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AEC Research and Development Report

TISK: A PROGRAM FOR CALCULATING
THERMAL NEUTRON SCATTERING KERNELS,
AND ITS APPLICATION TO H_2O

JUNE 1972

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June 1972

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COMPUTER CODE ABSTRACT

1. Name: TISK
2. Computer: The TISK Code is designed to operate on the UNIVAC 1108 computer system.
3. Problem Solved: The code computes either the thermal neutron scattering law $S(\alpha, \beta)$, or the zeroth and first Legendre moments ($\sigma_n(E_0 \rightarrow E)$, $n = 0, 1$) of the scattering cross section.
4. Method of Solution: The Egelstaff-Schofield representation of $S(\alpha, \beta)$ as a cosine transform is used. For $\sigma_n(E_0 \rightarrow E)$, this representation is integrated analytically over the angular variable to obtain a representation of $\sigma_n(E_0 \rightarrow E)$ itself as a cosine transform. Integrals over successive half-cycles of the cosine are evaluated using Simpson's integration with successive refinement of the partition. The resulting alternating series is summed using an Euler transform to minimize accrual of round-off error. When appropriate, the contributions to the integral from large values of t are evaluated from analytical expressions, with only the contributions from smaller t values being computed numerically. For large momentum transfers and large E_0 , asymptotic expansions of $S(\alpha, \beta)$ and $\sigma_n(E_0 \rightarrow E)$ are used instead. TISK performs these computations any user-supplied function routine for the width function $w(t)$. However, a versatile width generator is supplied with the code, and is based on a representation of the spectral function $\rho(\beta)$ as a sum of resonance-like peaks containing many adjustable parameters. In particular, a set of parameters for room temperature light water is available.

5. Restrictions on the Complexity of the Problem: As presently programmed, the number of energy groups must not exceed 101. Neither the number of α -values, nor the number of β -values must exceed 100.
6. Typical Running Time: Highly dependent on the complexity of the spectral function $\rho(\beta)$.
7. Unusual Features of the Program: Either energy groups, or energy points may be specified routinely. For the elastic case ($E = E_0$), the average of the $\sigma_n(E_0 \rightarrow E)$ over a narrow elastic group is computed directly, since the value at the point $E = E_0$ may be infinite. It is possible to evaluate the $\sigma_n(E_0 \rightarrow E)$ for a subset of the desired energy set, and to restart a run aborted for lack of time without loss of previously computed information.
8. Related and Auxiliary Programs: None.
9. Status: TISK is in use on the UNIVAC 1108 Computer, Computer Sciences Corporation, Richland, Washington.
10. References:
 - A. G. Gibbs and C. W. Lindenmeier. TISK: A Program for Calculating Thermal Neutron Scattering Kernels, and its Application to H₂O. BNWL-1675. Battelle-Northwest, Richland, Washington. June 1972.
 - A. G. Gibbs and C. W. Lindenmeier. "Analytical Evaluation of the Large Time Contribution to Neutron Scattering Cross Sections," in Neutron Thermalization and Reactor Spectra. I.A.E.A., Vienna, (1962).
 - P. A. Egelstaff and P. Schofield, Nucl. Sci. Engng. 12, 260 (1962).
11. Machine Requirements: 64 k memory, normal input, output, program, and punch units.
12. Programming Language Used: FORTRAN-V.

13. Operating System: UNIVAC 1108 computer with FORTRAN-V compiler and CSCX operating system.
14. User Information: The code and report may be obtained through the Argonne Code Center at Argonne National Laboratory.
15. Material Available: FORTRAN Source Deck, Sample Cases, Documentation.
16. Acknowledgment: This work was performed under U. S. Atomic Energy Commission Contract AT(45-1)-1830

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INTRODUCTION

Program TISK generates incoherent thermal neutron scattering kernels for reactor moderators using the Egelstaff-Schofield¹ representation. Either $S(\alpha, \beta)$ itself, or the zeroth and first Legendre moments of the scattering cross section ($\sigma_n(E_0 \rightarrow E)$, $n = 0, 1$) are computed. Both are generated from the width function $w(t)$ by direct numerical evaluation of the appropriate Fourier cosine transform. When the moments $\sigma_n(E_0 \rightarrow E)$ are desired, they are computed directly without the need for a prior computation, storage and integration of the S-function.

It is envisioned that the S-function option of TISK will be used in the analysis of scattering data to obtain the spectral function $\rho(\beta)$, while the moment-generating option will be used to provide scattering kernels for reactor analysis.

Program TISK has evolved over a period of several years, and represents the culmination of a number of efforts, first at the Hanford Laboratories, and later at Battelle-Northwest, related to neutron scattering cross sections and numerical methods.^{2,3,4,5}

In Part I of the present document, some general results are reviewed from the theory of slow neutron scattering, and computational methods are discussed. In Part II, the TISK program is presented

as a realization of the methods of Part I. In Part III, we outline a method for representing the spectral function as a sum of convenient analytical functions, and in Part IV, an application to H_2O is summarized.

Acknowledgement

During the evolution of program TISK, the authors have benefitted from the knowledge and experience of many co-workers. In particular, it is a pleasure to acknowledge the contributions of P. A. Ekstrom, D. A. Kottwitz, and K. B. Stewart.

PART I - THEORY

Scattering of slow neutrons

When slow neutrons interact with a system of atoms, the interactions require sufficient time for the neutrons to sense not only the presence, but also the velocities and accelerations of individual atoms. Thus, scattering cross sections for slow neutrons depend intimately on the detailed dynamics of the atomic motions.

A general formalism relating the double differential scattering cross section to the dynamical correlation functions which describe atomic motions was given by Van Hove⁶ in 1954. However, the Van Hove formalism is tractable only for highly idealized models of the atomic system, such as the free gas and the isotropic harmonic crystal. For the more complex scatterers of interest in thermal reactor design, some approximations are needed.

The analysis is considerably simplified if only incoherent scattering is considered since this component is related, in Van Hove's formalism, to the dynamics of single atoms. In contrast, coherent scattering depends on the correlated dynamics of pairs of atoms, and is thus much more difficult to calculate. Fortunately, many important moderators contain hydrogen, for which the ratio of coherent to incoherent scattering is only 0.022. Thus, rough approximations to the coherent component of homogeneous scatterers are sufficient. The present document is concerned with calculation of the all-important incoherent component of the scattering. However, the methods are applicable to that component even in cases when coherent scattering is significant.

The S-function

The incoherent scattering cross section (barns/eV steradian) is usually written as¹

$$(1) \quad \sigma_s(E_0 \rightarrow E, \theta) = \frac{\sigma_b}{4\pi kT} \left(\frac{E}{E_0} \right)^{\frac{1}{2}} e^{-\frac{\beta}{2}} S(\alpha, \beta)$$

Here, E_0 and E are the initial and final neutron energies, σ_b is the bound atom cross section, and

$$(2) \quad \alpha = \frac{E_0 + E - 2\sqrt{EE_0} \cos \theta}{AkT}$$

$$\beta = \frac{E - E_0}{kT}$$

The angle θ is the scattering angle in the laboratory system, A is the atomic mass, and T the temperature of the scattering material. The function $S(\alpha, \beta)$ defined by Equation (1) is called the scattering law. For the special cases of the free gas and harmonic crystal (and for some simple approximate models of liquids) $S(\alpha, \beta)$ can be written as a Fourier cosine transform.

$$(3) \quad S(\alpha, \beta) = \frac{1}{\pi} \int_0^{\infty} e^{-\alpha w(t)} \cos \beta t \, dt$$

Here, $w(t)$ is a function related to the time-dependent mean square displacement of an atom away from an initial position. This representation of S is exact only for the simple cases mentioned above. Nonetheless, this form is often assumed to provide an adequate representation in the general case provided that an appropriate $w(t)$ is used. Egelstaff and Schofield¹ showed how to obtain the $w(t)$ from experiment. First, a spectral function $\rho(\beta)$ is defined as

$$(4) \quad \rho(\beta) = \frac{1}{\pi\beta} \sinh \left(\frac{\beta}{2} \right) \cdot \int_0^{\infty} w''(t) \cos \beta t \, dt$$

For a cubic crystal, this function is identical to the distribution of normal modes, while Equation (4) serves to define $\rho(\beta)$ in general. If Equation (3) is integrated twice by parts and the limit $\alpha \rightarrow 0$ is taken, it follows that

$$(5) \quad \rho(\beta) = 2 \cdot \beta \cdot \sinh\left(\frac{\beta}{2}\right) \cdot \lim_{\alpha \rightarrow 0} \frac{S(\alpha, \beta)}{\alpha}$$

Thus, $\rho(\beta)$ can be obtained by extrapolating experimental data to small α . Once $\rho(\beta)$ is known, $w(t)$ can be obtained by inverting the cosine transform in Equation (4) to obtain an expression for $w''(t)$, and then integrating twice. The constants of integration are determined by the Placzek moment relations which imply that

$$(6) \quad w\left(\frac{i}{2}\right) = w'(0) = 0$$

The final result is

$$(7) \quad w(t) = \int_0^{\infty} \rho(\beta) \frac{[\cosh(\beta/2) - \cos \beta t]}{\beta \sinh(\beta/2)} d\beta$$

In summary, if experimental data is interpreted as in Equation (1) to obtain S , the result can be extrapolated as in Equation (5) to obtain ρ . The function w can then be calculated from Equation (7). Finally, S can be computed from Equation (3) and the cross section from Equation (1). This approach is not entirely circular since only discrete values of α need be considered to evaluate the limit in Equation (5), while S can be calculated for arbitrary α and β from Equation (3). Thus, the above method serves to interpolate and extrapolate experimental data. If the temperature dependence of ρ is known, temperature interpolation of S is also provided.

