

# Total Scattering Cross Section of Solids for Cold and Epithermal Neutrons

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Simple expressions are given which accurately describe the total cross section of solids at cold and epithermal neutron energies. They are intended to provide a consistent procedure for the evaluation of solid state effects, which must be subtracted from the experimental data when information is wanted on intrinsic nuclear properties. The formulae presented here are the asymptotic forms to which the full expressions reduce in those energy limits. A Debye model is adopted to describe the frequency spectrum of the solid. The present results are compared with some commonly used expressions as well as with the exact formalism. The effect of temperature is discussed and numerical calculations are presented for some cases.

## I. Introduction

The unique properties of thermal neutrons for the investigation of condensed matter have been recognized from the early days when neutron sources became available for research purposes. Since then, much work has been done on both experimental and theoretical aspects to fully exploit those properties, thus transforming their potentiality into a well established technique for the study of structure and dynamics of matter [1].

Besides the traditional field of atomic motion studied in liquids and solids, the availability of new powerful neutron sources, specialized moderators and advanced instruments has opened new horizons for the application of neutron techniques [2, 3]. Whether they involve the use of very cold neutrons aimed to determine some fundamental properties of the neutron itself [4] or epithermal neutrons to obtain information on nuclear properties, an accurate evaluation of the chemical binding effects is necessary to subtract their contribution from the experimental data.

The behaviour of the total scattering cross section as a function of the sample properties and the incident neutron energy is a basic information which can be predicted with a high degree of accuracy for polycrystalline solids over the whole

thermal range [5]. In the case of molecular liquids, such an evaluation can be performed by using either computer codes [6] or a semianalytical method [7]. However, for any problem requiring the evaluation of cross sections it is necessary to know the values of the corresponding nuclear constants  $\sigma_c$  (coherent) and  $\sigma_i$  (incoherent) which characterize the neutron-nucleus interaction [8].

Figure 1 shows the total cross section  $\sigma_T$  of Molybdenum at thermal energies as calculated by the code CRIPO [5] together with experimental

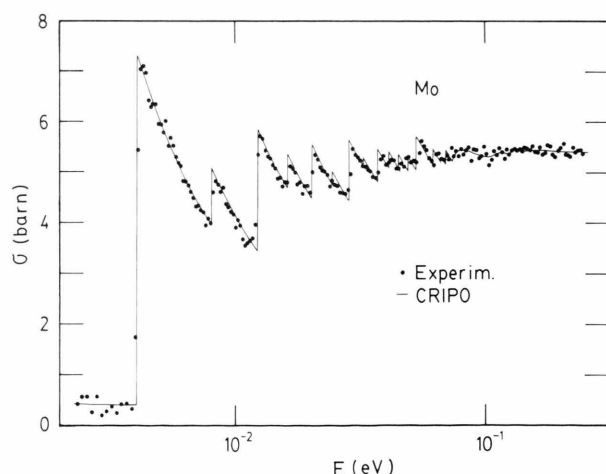


Fig. 1. The total cross section (absorption subtracted) of Molybdenum in the thermal neutron range. The experimental points are from [9] whereas the solid line is calculated using the CRIPO computer code.

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points [9]. Although CRIPO can provide results at cold or epithermal neutron energies as well, I consider it convenient to present the much simpler expressions to which the full formalism reduces at the extremes of the thermal range, thus offering to the experimentalist a compact – yet extremely accurate – set of formulae.

The incoherent approximation for the inelastic components of the total cross sections is used throughout this work as – according to Placzek's [10] arguments – the multiphonon terms which dominate the cross section at high energies do not contribute significantly to the interference (or coherent) effects; the situation at low energies is a more subtle matter but nonetheless the approximation is still a good one in most cases (Section IV). However, the elastic components – coherent and incoherent – are evaluated using their exact expressions and therefore no approximation is made on them.

## II. Basic Equations

The total cross section  $\sigma_T(E)$  corresponding to an incident neutron energy  $E$  can be written as

$$\sigma_T(E) = \sigma_s(E) + \sigma_r(E), \quad (1)$$

where  $\sigma_s(E)$  and  $\sigma_r(E)$  denote the contributions arising from scattering and reaction processes, respectively. Although (1) may look incomplete from a general point of view, it serves the purpose of explicitly isolating the scattering contribution, which we will concentrate ourselves on, from the rest.

The total cross section for scattering processes is

$$\sigma_s(E) = \sigma_c^* \cdot S_{\text{coh}}^{\text{el}}(E) + \sigma_i \cdot S_{\text{inc}}^{\text{el}}(E) + \sigma_c^* \cdot S_{\text{coh}}^{\text{inel}}(E) + \sigma_i \cdot S_{\text{inc}}^{\text{inel}}(E), \quad (2)$$

where  $\sigma_c$  and  $\sigma_i$  are the coherent and incoherent nuclear constants, whereas the functions  $S(E)$  contain the structure and dynamics of the sample system.

