m-1} j^2 \rho_j\right]$$

$$+ 3 \frac{2\Delta\omega^4}{N} \left(\frac{2kT}{\Delta\omega}\right)^2 \left[sh \frac{\Delta\omega}{2kT} - 2 \left(\frac{2kT}{\Delta\omega}\right) \left(ch \frac{\Delta\omega}{2kT} - 1\right)\right] \left[\sum_{j=1}^{m-1} j^2 f_j \; chj \frac{\Delta\omega}{2kT}\right]$$

$$+ 3 \frac{2\Delta\omega^3}{N} \left(\frac{2kT}{\Delta\omega}\right)^2 \left[ch \frac{\Delta\omega}{2kT} - 4\left(\frac{2kT}{\Delta\omega}\right) sh \frac{\Delta\omega}{2kT} + 6\left(\frac{2kT}{\Delta\omega}\right)^2 \left(ch \frac{\Delta\omega}{2kT} - 1\right)\right]$$

$$\times \left[\sum_{j=1}^{m-1} \rho_j\right] + \frac{2\Delta\omega^4}{N} \left(\frac{2kT}{\Delta\omega}\right)^2 \left[sh \frac{\Delta\omega}{2kT} - 6\left(\frac{2kT}{\Delta\omega}\right) ch \frac{\Delta\omega}{2kT} + 18 \left(\frac{2kT}{\Delta\omega}\right)^2 sh \frac{\Delta\omega}{2kT}\right.$$

$$\left. - 24 \left(\frac{2kT}{\Delta\omega}\right)^3 \left(ch \frac{\Delta\omega}{2kT} - 1\right)\right] \left[\frac{1}{2} f_0 + \sum_{j=1}^{m-1} f_j \; ch\, j \frac{\Delta\omega}{2kT}\right] \quad . \qquad (11)$$

In these expressions the first term is dominant. Evaluating other coefficients in front of Σ symbols, we gain accuracy expressing the needed parameters in power series of the small constant $\Delta\omega/2kT$.

At this stage we have computed $g(0)$, a_2, a_3, $f_j^{(1)}$, and the scaling factor. For graphite $g^{(0)}$, a_2, a_3, and $f_j^{(1)}$ are calculated separately for perpendicular vibrations using ρ_1, and for vibrations in the planes using ρ_2. Then, for every set of directions, ℓ, the appropriate quantities are found by interpolating linearly with ℓ^2 as described in Appendix C. Finally, for each ℓ the calculations proceed as is described in Chapters III, IV, and V.

III. THE MULTIPHONON EXPANSION

The multiphonon expansion of Eq. (2) is obtained by expanding $\exp \mu\gamma G(t)$ in a power series.

$$\sigma(E \rightarrow E', \theta) = (\sigma_b/8\pi^2)(E'/E)^{1/2} \exp \{[(E - E')/2kT] - \mu\gamma g(0)\}$$

$$\int_{-\infty}^{\infty} \exp i(E - E')t \, dt \sum_{n=0}^{\infty} \frac{(\mu\gamma)^n}{n!} [G(t)]^n \tag{12}$$

Using Eq. (6), with the understanding that $f_{-j} = f_j$, we can express

$$[G(t)]^n = \left(\frac{2 \sin\Delta\omega t/2}{\Delta\omega t}\right)^{2n} \left[\sum_{j=-m+1}^{m-1} f_j^{(1)} \exp ij\Delta\omega t\right]^n \tag{13}$$

as a product of two functions. The first function is independent of the specifications of the problem and has a Fourier transform which is an even function of the argument; this is nonvanishing only for argument values smaller than $n\Delta\omega$. In Appendix A we have computed a table of transform values for integral multiples of $\Delta\omega$:

$$\frac{\Delta\omega}{2\pi} \int_{-\infty}^{\infty} \left(\frac{2 \sin\Delta\omega t/2}{\Delta\omega t}\right)^{2n} \exp\left(-i \frac{\Delta\omega t}{2} 2\nu\right) dt = c_\nu^{(n)} \tag{14}$$

The second factor of Eq. (13) is a weighted sum of exponentials. By means of the abbreviation

$$\left[\sum_{j=-m+1}^{m-1} f_j^{(1)} \exp(ij\Delta\omega t)\right]^n = \sum_{j=-n(m-1)}^{n(m-1)} F_j^{(n)} \exp(ij\Delta\omega t) \quad , \qquad (15)$$

we find weighting factors $F_j^{(n)}$ by an iterative procedure:

$$F_j^{(n)} = \sum_{i=-m+1}^{m-1} f_i^{(1)} F_{j-i}^{(n-1)} \quad \text{for} \quad 0 \leq j \leq n(m-1), \ldots \qquad (16)$$

where it is understood that

$$F_{-j}^{(n)} = F_j^{(n)} \text{ and } F_j^{(n)} = 0 \text{ for } |j| > n(m-1) \quad .$$

Now substituting Eq. (15) into Eq. (13) and using Eq. (14), we obtain easily the Fourier transform of $[G(t)]^n$:

$$\frac{\Delta\omega}{\pi}\int_0^\infty dt \cos j\Delta\omega t \, [G(t)]^n = \sum_{\nu=-n+1}^{n-1} c_\nu^{(n)} F_{j-\nu}^{(n)} = f_j^{(n)} \quad , \qquad (17)$$

for $0 \leq j \leq n\ m-1$. Here again it will be understood that

$$f_{-j}^{(n)} = f_j^{(n)} \text{ and } f_j^{(n)} = 0 \text{ for } |j| \geq n\ m \quad .$$

Thus, the multiphonon contributions are determined using Eqs. (16) and (17).

This calculation of multiphonon contributions by means of Eqs. (16) and (17) is based on the assumption that f can be represented as weighted sum of an elementary function displaced repeatedly by a constant interval. The coefficients $c_\nu^{(n)}$ have been evaluated by assuming that this elementary function is rooflike. If Dirac's δ-function was chosen for the elementary function, the expressions for g(0), N, and a_2 would be much simplified, and Eq. (17) would be unnecessary. Only some simple modifications of present Eqs. (7), (8), (10), (11), and (14) would be needed if f was approximated by a step function.

IV. CALCULATIONS OF DIFFERENTIAL SCATTERING CROSS SECTION AND SCATTERING KERNEL

If E and E' are integral multiples of $\Delta\omega$:

$$E = i\Delta\omega; \quad E' = i'\Delta\omega \quad ,$$

the inelastic-scattering cross section may be obtained substituting Eq. (17) into Eq. (12):

$$\sigma(E = i\Delta\omega \rightarrow E' = i'\Delta\omega, \theta) = (\sigma_b/4\pi\Delta\omega)(i'/i)^{1/2}\{\exp[(i-i')\frac{\Delta\omega}{2kT} - \mu\gamma g(0)]\}\left[\sum_{n=1}^{\infty}\frac{1}{n!}(\mu\gamma)^n f^{(n)}_{(i-i')}\right] \qquad (18)$$

The leading term in Eq. (12) for $n = 0$ is a Dirac δ-function and represents purely elastic cross section:

$$\sigma_{el}(E = i\Delta\omega \rightarrow E' = E, \theta) = (\sigma_b/4\pi)\exp[-2\mu g(0)\Delta\omega\, i(1-\cos\theta)] \ . \qquad (19)$$

Since contributions of only 25 phonons have been considered in evaluating the sum of Eq. (18), we assume that remaining terms a_{26}, a_{27}, . . . decrease in geometric progression, and to the sum of 25 terms we add the value of estimated remainder:

$$R = \frac{a_{25}^2}{a_{24} - a_{25}} \quad ,$$

if it is smaller than 10% of the sum. Otherwise, convergence is considered unsatisfactory. Actually, the remaining terms decrease somewhat faster than in geometric progression, and values obtained are slight overestimates.