Legendre moments of the cross section

Many computer codes for reactor analysis do not require complete knowledge of $\sigma_s(E_0 \rightarrow E, \theta)$ but only of the first few Legendre moments

$$(8) \quad \sigma_n(E_0 \rightarrow E) = 2\pi \int_{-1}^1 P_n(\cos \theta) \cdot \sigma_s(E_0 \rightarrow E, \theta) d(\cos \theta)$$

These moments can be evaluated in two different ways: If S is available at the desired temperature, the integral in Equation (8) can be carried out numerically using Equation (1) and tabulated values of S . This is the approach used by the FLANGE code.⁷ Alternatively, the integral representation of S (Equation (3)) can be substituted into Equation (8) and the orders of integration interchanged. Since α is a linear function of $\cos \theta$, the integration over $\cos \theta$ can be carried out analytically. If we define

$$(9) \quad B(E, E_0) = \frac{E_0 + E}{AkT}, \quad C(E_0, E) = \frac{2\sqrt{EE_0}}{AkT}$$

then

$$(10) \quad \alpha = B - C \mu$$

In carrying out the integration over $\cos \theta$, the integral representation of the modified spherical Bessel functions is used

$$(11) \quad i_n(x) = \frac{1}{2} \int_{-1}^1 P_n(\mu) e^{x\mu} d\mu$$

In particular

$$i_0(x) = \frac{\sinh x}{x}$$

$$(12) \quad i_1(x) = \frac{1}{x} \left(\cosh x - \frac{\sinh x}{x} \right)$$

$$i_{n+1}(x) = i_{n-1}(x) - \frac{(2n+1)}{x} i_n(x) \quad (n \geq 1)$$

The final result is a representation of the cross section as a Fourier cosine transform

$$(13) \quad \sigma_n(E_0 \rightarrow E) = \frac{\sigma_b}{\pi kT} \left(\frac{E}{E_0} \right)^{\frac{1}{2}} e^{-\frac{\beta}{2}} \times \int_0^{\infty} \cos \beta t e^{-Bw(t)} i_n(Cw(t)) dt$$

It is the cosine transform approach of Equation (13) which is pursued here.

Enhanced convergence of integrals

The form of $w(t)$ at large t has a profound effect both on the shape of S and σ_n near $\beta = 0$ and on the rate of convergence of the integrals in Equations (3) and (13). Since $w(t)$ is related to the mean square displacement of an atom, its asymptotic form at large t is one of the following

$$(14a) \quad w(t) \sim w_{\infty}(t) = \begin{cases} Jt^2 + \frac{K}{4}, & \text{gas} \\ 2 dt, & \text{liquid} \\ W, & \text{solid} \end{cases}$$

Here, J , K , d , and W are appropriate constants. Sometimes a more complicated liquid function is used,

$$(14b) \quad w_{\infty}(t) = 2 d \left(t^2 + c^2 + \frac{1}{4} \right)^{\frac{1}{2}} - e$$

Here, d , c , and e are appropriate constants.

For certain ranges of E_0 and E (or α and β) the integrals in Equations (3) and (13) may include substantial contributions from large values of t , where $w(t)$ has one of the asymptotic forms noted in Equations (14). In these cases it is advantageous to add and subtract the asymptotic form under the integral sign, i.e. Equation (3) becomes

$$(15) \quad S(\alpha, \beta) = S_{\infty}(\alpha, \beta) + \frac{1}{\pi} \int_0^{\infty} \left[e^{-\alpha w(t)} - e^{-\alpha w_{\infty}(t)} \right] \cos \beta t dt$$

with

$$(16) \quad S_{\infty}(\alpha, \beta) = \frac{1}{\pi} \int_0^{\infty} e^{-\alpha w_{\infty}(t)} \cos \beta t dt$$

Similarly, Equation (13) becomes

$$(17) \quad \sigma_n(E_0 \rightarrow E) = \sigma_{n,\infty}(E_0 \rightarrow E) + \frac{\sigma_b}{\pi kT} \left(\frac{E}{E_0}\right)^{\frac{1}{2}} e^{-\frac{\beta}{2}} \times \\ \int_0^{\infty} \cos \beta t \left\{ e^{-Bw(t)} i_n(Cw(t)) - e^{-Bw_{\infty}(t)} i_n(Cw_{\infty}(t)) \right\} dt$$

where

$$(18) \quad \sigma_{n,\infty}(E_0 \rightarrow E) = \frac{\sigma_b}{\pi kT} \left(\frac{E}{E_0}\right)^{\frac{1}{2}} e^{-\frac{\beta}{2}} \int_0^{\infty} \cos \beta t e^{-Bw_{\infty}(t)} i_n(Cw_{\infty}(t)) dt$$

since $w_{\infty}(t)$ is generally a simple function of t , it is often possible to evaluate S_{∞} and $\sigma_{n,\infty}$ in closed form. The results for the forms of $w_{\infty}(t)$ shown in Equation (14) are listed in Appendix I. In situations where S or σ_n have major contributions from large values of t , Equations (15) and (17) provide a more rapid and accurate means of computing S and σ_n than do Equations (3) and (13).

Experience indicates that for calculations of S , Equation (15) is preferred when α is sufficiently small. Similarly, for calculation of $\sigma_n(E_0 \rightarrow E)$, Equation (17) is preferable for sufficiently small E . The precise switching points depend on the details of $\rho(\beta)$.

Numerical evaluation of cosine transforms

As noted above, both S and σ_n can be expressed as Fourier cosine transforms. To outline the method used here for their numerical evaluation, consider a general cosine transform

$$(19) \quad F(\beta) = \int_0^{\infty} f(t) \cos \beta t dt$$

Numerical evaluation of $F(\beta)$ for $\beta > 0$ may pose some difficulty, particularly at large β , where contributions from successive half-cycles of the cosine may be of opposite sign, and large round-off errors may accumulate. In order to confront the problem of large cancellations directly, $F(\beta)$ is written as a sum of contributions from successive half cycles:

$$(20) \quad F(\beta) = \sum_{n=0}^{\infty} G_n(\beta)$$

where

$$(21) \quad G_n(\beta) = \int_{(n - \frac{1}{2}) \frac{\pi}{\beta}}^{(n + \frac{1}{2}) \frac{\pi}{\beta}} f(t) \cos t \, dt$$

(for $n = 0$, the lower limit is replaced by zero) If the terms G_n are evaluated by a quadrature rule, with successive refinement of the partition until some specified precision is reached, then the problem of evaluating the slowly convergent integral in Equation (19) is replaced by the problem of summing the slowly convergent series in Equation (20). A particularly useful technique for summing such a series is provided by the Euler-Van Wijngaarden transformation⁸ which can be written as

$$(22) \quad \sum_{n=0}^{\infty} G_n = G_0 + G_1 + \dots + G_{n-1} + \frac{1}{2} \sum_{j=0}^{\infty} M^j G_n$$

Here, M is the forward mean operator, defined by

$$(23) \quad M G_i = \frac{1}{2} (G_i + G_{i+1})$$

The algorithm (22) is equivalent to the direct summation of the first n terms of the series, followed by Euler transformation of the rest. The success of the Euler transformation is due to the observation that when an alternating series is slowly convergent, the series composed of averages of successive terms often converges much faster. While use of the Euler

transformation does not completely eliminate the problem of cancellations, it at least minimizes their effect. This approach has been used with success by Ekstrom⁴ in the computer program FTRANS, which evaluates general sine and cosine transforms.

As a measure of the success of the above method in a particular case, the number of significant figures in the result can be estimated as follows: Since rounding errors accrued in evaluating the integrand of Equation (19) are of random magnitude and sign, the absolute error in a numerical approximation to the integral may be estimated as

$$(24) \quad A.E. = K. \int_0^{\infty} |f(t) \cos \beta t| dt$$

where K is approximately 10^{-8} for an eight figure machine. The relative error is then approximately

$$(25) \quad R.E. = \frac{K. \int_0^{\infty} |f(t) \cos \beta t| dt}{\left| \int_0^{\infty} f(t) \cos \beta t dt \right|}$$

(this can be quite large, since the integrand changes sign frequently)
An estimate of the number of significant figures in the result is thus

$$(26) \quad S.F. = -\log_{10} (R.E.)$$

The explicit formulas which result when the above method is applied to the computation of S and σ_n from Equations (3) and (13) are given below

$$(27) \quad S(\alpha, \beta) = \frac{1}{\pi} \sum_{n=0}^{\infty} G_n(\beta)$$

with

$$(28) \quad G_n(\beta) = \int_{(n-\frac{1}{2}) \frac{\pi}{\beta}}^{(n+\frac{1}{2}) \frac{\pi}{\beta}} e^{-\alpha w(t)} \cos \beta t dt$$

$$(29) \quad \sigma_n (E_0 \rightarrow E) = \frac{\sigma_b}{\pi kT} \left(\frac{E}{E_0} \right)^{\frac{1}{2}} e^{\frac{\beta}{2}} \sum_{j=0}^{\infty} G_j (\beta)$$

with

$$(30) \quad G_j (\beta) = \frac{1}{|\beta|} \int_{(j-\frac{1}{2})\pi}^{(j+\frac{1}{2})\pi} \cos \tau e^{-Bw\left(\frac{\tau}{|\beta|}\right)} i_n \left(Cw \left(\frac{\tau}{|\beta|} \right) \right) d\tau$$

Analogous expressions result when the same method is applied to evaluate the integrals in Equations (15) and (17).

The elastic case, $E = E_0$ ($\beta = 0$)

For $E = E_0$, Equations (3) and (13) reduce to

$$(31) \quad S(\alpha, 0) = \frac{1}{\pi} \int_0^{\infty} e^{-\alpha w(t)} dt$$

$$(32) \quad \sigma_n (E_0 \rightarrow E_0) = \frac{\sigma_b}{\pi kT} \int_0^{\infty} e^{-Bw(t)} i_n(Cw(t)) dt$$

It follows from Equation (14) that the asymptotic forms of the integrands in Equations (31) and (32) are

$$(33) \quad e^{-\alpha w(t)} \sim \begin{cases} e^{-\alpha J t^2} & , \text{ gas} \\ e^{-2\alpha d t} & , \text{ liquid} \\ \text{constant} & , \text{ solid} \end{cases}$$

$$(34) \quad e^{-Bw(t)} i_n(Cw(t)) \sim \begin{cases} \frac{1}{t^2} & , \text{ gas} \\ \frac{1}{t} & , \text{ liquid} \\ \text{constant} & , \text{ solid} \end{cases}$$

Thus, $S(\alpha, 0)$ is finite for a gas and liquid, but has a delta-function singularity for a solid. Furthermore, $\sigma_n(E_0 \rightarrow E)$ is finite for a gas, has a logarithmic singularity for a liquid, and has a delta-function singularity for a solid. The evaluation of $S(\alpha, 0)$ for the gas and liquid cases is straightforward. If a step length Δ is chosen, (e.g. such that the integrand decays by approximately one-half each time t increases by Δ) then Equation (31) can be written as

$$(35) \quad S(\alpha, 0) = \frac{1}{\pi} \sum_{n=0}^{\infty} \int_{n \cdot \Delta}^{(n+1) \cdot \Delta} e^{-\alpha W(t)} dt$$

Each integral is then evaluated by a quadrature rule to within some specified tolerance, and terms are included in the sum until they become negligible.