In (2) the asterisk attached to  $\sigma_c$  is a remainder that this quantity is also dependent on neutron energy via the effect of neutron-electron interaction, Schwinger scattering and nuclear resonance contributions [11]. Also, I will assume a Debye spectrum, with a characteristic temperature  $\theta_D$ , to

represent the eigenfrequency distribution of the solid.

### II.1. The Elastic Components

The elastic coherent contribution to the total cross section of a polycrystalline solid is given by

$$S_{\text{coh}}^{\text{el}}(E) = \frac{\pi^2 \hbar^2}{2m E v_0} \sum_{\tau \neq 0}^{< 2k} \frac{w(\tau)}{\tau} \exp \left\{ -\frac{3 \hbar^2 \Phi_1(\theta)}{2M k_B \theta_D} \tau^2 \right\}, \quad (3)$$

where  $v_0$  is the volume of the unit cell,  $w(\tau)$  the multiplicity of reciprocal lattice vectors of modulus  $\tau$ ,  $k$  the incident neutron wavevector ( $E = \hbar^2 k^2 / 2m$ ) and  $\Phi_1(\theta)$  a function of  $\theta = T / \theta_D$  which is defined in the Appendix.  $M$  and  $m$  are the scattering nuclei and neutron masses, respectively.

The elastic incoherent part of the cross section is

$$S_{\text{inc}}^{\text{el}}(E) = \frac{1}{12} \left( \frac{M}{m} \right) \frac{k_B \theta_D}{E \Phi_1(\theta)} \cdot \left[ 1 - \exp \left\{ -12 \left( \frac{m}{M} \right) \frac{E}{k_B \theta_D} \Phi_1(\theta) \right\} \right]. \quad (4)$$

It is easy to show (e.g. [12]) that (3) reduces to the incoherent form (4) if the sum is replaced by an integral in the limit of  $k \rightarrow \infty$ . However, this is only an upper limit for the exact expression (3), as can be shown either theoretically [13, 14] or by numerical calculations using the computer code CRIPO. This matter is further discussed in Section III.

### II.2. The Inelastic Components

As it was stated previously, the incoherent approximation in the inelastic contributions is a very good one for neutron energies above  $\sim 0.4$  eV [14], and therefore I will describe both (coherent plus incoherent) components by  $(\sigma_c^* + \sigma_i) \cdot S_{\text{inc}}^{\text{inel}}(E)$ .

Neither a phonon nor a mass expansion is adequate for the evaluation of  $S_{\text{inc}}^{\text{inel}}(E)$ , but Placzek [10] pointed out that a rapidly converging mass expansion is obtained for the total cross section

$$S_{\text{inc}}^{\text{tot}}(E) = S_{\text{inc}}^{\text{el}}(E) + S_{\text{inc}}^{\text{inel}}(E), \quad (5)$$

so that the best prescription is to obtain  $S_{\text{inc}}^{\text{inel}}(E)$  from the difference of (5) and (4).

The general expression of this expansion is

$$S_{\text{inc}}^{\text{tot}}(E) = \sum_{n=0}^{\infty} \left( \frac{1}{A} \right)^n A_n(E, \theta) \quad (6)$$

with

$$A_n(E, \theta) = \frac{1}{4x^2} \cdot \frac{3^n}{(n+1)} \sum_{l=0}^n a_l^{(n)}; \quad A_0(E, \theta) = 1 \quad (7)$$

and

$$a_l^{(n)} = \frac{\{-\Phi_1(\theta)\}^{n-l}}{l!(n-l)!} \prod_{j=1}^l \int_{-1}^1 d\varepsilon_j \varepsilon_j (e^{\varepsilon_j/\theta} - 1)^{-1} \cdot \{(x+x')^{2n+2} - (x-x')^{2n+2}\}. \quad (8)$$

I am using the notation

$$x^2 = E/k_B \theta_D, \quad A = M/m.$$

In (8) it is understood that

$$x' = \begin{cases} x^2 + \sum_{j=1}^l \varepsilon_j & \text{if } \sum_{j=1}^l \varepsilon_j > -x^2, \\ x' = 0 & \text{otherwise,} \end{cases} \quad (9)$$

and this condition will effectively modify the integration limits in the definition of  $a_l^{(n)}$ .

We will stop at this point the consideration of the exact form of  $S_{\text{inc}}^{\text{tot}}(E)$  to concentrate in its behaviour at epithermal neutron energies.