Instead of the differential scattering cross section, we may evaluate the scattering kernel S.[7] This is a function of energy and momentum change, and is connected with the differential scattering cross section by

$$\sigma(E \rightarrow E', \theta) = S(\sigma_b/4\pi)(E'/E)^{1/2}(kT)^{-1}\cdot\exp[(E - E')/2kT] \quad .$$

Using Eq. (18) we see that

$$S = \frac{kT}{\Delta\omega}\exp[-\mu\gamma g(0)]\sum_{n=1}^{\infty}\frac{(\mu\gamma)^n}{n!}f^{(n)}_{(E-E')/\Delta\omega} \quad . \qquad (20)$$

And it can be computed easily for any change of momentum and energy change in integer multiples of $\Delta\omega$. Egelstaff[7] prefers to consider S as a function of two dimensionless parameters: one proportional to the change of momentum, squared,

$$\alpha = \mu\gamma/kT \quad ,$$

another proportional to the change in energy:

$$\beta = |E - E'|/kT.$$

Thus our calculation may be used to evaluate S for any given α and for any sequence of values β, till Eq. (20) stops converging according to our criterion.

Quite often for evaluation of the cross section the Placzek[8] expansion is used. It consists of expanding $\exp\{\mu\gamma[g(t) - g(0)]\}$ in power series of μ and performing the Fourier transform term by term. This expansion has been found very convenient for evaluation of the total cross section. We can understand that this should be so by keeping γ constant and integrating over all real values of energy change ϵ. Then

$$\int d\epsilon \int (\exp i\epsilon t) \{\exp \mu\gamma[g(t) - g(0)]\} dt = 2\pi \quad ,$$

and we need only the first term of power series in $\mu (n = 0)$ to evaluate this integral. Similarly, if we again (incorrectly) let ϵ assume all positive and negative values, we need only $(n + 1)$ terms to evaluate the n-th moment:

$$\int \epsilon^n d\epsilon \int (\exp i\epsilon t) \{\exp[\mu\gamma(g(t) - g(0))]\} dt \quad .$$

However, the Placzek expansion converges poorly for purely elastic cross sections:

$$\int (\exp i\epsilon t) \{\exp[-\mu\gamma g(0)]\} dt \quad ,$$

and therefore converges poorly for purely inelastic cross section. Indeed, if one uses only a number of terms of order $\mu\gamma\, g(0)$ (when it is large), either the elastic or total inelastic cross section becomes negative. Since here we are interested in the value of the cross section for a specified energy change, we have preferred multiphonon expansion with considerably better prospects for convergence as seen in the Appendix B.

V. CALCULATION OF MULTIGROUP INELASTIC MATRICES AND TRANSPORT CROSS SECTIONS

To obtain the multigroup inelastic matrices and transport cross sections, we perform the integration over direction of scattering, θ, analytically. Either the multiphonon expansion is used if it converges satisfactorily, or an asymptotic expression is used. Integration over final energies and averaging over initial energies is performed numerically.

A. Calculation by Multiphonon Expansion

Integrating Eq. (18) over the angle of scattering, we obtain

$$\sigma(i\Delta\omega \rightarrow i'\Delta\omega) = [\sigma_b/4\mu g(0)(\Delta\omega)^2 i]\exp(i-i')\Delta\omega/2kT \sum_{n=1}^{\infty}[g(0)]^{-n} f^{(n)}_{(i-i')}$$

$$\Big(\Big\{\exp[-\mu g(0)\Delta\omega(\sqrt{i}-\sqrt{i'})^2]\Big\}\Big\{1+\frac{1}{1!}\mu g(0)\Delta\omega(\sqrt{i}-\sqrt{i'})^2+\ldots+\frac{1}{n!}[\mu g(0)\Delta\omega(\sqrt{i}-\sqrt{i'})^2]^n\Big\}$$

$$-\Big\{\exp[-\mu g(0)\Delta\omega(\sqrt{i}+\sqrt{i'})^2]\Big\}\Big\{1+\frac{1}{1!}\mu g(0)\Delta\omega(\sqrt{i}-\sqrt{i'})^2+\ldots+\frac{1}{n!}[\mu g(0)\Delta\omega(\sqrt{i}+\sqrt{i'})^2]^n\Big\}\Big). \tag{21}$$

Similarly, integration over θ of the purely elastic cross section, Eq. (19), gives

$$\sigma_{el}(i\Delta\omega) = [\sigma_b/4\mu g(0)\Delta\omega i]\{1-\exp[-4\mu g(0)\Delta\omega i]\} \quad . \tag{22}$$

We evaluate Eq. (21) using 25 terms and estimate the remainder by means of the assumption that neglected terms decrease in geometric progression as in Chapter IV. If the remainder turns out to large, we switch to the asymptotic formula of section B below. As seen in Appendix B, the multiphonon expansion is expected to be good even at very high energies if the energy change is not large and a sufficient number of phonons has been used; $(25=)\ n_{max} \gtrsim 4a_2 g(0)$.

In this part we evaluate also the transport cross section. We define the contribution of inelastic scattering to the transport cross section as

$$\sigma''_{tr}(E) = \int dE'\,\sigma_{tr}(E\rightarrow E') = \int dE' \int \sigma(E\rightarrow E',\theta)\,(1-\cos\theta)\,2\pi d\cos\theta \quad .$$

And we obtain $\sigma_{tr}(E\rightarrow E')$ using Eq. (18):

$$\sigma_{tr}(E\rightarrow E') = [\sigma_b/8\mu^2 g(0)^2\Delta\omega^3 i^{3/2} i'^{1/2}]\exp[(i-i')\Delta\omega/2kT]$$

$$\sum_{n=1}^{\infty}\Big\{n[g(0)]^{-n+1} f^{(n-1)}_{(i-i')} - \mu g(0)\Delta\omega(\sqrt{i}-\sqrt{i'})^2\cdot[g(0)]^{-n} f^{(n)}_{(i-i')}\Big\}$$

$$\Big(\Big\{\exp[-\mu g(0)\Delta\omega(\sqrt{i}-\sqrt{i'})^2]\Big\}\Big\{1+\frac{1}{1!}\mu g(0)\Delta\omega(\sqrt{i}-\sqrt{i'})^2+\ldots+\frac{1}{n!}[\mu g(0)\Delta\omega(\sqrt{i}-\sqrt{i'})^2]^n\Big\}$$

$$-\Big\{\exp[-\mu g(0)\Delta\omega(\sqrt{i}+\sqrt{i'})^2]\Big\}\Big\{1+\frac{1}{1!}\mu g(0)\Delta\omega(\sqrt{i}+\sqrt{i'})^2+\ldots+\frac{1}{n!}[\mu g(0)\Delta\omega(\sqrt{i}+\sqrt{i'})^2]^n\Big\}\Big) \quad , \tag{23}$$

where it is understood that $f^{(0)}_{(i-i')} = 0$. Since evaluation of Eq. (23) may be performed at the same time as evaluation of Eq. (21), not much additional computation is required. Also, the computation may be arranged so that evaluation of the long sum is done only for $i > i'$ and the results used for upscattering, $i' > i$. Later integration over final energies of the transport cross section is described. To this sum we add also the contribution of purely elastic scattering:

$$\sigma_{tr,el} = [\sigma_b/8(\mu g(0)\Delta\omega i)^2] \cdot \{1 - [1 + 4\mu g(0)\Delta\omega i] \exp[-4\mu g(0)\Delta\omega i]\} \tag{24}$$