For a solid, $S(\alpha, 0)$ is infinite, having the character of a delta-function rising above a smooth inelastic background. This decomposition is exhibited explicitly if, instead of Equation (3), Equation (15) is used. For the case of a solid, Equation (15) becomes

$$(36) \quad S(\alpha, \beta) = e^{-\alpha W} \delta(\beta) + \frac{1}{\pi} \int_0^{\infty} [e^{-\alpha W(t)} - e^{-\alpha W}] \cos \beta t dt$$

Near $\beta = 0$, this gives

$$(37) \quad S(\alpha, \beta) = e^{-\alpha W} \delta(\beta) + \frac{1}{\pi} \int_0^{\infty} [e^{-\alpha W(t)} - e^{-\alpha W}] dt$$

The integral term here can be evaluated in a manner analogous to Equation (35), leading to an explicit representation of $S(\alpha, \beta)$ near $\beta = 0$ for the solid case.

For $\sigma_n (E_0 \rightarrow E)$, a procedure analogous to that outlined above could be followed. However, we choose to develop a different approach here. In practice, the value of σ_n at the point $E = E_0$ is not of great interest. What is needed for reactor analysis is the average of σ_n over a narrow energy group centered about $E = E_0$, i.e.

$$(38) \quad \sigma_n (E_0 \rightarrow E) = \frac{1}{\Delta E} \int_{-\frac{\Delta E}{2}}^{\frac{\Delta E}{2}} \sigma_n (E_0 \rightarrow E) dE$$

Determination of the appropriate ΔE values is discussed in a later section. If Equation (13) is used in Equation (38), and the orders of integration are interchanged, then for the case of narrow energy groups it is possible to write $\bar{\sigma}_n$ in the form

$$(39) \quad \bar{\sigma}_n (E_0 \rightarrow E) = \int_0^{\infty} g_n (E_0, \Delta E, w(t)) dt$$

where g_n is a known function, given in Appendix II. The integral in Equation (39) can be evaluated by breaking it into steps of length Δ , analogous to Equation (35); it converges for all cases of interest: gas, liquid and solid. An enhanced rate of convergence can be obtained by adding and subtracting the large t form of the integrand, i.e.

$$(40) \quad \bar{\sigma}_n (E_0 \rightarrow E_0) = \bar{\sigma}_{n,\infty} (E_0 \rightarrow E_0) + \int_0^{\infty} [g_n (E_0, \Delta E, w(t)) - g_n (E, \Delta E, w_{\infty}(t))] dt$$

Here,

$$(41) \quad \bar{\sigma}_{n,\infty} (E_0 \rightarrow E) = \int_0^{\infty} g_n (E_0, \Delta E, w_{\infty}(t)) dt$$

Values of $\bar{\sigma}_{n,\infty}$ are also given in Appendix II for various forms of $w_\infty(t)$. Once again, the integral in Equation (40) can be evaluated in a manner analogous to Equation (35).

Asymptotic results for large α , β and E_0

For large values of α , β , or E_0 , the computation of S and σ_n may be expedited by using asymptotic expansions. For large α , Egelstaff and Schofield¹ have derived an expansion of S by the method of steepest descents. The appropriate saddle point $z = i\tau$ is defined by

$$(42) \quad w'(i\tau) = i \beta/\alpha$$

For $\beta/\alpha = 0$, the root is at $\tau = 0$, while for $\beta/\alpha = 1$, the root is at $\tau = 1/2$. If we define

$$(43) \quad g(\tau) = -i w'(i\tau) = \int_0^\infty \frac{\sinh \frac{\beta\tau}{2}}{\sinh \frac{\beta}{2}} \rho(\beta) d\beta$$

then τ can be evaluated by Newton's method from the iterative scheme

$$(44) \quad \tau_{n+1} = \tau_n - \frac{g(\tau_n) - \beta/\alpha}{g'(\tau_n)}$$

Once τ is determined, the asymptotic expansion of S proceeds through the following sequence of computations. First, let

$$(45) \quad f_n(\tau) = \begin{cases} -w(i\tau) & , n = 0 \\ -iw'(i\tau) & , n = 1 \\ w''(i\tau) & , n = 2 \\ iw^{(3)}(i\tau) & , n = 3 \\ -w^{(4)}(i\tau) & , n = 4 \end{cases}$$

Then, define

$$(46) \quad C_1(\tau) = \frac{1}{8} (f_4/f_2) - \frac{5}{24} (f_3/f_2)^2$$

Finally

$$(47) \quad S(\alpha, \beta) \sim (2\pi\alpha f_2(\tau))^{-\frac{1}{2}} e^{-\alpha(\tau f_1(\tau) - f_0(\tau))} \left(1 + \frac{1}{\alpha f_2(\tau)} C_1(\tau) + O(\alpha^{-2})\right)$$

Higher order terms are given by Egelstaff and Schofield, but will not be necessary for sufficiently large α . When applicable, Equation (47) provides a much faster computation of S than does Equation (3).

For $\sigma_n (E_0 \rightarrow E)$, application of the short collision time expansion leads to the result that σ_n is formally identical to the corresponding σ_n for a free gas at an effective temperature $\bar{T}$ chosen so that the average atomic kinetic energy is $3/2 k \bar{T}$. It can be shown that⁹

$$(48) \quad \bar{T} = T \cdot \int_0^\infty \frac{\beta}{2} \cdot \coth \frac{\beta}{2} \cdot \rho(\beta) d\beta$$

The expressions for the first two moments for the free gas at temperature T follow from Equation (13) with $w(t) = t^2 + 1/4$:

$$(49a) \quad \sigma_0 (E_0 \rightarrow E) = \left(\frac{\sigma_b A}{8E_0} \right) \left\{ \left[\text{Erf}(X_1) - \text{Erf}(X_2) \right] + e^{-\beta} \left[\text{Erf}(X_3) - \text{Erf}(X_4) \right] \right\}$$

$$(49b) \quad \sigma_1(E_0 \rightarrow E) = \frac{\sigma_b A^2 kT}{4\sqrt{\pi} E_0 \sqrt{E E_0}} \left\{ \left[\sqrt{B+C} e^{-X_1^2} - \sqrt{B-C} e^{-X_2^2} \right] - \frac{\sqrt{\pi}}{4} \left[(2-B-\beta) \left[\text{Erf}(X_1) - \text{Erf}(X_2) \right] + (2-B+\beta) e^{-\beta} \left[\text{Erf}(X_3) - \text{Erf}(X_4) \right] \right] \right\}$$

Here, B, C, and β are in Equations (2) and (9), and

$$\begin{aligned} x_1 &= \frac{1}{2} \left(\sqrt{B+C} + \frac{\beta}{\sqrt{B+C}} \right) & , & & x_3 &= \frac{1}{2} \left(\sqrt{B+C} - \frac{\beta}{\sqrt{B+C}} \right) \\ x_2 &= \frac{1}{2} \left(\sqrt{B-C} + \frac{\beta}{\sqrt{B-C}} \right) & & & x_4 &= \frac{1}{2} \left(\sqrt{B-C} - \frac{\beta}{\sqrt{B-C}} \right) \end{aligned}$$

If both β and E are sufficiently large, these expressions, with T replaced by $\bar{T}$, provide an accurate computation of $\sigma_n (E_0 \rightarrow E)$ in much less time than required with Equation (13).

Energy group widths and the integrated cross sections

Codes for reactor analysis require not only the differential cross sections $\sigma_n (E_0 \rightarrow E)$, but also the integrated cross sections

$$(50) \quad \sigma_n (E) = \int_0^{\infty} \sigma_n (E \rightarrow E') dE'$$

These cross sections may be obtained by experiment, or by integrating the computed differential cross sections. Comparison of the computed and measured $\sigma_n (E)$ provides an additional check on the adequacy of the $\rho(\beta)$ used in the computation. Program TISK provides for a calculation of the integrated cross sections by either of two methods, depending on whether the user specifies a set of energy groups or a set of energy points.

If energy group boundaries are specified, say $0 < EG_1 < EG_2 < \dots < EG_N$, then the group widths are obviously given by

$$(51) \quad \Delta E_1 = EG_1$$

$$\Delta E_n = EG_n - EG_{n-1}, \quad n=2,3,\dots,N$$

Program TISK then locates the midpoint of each energy group:

$$(52) \quad E_1 = EG_1/2$$

$$E_n = (EG_n + EG_{n-1})/2$$

and computes the point-to-point kernels $\sigma_n(E_i \rightarrow E_j)$. The integral in Equation (50) is then approximated by the quadrature rule

$$(53) \quad \sigma_n(E_i) = \sum_{j=1}^N \sigma_n(E_i \rightarrow E_j) \Delta E_j$$

If instead, energy points $E_1 < E_2 < \dots < E_N$ are specified in the input, then program TISK computes the $\sigma_n(E_i \rightarrow E_j)$ for the given energies. An additional energy point is obtained by noting that Equation (13) implies that $\sigma_n(E_0 \rightarrow 0) = 0$. Using these $N + 1$ values of $\sigma_n(E_0 \rightarrow E)$, and computing the integral with trapezoidal integration logic again leads to Equation (53), but with the appropriate ΔE_n now given by

$$(54) \quad \Delta E_1 = E_2/2$$

$$\Delta E_n = (E_{n+1} - E_{n-1})/2, \quad n = 2, 3, \dots, N-1$$

$$\Delta E_N = (E_N - E_{N-1})/2$$

The above integration schemes are only two of many possible ones. To allow for flexibility, the computation of the ΔE_j and the summation in Equation (53) are carried out by separate subroutines (DELTA E and ADDUP). These are easily replaced if the user prefers a different integration logic.

The ΔE_j computed above are used not only in the calculation of the integrated cross sections, but also in the computation of the group averaged cross sections described earlier.

In addition to computing $\sigma_0(E)$ and $\sigma_1(E)$, program TISK uses these results to compute both the transport cross section

$$(55) \quad \sigma_{tr}(E) = \sigma_0(E) - \sigma_1(E)$$

and the average cosine of the scattering angle

$$(56) \quad \bar{\mu}(E) = \sigma_1(E) / \sigma_0(E)$$

at each energy point.