### III. Asymptotic Forms in the Epithermal Neutron Range

#### III.1. The Total Incoherent Cross Section

The results which I present in this section usually have a much wider range of validity than the one stated in the heading, as the required condition is

$$x^2 = E/k_B \theta_D \gg 1. \quad (10)$$

Under this hypothesis, I obtained – after some lengthy algebra – the following expressions for the asymptotic limits of the first  $A_n(E, \theta)$ :

$$\begin{aligned} A_0 &= 1, \\ A_1 &\simeq -2 + \frac{1}{x^2} \cdot \frac{3}{4} \Phi_3(\theta), \\ A_2 &\simeq 3 - \frac{1}{x^2} \cdot \frac{3}{2} \Phi_3(\theta), \\ A_3 &\simeq -4 + \frac{1}{x^2} \cdot \frac{9}{4} \Phi_3(\theta). \end{aligned} \quad (11)$$

According to (6) it follows that

$$S_{\text{inc}}^{\text{tot}}(E) \simeq 1 + \sum_{n=1}^{\infty} (-1)^n \frac{(n+1)}{A^n} + \frac{1}{x^2} \cdot \frac{3}{4} \Phi_3(\theta) \sum_{n=1}^{\infty} (-1)^{n+1} \frac{n}{A^n}$$

or

$$S_{\text{inc}}^{\text{tot}}(E) \simeq \left( \frac{A}{A+1} \right)^2 \left\{ 1 + \frac{3}{4A} \Phi_3(\theta) \frac{1}{x^2} \right\}. \quad (12)$$

This formula gives an excellent approximation to the total incoherent cross section. For aluminium ( $\theta_D = 358$  K) at  $T = 300$  K there is a maximum relative discrepancy of  $4 \times 10^{-3}$  in the whole region of  $x \geq 1$  ( $E \geq 0.031$  eV); at 1 eV that discrepancy is about  $5 \times 10^{-4}$ , and it is of course even smaller at higher energies.

The function  $\Phi_3(\theta)$  (see Appendix) varies with  $\theta$  as shown in Fig. 2, and it is given in Table 1 for  $\theta$  between 0.05 and 2. According to its definition it is easy to verify that  $\Phi_3$  tends to  $1/4$  as  $\theta \rightarrow 0$  and then

$$S_{\text{inc}}^{\text{tot}}(E)_{T \rightarrow 0} \cong \left( \frac{A}{A+1} \right)^2 \left\{ 1 + \frac{3}{16A} \frac{k_B \theta_D}{E} \right\}, \quad (13)$$

thus showing that a sort of Doppler correction still exists in this limit, originated in the zero-point kinetic energy of the lattice.

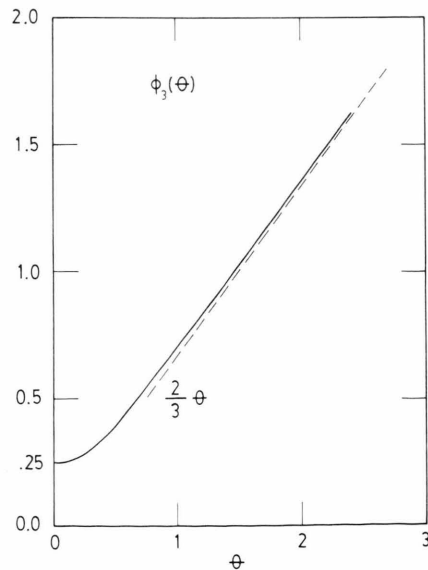


Fig. 2. The function  $\Phi_3(\theta)$ . The dashed line represents the asymptotic form for large values of  $\theta$ .

Table 1. The functions  $\Phi_1$ ,  $\Phi_3$  and  $g_2$  defined by (A.1) and (25), respectively, as a function of  $\theta = T/\theta$ .