B. Calculation by an Asymptotic Expression

When energy change and initial energy are large, the multiphonon expansion fails to converge, and we use an asymptotic expression to calculate $\sigma(E \to E')$. The asymptotic expression can be obtained in a closed form by integrating Eq. (2) over the directions of scattering:

$$\sigma(E \to E') = (\sigma_b/8\pi\mu E) \int_{-\infty}^{+\infty} \left\{\exp\left[- i(E - E')\left(t + \frac{i}{2kT}\right)\right]\right\} \frac{\exp\{\mu(\sqrt{E} + \sqrt{E'})^2 [G(t) - g(0)]\} - \exp\{\mu(\sqrt{E} - \sqrt{E'})^2 [G(t) - g(0)]\}}{G(t) - g(0)} dt \; . \tag{26}$$

We know that for very large energies the cross section approaches the cross section of a free atom. The downscattering cross section is appreciable only when $E - E' \lesssim (\sqrt{E} + \sqrt{E'})^2$ and very nearly vanishes for larger energy losses. Thus, it seems that the behavior of the cross section in the drop-off region is most important when energies are not so very high. In this region the integral of the first term is very much larger than the integral of the second term ($\mu < 1$), as one can see clearly by trying to apply the method of steepest descent. To obtain the first term we expand G(t) in Taylor series about the point $t = -i/2kT$:

$$G(t) = g(0) + i\left(t + \frac{i}{2kT}\right) - \frac{1}{2!} a_2 \left(t + \frac{i}{2kT}\right)^2 - \frac{i}{3!} a_3 \left(t + \frac{i}{2kT}\right)^3 + \frac{1}{4!} a_4 \left(t + \frac{i}{2kT}\right)^4 + \ldots \; , \tag{27}$$

where

$$g(0) = \int d\omega \rho(\omega) \left(\coth \frac{\omega}{2kT}\right) \frac{1}{\omega} \qquad a_2 = \int d\omega \rho(\omega) \left(\coth \frac{\omega}{2kT}\right) \omega$$

$$1 = \int d\omega \rho(\omega) \qquad a_3 = \int d\omega \rho(\omega) \; \omega^2$$

are constants evaluated in Chapter II.

Now, if we substitute Eq. (27) into the integrand and introduce a new variable of integration,

$$x = \sqrt{\frac{1}{2}\,\mu(\sqrt{E} + \sqrt{E'})^2\, a_2}\,\left(t + \frac{i}{2kT}\right),$$

we see that the integral in Eq. (26) is very nearly equal to

$$\int dt \frac{\exp\left\{-i(E - E')\left(t + \frac{i}{2kT}\right) + \mu(\sqrt{E} + \sqrt{E'})^2\,[G(t) - g(0)]\right\}}{G(t) - g(0)} =$$

$$\int \left\{ix - \sqrt{\frac{a_2}{2\mu(\sqrt{E} + \sqrt{E'})^2}}\, x^2 - \frac{a_2}{2\mu(\sqrt{E} + \sqrt{E'})^2}\,\frac{2}{3}\, i\,\frac{a_3}{a_2^2}\, x^3 + \ldots\right\}^{-1}$$

$$\cdot \exp\left\{-\, 2\,\frac{\sqrt{E} - \sqrt{E'} - \mu(\sqrt{E} + \sqrt{E'})}{\sqrt{2\mu a_2}}\, ix - x^2 - \sqrt{\frac{a_2}{2\mu(\sqrt{E} + \sqrt{E'})^2}}\,\frac{2}{3}\, i\,\frac{a_3}{a_2^2}\, x^3\right.$$

$$\left. + \frac{a_2}{2\mu(\sqrt{E} + \sqrt{E'})^2}\,\frac{1}{3}\,\frac{a_4}{a_2^3}\, x^4 + \ldots\right\} dx \quad .$$

If we assume now that

$$\frac{\sqrt{E} - \sqrt{E'} - \mu(\sqrt{E} + \sqrt{E'})}{\sqrt{2\mu a_2}} = \eta \tag{28}$$

is finite, while $2\mu(\sqrt{E} + \sqrt{E'})^2/a_2 \to \infty$, and expand the integrand in power series, we find that leading term reduces to a standard form.(9) The value of the integral can be obtained easily from the integral

$$\int_{-\infty}^{\infty} dx \exp\,[-2i\eta\, x - x^2] = \sqrt{\pi}\exp\,(-\eta^2)$$

by integration with respect to the parameter η. The constant of integration is determined from consideration of the value of the integral for large positive η. Then the method of steepest descent shows that the integral vanishes when the path of integration is below the pole. We obtain, thus,

$$\int \frac{dx}{ix} \exp\,[-2i\eta x - x^2] = \pi(1 - \mathrm{erf}\,\eta) \quad . \tag{29}$$

Integration of succeeding terms is elementary. Collecting the terms, we obtain for $E > E'$,

$$\sigma(E \rightarrow E') = (\sigma_b/8\mu E)\left\{1 - \operatorname{erf}\eta - \sqrt{\frac{1}{\pi}}\sqrt{\frac{a_2}{2\mu(\sqrt{E} + \sqrt{E'})^2}}\, e^{-\eta^2} \cdot \left[1 + \frac{a_3}{3a_2^2} - \frac{2a_3}{3a_2^2}\eta^2\right]\right.$$

$$+ \sqrt{\frac{1}{\pi}}\left(\frac{a_2}{2\mu(\sqrt{E} + \sqrt{E'})^2}\right) e^{-\eta^2}\left[\left(1 - \frac{2}{3}\frac{a_3}{a_2^2} - \frac{1}{2}\frac{a_4}{a_2^3} + \frac{5}{6}\frac{a_3^2}{a_2^4}\right)\eta\right.$$

$$\left.\left. + \left(\frac{1}{3}\frac{a_4}{a_2^3} - \frac{10}{9}\frac{a_3^2}{a_2^4}\right)\eta^3 + \frac{2}{9}\frac{a_3^2}{a_2^4}\eta^5\right] + \ldots\right\} \quad . \qquad (30)$$

Equation (30) is considered unsatisfactory and not usable when η becomes so large and positive that the second term is larger in absolute value than the first. Neglected values are considered vanishingly small. In practice, we have neglected the last term for simplicity, and we have used Eq. (30) only for downscattering. Upscattering has been obtained from Eq. (30) by means of detailed balance:

$$\sigma(E' \rightarrow E) = \sigma(E \rightarrow E')\frac{E}{E'}\exp\left[-(E - E')/kT\right] \quad .$$