Corrections for oxygen scattering in H₂O

One of the most important moderators is H₂O, in which a minor correction must be added to account for the scattering by oxygen. In the past, this has usually been done by treating oxygen as an ideal gas at temperature T. But since the oxygen and hydrogen are bound together in the same molecule, we suspect that a better tactic is to treat the oxygen as an ideal gas at the effective temperature $\bar{T}$, rather than the thermodynamic temperature T. If we express α and β in terms of the actual temperature and hydrogen mass, as is usual, and write the S-function for H₂O as an effective S per hydrogen atom, the result is

$$(57) \quad S(\alpha, \beta) = S_H(\alpha, \beta) + \frac{\sigma_{b,0}}{2\sigma_{b,H}} \frac{\exp\left(-\frac{|\beta|}{2} - \left(\frac{\alpha}{16} - |\beta|\right)^2 / \left(\frac{\alpha\bar{T}}{4T}\right)\right)}{\sqrt{\pi\alpha\bar{T}/4T}}$$

Here, $S_H(\alpha, \beta)$ is computed from Equation (3) and the appropriate $\rho(\beta)$ for water.

PART II - DESCRIPTION OF CODE

A realization of the procedure outlined in Part I is described here. The resulting package, TISK, consists of two main programs. These are program TSKESS which controls the evaluation of $S(\alpha, \beta)$, and program TSKSIG which controls the evaluation of $\sigma_n(E_0 \rightarrow E)$ for $n = 0$ and $n = 1$. Both of these main programs call upon a common set of subroutines and function routines. The main programs, and most of the subprograms, are applicable to all scatterers for which $S(\alpha, \beta)$ can be represented as in Equation (3). Program TISK is written in Fortran V for the Univac 1108.

Computation of $S(\alpha, \beta)$ - Program TSKESS

The program TSKESS reads input as a NAMELIST (see input instructions), including temperature T and values of α and β . The computation of S proceeds using the following routines.

1. GAS, TAU, WIT. If α is sufficiently large, S is evaluated from Equation (47) by a subroutine GAS. The saddle point is located by a function routine TAU using Equation (44) with $\tau = 1/2$ as a starting guess. Values of $f_n(\tau)$, Equation (45), are generated by a function routine WIT.
2. INFIN, SIMPS, FAMDR. If α is not large, but β is zero, then S is evaluated as in Equation (35) by a subroutine INFIN. The individual integrals in the sum are evaluated by a Simpson integration routine SIMPS. Some of the operations in SIMPS require numeric rounding, which is done by a routine FAMDR.

3. SZER1, MOMENT, GEE, JNT/JDIFF, WIDTH, WASYM. If α is not large or β is not zero, S is evaluated from one of the two equations (3) or (15). When α is sufficiently small, Equation (15) is used, in which case $S_{\infty}(\alpha, \beta)$ is first evaluated by a subroutine SZER1, using the appropriate analytical expression from Appendix I. In either case, the integral (Equation (3) or Equation (15)) is evaluated as in Equations (28) and (22). The Euler sum is accumulated by a subroutine MOMENT. The individual terms G_j are evaluated by a subroutine GEE, using Simpson's rule with successive refinement of the partition. The integrands required by GEE are evaluated by subroutines JNT (if Equation (3) is used) or JDIFF (if Equation (15) is used). Both of these call the function WIDTH for $w(t)$ and a function WASYM for $w_{\infty}(t)$.
4. SOXY. For the case of H_2O , an oxygen contribution may, if desired, be computed, using Equation (57), by the routine SOXY. This contribution is added to the value of S computed above.
5. LINES. In the output of program TSKESS, lines and pages are counted by the routine LINES.

The output of TSKESS consists of (1) the temperature T , (2) the atomic mass A , 3) any information written out by PARMS, 4) for each value of β , a table displaying as a function of α , S , S/α , $2\beta \sinh\left(\frac{\beta}{2}\right)S/\alpha$ and an estimate of significant figures in S . The above information can also be output on tape or on punched cards.

Computation of $\sigma_n(E_0 \rightarrow E)$ - Program TSKSIG

The program TSKSIG reads input as a NAMELIST (see input instructions) including temperature T , free atom cross section σ_f ($\sigma_f = \left(\frac{A}{A+1}\right)^2 \sigma_b$) and energies E . The computation of $\sigma_n(E_0 \rightarrow E)$ proceeds using the following routines.

1. GAS. If both β and E_0 are sufficiently large, the σ_n are evaluated by a subroutine GAS, using Equations (49).
2. SZER1, ELAST, INFIN, SIMPS, FAMDR, E2EINT. If GAS is not used, but $E = E_0$ then the $\bar{\sigma}_n(E_0 \rightarrow E_0)$ are evaluated as in Equation (40). First, the $\bar{\sigma}_{n,\infty}(E_0 \rightarrow E_0)$ are evaluated by the subroutine SZER1, using the appropriate analytical expression from Appendix II. Next, the integral term in Equation (40) is evaluated by the same method as in Equation (35). The sum is accumulated by a subroutine INFIN and individual integrals in the sum are evaluated by a Simpson integration routine SIMPS. Some of the operations in SIMPS require numeric rounding which is done by a routine FAMDR. The integrands required by SIMPS are evaluated by a function routine E2EINT.
3. MOMENT, SZER1, GEE, JNT/JDIFF, WIDTH, WASYM. If neither of the above cases is applicable, the $\sigma_n(E_0 \rightarrow E)$ are evaluated from one of the equations (13) or (17). If E is sufficiently small, Equation (17) is used, in which case $\sigma_{n,\infty}(E_0 \rightarrow E)$ is first evaluated by the routine SZER1 from the analytical expressions in Appendix I. In either case, the integral (Equation (13) or (17)) is evaluated as in Equations (28) and (20). The Euler sum is

accumulated by a subroutine MOMENT. The individual terms G_j are evaluated by a subroutine GEE using Simpson integration with successive refinement of the partition. The integrands are evaluated by the subroutine JNT (if Equation (13) is used) or JDIFF (if Equation (17) is used). Both of these routines call WIDTH to obtain $w(t)$ and WASYM to obtain $w_{\infty}(t)$.

4. DELTAE, ADDUP. After computing the differential cross sections as above, the integrated cross sections are computed as in Equation (53) by the routine ADDUP. The ΔE_j are generated as in Equations (51) or (54) by the routine DELTAE.

5. AUS, LINES, PRINT. In the output, lines and pages are counted by the routine LINES. The $\sigma_n(E_0 \rightarrow E)$ are written out by AUS, and the $\sigma_n(E)$ by PRINT.

The output of TSKSIG consists of (1) the temperature T , (2) the atomic mass A , (3) the free atom cross section, (4) any information written out by PARMS, (5) a list, with entries for each energy pair, of $\frac{\sigma_0(E_0 \rightarrow E)}{\sigma_f}$ and $\frac{\sigma_1(E_0 \rightarrow E)}{\sigma_f}$, and significant figure estimates, (6) $\sigma_0(E_0 \rightarrow E)$ and $\sigma_1(E_0 \rightarrow E)$ written out in a matrix array, (7) tables of $\sigma_0(E)$, $\sigma_1(E)$, $\sigma_{tr}(E)$, and $\bar{\mu}(E)$. The above information can also be output on tape or on punched cards.

Function routings

In addition to the major routines listed above, several function routines are called frequently:

1. COSH , SINH , TANH - evaluate the hyperbolic functions.
2. SHOX - evaluates the spherical Bessel function

$$j_0(x) = \sinh(x)/x,$$
3. HYPER - evaluates the spherical Bessel function $j_i(x)$,
4. EXK1 (x,y) evaluates the function $x K_1(x) e^y$
5. ERF - evaluates the error function
6. DELERF (x,y,z) - evaluates the function

$$e^x (\text{Erf}(y) - \text{Erf}(z)).$$

Error Checking routine

In addition to supplying an estimate of significant figures, program TISK also checks frequently for overflow and attempted division by zero. The subroutine ERRCHK¹⁰ calls the system routines OVERFL and DVCHK for this purpose. ERRCHK is called at the end of each routine, and a RETURN 0 is called if an overflow or attempted division by zero is detected.

Convergence criteria

In the subroutine MOMENT, which accumulates terms in the Euler sum (cf. Equations (27), and (29)), terms are added until the ratio of the last term to the accumulated sum is less in absolute value than an input number, TOLS (4).

In the subroutine GEE, which evaluates the individual terms in the Euler sum, each term G_j is evaluated to a precision of 1×10^{-6} or, when it occurs sooner, until the ratio of the change in the G_j resulting from the most recent partition refinement to the accumulated sum in MOMENT is less in absolute value than an input number, TOLS (3). Thus, if the last few G_j contribute only little to the sum, they need not be evaluated to high accuracy.

In the evaluation of the group average elastic kernels, terms are accumulated by INFIN (cf. Equation (35)) until the ratio of the most recent contribution to the accumulated sum is less in absolute value than an input number, TOLS (2). For the computation of $S(\alpha, 0)$, the values are accumulated by INFIN until the corresponding ratio is less in absolute value than another input number, TOLS (1).

Convergence problems and approximations

Program TISK monitors a number of its own computations and writes an appropriate warning message if a possible difficulty in convergence is noted. These are described here.

If the Euler sum (cf. Equations (27), (29)) accumulated by MOMENT in the computation of $\sigma_n(E_0 \rightarrow E)$ or $S(\alpha, \beta)$ does not converge after thirty terms, the index n of the moment (zero for $S(\alpha, \beta)$) and the ratio of the most recent term to the accumulated sum are written out with the following message:

"() - MOMENT DID NOT CONVERGE; LAST TERM/SUM = ____."

The most recent value of the sum is used in subsequent calculations.

If an individual term G_j (cf. Equations (28), (30)) in the Euler sum for $\sigma_n (E_0 \rightarrow E)$ or $S (\alpha, \beta)$ has not been evaluated to within the desired tolerance after fourteen doublings of the partition for the Simpson integration, then the term index j , the moment index n (zero for $S (\alpha, \beta)$) and the fractional change in the term G_j produced by the most recent partition refinement are written out with the message,

"GEE (___) DID NOT CONVERGE FOR (___) - MOMENT, $(G(N)-G(N-1))/G(N) =$
_____".

The most recent value of G_j is used in subsequent calculations

In the computation of group average elastic cross sections, or of $S (\alpha, 0)$, as in Equation (35), if the sum has not converged to within the specified tolerance after fifty terms, INFIN writes out the ratio of the most recent term to the accumulated sum with the following message:

"INFIN DID NOT CONVERGE AFTER 50 TERMS; LAST TERM/SUM = _____".

The most recent value of the sum is used in subsequent calculations.

If an individual integral in the sum accumulated by INFIN (cf. Equations (35), (37)) has not been evaluated to the desired accuracy after twelve doublings of the partition for the Simpson integration, then the interval of integration and the change in the integral produced by the most recent partition refinement are written out with the message

"SIMPS DID NOT CONVERGE ON INTERVAL ___ TO ___; $(OLD - NEW)/NEW =$ _____".

The most recent value of the integral is used in subsequent calculations.