| $\theta$ | $\Phi_1$ | $\Phi_3$ | $g_2$   |
|----------|----------|----------|---------|
| 0.05     | 0.50822  | 0.25008  | 0.00010 |
| 0.10     | 0.53289  | 0.25129  | 0.00118 |
| 0.15     | 0.57358  | 0.25596  | 0.00461 |
| 0.20     | 0.62835  | 0.26568  | 0.01115 |
| 0.25     | 0.69407  | 0.28029  | 0.02056 |
| 0.30     | 0.76781  | 0.29888  | 0.03227 |
| 0.35     | 0.84733  | 0.32052  | 0.04571 |
| 0.40     | 0.93103  | 0.34444  | 0.06044 |
| 0.45     | 1.01783  | 0.37008  | 0.07614 |
| 0.50     | 1.10695  | 0.39704  | 0.09259 |
| 0.55     | 1.19785  | 0.42502  | 0.10960 |
| 0.60     | 1.29014  | 0.45381  | 0.12707 |
| 0.65     | 1.38352  | 0.48323  | 0.14489 |
| 0.70     | 1.47780  | 0.51317  | 0.16300 |
| 0.75     | 1.57280  | 0.54353  | 0.18134 |
| 0.80     | 1.66839  | 0.57425  | 0.19988 |
| 0.85     | 1.76448  | 0.60525  | 0.21859 |
| 0.90     | 1.86098  | 0.63650  | 0.23743 |
| 0.95     | 1.95784  | 0.66798  | 0.25639 |
| 1.00     | 2.05501  | 0.69961  | 0.27545 |
| 1.05     | 2.15244  | 0.73141  | 0.29459 |
| 1.10     | 2.25009  | 0.76334  | 0.31381 |
| 1.15     | 2.34795  | 0.79539  | 0.33310 |
| 1.20     | 2.44598  | 0.82755  | 0.35245 |
| 1.25     | 2.54416  | 0.85980  | 0.37184 |
| 1.30     | 2.64248  | 0.89213  | 0.39128 |
| 1.35     | 2.74093  | 0.92453  | 0.41076 |
| 1.40     | 2.83948  | 0.95700  | 0.43028 |
| 1.45     | 2.93813  | 0.98953  | 0.44983 |
| 1.50     | 3.03687  | 1.02211  | 0.46941 |
| 1.55     | 3.13569  | 1.05473  | 0.48902 |
| 1.60     | 3.23459  | 1.08740  | 0.50865 |
| 1.65     | 3.33355  | 1.12011  | 0.52830 |
| 1.70     | 3.43257  | 1.15286  | 0.54797 |
| 1.75     | 3.53164  | 1.18564  | 0.56766 |
| 1.80     | 3.63077  | 1.21845  | 0.58736 |
| 1.85     | 3.72994  | 1.25129  | 0.60709 |
| 1.90     | 3.82916  | 1.28415  | 0.62682 |
| 1.95     | 3.92842  | 1.31704  | 0.64657 |
| 2.00     | 4.02771  | 1.34995  | 0.66633 |

On the other hand, at very high temperatures  $\theta \rightarrow \infty$  and  $\Phi_3 \rightarrow \frac{2}{3}\theta$ , therefore from (12):

$$S_{\text{inc}}^{\text{tot}}(E)_{T \rightarrow \infty} \cong \left( \frac{A}{A+1} \right)^2 \left\{ 1 + \frac{1}{2A} \frac{k_B T}{E} \right\}, \quad (14)$$

which we recognize as the commonly used expression for  $S_{\text{inc}}^{\text{tot}}(E)$ , corresponding to a gas of particles of mass  $M$  in equilibrium at a temperature  $T$ .

### III.2. The Correction to the Incoherent Approximation in the Elastic Components

Placzek et al. [13, 15] have shown that for large  $k$ , the correction  $\delta S$  is given by

$$\delta S = S_{\text{inc}}^{\text{el}}(E) - S_{\text{coh}}^{\text{el}}(E) \cong \frac{\lambda^2}{8\pi v_0^{2/3}} I \quad (15)$$

with  $I$  being a lattice structure and temperature dependent coefficient with a typical value  $I \cong 2.88$  [14]. Rewriting (15) as

$$\delta S \cong (8\pi v_0^{2/3})^{-1} J/E, \quad (16)$$

the typical value of  $J$  should be  $\sim 0.2356$ . Using the code CRIPO I calculated  $\delta S(E)$  for  $Al$ , and the results in the energy range from 0.125 eV to 1 eV are shown in Fig. 3 as a function of  $E^{-1}$ ; I found in this case that (16) is a very good representation of the difference  $S_{\text{inc}}^{\text{el}} - S_{\text{coh}}^{\text{el}}$ , with a value  $J = 0.2344$ . It is concluded that the time consuming exact expression (3) of the elastic coherent component can be very well approximated in the epithermal range by

$$S_{\text{coh}}^{\text{el}}(E) \cong S_{\text{inc}}^{\text{el}}(E) - \delta S(E). \quad (17)$$

Summarizing the previous results, for the evaluation of the different components of the total (scattering) cross section of solids in the epithermal neutron energy range, I propose to use the following prescription:

- Evaluate  $S_{\text{inc}}^{\text{el}}(E)$  from (4),
- Evaluate  $S_{\text{inc}}^{\text{tot}}(E)$  from (12),
- Obtain  $S_{\text{inc}}^{\text{inel}}(E)$  as  $S_{\text{inc}}^{\text{tot}}(E) - S_{\text{inc}}^{\text{el}}(E)$ ,