For large energies $\sigma_{tr}(E \rightarrow E')$ can be calculated in a very similar way. Direct integration using Eq. (2) for $\sigma(E \rightarrow E', \theta)$ gives

$$\sigma_{tr}(E \rightarrow E') = \int \sigma(E \rightarrow E', \theta)(1 - \cos\theta)\, 2\pi d\cos\theta = (\sigma_b/8\pi\mu E)\int \frac{dt \exp\left[-i(E - E')\left(t + \frac{i}{2kT}\right)\right]}{G(t) - g(0)}$$

$$\cdot \left\{\left[2 - \frac{1}{2\mu\sqrt{E E'}\,[G(t) - g(0)]}\right]\exp\left[\mu(\sqrt{E} + \sqrt{E'})^2(G(t) - g(0))\right]\right.$$

$$\left. - \frac{1}{2\mu\sqrt{E E'}\,[G(t) - g(0)]}\exp\left[\mu(\sqrt{E} - \sqrt{E'})^2(G(t) - g(0))\right]\right\} \quad .$$

Here again the integral of the second term is very small, and we can evaluate the first term by the same procedure as previously. An additional singular integral is encountered and is evaluated by integrating Eq. (29) with respect to the parameter η:

$$\int \frac{dx}{x^2}\exp(-2i\eta x - x^2) = 2\pi\left\{\eta[1 - \operatorname{erf}\eta] - \frac{1}{\sqrt{\pi}}\exp(-\eta^2)\right\} \quad .$$

The result of this integration is a sum of two series. The first one is just twice the series of Eq. (30), representing predominantly backward scattering for $E - E' \gtrsim \mu(\sqrt{E} + \sqrt{E'})^2$. The second series represents the deviation from backward scattering and tends to cancel the value of the first series when $E' \rightarrow E$ and scattering becomes nearly forward. Thus, simultaneously with Eq. (30), we may evaluate also

$$\sigma_{tr}(E \rightarrow E') = (\sigma_b/4\mu E)\Bigg(1 - \mathrm{erf}\,\eta - \sqrt{\frac{a_2}{2\pi\mu(\sqrt{E}+\sqrt{E'})^2}}\; e^{-\eta^2}\left[1 + \frac{a_3}{3a_2^2} - \frac{2a_3}{3a_2^2}\eta^2\right] + \ldots$$

$$- \sqrt{\frac{(\sqrt{E}+\sqrt{E'})^2 a_2}{8\mu E E'}}\Bigg\{\eta(\mathrm{erf}\,\eta - 1) + \frac{1}{\sqrt{\pi}}e^{-\eta^2} + \sqrt{\frac{a_2}{2\pi\mu(\sqrt{E}+\sqrt{E'})^2}}$$

$$\left[\sqrt{\pi}\,(\mathrm{erf}\,\eta - 1) + \frac{a_3}{3a_2^2}\,\eta\, e^{-\eta^2}\right] + \ldots\Bigg\}\Bigg) \tag{31}$$

C. Integration over Final Energies and Averaging over Initial Energies

To develop multigroup scattering cross sections, we numerically integrate over final energies E' and average over initial energies E by means of Simpson's rule. Thus, in every energy group there has to be an even number of elementary intervals. At first, integrations over E' are performed for every value of E. The results of these integrations, for every value of E, are inelastic cross sections for every energy group and scattering contribution to the transport cross section σ^{i}_{tr}. To obtain the latter, we integrate over E' of Eqs. (23) or (31) and add the elastic contribution Eq. (24). To economize the calculations, for every pair of values, E and E', the evaluation of inelastic cross section and transport cross section for up- and down-scattering is done at the same time, and the results are multiplied with appropriate coefficients and accumulated. Integration begins with $E = E' = \Delta\omega$. Then E is kept the same and E' increases till maximum value is reached or the asymptotic formula Eq. (30) fails and the cross section is considered negligible for larger values of E'. At the end of this step, we have a complete set of cross sections for $E = \Delta\omega$. In the next step, we start with $E = E' = 2\Delta\omega$ and end up with a complete set of cross sections for $E = 2\Delta\omega$. We continue in this way, always starting evaluation on the diagonal, till the maximum value of E is reached.

After finishing integration over E', with the first value of ℓ, we pick up the next value of ℓ, as explained in Appendix C. Interpolation takes place for new values of contstants $f_j^{(1)}$, g(0), a_2, and a_3; we repeat the calculations of Chapter V sections A and B, and integrate over final energy E'. The results of this integration are immediately multiplied with appropriate weighting factor for each ℓ and immediately added to the previous values.

Final results may be used to obtain standard multigroup cross-section sets for reactor regions having various flux shapes. In this, last, part of the procedure, the complete transport cross section:

$$\sigma_{tr} = \sigma'_{tr} + \sigma_c$$

is calculated. The capture cross section is assumed to be proportional to $E^{-1/2}$, and its value for 2,200 m/sec neutrons is assumed as given. Then σ_c, the diffusion coefficient $(1/3\sigma_{tr})$, and the inelastic scattering cross sections for every group of final energy E' are averaged in every group of initial energy E, weighting each with a chosen flux. So far three forms of the flux have been chosen in each group:

1. Hardened Maxwellian:

$$\phi \propto (CE/kT) \exp(-CE/kT),$$

where C is a number somewhat larger than one. This form is convenient for groups of lower energy.

2. The flux is assumed to be proportional to the N-th power of energy:

$$\phi \propto (E/kT)^N \quad .$$

3. The flux is given numerically for every value of energy within the group, for which cross sections are calculated.

Calculation of the cross sections for every couple of E and E' that can be expressed in integral multiples of $\Delta\omega$ may be too time consuming and, indeed, unnecessary if energies are large. From the leading term in Eq.(30) we see that the extent of the drop-off region at large energies is proportional to the square root of the initial energy. Thus, at high energies, the elementary interval of integration may be allowed to increase proportionally to the square root of energy. The increase, however, must be such that the number of elementary integration intervals in every group is even.

Appendix A

EVALUATION OF $c_\nu^{(n)}$

After a change of integration variable Eq. (14) can be written as

$$c_\nu^{(n)} = \frac{1}{\pi} \int_{-\infty}^{+\infty} \left(\frac{\sin x}{x}\right)^{2n} \exp(-2i\nu x)\, dx \quad . \tag{A-1}$$

This integral can be evaluated exactly by changing slightly the path of integration to avoid x = 0, expanding $(\sin x)^{2n}$ in power series of exp ix and finding the residue of each term. In this way we obtain[10]

$$c_\nu^{(n)} = \frac{1}{(2n-1)!} \left[(n-\nu)^{2n-1} - \binom{2n}{1}(n-\nu-1)^{2n-1} + \binom{2n}{2}(n-\nu-2)^{2n-1} - \binom{2n}{3}(n-\nu-3)^{2n-1} + \ldots + (-1)^{n-\nu-1}\binom{2n}{n-\nu-1}(1)^{2n-1}\right] . \tag{A-2}$$

We see also while deriving this formula that $c_\nu^{(n)} = 0$ for $|\nu| \geq n$. Further, we can show simply, starting with Eq. (A-1) and summing over all integer values of ν, that

$$c_0^{(n)} + 2 \sum_{\nu=1}^{n-1} c_\nu^{(n)} = 1 \quad . \tag{A-3}$$

Table A-1 contains values of $c_\nu^{(n)}$ derived by direct evaluation of Eq. (A-2). All values contained therein satisfy Eq. (A-3) coincident with 8-place accuracy. For $1 \leq n \leq 11$, values of $(2n-1)!\, c_\nu^{(n)}$ were found exactly. By this time, however, the calculations were involving numbers as high in order of magnitude as 10^{22}. The ensuing calculations ($12 \leq n \leq 25$) were continued with the intention of guaranteeing only 8-place accuracy.

n	ν	Digits Lost
5	0	1
10	0	3
15	0	4
20	0	6
25	0	8
25	5	4
25	10	1
25	15	1
25	20	0

Since the series in Eq. (A-2) is alternating in sign and since the binomial coefficients increase with successive terms, there was a tendency toward cancellation dependent upon the values of n and ν. For a given value of n this tendency reduced with increasing values of ν. It increased, however, with increasing values of n. The adjoining tabulation is intended to exemplify this effect. The third column designates the number of digits lost from the largest term in the respective series.