In the computations for group average elastic cross sections, the expressions (see Appendix II) are not accurate if $\Delta E/2E_0$ is not small compared to 1. If this ratio exceeds 0.25, the following message is written:

" $\Delta E/2E_0 = \text{____}$, THUS, GROUP AVERAGE ELASTIC KERNEL IS ONLY APPROXIMATE."

The elastic kernel will, nonetheless, be evaluated using the approximate expressions.

Model-dependent routines

The four model-dependent routines are DATA, PARMS, WIDTH, and WIT. In general, these routines may be supplied by the user; however, a set applicable to a wide range of scatterers, including H_2O , is included with the TISK package. This particular set is described in Parts III and IV below. A description of the routines in the general case is given below.

WIDTH - This routine generates the function $w(t)$, either from analytical expressions or by direct numerical integration as in Equation (7).

WIT - This is a block data routine containing the following:

- (a) Mass of scattering nucleus in units of neutron mass, stored in a common block labeled /A/.
- (b) An integer (0 through 3) stored in a common block labeled /CHOICE/. If $I=0$, S and σ_n will be computed from Equations (3) and (13). If $I > 0$, Equations (15) and (17)

will be used instead when advantageous. The asymptotic form of $w(t)$ is signalled by the value of I . If $I = 1$, it is $J t^2 + K/4$, if $I = 2$, it is $2 d t$, and if $I = 3$, it is $2 d (t^2 + c^2 + 1/4)^{1/2} - e$.

(c) If $w(t)$ is a diffusive width function, appropriate parameters, d , c , c^2 and e must be stored in a common block labelled /PTE/.

(d) If $w(t)$ is a gas like width function, appropriate parameters J and K must be stored in a common block labelled /PJK/.

(e) A specification of $\rho(\beta)$, either as pointwise data or as parameters for fitting functions. Data for more than one temperature may be included. This data is placed in common accessible to PARMS, WIDTH, and WIT as needed.

PARMS - This routine allows for manipulation of numbers from DATA and from input to produce the following:

(a) Any parameters used by WIDTH and WIT, stored in common blocks accessible to these routines.

(b) The ratio of $\bar{T}$ to T , stored in a common block labeled /TRATIO/

(c) Information on step size and partition used in evaluating integrals, in particular:

(1) The step size used to evaluate $S(\alpha, 0)$ in Equation (35) expressed as $\text{step} = \text{STP}/\alpha$

(2) The initial partition M used to evaluate each integral G_j in Equations (28) and (30).

This is defined through a number STRSIM as

$$M = \text{INT } |\text{STRSIM}/\beta|$$

(3) The value of j beyond which the initial partition used to evaluate G_j can be reduced to four. This is defined in terms of a number of TCH as $(j - \frac{1}{2}) \geq \text{TCH} \cdot |\beta|$.

The numbers STP, STRSIM, and TCH are stored in a common block labeled /STR/

(d) Information on when asymptotic expressions are to be used, and when large t parts of integrals should be treated separately, in particular:

(1) The value of α above which S is evaluated from Equation (47); this is called SU

(2) The value of α below which S is evaluated from Equation (15) rather than Equation (3). This is called SLS.

(3) The value of E below which $\sigma_n(E_0 \rightarrow E)$ is evaluated from Equation (17) rather than Equation (13). This is called SLSIG.

(4) The values of β (GOGAS) and E (EGAS) above which σ_n is evaluated from Equations (49).

The numbers SU, SLS, SLSIG, GOGAS, and EGAS are stored in a common block labelled /SWITCH/.

(e) In the case of a gas-like width function, one additional set of numbers is needed. These are:

$$RKA = (K/A)^{1/2}$$

$$RAJ = (A/J)^{1/2}$$

$$RKJ = (K/J)^{1/2}$$

$$RRJK = (JK)^{-1/2}$$

These numbers are stored in a common block labelled /RRR/.

Any of the model dependent routines have access to the temperature (in eV) through a common block /T/, while the atomic mass is available through a block labeled /A/.

It should be noted that there is some flexibility in the choice of routines which define the contents of /STR/ and /SWITCH/. If these are simply given as numbers, rather than being computed from $\rho(\beta)$, then they may be included in DATA. Similarly, if the parameters J, K, d, c and e must be computed from $\rho(\beta)$ then they may be assigned in PARMS rather than in DATA.

Testing of Program TISK

In order to verify the logic of program TISK, several tests were devised. First, to check the routines which compute and accumulate the

terms of the Euler sum, programs TSKESS and TSKSIG were run with the simple width function $w(t) = t^2 + 1/4$, corresponding to the ideal gas. Results agreed to several figures with the known analytical expressions for this case. Additional tests were based on the scattering model for water described in Part IV. In addition to reconstructing experimental scattering data, the internal consistency of the code was checked by comparing direct computations (Eqs. (3), (13)) with computations using large-time subtraction (Eqs. (15), (17)) and, where applicable, with computations using the asymptotic expressions (Eqs. (47),(49)). Excellent agreement was found in all cases.

Input Instructions - program TSKESS

The input of program TSKESS is in the standard Fortran NAMELIST format (see sample case). The NAMELIST is called TISKS, and consists of the following:

- DENT - Up to 60 alphanumeric characters identifying the case.
- TEMP - Temperature in degrees Kelvin
- ISOXY - An integer, 1 if an oxygen contribution is to be added
(for the case of H_2O) to $S(\alpha, \beta)$; zero otherwise.
- NPCH - An integer, 1 if card output is desired, 0 otherwise.
- NTAPE - An integer, 1 if tape output is desired, 0 otherwise.
- NA - Number of alpha values.
- NB - Number of beta values.
- ALPHA - List of alpha values.
- BETA - List of beta values.

ETOL - List of (four) tolerances to be used in computation
(see Convergence Criteria section, above).

All information on the spectral function is included in the
block data routine DATA (see model-dependent routines, above).

Input instructions - program TSKSIG

The input of program TSKSIG is in the standard Fortran NAMELIST
format (see sample case). The NAMELIST is called TISK, and contains the
following:

- DENT - Up to 60 alphanumeric characters identifying the case.
- TEMP - Temperature in degrees Kelvin
- SIGF - Free atom cross section, arbitrary units.
- NM - Number of highest moment required (0 or 1).
- NE - The absolute value of NE is the number of energies or
groups. If NE is negative, energy points are given; if
NE is positive, energy group boundaries are given.
- E - List of energies (or group boundaries) in ascending order.
- NSTART - An integer, 0 for a normal run, 1 for a restart run.
- NMIN - The energy pair with which the computation begins (1 for
a normal run).
- NPAIR - The number of E pairs for which cross sections are to
be computed (at least $|NE|(|NE| + 1)/2$ for a complete
matrix).
- NEL - An integer, 0 if elastic points ($E = E_0$) are to be
skipped; 1 if they are to be computed.
- NINT - An integer, 0 if the integrated cross sections are not
to be computed, 1 if they are.

- NTAPE - An integer, 1 if tape output is desired, 0 otherwise.
- NPCH - An integer, 1 if card output is desired, 0 otherwise.
- ETOL - A set of (four) tolerances to be used in the computation
(see Convergence Criteria section, above).

All information on the spectral function is included in the block data routine DATA (see model-dependent routines, above).

Sampling and Restart Options of Program TSKSIG

Since the time required to compute a scattering kernel is highly dependent on the complexity of the spectral function and on the particular set of energies used, it is difficult to give precise estimates of running time. In order to allow the user the freedom to experiment, program TSKSIG has provisions for running a subset of a given energy mesh, and for restarting a run which has not been completed because of lack of time.

If an energy mesh $E_1 < E_2 < \dots < E_N$ has been given, then the cross sections are computed in the order $\sigma(E_1 \rightarrow E_1)$, $\sigma(E_2 \rightarrow E_1)$, $\sigma(E_2 \rightarrow E_2)$, $\sigma(E_3 \rightarrow E_1)$, $\sigma(E_3 \rightarrow E_2)$, $\sigma(E_3 \rightarrow E_3)$, etc. If it is desired to sample the results by beginning the computation with the n^{th} energy pair and computing for the next N pairs, then in the input list, set $NMIN = n$, and $NPAIR = N$. (see input instructions).

In order to allow for restarting a run which has not been completed, it is first necessary that card output have been obtained for that run ($NPCH = 1$ in original input list). For every five energy pairs, and each moment, a card will have been punched listing the number of

the first energy pair, the moment index (0 or 1) and the five computed values of cross sections (Format 2I5, 5E12.5). In order to restart the run, simply resubmit the original input cards, changing (if necessary) only NSTART to be 1. After the original input cards, append the punched cards obtained in the original run. Program TSKSIG will then call a subroutine RESTRT to read in the new punched cards and determine the appropriate starting point for the computation to resume.

PART III - REPRESENTATION OF THE SPECTRAL FUNCTION $\rho(\beta)$

For most scatterers of interest, the spectral function $\rho(\beta)$ has the form of a series of resonance-like peaks corresponding to (hindered) translations, rotations and vibrations of the molecule. Lindenmeier^{2,3} has suggested that the experimental $\rho(\beta)$ be fit with a series of analytical functions for which the integral in Eq.(7) leading to $w(t)$ can be carried out in closed form, thus eliminating the need for a time-consuming and possibly inaccurate numerical evaluation of $w(t)$. The fitting functions have the form

$$(56) \quad \rho_i(\beta) = \frac{1}{N_i} \beta \sinh \frac{\beta}{2} \left[e^{-\frac{(\beta-\gamma_i)^2}{4\delta_i}} + e^{-\frac{(\beta+\gamma_i)^2}{4\delta_i}} \right]$$

where N_i is chosen so that

$$(57) \quad \int_0^{\infty} \rho_i(\beta) d\beta = 1$$

i.e.

$$(58) \quad N_i = 2\sqrt{\pi\delta_i} e^{\delta_i/4} \left[\gamma_i \sinh \frac{\gamma_i}{2} + \delta_i \cosh \frac{\gamma_i}{2} \right]$$

For positive β , each $\rho_i(\beta)$ has a peak centered at approximately $\beta = \gamma_i + \delta_i$. The full width at half maximum is approximately $4\sqrt{\ln 2} \sqrt{\delta_i}$.