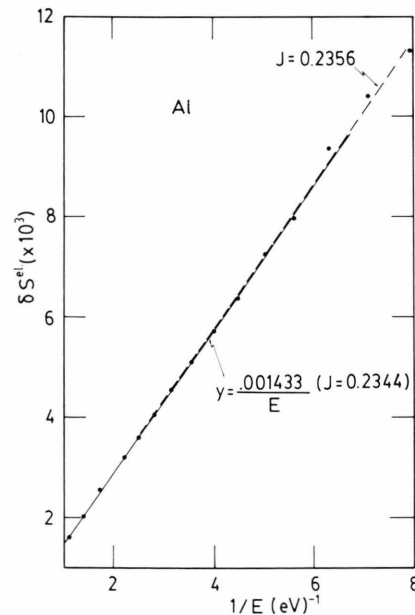


Fig. 3. The difference between the elastic (coherent and incoherent) components of the cross section at epithermal neutron energies. The dots are results from a CRIPO calculation (see text for details).

d) Evaluate  $\delta E(E)$  from (16), using a typical value  $J \cong 0.235$  or extracting the value corresponding to a given material from a CRIPO run.

e) Obtain  $S_{\text{coh}}^{\text{el}}(E)$  as  $S_{\text{inc}}^{\text{el}}(E) - \delta S(E)$ .

On the other hand, the total cross section is given directly by

$$\sigma_s(E) = \sigma_c^* [S_{\text{inc}}^{\text{tot}}(E) - \delta S(E)] + \sigma_i S_{\text{inc}}^{\text{tot}}(E), \quad (18)$$

which is a form amenable for the use of fitting procedures if there is an unknown quantity (usually  $\sigma_i$  [12]).

### III.3. Extension to Compounds

Consider for simplicity the case of a binary compound, with concentration  $C_x$  and  $C_y$  of nuclei  $X$  and  $Y$ , each with masses  $M_x$  and  $M_y$  and scattering properties  $\{b_x\}$  and  $\{b_y\}$ , respectively.

The scattering cross sections of the compound are given by

$$\bar{\sigma}_c = 4\pi (C_x b_x + C_y b_y)^2 \quad \text{and} \quad (19)$$

$$\sigma_i = 4\pi [(C_x b_x^2 + C_y b_y^2) - (C_x b_x + C_y b_y)^2] + (C_x \sigma_i^x + C_y \sigma_i^y),$$

whereas the effective mass  $\bar{M}$  is

$$\frac{(\bar{\sigma}_c + \bar{\sigma}_i)}{\left(1 + \frac{1}{\bar{M}}\right)^2} = C_x \frac{(\sigma_c^x + \sigma_i^x)}{\left(1 + \frac{1}{M_x}\right)^2} + C_y \frac{(\sigma_c^y + \sigma_i^y)}{\left(1 + \frac{1}{M_y}\right)^2}. \quad (20)$$

If there is an unknown quantity, for example  $\sigma_i^y$ , we can express  $\bar{M}$  as  $\bar{M}(\sigma_i^y)$  from (20) and then obtain  $\sigma_i^y$  by fitting (18) to the experimental data after the use of  $\bar{A} = \bar{M}/m$  in (14).

## IV. Cross Sections at Cold Neutron Energies

At neutron energies below the thermal range, the inelastic component of the scattering cross section is dominated by the one-phonon contribution. The validity of the incoherent approximation [4] is usually assumed although it has been shown [14] that corrections as big as 15% could be necessary in special circumstances.

It is easy to show that the incoherent one-phonon contribution to the total cross section at all neutron energies and temperatures is given by

$$S_{\text{inc}}^{\text{inel}(1)}(E) = [2x^2 \Phi_1(\theta)]^{-1} \int_{\max(-1, -x^2)}^1 d\varepsilon I(\varepsilon) (e^{\varepsilon/\theta} - 1)^{-1}, \quad (21)$$

where

$$I(\varepsilon) = \exp \left\{ -\frac{3\Phi_1(\theta)}{A} (2x^2 + \varepsilon) \right\} \cdot \left\{ \left[ \frac{A}{3\Phi_1(\theta)} + 2x^2 + \varepsilon \right] \cdot \sinh \left[ 6x(x^2 + \varepsilon)^{1/2} \frac{\Phi_1(\theta)}{A} \right] - 2x(x^2 + \varepsilon)^{1/2} \cdot \cosh \left[ 6x(x^2 + \varepsilon)^{1/2} \frac{\Phi_1(\theta)}{A} \right] \right\}. \quad (22)$$