Table A-1

COEFFICIENTS OF $c_\nu^{(n)}$

n	ν	$c_\nu^{(n)} \times 10^q$	q
1	0	1.000 0000	0
2	0	6.666 6667	1
	1	1.666 6667	1
3	0	5.500 0000	1
	1	2.166 6667	1
	2	8.333 3333	3
4	0	4.793 6507	1
	1	2.363 0952	1
	2	2.380 9523	2
	3	1.984 1269	4
5	0	4.304 1776	1
	1	2.431 4925	1
	2	4.025 5731	2
	3	1.383 3774	3
	4	2.755 7319	6
6	0	3.939 2556	1
	1	2.439 6028	1
	2	5.520 2020	2
	3	3.823 8786	3
	4	5.100 6092	5
	5	2.505 2108	8
7	0	3.653 7086	1
	1	2.417 8841	1
	2	6.797 4968	2
	3	7.312 2366	3
	4	2.376 2984	4
	5	1.313 3086	6
	6	1.605 9043	10
8	0	3.422 4025	1
	1	2.381 2319	1
	2	7.859 5252	2
	3	1.150 2274	2
	4	6.485 4898	4
	5	1.057 2004	5
	6	2.504 5990	8
	7	7.647 1635	13
9	0	3.230 0939	1
	1	2.337 3674	1
	2	8.731 1640	2
	3	1.607 3921	2
	4	1.330 8125	3
	5	4.182 1548	5
	6	3.564 3941	7
	7	3.684 5271	10
	8	2.811 4572	15
10	0	3.066 9310	1
	1	2.290 4565	1
	2	9.441 9298	2
	3	2.078 1149	2

n	ν	$c_\nu^{(n)} \times 10^q$	q
10	4	2.291 8669	3
	5	1.134 1319	4
	6	2.069 3993	6
	7	9.468 3295	9
	8	4.309 8160	12
	9	8.220 6352	18
11	0	2.926 2269	1
	1	2.242 8008	1
	2	1.001 9429	1
	3	2.545 1983	2
	4	3.511 1077	3
	5	2.436 1241	4
	6	7.486 5178	6
	7	8.158 7910	8
	8	2.038 3683	10
	9	4.104 7002	14
	10	1.957 2941	20
12	0	2.803 2619	1
	1	2.195 6830	1
	2	1.048 7418	1
	3	2.997 4159	2
	4	4.952 3095	3
	5	4.473 1411	4
	6	2.022 5084	5
	7	3.967 9867	7
	8	2.634 6734	9
	9	3.633 8306	12
	10	3.244 8470	16
	11	3.868 1701	23
13	0	2.694 5977	1
	1	2.149 8081	1
	2	1.086 5617	1
	3	3.427 9354	2
	4	6.573 0455	3
	5	7.344 9505	4
	6	4.485 9427	5
	7	1.356 7864	6
	8	1.734 3915	8
	9	7.116 6678	11
	10	5.456 8031	14
	11	2.163 2358	18
	12	6.446 9503	26
14	0	2.597 6616	1
	1	2.105 5470	1
	2	1.117 0135	1
	3	3.833 0006	2
	4	8.330 7168	3
	5	1.110 0319	3
	6	8.639 5093	5
	7	3.656 2192	6
	8	7.545 8578	8
	9	6.381 8009	10
	10	1.634 7825	12
	11	6.999 6612	16

n	ν	$c_\nu^{(n)} \times 10^q$	q
14	12	1.232 6137	20
	13	9.183 6902	29
15	0	2.510 4851	1
	1	2.063 0735	1
	2	1.141 4048	1
	3	4.210 9370	2
	4	1.018 5923	2
	5	1.574 3122	3
	6	1.497 4195	4
	7	8.304 3229	6
	8	2.481 8502	7
	9	3.549 3851	9
	10	2.009 1861	11
	11	3.236 5913	14
	12	7.760 2485	18
	13	6.071 9897	23
	14	1.130 9962	31
16	0	2.431 5338	1
	1	2.022 4454	1
	2	1.160 7955	1
	3	4.561 4397	2
	4	1.210 4051	2
	5	2.124 1798	3
	6	2.392 9595	4
	7	1.659 4236	5
	8	6.676 1530	7
	9	1.430 3578	8
	10	1.434 6824	10
	11	5.483 9277	13
	12	5.584 3506	16
	13	7.510 8451	20
	14	2.611 6085	25
	15	1.216 1250	34
17	0	2.359 5908	1
	1	1.983 6513	1
	2	1.176 0460	1
	3	4.885 0747	2
	4	1.405 5748	2
	5	2.753 9276	3
	6	3.586 6647	4
	7	3.003 3305	5
	8	1.544 3189	6
	9	4.572 7586	8
	10	7.108 2216	10
	11	5.048 2095	12
	12	1.311 8221	14
	13	8.475 7895	18
	14	6.401 6643	22
	15	9.892 4570	28
	16	1.151 6335	38
18	0	2.293 6771	1
	1	1.946 6400	1
	2	1.187 8567	1
	3	5.182 9380	2

n	ν	$c_\nu^{(n)} \times 10^q$	q
18	4	1.601 6790	2
	5	3.456 1876	3
	6	5.105 4171	4
	7	5.025 2908	5
	8	3.177 8930	6
	9	1.228 4490	7
	10	2.708 7243	9
	11	3.084 8030	11
	12	1.562 9703	13
	13	2.775 4497	16
	14	1.140 7854	19
	15	4.841 7295	24
	16	3.325 1955	30
	17	9.677 5929	41
19	0	2.232 9949	1
	1	1.911 3383	1
	2	1.196 8001	1
	3	5.456 4285	2
	4	1.796 7629	2
	5	4.222 6622	3
	6	6.966 6316	4
	7	7.891 4769	5
	8	5.958 7571	6
	9	2.883 1681	7
	10	8.474 0266	9
	11	1.404 9088	10
	12	1.181 4668	12
	13	4.296 4269	15
	14	5.234 1896	18
	15	1.371 1634	21
	16	3.271 4818	26
	17	9.985 5722	33
	18	7.265 4602	44
20	0	2.176 8871	1
	1	1.877 6616	1
	2	1.203 3457	1
	3	5.707 0915	2
	4	1.989 2809	2
	5	5.044 6835	3
	6	9.178 7613	4
	7	1.176 2589	4
	8	1.036 1473	5
	9	6.076 5838	7
	10	2.274 1955	8
	11	5.130 2689	10
	12	6.446 3349	12
	13	4.029 0598	14
	14	1.056 6743	16
	15	8.858 2888	20
	16	1.480 8858	23
	17	1.986 7421	28
	18	2.695 1612	35
	19	4.902 4697	47
21	0	2.124 8065	1
	1	1.845 5211	1