The corresponding $w_i(t)$ are found from Eq. (7) to be

$$(59) \quad w_i(t) = A_i - B_i e^{-\delta_i t^2} \cos \gamma_i t$$

where

$$(60) \quad A_i = \frac{\cosh \frac{\gamma_i}{2}}{\gamma_i \sinh \frac{\gamma_i}{2} + \delta_i \cosh \frac{\gamma_i}{2}}$$

$$(61) \quad B_i = \frac{e^{-\delta_i/4}}{\gamma_i \sinh \frac{\gamma_i}{2} + \delta_i \cosh \frac{\gamma_i}{2}}$$

For β very near zero, $\rho(\beta)$ may have an additional peak corresponding to a free or hindered translation of the molecule. The peak is absent for a solid, while for a gas it has the form of a delta function:

$$(62) \quad \rho_0(\beta) = J \cdot \delta(\beta)$$

with J a constant. The corresponding contribution to $w(t)$ is

$$(63) \quad w_0(t) = J \cdot (t^2 + 1/4)$$

For a liquid, the precise form of $\rho(\beta)$ near $\beta = 0$ is not known, but Egelstaff and Schofield² have suggested

$$(64) \quad \rho_0(\beta) = \frac{4d}{\pi} \frac{\sinh \beta/2}{\beta} x K_1(x)$$

with

$$x = (c^2 + 1/4)^{1/2} \beta$$

and d and c constants. The corresponding contribution to $w(t)$ is

$$(65) \quad w_0(t) = 2d \left[(t^2 + c^2 + 1/4)^{1/2} - c \right].$$

Combining the small $-\beta$ peak with a sum of resonances with weights $1/M_i$ leads to

$$(66) \quad \rho(\beta) = \rho_0(\beta) + \sum_{i=1}^N \frac{1}{M_i} \rho_i(\beta)$$

and, correspondingly,

$$(67) \quad w(t) = w_0(t) + \sum_{i=1}^N \frac{1}{M_i} w_i(t)$$

This form of $w(t)$ is easily programmed into the function routine WIDTH. The derivatives are also easily computed analytically; since

$$\begin{aligned}
 w_i'(t) &= B_i e^{-\delta_i t^2} \left[\gamma_i \sin \gamma_i t + 2t\delta_i \cos \gamma_i t \right] \\
 w_i''(t) &= B_i e^{-\delta_i t^2} \left[(\gamma_i^2 + 2\delta_i - 4\delta_i^2 t^2) \cos \gamma_i t \right. \\
 &\quad \left. - 4\delta_i \gamma_i t \sin \gamma_i t \right] \\
 (68) \quad w_i'''(t) &= B_i e^{-\delta_i t^2} \left[(12\delta_i^2 \gamma_i t^2 - 6\delta_i \gamma_i - \gamma_i^3) \sin \gamma_i t \right. \\
 &\quad \left. - (12\delta_i^2 t + 6\delta_i \gamma_i^2 t - 8\delta_i^3 t^3) \cos \gamma_i t \right] \\
 w_i^{(4)}(t) &= B_i e^{-\delta_i t^2} \left\{ \left[8\delta_i \gamma_i t (\gamma_i^2 + 6\delta_i - 4\delta_i^2 t^2) \right] \sin \gamma_i t \right. \\
 &\quad \left. - \left[8\delta_i^2 t^2 (12\delta_i^2 t^2 - 6\delta_i - 3\gamma_i^2) \right. \right. \\
 &\quad \left. \left. - 12\delta_i^2 - 12\delta_i \gamma_i^2 - \gamma_i^4 \right] \cos \gamma_i t \right\}
 \end{aligned}$$

If higher order derivatives are required, they may be obtained through a recursion relation. Again, defining $t = i\tau$ we have

$$w_i(i\tau) = A_i - B_i P(\tau),$$

where

$$(69) \quad P(\tau) = \cosh(\gamma_i \tau) e^{\delta_i \tau^2}.$$

Then, taking n derivatives gives

$$w_i^{(n)}(t) = -B_i (-i)^n P^{(n)}(\tau), \quad (n \geq 1).$$

Define

$$Q = \sinh(\gamma_i \tau) e^{\delta_i \tau^2}$$

Then the n^{th} derivative of P will have the form

$$(70) \quad P^{(n)}(\tau) = a_n(\tau) P(\tau) + b_n(\tau) Q(\tau)$$

where $a_n(\tau)$ and $b_n(\tau)$ are polynomials in τ . Expressing the n^{th} derivative in terms of the $(n-1)^{\text{th}}$ gives

$$P^{(n)}(\tau) = \frac{d}{d\tau} P^{(n-1)}(\tau) =$$

$$a_{n-1}(\tau) P'(\tau) + a'_{n-1}(\tau) P(\tau) + b_{n-1}(\tau) Q'(\tau) + b'_{n-1}(\tau) Q(\tau) .$$

However,

$$P'(\tau) = \gamma Q(\tau) + 2\delta\tau P(\tau)$$

and

$$Q'(\tau) = \gamma P(\tau) + 2\delta\tau Q(\tau)$$

so that

$$(71) \quad a_n = a'_{n-1} + 2\delta\tau a_{n-1} + \gamma b_{n-1}$$

and

$$b_n = b'_{n-1} + 2\delta\tau b_{n-1} + \gamma a_{n-1} .$$

Now, let

$$a_n(\tau) = \sum_{p=0}^n \alpha_{n,p} \tau^p$$

and

$$b_n(\tau) = \sum_{p=0}^n \beta_{n,p} \tau^p .$$

Then

$$\sum_{p=0}^n \alpha_{n,p} \tau^p = \left\{ \sum_{p=1}^n p \alpha_{n-1,p} \tau^{p-1} + 2\delta \sum_{p=0}^n \alpha_{n-1,p} \tau^{p+1} + \gamma \sum_{p=0}^n \beta_{n-1,p} \tau^p \right\}$$

and similarly for b_n .

Equating terms in τ^p gives

$$(72) \quad \alpha_{n,p} = (p+1) \alpha_{n-1,p+1} + 2\delta \alpha_{n-1,p-1} + \gamma \beta_{n-1,p}$$

$$\beta_{n,p} = (p+1) \beta_{n-1,p+1} + 2\delta \beta_{n-1,p-1} + \gamma \alpha_{n-1,p}.$$

Noting that the initial conditions are $a_0 = 1$ and $b_0 = 0$, we find

$$\alpha_{n,p} = 0, \quad n+p \text{ odd}$$

$$\beta_{n,p} = 0, \quad n+p \text{ even}.$$

This suggests defining

$$\begin{aligned} c_{n,p} &= \alpha_{n,p} \tau^p, \quad n+p \text{ even} \\ &= \beta_{n,p} \tau^p, \quad n+p \text{ odd.} \end{aligned}$$

From equation (72), the $c_{n,p}$ are seen to satisfy

$$(73) \quad c_{n,p} = \frac{(p+1)}{\tau} c_{n-1,p-1} + 2\delta\tau c_{n-1,p+1} + \gamma c_{n-1,p}$$

where

$$c_{0,0} = 1, \quad c_{1,0} = \gamma, \quad c_{1,1} = 2\delta\tau.$$

The n^{th} derivative of $w_i(i\tau)$ is thus

$$(74) \quad w_i^{(n)}(i\tau) = -B_i (-i)^n \left\{ P(\tau) \cdot \sum_{\substack{p=0 \\ (n+p) \\ \text{even}}}^n c_{n,p} \right. \\ \left. + Q(\tau) \cdot \sum_{\substack{p=0 \\ (n+p) \\ \text{odd}}}^n c_{n,p} \right\}.$$

These are easily programmed into the routine WIT. Similarly, a closed form expression for $\bar{T}$ follows from Eq. (48).

$$(75) \quad \left(\frac{\bar{T}}{T} \right) = \left\{ \frac{d}{c} \left(1 + \frac{1}{4c^2} \right) \right\} \\ + \sum_{i=1}^N \frac{\delta_i \gamma_i \sinh \frac{\gamma_i}{2} + \left(\frac{\gamma_i^2}{2} + \delta_i + \frac{\delta_i^2}{2} \right) \cosh \frac{\gamma_i}{2}}{M_i \left(\gamma_i \sinh \frac{\gamma_i}{2} + \delta_i \cosh \frac{\gamma_i}{2} \right)}.$$

It must be emphasized that the above expressions are not the only ones that may be used with TISK. However, the flexible sum of resonance peaks with many adjustable parameters can be made to fit most experimental spectral functions quite well, and the analytical expressions for $w(t)$ and its derivatives, and for $\bar{T}$, are easily programmed and efficient computation is guaranteed. Thus, this approach will usually be preferred.

An additional merit of the present representation scheme is that the parameters STP, STRSIM and TCH (see description of PARMS above) which regulate the step size and initial partition used to evaluate integrals in GEE are easily obtained.

To obtain STP, we note that in evaluating $S(\alpha, 0)$ from Eq. (35), it is reasonable to choose the step size Δ so that the integrand decays by one half for each time step of duration Δ . Requiring $\exp(-\alpha[w(\Delta) - w(0)]) = 1/2$ and estimating $w(t)$ by $2 \int_0^t d\tau$ leads to the estimate $\Delta = \ln 2 / 2d\alpha$, so that $STP = \ln 2 / 2d$.

To obtain STRSIM, we note that in evaluating G_j from Eq. (30), it is desired to pick an initial partition for an interval of length $\pi/|\beta|$. If we require that the partition be fine enough so that the period of the fastest of the oscillatory terms $(\cos(\frac{\gamma_i t}{|\beta|}))$ in $w(t/|\beta|)$ contains at least four mesh points, then the interval must be partitioned into at least $\frac{2\gamma_{\max}}{|\beta|}$ subintervals. Since this is not generally an integer, we take $M = \text{INT} \left\lceil \frac{2\gamma_{\max}}{|\beta|} \right\rceil$, so that $STRISM = 2\gamma_{\max}$.

To obtain TCH, we note that the oscillating parts of $w(t/|\beta|)$ decay as $\exp(-\delta_j t^2 / \beta^2)$. For t large enough, these terms vanish and $w(t/|\beta|)$ has much less structure. The partition can then be relaxed, say to $M = 4$. For G_j , the exponential terms in $w(t/|\beta|)$ are certainly less than 0.001 if

$$\delta_{\min} \left(\frac{(j-1/2)\pi}{|\beta|} \right)^2 > \ln(.001), \text{ i.e., if } (j-1/2) \geq \frac{(-\ln(.001))^{1/2} |\beta|}{\pi \sqrt{\delta_{\min}}}.$$

Thus, we take $TCH = 0.8366 / \sqrt{\delta_{\min}}$.