The phonon annihilation contribution in (21) corresponds to  $\varepsilon > 0$  whereas the creation part is given by  $\varepsilon < 0$ . The mass expansion of  $S_{\text{inc}}^{\text{inel}(1)}$  can be written directly from (6), by summing up the contributions involving  $a_1^{(n)}$ . Then we find

$$S_{\text{inc}}^{\text{inel}(1)} = \frac{3}{A} \left\{ \frac{1}{x} g_2 + 2x g_1 \right\} - \frac{3}{A^2} \Phi_1(\theta) \left\{ \frac{3}{x} g_3 + 16x g_2 + 16x^3 g_1 \right\} + \frac{27}{A^3} \Phi_1^2(\theta) \left\{ \frac{1}{2x} g_4 + 5x g_3 + 12x^3 g_2 + 8x^5 g_1 \right\}, \quad (23)$$

where the  $g$ 's are functions which depend on both  $x$  and  $\theta$ :

$$g_m = \int_{\max(-1, -x^2)}^1 d\varepsilon \varepsilon^m (x^2 + \varepsilon)^{1/2} (e^{\varepsilon/\theta} - 1)^{-1}. \quad (24)$$

It is by taking only the first term in the first bracket on the r.h.s. of (23) and furthermore assuming that  $\theta$  is not much smaller than unity, that the commonly adopted form of  $S_{\text{inc}}^{\text{inel}(1)}$  [4, 14] is found. Incidentally, we must note that "1/x" terms also appear in the higher powers of  $A^{-1}$ , which indicates that they must be included if a precise evaluation at low energies is pursued, mostly if a light nucleus is involved.

At neutron energies much lower than the characteristic "Debye energy"  $k_B \theta_D$ ,  $x \sim 0$  and therefore we can neglect the contribution from phonon creation such that

$$g_m \approx \int_0^1 d\varepsilon \varepsilon^{m+1/2} (e^{\varepsilon/\theta} - 1)^{-1}. \quad (25)$$

It is easy to show that  $g_m$  can be represented by the series

$$g_m = -\frac{1}{2}(m+3/2)^{-1} + \theta \left\{ (m+1/2)^{-1} + \sum_{k=1}^{\infty} (-1)^{k+1} \cdot \frac{B_k}{(2k)!} (m+1/2+2k)^{-1} \cdot \theta^{-2k} \right\}, \quad (26)$$

which converges for  $\theta = T/\theta_D > 1/(\pi e) \sim 0.12$ . The  $B_k$  are the Bernoulli numbers. Clearly the behaviour of all  $g_m$  and hence  $S_{\text{inc}}^{\text{inel}(1)}$  is proportional to  $T$  at high temperatures.

For  $\theta \ll 1$  another expansion is in order. Starting again from (25),

$$g_m = \theta \log(1 - e^{-1/\theta}) + (m+1/2) \theta \sum_{n=1}^{\infty} \frac{1}{n} \int_0^1 d\varepsilon \varepsilon^{m-1/2} e^{-n\varepsilon/\theta}.$$

The integrals are of the form  $\int_0^{n/\theta} dy y^{m-1/2} e^{-y}$ , and then one can extend the upper limit to infinity as  $\theta \ll 1$ . This leads immediately to the result

$$g_m = \theta \log(1 - e^{-1/\theta}) + (m+1/2) \Gamma(m+1/2) \zeta(m+3/2) \theta^{m+3/2}, \quad (27)$$

which shows the  $T^{7/2}$  behaviour of  $S_{\text{inc}}^{\text{inel}}$  at low temperature due to the leading term  $g_2/x$  in (23).

A very useful approximation to the  $g_m$ 's, valid for  $\theta \geq 0.5$ , is given by

$$g_m = \{1 - [r(\theta) + 1]^{-1}\} \cdot \frac{\theta}{(m+1/2)} \quad (28)$$

with  $r(\theta) = b(\theta - a)$  and

$$b = 2(m+3/2)/(m+1/2), \\ a = 1/b - B_1(m+2)/(m+5/2). \quad (29)$$

The results of this approximation are compared in Fig. 4 with numerical results from (25) for  $m=1$  to 4. It is seen that good agreement is achieved over the range for which the prescription of (28) is proposed ( $\theta \geq 0.5$ ).

With this information at hand, and the fact that the term containing  $g_2$  is the leading one at very low energies in the mass expansion, I propose to calculate the  $g_m$ 's other than  $g_2$  according to

$$g_m/g_2 = 5/(2m+1),$$

which when replaced in (23) gives us a simple formula for the one-phonon cross section:

$$S_{\text{inc}}^{\text{inel}(1)} \cong g_2(\theta) \left\{ \frac{1}{x} \left( \frac{3}{A} \right) \cdot \left[ 1 - \left( \frac{3}{A} \right) \Phi_1 \frac{5}{7} + \left( \frac{3}{A} \right)^2 \Phi_1^2 \frac{5}{18} \right] + x \left( \frac{3}{A} \right) \left[ \frac{10}{3} - \left( \frac{3}{A} \right) \Phi_1 \frac{16}{3} + \left( \frac{3}{A} \right)^2 \Phi_1^2 \frac{25}{7} \right] \right\}. \quad (30)$$

It is shown in the next section that this expression constitutes an excellent approximation to the exact formula (21) in the cold neutron energy region, where the inelastic component of the cross section is controlled by the one-phonon contribution. For the sake of completeness, the values of  $\Phi_1(\theta)$  and  $g_2(\theta)$  are given in Table 1 up to  $\theta = 2$ ; beyond this value it is satisfactory to use  $\Phi_1(\theta \geq 2) = 2\theta$  and  $g_2(\theta \geq 2)$  calculated from (28).