n	ν	$c_\nu^{(n)} \times 10^q$	q
21	2	1.207 8808	1
	3	5.936 5216	2
	4	2.178 0373	2
	5	5.913 6241	3
	6	1.174 2268	3
	7	1.678 6922	4
	8	1.693 1210	5
	9	1.173 4829	6
	10	5.400 8861	8
	11	1.577 7967	9
	12	2.753 5017	11
	13	2.639 7162	13
	14	1.232 7358	15
	15	2.340 6061	18
	16	1.353 3108	21
	17	1.445 0840	25
	18	1.090 2884	30
	19	6.573 5640	38
	20	2.989 3107	50
22	0	2.076 2933	1
	1	1.814 8278	1
	2	1.210 7259	1
	3	6.146 2968	2
	4	2.362 1280	2
	5	6.821 1776	3
	6	1.465 0822	3
	7	2.309 5246	4
	8	2.626 5640	5
	9	2.108 2343	6
	10	1.161 1275	7
	11	4.230 9608	9
	12	9.722 9842	11
	13	1.321 4473	12
	14	9.719 2876	15
	15	3.406 1660	17
	16	4.696 5446	20
	17	1.876 1225	23
	18	1.280 4183	27
	19	5.433 3385	33
	20	1.455 9388	40
	21	1.655 2108	53
23	0	2.030 9579	1
	1	1.785 4951	1
	2	1.212 1472	1
	3	6.337 9400	2
	4	2.540 8901	2
	5	7.759 5416	3
	6	1.789 2568	3
	7	3.079 7509	4
	8	3.899 4517	5
	9	3.565 1334	6
	10	2.298 9024	7
	11	1.014 6704	8
	12	2.949 2901	10
	13	5.366 7858	12
	14	5.712 6175	14

n	ν	$c_\nu^{(n)} \times 10^q$	q
23	15	3.238 6105	16
	16	8.548 1443	19
	17	8.580 3055	22
	18	2.371 1955	25
	19	1.034 7610	29
	20	2.469 7009	35
	21	2.941 2906	43
	22	8.359 6509	57
24	0	1.988 4680	1
	1	1.757 4395	1
	2	1.212 3671	1
	3	6.512 8957	2
	4	2.713 8567	2
	5	8.721 5228	3
	6	2.145 1351	3
	7	3.998 1124	4
	8	5.575 9006	5
	9	5.727 3232	6
	10	4.247 5324	7
	11	2.218 2792	8
	12	7.903 5283	10
	13	1.844 3836	11
	14	2.672 6183	13
	15	2.238 8184	15
	16	9.821 6928	18
	17	1.958 2622	20
	18	1.433 7300	23
	19	2.743 7287	27
	20	7.658 1532	32
	21	1.028 0904	37
	22	5.441 7959	46
	23	3.866 6285	60
25	0	1.948 5379	1
	1	1.730 5825	1
	2	1.211 5719	1
	3	6.672 5185	2
	4	2.880 7194	2
	5	9.700 5958	3
	6	2.530 7828	3
	7	5.071 0586	4
	8	7.719 2246	5
	9	8.805 3919	6
	10	7.400 4034	7
	11	4.486 6942	8
	12	1.911 1153	9
	13	5.531 2635	11
	14	1.042 1160	12
	15	1.208 3763	14
	16	7.998 9178	17
	17	2.724 4682	19
	18	4.113 3833	22
	19	2.200 0616	25
	20	2.917 6807	29
	21	5.209 7672	34
	22	3.934 0199	40
	23	9.254 7548	49
	24	1.643 9747	63

If n is large and $c_\nu^{(n)}$ appreciable, the Central Limit Theorem can be used.[6] The values predicted by the Central Limit Theorem are obtained by the following replacement in Eq. (A-1):

$$\frac{\sin x}{x} \rightarrow \exp\left(-\frac{1}{6}x^2\right) ,$$

so that in this approximation

$$c_\nu^{(n)} \approx \frac{1}{\pi}\int_{-\infty}^{\infty} dx \exp\left(-\frac{1}{6}x^2 - 2i\nu x\right) = \sqrt{\frac{3}{\pi n}} \exp\left(-\frac{3\nu^2}{n}\right) .$$

Numerical values obtained with this approximation with n = 25 have been computed and displayed along with the correct values in Table A-II. Agreement is definitely poor for larger values of ν.

Table A-II

EVALUATION OF $c_{\nu}^{(25)} \times 10^{q}$ BY ALTERNATIVE METHODS

ν	By the Longhand Method	q	By the Theorem of Central Limits	q	By the Method of Steepest Descent	q	$-\frac{1}{2n}\left[\frac{1}{8}\frac{f_0^{IV}}{(f_0'')^2} - \frac{5}{24}\frac{(f_0''')^2}{(f_0'')^3}\right]$
0	1.949	1	1.954	1	1.949	1	0.0030
1	1.731	1	1.733	1	1.730	1	0.0030
2	1.212	1	1.209	1	1.210	1	0.0030
3	6.673	2	6.637	2	6.659	2	0.0031
4	2.881	2	2.865	2	2.883	2	0.0031
5	9.701	3	9.730	3	9.670	3	0.0031
6	2.531	3	2.599	3	2.527	3	0.0032
7	5.071	4	5.462	4	5.048	4	0.0032
8	7.719	5	9.029	5	7.745	5	0.0033
9	8.805	6	1.174	5	8.829	6	0.0033
10	7.400	7	1.201	6	7.419	7	0.0034
11	4.487	8	9.662	8	4.464	8	0.0035
12	1.911	9	6.115	9	1.902	9	0.0036
13	5.531	11	3.045	10	5.534	11	0.0037
14	1.042	12	1.192	11	1.041	12	0.0038
15	1.208	14	3.673	13	1.207	14	0.0038
16	7.999	17	8.902	15	7.965	17	0.0037
17	2.724	19	1.697	16	2.710	19	0.0035
18	4.113	22	2.545	18	4.096	22	0.0031
19	2.200	25	3.002	20	2.200	25	0.0026
20	2.918	29	2.785	22	2.914	29	0.0022
21	5.210	34	2.033	24	5.218	34	0.0018
22	3.934	40	1.167	26	3.930	40	0.0017
23	9.255	49	5.272	29	9.234	49	0.0017
24	1.644	63	1.873	31	1.645	63	0.0017

A better approximation procedure for the whole range of values ν/n would be the Method of Steepest Descent. By this method, the extremum of the function $2n \ln \frac{\sin x}{x} - 2\nu x i$ is obtained, the path of integration is shifted to pass through this maximum, and the integral is evaluated under the assumption that ν/n remains constant while n increases towards infinity. The extremum τ_0 of our function is found to lie on an imaginary axis, and its position is obtained by differentiating

$$f(\tau) = \ln \operatorname{sh} \tau - \ln \tau \quad ,$$

and, equating the result to ν/n,

$$f'(\tau_0) = \coth \tau_0 - \frac{1}{\tau_0} = \frac{\nu}{n} \quad . \qquad \text{(A-4)}$$