An approximate temperature interpolation of $\rho(\beta)$ over a narrow range of T about the experimental temperature is provided by the observation that, for a harmonic crystal, the normal mode distribution is independent of T when expressed in frequency units, i.e.,

$\rho(\omega) = \rho(\beta) \left| \frac{d\beta}{d\omega} \right|$ with $\rho = \frac{\hbar\omega}{kT}$. For the $\rho_i(\beta)$, this is equivalent to taking $\gamma_i T$ and $\delta_i T$ to be independent of temperature. Since $\rho(\beta)$ is constant only for the harmonic crystal, and not in general, this approximation will not be adequate for extrapolating to temperatures far removed from the experimental one. In these cases, it will be necessary to use data for a number of temperatures to determine the appropriate T -dependence of the fitting parameters.

PART IV - APPLICATION TO H₂O

In order to obtain a scattering kernel for room temperature water, the fitting functions of Part III were applied to the measured $\rho(\beta)$ of Haywood¹¹ and Harling¹². Since the Haywood experiment was sensitive primarily to the low range of beta, while the Harling experiment was sensitive primarily to the intermediate range of beta ($3 < \beta < 11$), we chose the fitting parameters to match the Haywood data for $\beta < 3$ and the Harling data for $\beta > 3$. Five resonances were used to fit the data between $0.25 < \beta < 11$, and an additional resonance was added to represent the unresolved vibrational modes at $\beta \approx 17$. For the unresolved diffusive peak at $\beta = 0$, we used the Egelstaff-Schofield expression with $d = 0.04$ (consistent with the measured diffusion coefficient of water) and $c = 100$ (as recommended by Egelstaff and Schofield). The final choice of resonance fitting parameters is

i	M_i	center $(\gamma_i + \delta_i)kT$	full width $(4\sqrt{\lambda n^2} \sqrt{\delta_i})kT$
1	35.8	0.0087 (eV)	0.0159 (eV)
2	95.0	0.0287	0.011
3	2.94	0.0638	0.058
4	5.25	0.174	0.110
5	9.10	0.206	0.023
6	3.1188	0.459	0.070

The above choices reproduce the experimental data fairly well. The treatment of oxygen as an ideal gas at temperature $\bar{T}$, rather than temperature T , greatly improves the agreement with the data at large α .

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APPENDIX I

 $S(\alpha, \beta)$ and $\sigma_n(E_0 \rightarrow E)$ for simple $w(t)$

When $w(t)$ is simple, the integrals in Eqs. (3) and (13) can be evaluated in closed form. In particular, we obtain analytical expressions for $S_\infty(\alpha, \beta)$ and $\sigma_{n,\infty}(E_0 \rightarrow E)$. In all of the expressions below, B , C and β are defined in Eqs. (2) and (9).

1. For $w(t) = Jt^2 + K/4$ (J, K constants)

$$S(\alpha, \beta) = \frac{1}{\sqrt{4\pi J\alpha}} \exp \left(-\frac{K}{4}\alpha - \frac{\beta^2}{4J\alpha} \right)$$

$$\begin{aligned} \sigma_0(E_0 \rightarrow E) &= \frac{\sigma_b A}{8E_0} e^{-\beta/2} \left\{ e^{\sqrt{\frac{K}{J}} \frac{\beta}{2}} [\text{Erf}(y_1) - \text{Erf}(y_2)] \right. \\ &\quad \left. + e^{-\sqrt{\frac{K}{J}} \frac{\beta}{2}} [\text{Erf}(y_3) - \text{Erf}(y_4)] \right\} \\ \sigma_1(E_0 \rightarrow E) &= \frac{\sigma_b A}{8E_0} \frac{e^{-\beta/2}}{C\sqrt{JK}} \left\{ \frac{4}{\sqrt{\pi K}} [\sqrt{B+C} e^{-y^2} - \sqrt{B-C} e^{-y^2}] \right. \\ &\quad + \left(\frac{2}{K} - B - \frac{\beta}{\sqrt{JK}} \right) e^{\sqrt{\frac{K}{J}} \frac{\beta}{2}} [\text{Erf}(y_2) - \text{Erf}(y_1)] \\ &\quad \left. + \left(\frac{2}{K} - B + \frac{\beta}{\sqrt{JK}} \right) e^{-\sqrt{\frac{K}{J}} \frac{\beta}{2}} [\text{Erf}(y_4) - \text{Erf}(y_3)] \right\} \end{aligned}$$

In the above expressions,

$$y_1 = \frac{1}{2} \left(\sqrt{K(B+C)} + \frac{\beta}{2\sqrt{J(B+C)}} \right), \quad y_3 = \frac{1}{2} \left(\sqrt{K(B+C)} - \frac{\beta}{2\sqrt{J(B+C)}} \right)$$

$$y_2 = \frac{1}{2} \left(\sqrt{K(B-C)} + \frac{\beta}{2\sqrt{J(B-C)}} \right), \quad y_4 = \frac{1}{2} \left(\sqrt{K(B-C)} - \frac{\beta}{2\sqrt{J(B-C)}} \right)$$

2. For $w(t) = 2 \, dt$ (d constant)

$$S(\alpha, \beta) = \frac{1}{\pi} \frac{2d\alpha}{(2d\alpha)^2 + \beta^2}$$

$$\sigma_0(E_0 \rightarrow E) = \frac{\sigma_b A}{16 \pi d E_0} e^{-\beta/2} \ln \left(\frac{[2d(B+C)]^2 + \beta^2}{[2d(B-C)]^2 + \beta^2} \right)$$

$$\sigma_1(E_0 \rightarrow E) = \frac{B}{C} \sigma_0(E_0 \rightarrow E)$$

$$+ \frac{\sigma_b A}{16 \pi d E_0} e^{-\beta/2} \left(\frac{\beta}{dC} \left[\tan^{-1} \left(\frac{2d(B+C)}{\beta} \right) - \tan^{-1} \left(\frac{2d(B-C)}{\beta} \right) \right] - 1 \right)$$

3. For $w(t) = W$ (W constant)

$$S(\alpha, \beta) = e^{-\alpha W} \delta(\beta)$$

$$\sigma_n(E_0 \rightarrow E) = \frac{\sigma_b}{2kT} e^{-BW} i_n(CW) \cdot \delta(\beta)$$

4. For $w(t) = 2 \, d [(t^2 + c^2 + 1/4)^{1/2} - a]$ (d, a constants)

$$S(\alpha, \beta) = \frac{2d\alpha e^{2da\alpha}}{\pi[(2d\alpha)^2 + \beta^2]} \cdot x K_1(x),$$

$$x = [(c^2 + 1/4) ((2d\alpha)^2 + \beta^2)]^{1/2}$$

Expressions for $\sigma_n(E_0 \rightarrow E)$ have not been obtained for this $w(t)$.

APPENDIX II

Group Average Elastic Cross Sections

For narrow energy groups, the group average elastic cross sections $\overline{\sigma}_n(E_0 \rightarrow E_0)$ can be computed as follows. From Eq. (2) and (9),

$$B = \left(\frac{2E_0}{AkT} \right) \left(1 + \frac{kT\beta}{2E_0} \right)$$

$$C = \left(\frac{2E_0}{AkT} \right) \left(1 + \frac{kT\beta}{E_0} \right)^{1/2}$$

Thus,

$$B + C = \left(\frac{4E_0}{AkT} \right) \left(1 + O\left(\frac{\beta kT}{2E_0} \right) \right)$$

$$B - C = \left(\frac{kT\beta^2}{4AE_0} \right) \left(1 + O\left(\frac{\beta kT}{2E_0} \right) \right)$$

Ignoring terms of order $\frac{\beta kT}{2E_0}$, and using these expressions in Eq. (13) leads to

$$\sigma_0(E_0 \rightarrow E) \simeq \left(\frac{\sigma_b A}{2\pi E_0} \right) \int_0^\infty \frac{1}{2w(t)} e^{-\beta/2} \cos \beta t$$

$$\left\{ e^{-\left(\frac{kT\beta^2}{4AE_0} \right)} w(t) - e^{-\left(\frac{4E_0}{AkT} \right)} w(t) \right\} dt$$

for E near E_0 . To compute the group average, let $\Delta\beta = \Delta E/kT$ and average the above equation over $\Delta\beta$. Interchanging orders of integration leads to

$$\overline{\sigma}_0(E_0 \rightarrow E) = \left(\frac{\sigma_b A}{2\pi E_0} \right) \int_0^\infty \frac{1}{2w(t)} \left[1 + e^{-\left(\frac{4E_0}{AkT} \right) w(t)} K(t, \Delta\beta) \right] dt$$

where

$$\begin{aligned} K(t, \Delta\beta) &= \frac{1}{\Delta\beta} \int_{-\frac{\Delta\beta}{2}}^{\frac{\Delta\beta}{2}} e^{-\beta/2} \cos \beta t \, d\beta \\ &= \left[\frac{\sinh(\Delta\beta/4)}{\Delta\beta} \cdot \cos\left(\frac{\Delta\beta t}{2}\right) + \cosh\left(\frac{\Delta\beta}{4}\right) \frac{t \sin\left(\frac{\Delta\beta t}{2}\right)}{(\Delta\beta/2)} \right] \cdot \left(t^2 + \frac{1}{4}\right)^{-1} \end{aligned}$$

and

$$I = \frac{1}{\Delta\beta} \int_{-\frac{\Delta\beta}{2}}^{\frac{\Delta\beta}{2}} e^{-\beta/2} \cos \beta t \, e^{-\left(\frac{kT}{4AE_0} \right) w(t) \beta^2} \, d\beta$$

Since $\Delta\beta$ is small, I can be approximated by

$$I \simeq e^{-\frac{kTw(t) \langle \beta^2 \rangle}{4AE_0}} K(t, \Delta\beta)$$

where

$$\langle \beta^2 \rangle \equiv \frac{\int_{-\frac{\Delta\beta}{2}}^{\frac{\Delta\beta}{2}} \beta^2 e^{-\beta/2} \, d\beta}{\int_{-\frac{\Delta\beta}{2}}^{\frac{\Delta\beta}{2}} e^{-\beta/2} \, d\beta} = 8 + \frac{(\Delta\beta)^2}{4} - 2\Delta\beta \coth\left(\frac{\Delta\beta}{4}\right)$$

The final result is

$$\overline{\sigma}_0(E_0 \rightarrow E) = \int_0^\infty g_0(E_0, \Delta E, w(t), t) \, dt$$

where

$$g_0(E_0, \Delta E, w(t), t) = \left(\frac{\sigma_b A}{4\pi E_0} \right) \cdot \frac{1}{w(t)} \cdot \left\{ e^{-\frac{kT \langle \beta^2 \rangle}{4AE_0} w(t)} - e^{-\left(\frac{4E_0}{AkT} \right) w(t)} \right\} \cdot K(t, \Delta \beta) .$$

Applying identical approximations to $\overline{\sigma_1}(E_0 \rightarrow E_0)$ leads to

$$\overline{\sigma_1}(E_0 \rightarrow E_0) = \int_0^\infty g_1(E_0, \Delta E, w(t), t) dt$$

where

$$g_1(E_0, \Delta E, w(t), t) = \left(\frac{\sigma_b A}{2\pi E_0} \right) \frac{1}{w(t)} \cdot \left\{ e^{-\left(\frac{kT \langle \beta^2 \rangle}{4AE_0} \right) w(t)} \left(1/2 - \frac{AkT}{4E_0 w(t)} \right) + e^{-\left(\frac{4E_0}{AkT} \right) w(t)} \left(1/2 + \frac{AkT}{4E_0 w(t)} \right) \right\} \cdot K(t, \Delta \beta) .$$

Appendix III

Sample Cases

INPUT - PROGRAM TSKESS

'MT FR5 DATA,DATA

BLOCK DATA

C SAMPLE CASE
C LIGHT WATER, T = 293 K,
C SIX RESONANCE FIT TO RHO(BETA).
C RESONANCE WEIGHT = 1/AM(I),
C RESONANCE PEAK AT AL(I) (EV),
C RESONANCE WIDTH (FWHM) = WTH(I) (EV).