The incoherent approximation is a good one in normal circumstances and in that case we can write

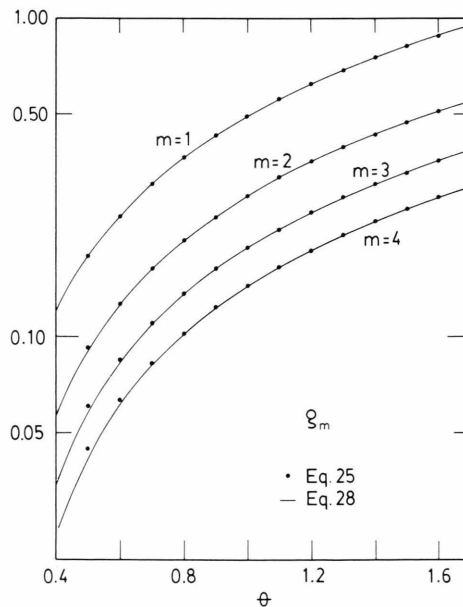


Fig. 4. The behaviour of  $g_m(\theta)$  for  $m=1$  to 4 and  $\theta = T/\theta_D \geq 0.4$ . The circles are the exact results from (25) whereas the solid lines correspond to the approximation (28).



the total (scattering) cross section as

$$\sigma_s(E) = \sigma_i S_{\text{inc}}^{\text{el}}(E) + (\sigma_c^* + \sigma_i) S_{\text{inc}}^{\text{inel}(1)}(E), \quad (31)$$

with  $S_{\text{inc}}^{\text{el}}$  given by (4) and  $S_{\text{inc}}^{\text{inel}(1)}$  calculated according to (30).

## V. Numerical Results and Discussion

Let us consider first a situation involving epithermal neutrons. To visualize the effect of the “Doppler term” in (12), the difference between  $S_{\text{inc}}^{\text{inel}}$  and the free atom limit,

$$\Delta(E, \theta) = \frac{3A}{4(A+1)^2} \cdot \Phi_3(\theta) \cdot \frac{k_B \theta_D}{E}, \quad (32)$$

is shown in Fig. 5 for Beryllium at different temperatures. The value  $\theta_D = 1031$  K [16] has been used in all cases. It is evident that the usual correction (14), indicated by dashed lines, only approximates the “correct” results (solid lines) at high temperatures and underestimating the latter by a factor of 5 at the lowest temperature considered. Admittedly this is a small correction ( $10^{-2}$ – $10^{-3}$ ) as compared to unity and decreases as  $1/A$  as the mass increases, but (12) is so simple that its use is recommended in accurate work.

To discuss some aspects of the cross section at cold neutron energies, I have chosen Vanadium as a convenient example. With a Debye temperature  $\theta_D \cong 390$  K [16] we have  $\theta \cong 0.75$  at room temperature ( $T = 293$  K). Below  $10^{-3}$  eV the total scattering cross section is completely represented by the elastic and one-phonon contributions [17] and furthermore, it is entirely incoherent ( $\sigma_c/\sigma_i \cong 0.003$ ).

In Fig. 6 the inelastic (one-phonon) component  $S_{\text{inc}}^{\text{inel}(1)}(E)$  is shown, as calculated from its exact expression (Curve A, (21)), the proposed mass expansion (Curve B, (30)) and from the commonly employed truncated series as given by formula (4.1) of [4] (Curve C). Above  $10^{-3}$  eV, curve B clearly separates from the exact result due to the neglect of phonon-creation processes or, more precisely, by the use of the approximation (25) to represent the complete expression (24). At lower energies however, our very simple mass expansion (30) provides an excellent description of the exact curve A.

As far as curve C is concerned, we must remember that it is originated by an expression of the form

$$S_{\text{inc}}^{\text{inel}(1)} \cong \frac{3}{A} \frac{g_2}{x}, \quad (30)$$

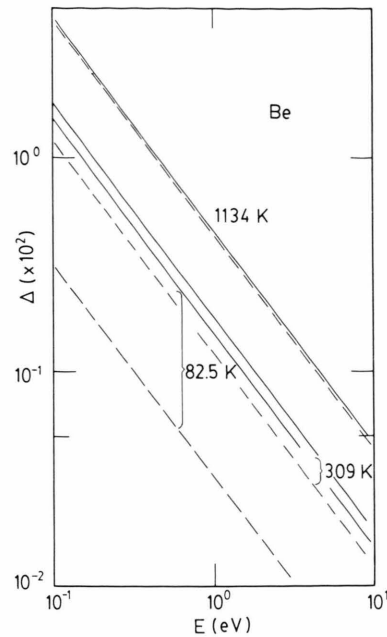


Fig. 5. The correction term  $\Delta(E, \theta)$  for Beryllium at different temperatures (see text for details).