From this equation τ_0 was found for every value of ν/n, and $c_\nu^{(n)}$ was computed according to the formula

$$\ln c_\nu^{(n)} = 2nf_0 - \frac{1}{2}\ln n\pi f_0 + \frac{1}{2n}\left[\frac{1}{8}\frac{f_0^{IV}}{(f_0'')^2} - \frac{5}{24}\frac{(f_0''')^2}{(f_0'')^3}\right] + \ldots \quad , \text{(A-5)}$$

where the values of f and its derivatives have to be evaluated at $\tau = \tau_0$. The results of this calculation with n = 25 are also displayed in Table A-II. It is evident that this procedure gives reasonable agreement over the whole range of values of ν/n. The disagreement between these approximate values and the exact values is due, at least in part, to insufficient accuracy in the determination of τ_0 from Eq. (A-4) (four places were used most of the time). In Table A-II we have given also the value of the last term used in Eq. (A-5). One certainly should expect the fractional error in $c_\nu^{(n)}$ due to truncation of series Eq. (A-5) to be less than the last term used.

Appendix B

THE METHOD OF STEEPEST DESCENT AND CONVERGENCE OF MULTIPHONON EXPANSION

For large energy values we have used formulae based upon a Taylor series expansion of G about the point $t = -i/2kT$. This expansion gave reasonable approximation in the vicinity of $E-E' \approx \mu(\sqrt{E} + \sqrt{E'})^2$; however, the error is considerable for other values of the ratio E'/E. As we have seen in Appendix A, we can expect good accuracy for any ratio E'/E if we use an expansion of G about a variable point $t = -i\tau$ chosen to obtain the steepest descent in the integrand. Formulae obtained by this method are difficult to evaluate numerically. But they present a clear picture of the cross section at large momentum transfers, when multiphonon expansion requires many terms.

In the method of steepest descent, we use a Taylor expansion of G(t) about a variable point, $t = -i\tau$, on the imaginary axis:

$$G(t) = G + G'i(t+i\tau) - \frac{1}{2!} G''(t+i\tau)^2 - \frac{1}{3!} G'''i(t+i\tau)^3 + \frac{1}{4!} G^{iv}(t+i\tau)^4 + \ldots \quad , \qquad \text{(B-1)}$$

where coefficients

$$G^{(n)} = \frac{d^n}{d\tau^n} \int \frac{d\omega\, \rho(\omega)}{\omega \operatorname{sh} \omega/2kT} \operatorname{ch} \omega\tau$$

are all positive. To evaluate $\sigma(E \rightarrow E', \theta)$, a value of τ is chosen so that the integrand in Eq. (2) is an extremum:

$$E - E' = \mu\gamma G' \quad . \qquad \text{(B-2)}$$

Upon introducing a new variable of integration,

$$x = \sqrt{\frac{1}{2}\mu\gamma G''}\,(t+i\tau)$$

and expanding the integrand in Eq. (2) in powers of $\sqrt{G''/2\mu\gamma}$, we obtain

$$\int dt \exp\left\{-(E-E')\, i\left(t + \frac{i}{2kT}\right) + \mu\gamma[G(t) - g(0)]\right\} = \sqrt{\frac{2}{\mu\gamma G''}} \int dx \exp$$

$$\left\{-\mu\gamma G'\left(\tau - \frac{1}{2kT}\right) + \mu\gamma\,[G - g(0)] - x^2 - \sqrt{\frac{G''}{2\mu\gamma}}\,\frac{2}{3}\, i\, \frac{G'''}{G''^2}\, x^3 + \left(\frac{G''}{2\mu\gamma}\right)\frac{1}{3}\,\frac{G^{iv}}{G''^3}\, x^4 + \ldots\right\}$$

$$= \sqrt{\frac{2}{\mu\gamma G''}} \exp\left\{\mu\gamma\left[-G'\left(\tau - \frac{1}{2kT}\right) + G - g(0)\right]\right\} \cdot \int dx\, e^{-x^2}$$

$$\left\{1 - \sqrt{\frac{G''}{2\mu\gamma}}\,\frac{2}{3}\, i\, \frac{G'''}{G''^2}\, x^3 + \left(\frac{G''}{2\mu\gamma}\right)\left[\frac{1}{3}\,\frac{G^{iv}}{G''^3}\, x^4 - \frac{2}{9}\,\frac{G'''^2}{G''^4}\, x^6\right] + \ldots\right\} \quad .$$

Thus, after integration, we have

$$\sigma(E \rightarrow E', \theta) = (\sigma_b/8\pi^2)(E'/E)^{1/2}(4\pi/2\mu\gamma G'')^{1/2}$$

$$\cdot \exp\left\{\mu\gamma\left[-G'\left(\tau - \frac{1}{2kT}\right) + G - g(0)\right]\right\}$$

$$\cdot \left\{1 + \frac{G''}{2\mu\gamma}\left[\frac{3}{12}\frac{G^{iv}}{G''^3} - \frac{5}{12}\frac{G'''^2}{G''^4}\right] + \ldots\right\} \quad , \qquad \text{(B-3)}$$

a convenient expression for large momentum transfers when multiphonon expansion becomes impractical.

By contemplation of Eq. (B-3) we can make a judgment on the number of phonons necessary to obtain the differential cross section. It is reasonable to expect that, when Eq. (B-3) is approximately valid, this number is roughly equal to the number of terms required in the power series expansion of exp $(\mu\gamma G)$. Thus the largest contribution is expected for $n = \mu\gamma G$. Since

$$\frac{d^2}{dn^2} \ln \frac{1}{n!} (\mu\gamma G)^n \approx -\frac{1}{\mu\gamma G} \quad ,$$

one would obtain the value of the exponential within about two per cent if one uses

$$n_{max} = (\sqrt{\mu\gamma G} + 1)^2 \quad . \qquad \text{(B-4)}$$

Actually, applying the method of steepest descent to each term of the phonon expansion we see that the "half-width" is somewhat smaller and that

$$n_{max} = \left[\sqrt{\mu\gamma G} + \sqrt{1 - (G'^2/GG'')}\right]^2 \qquad \text{(B-5)}$$

would be satisfactory. Thus, for large $\mu\gamma G$ only comparatively small number of phonons at the end of expansion contribute significantly towards the sum. The second term in Eq. (B-3) is then

$$\frac{1}{12}\frac{1}{\mu\gamma G}\frac{3G^{iv}G'' - 5G'''^2}{2G''^3} G \approx \frac{1}{12 n_{max}} \frac{3G^{iv}G'' - 5G'''^2}{2G''^3} G \quad .$$

If τ (and the ratio $|E-E'|/\mu\gamma$) is very large, this term is approximately equal to $-1/12n_{max}$, and Eq. (B-3) joins quite smoothly our expansion of n_{max}(=25) phonons. However, for smaller τ this term can be considerably larger in absolute value. In such cases, one could try to approximate every multiphonon term by a Gaussian (or modified Gaussian) distribution. And, indeed, one can demonstrate(2) that such an approximation is good for individual terms. However, the number of terms required for evaluation of $\sigma(E \rightarrow E', \theta)$

is large. And, since the Gaussian distribution depends only on the second derivative of G, it cannot be depended upon to yield correctly the second term of Eq. (B-3), which requires knowledge of higher derivatives. Thus, at present we remain with the unpleasant need to evaluate exactly many terms in multiphonon expansion in some cases (as for graphite at high temperatures) if we want to join smoothly the method of steepest descent to the multiphonon expansion.