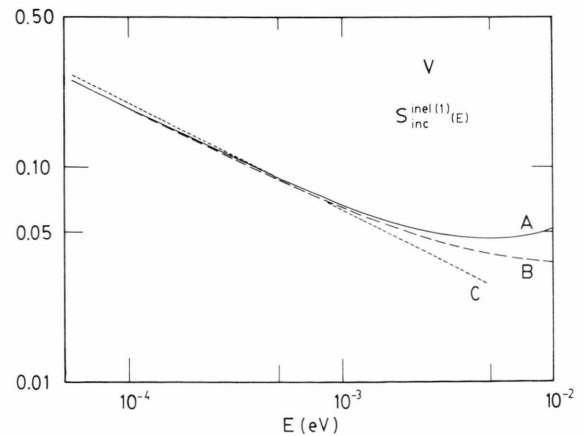


Fig. 6. The inelastic (one-phonon) incoherent cross section of Vanadium at cold neutron energies. Curve A is an exact calculation, curve B is the proposed mass expansion (30) and curve C is the commonly used “ $1/v$ ” approximation.

with  $g_2$  given by the (truncated) series of (26). Although the  $g_2$  thus obtained gives an accurate estimation of (25) for this  $\theta$ , a discrepancy is observed at low energies with respect to curves A and B. It can be shown that such a discrepancy is entirely due to the neglect of the next important term (compared to 1)

$$\sim -\left(\frac{3}{A}\right) \Phi_1(\theta) \frac{5}{7},$$

which therefore proves to be significant (6.7%) even in this case of a medium mass material ( $M = 50.942$  amu).

In view of the present availability of advanced techniques for total cross section measurements [4, 11, 18] and motivated by the corresponding requirement of accurate procedures for data analysis, I tried in this work to develop some expressions to which the full theory reduces at cold and epithermal neutron energies. I hope that experimentalists working in the field will find those simple and precise expressions to be a useful tool in the data analysis process.

## Appendix

The functions  $\Phi_m(\theta)$  are defined by

$$\Phi_m(\theta) = \int_{-1}^1 d\varepsilon \varepsilon^m (e^{\varepsilon/\theta} - 1)^{-1}. \quad (\text{A.1})$$

They can be accurately evaluated in terms of the expressions

$$\Phi_m(\theta) = \frac{(-1)^{m+1}}{m+1} + I_m [(-1)^{m+1} + 1], \quad (\text{A.2})$$

where

$$I_m = \theta \log(1 - e^{-1/\theta}) + \theta^{m+1} m! \zeta(m+1) - \sum_{n=1}^{\infty} a_{n,m}. \quad (\text{A.3})$$

In this formula,  $\zeta$  is the Riemann Zeta-function,

$$\zeta(m) = \sum_{n=1}^{\infty} \frac{1}{n^m},$$

and the coefficients  $a_{n,m}$  are defined by

$$a_{n,m} = e^{-n/\theta} \sum_{k=1}^m \theta^{k+1} m(m-1)\dots(m-k+1) n^{-(k+1)}. \quad (\text{A.4})$$

Clearly, from (A.2) for  $m$  even (and for all  $\theta$ ):

$$\Phi_m(\theta) = \frac{-1}{m+1}, \quad m \text{ even.}$$

For odd  $m$ , the evaluation of  $I_m$  according to (A.3) is required although in this case the Zeta-function is given directly in terms of the Bernoulli numbers  $B_k$ :

$$\zeta(2k) = \frac{2^{2k-1} \pi^{2k}}{(2k)!} B_k \quad (k = 1, 2, 3, \dots).$$

It is also seen from (A.3) that  $I_m \rightarrow 0$  as  $\theta \rightarrow 0$  and so,

$$\Phi_m(\theta)_{\theta \rightarrow 0} \rightarrow \frac{(-1)^{m+1}}{m+1}. \quad (\text{A.5})$$

The limiting form in the case  $\theta \gg 1$  is easily obtained from the definition (A.1):

$$\Phi_m(\theta \gg 1) \cong \theta \cdot \int_{-1}^1 d\varepsilon \varepsilon^{m-1} = \frac{\theta}{m} [1 - (-1)^m], \quad (\text{A.6})$$

and therefore  $\Phi_m(\theta \gg 1) \cong \frac{2}{m} \cdot \theta$  ( $m$  odd).

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