In evaluation of $\sigma(E \rightarrow E')$ we encounter also both multiphonon expansion and an asymptotic expression. Multiphonon expansion here needs to be used also at very high initial energies if energy loss is not large. When $|E-E'|$ is fixed finite and $\mu(\sqrt{E}+\sqrt{E'})^2$ keeps increasing, we can no longer nelgect the second term in Eq. (26). (The asymptotic expansion for it does not "converge.") Indeed the appropriate procedure for such a case would be to neglect the first term, since $\mu(\sqrt{E}+\sqrt{E'})^2$ is large and $[G(t) - g(0)]$ is negative. Since

$$\mu(\sqrt{E}-\sqrt{E'})^2 = \mu(E-E')^2/(\sqrt{E}+\sqrt{E'})^2$$

is small when $|E-E'|$ is finite and $(\sqrt{E}+\sqrt{E'})^2$ is large, we can expand our integrand in a power series in μ:

$$-\frac{\exp\left\{\mu(\sqrt{E}-\sqrt{E'})^2\,[G(t)-g(0)]\right\}}{G(t)-g(0)} = -\frac{1}{G(t)-g(0)} - \frac{\mu(E-E')^2}{(\sqrt{E}+\sqrt{E'})^2}$$
$$- \frac{1}{2}\frac{\mu^2(E-E')^4}{(\sqrt{E}+\sqrt{E'})^4}\,[G(t)-g(0)] - \ldots$$

and integrate term by term. Fourier transformation of

$$\frac{1}{g(0)-G(t)} - \frac{1}{g(0)}$$

will now give the main inelastic contribution. Thus, the inelastic cross section is approximately equal to

$$\sigma(E\rightarrow E') \approx (\sigma_b/8\pi\mu E)\int dt \exp - (E-E')\left(t+\frac{i}{2kT}\right)\left[\frac{1}{g(0)-G(t)} - g(0)\right]$$
$$= (\sigma_b/8\pi\mu E)\frac{1}{g(0)}\cdot\int dt \exp\left[-(E-E')\left(t+\frac{i}{2kT}\right)\right]\sum_{n=1}^{\infty}\left[\frac{G(t)}{g(0)}\right]^2 \ldots \qquad \text{(B-6)}$$

Since the nearest zero of $g(0) - G(t)$ is located at $t = -i/2kT$, for large values of $(E-E')$, Eq. (B-6) gives correct value for the inelastic cross section: $(\sigma_b/4\mu E)$. The same value, of course, is obtained also from Eq. (30) when $\mu(\sqrt{E}+\sqrt{E'})^2$ is large and η is large negative.

Applying the method of steepest descent to each term of Eq. (B-6), we see that the largest term, S_n, is obtained for $n = g(0)\ |E-E'|$. If n is large,

$$\frac{d^2}{dn^2} \ln S_n \approx -\frac{1}{g(0)\ |E-E'|} \frac{1}{a_2 g(0)-1} \quad .$$

Thus

$$n_{max} = \left(\sqrt{|E-E'|\ g(0)} + \sqrt{a_2 g(0)-1}\right)^2 \qquad \text{(B-7)}$$

terms should be satisfactory for the evaluation of Eq. (B-6). When the first term in Eq. (B-7) becomes smaller than the second, the number of phonons given by Eq. (B-7) is insufficient. It seems that one needs about $4[a_2 g(0)-1]$ terms even for small energy loss. Moreover, we believe also that for $|E-E'| \gtrsim a_2$ Eq. (B-6) will have approached its limiting value. Thus, if we use $n_{max} \gtrsim 4a_2 g(0)$, we should have a fairly smooth transition between multi-phonon expansion and the asymptotic expression.

Appendix C

AVERAGING OVER DIRECTIONS OF POLARIZATION FOR GRAPHITE

For calculation of the scattering cross section from polycrystalline graphite ρ used in the initial formula, Eq. (2), can be represented as an interpolation:

$$\rho = \rho_1 \ell^2 + \rho_2 (1 - \ell^2) \quad , \tag{C-1}$$

between frequency distribution perpendicular to the planes of crystal lattice, ρ_1, and frequency distribution in the planes, ρ_2.[3] The scattering cross section then is obtained upon integration of the final results for cross section over the directions of lattice orientation, $0 \leq \ell \leq 1$. Actually, in Chapter II, calculations of $f_j^{(1)}$, $g(0)$, a_2, and a_3 are performed separately for both sets of values ρ_{1j} and ρ_{2j}, and a common scaling factor is determined. Then, for every needed value of ℓ appropriate quantities $f_j^{(1)}$, $g(0)$, a_2, and a_3 are determined by an interpolation procedure, Eq. (C-1).

Since evaluation of the cross section is a quite elaborate and long process, we have chosen a Gaussian[11,12] integration process. We notice here that our integrand is an even function of ℓ. Thus, if we would expand the limits of integration from -1 to +1, we would not need actually to calculate the values of the integrand for negative values of ℓ. Thus (considering only Gaussian integration schemes with even numbers of values for ℓ), we see that by actually calculating the integrand value at n points we approximate the integrand with a polynomial of degree 4n-1. (Or, we can say that we approximate our integrand with a polynomial which coincides with the integrand at 3n points, of which 2n are chosen arbitrarily.) We can see easily that this integration scheme is exact for a Placzek expansion (in powers of μ) that neglects terms with μ^{2n} and higher powers. It is also exact for expansion of S in a power series of α up to and including the term with α^{2n-1}. These considerations lead us to believe that only a few points are needed for quite satisfactory integration over ℓ. Indeed, in several previous calculations graphite has been approximated by a cubic crystal, using only the total frequency spectrum, and thus essentially using only one point in our Gaussian integration scheme. Upon contemplating the increase of accuracy obtained by using the Placzek expansion, we believe that the additional labor required in using at least two points is well justified. The values of ℓ and corresponding weighting coefficients[13] have been given in Table C-I.

Table C-I

CONSTANTS FOR GAUSSIAN INTEGRATION
OF AN EVEN FUNCTION

n	$\ell_i^{(n)}$	$W_i^{(n)}$
1	0.57735027	1.00000000
2	0.33998104	0.65214515
	0.86113631	0.34785485
3	0.23861919	0.46791393
	0 66120939	0.36076157
	0.93246951	0.17132449
4	0.18343464	0.36268378
	0.52553241	0.31370665
	0.79666648	0.22238103
	0.96028986	0.10122854
5	0.14887434	0.29552422
	0.43339539	0.26926672
	0.67940957	0.21908636
	0.86506337	0.14945135
	0.97390653	0.06667134

ACKNOWLEDGMENTS

The author is grateful to Professor R. Courant, Dr. E. H. Bareiss and Mr. H. Greenspan for several stimulating discussions. He is also indebted to Mr. L. C. Kvitek whose very tedious numerical calculations are reported in Appendix A.

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