COMMON/A/AMASS

COMMON/CHOICE/CHOICE

COMMON/PTE/PD,PC,PCS,PE

COMMON/SCPS/N,AM(10),AL(10),WTH(10)

COMMON/SWITCH/SU,SLS,SLSIG,GOGAS,EGAS

DATA AMASS/1./, PC/100./, PD/0.04/

DATA N./6/

DATA (AM(I),AL(I),WTH(I),I=1,6)/35.8, .0087, .0159, 95.0, .0287,

2 0.011,2.94, .0638, .0580, 5.25, .174, .110, 9.1, .206, .023,

3 3.1188, 0.459, 0.070 /

DATA SU/30./, SLS/1./,SLSIG/0.025/,GOGAS/25./,EGAS/1.0/

DATA CHOICE/3/

END

' XQT TSKESS

\$TISKS DENT=50H TISK, WATER 293K, 6 RES FIT TO RHO(BETA).

TEMP=293., ISOXY=0, NA=4, NB=4,

ALPHA=5., 10., 15., 20.,

BETA=1., 2., 5., 10.,

ETOL=5.E-5, 5.E-4, 5.E-5, 5.E-4

\$

-50-

BNWL-1675

OUTPUT -PROGRAM TSKESS

PROGRAM TSKESS

TISK, WATER 293K, 6 RES FIT TO RHO(BETA).

TEMPERATURE = 2.9300000+02 OR 2.5246286-02EV

MASS OF SCATTERING NUCLEUS = 1.0000000+00

FITTING PARAMETERS FOR RHO(BETA)

D = 4.0000000-02

C = 1.0000000+02

REGION	WEIGHT	ENERGY	WIDTH
1	3.5800000+01	8.6999998-03	1.5900000-02
2	9.5000000+01	2.8700000-02	1.1000000-02
3	2.9400000+00	6.3800000-02	5.7999999-02
4	5.2500000+00	1.7400000-01	1.1000000-01
5	9.0999999+00	2.0600000-01	2.3000000-02
6	3.1188000+00	4.5900000-01	6.9999999-02

$W(T) = 2D(\text{SQRT}(T*T+C*C+1/4)-C) + \text{SUM}(A(I)-B(I)*\text{EXP}(-\text{DEL}(I)*T*T)*\text{COS}(\text{GAM}(I)*T))$

I	A(I)	B(I)	DEL(I)	GAM(I)
1	3.3621503-01	3.2928840-01	3.5765032-02	3.0884011-01
2	1.7970360-02	1.5414276-02	1.7117871-02	1.1196830+00
3	1.6513760-01	9.3166629-02	4.7590511-01	2.0511993+00
4	2.7871284-02	2.7102178-03	1.7117871+00	5.1803157+00
5	1.3475787-02	4.6423471-04	7.4837632-02	8.0847783+00
6	1.7635887-02	4.7289027-06	6.9320302-01	1.7487689+01

IRATIO = .4693617+01

BETA = 1.0000000+00

ALPHA	S-FUNCTION	S/ALPHA	2B.SH(B/2).S/AL	EST.SIG.FIGS.
5.0000000+00	6.2161605-02	1.2432321-02	1.2956848-02	7.4634894+00
1.0000000+01	3.6682934-02	3.6682934-03	3.8230608-03	7.8929206+00
1.5000000+01	1.6959202-02	1.1306134-03	1.1783147-03	7.9873002+00
2.0000000+01	7.5492105-03	3.7746052-04	3.9338581-04	8.0119299+00

BETA = 5.0000000+00

ALPHA	S-FUNCTION	S/ALPHA	2B.SH(B/2).S/AL	EST.SIG.FIGS.
5.0000000+00	3.7358573-03	7.4717146-04	4.5205400-02	6.5388596+00
1.0000000+01	4.6243049-03	4.6243048-04	2.7977990-02	7.2193052+00
1.5000000+01	3.5365634-03	2.3577090-04	1.4264621-02	7.5384990+00
2.0000000+01	2.2366958-03	1.1183479-04	6.7662335-03	7.7089773+00

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BETA = 1.0000000+01

ALPHA	S-FUNCTION	S/ALPHA	2B.SH(B/2).S/AL	EST.SIG.FIGS.
5.0000000+00	1.3816100-04	2.7632199-05	4.1007958-02	5.1234374+00
1.0000000+01	2.5191256-04	2.5191256-05	3.7385440-02	6.0181922+00
1.5000000+01	2.7221692-04	1.8147794-05	2.6932491-02	6.5040286+00
2.0000000+01	2.3315640-04	1.1657820-05	1.7300953-02	6.8204056+00

BETA = 2.0000000+00

ALPHA	S-FUNCTION	S/ALPHA	2B.SH(B/2).S/AL	EST.SIG.FIGS.
5.0000000+00	3.2142192-02	6.4284384-03	3.0218834-02	7.2878824+00
1.0000000+01	2.2615780-02	2.2615780-03	1.0631236-02	7.7778993+00
1.5000000+01	1.2218800-02	8.1458668-04	3.8292129-03	7.9266610+00
2.0000000+01	6.0340883-03	3.0170441-04	1.4182535-03	7.9830234+00

BNM-1675

Because of the space required, we have elected not to reproduce the output for a completely realistic case of program TISKSIG here. Rather, we have run TSKSIG for the lowest ten energy points of a standard 101 group mesh. While this provides a suitable test case, it does mean that the resulting integrated cross sections, and the corresponding average cosines are not computed accurately here.

INPUT - PROGRAM TSKSIG

IMT FR5 DATA,DATA

BLOCK DATA

C SAMPLE CASE
C LIGHT WATER, T = 293 K,
C SIX RESONANCE FIT TO RHO(BETA).
C RESONANCE WEIGHT = 1/AM(I),
C RESONANCE PEAK AT AL(I) (EV),
C RESONANCE WIDTH (FWHM) = WTH(I) (EV).

COMMON/A/AMASS

COMMON/CHOICE/CHOICE

COMMON/PTE/PD,PC,PCS,PE

COMMON/SCPS/N,AM(10),AL(10),WTH(10)

COMMON/SWITCH/SU,SLS,SLSIG,GOGAS,EGAS

DATA AMASS/1./, PC/100./, PD/0.04/

DATA N /6/

DATA (AM(I),AL(I),WTH(I),I=1,6)/35.8, .0087, .0159, 95.0, .0287,

2 0.011,2.94, .0638, .0580, 5.25, .174, .110, 9.1, .206, .023,

3 3.1188, 0.459, 0.070 /

DATA SU/30./, SLS/1./,SLSIG/0.025/,GOGAS/25./,EGAS/1.0/

DATA CHOICE/2/

END

XQT TSKSIG

\$TISK DENT=50H TISK,WATER 293K 6RES FIT TO RHO(BETA)

TEMP=293., SIGF=1.0, NM=1,

NE=-10,

E=0.001, 0.002, 0.004, 0.0065, 0.01, 0.015, 0.02, 0.0253, 0.033, 0.041,

NSTART=0, NMIN=1, NPAIR=200, NEL=1, NINT=1, NTAPE=0, NPCH=0,

ETOL=5.E-5,-5.E-4,-5.E-5,-5.E-4

\$

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BNWL-1675

OUTPUT-PROGRAM TSKSIG

TEMPERATURE = 2.9300000+02 OR 2.5246286+02EV

MASS OF SCATTERING NUCLEUS = 1.0000000+00

FREE ATOM SCATTERING CROSS SECTION = 1.0000000+00

FITTING PARAMETERS FOR RHO(BETA)

D = 4.0000000-02

C = 1.0000000+02

REGION	WEIGHT	ENERGY	WIDTH
1	3.5800000+01	8.6999998-03	1.5900000-02
2	9.5000000+01	2.8700000-02	1.1000000-02
3	2.9400000+00	6.3000000-02	5.7999999-02
4	5.2500000+00	1.7400000-01	1.1000000-01
5	9.0999999+00	2.0600000-01	2.3000000-02
6	3.1188000+00	4.5900000-01	6.9999999-02

$w(T) = 2D(\text{SGRT}(T+1+C+C+1/4)-C) + \text{SUM}(A(I)-B(I)*\text{EXP}(-\text{DEL}(I)*T*T)*\text{COS}(GAM(I)*T))$

	A(I)	B(I)	DEL(I)	GAM(I)
1	3.3621503-01	3.2928840-01	3.5765032-02	3.0884011-01
2	1.7970360-02	1.5414276-02	1.7117871-02	1.1196830+00
3	1.6513760-01	9.3166629-02	4.7590511-01	2.0511993+00
4	2.7871284-02	2.7102178-03	1.7117871+00	5.1803157+00
5	1.3475787-02	4.6423471-04	7.4837632-02	8.0847783+00
6	1.7635887-02	4.7289027-06	6.9320302-01	1.7487689+01

TR, TIO = .4693617+01

	EZERO	EFINAL	SIG0	SIG1	FIG0	FIG1
1	1.000000-03	1.000000-03	3.703238+03	1.059797+02	3.500000+00	3.500000+00
2	2.000000-03	1.000000-03	3.081823+01	-1.257021+01	7.452358+00	7.525429+00
3	2.000000-03	2.000000-03	2.384826+03	9.745685+01	3.500000+00	3.500000+00
4	4.000000-03	1.000000-03	3.961853+00	-9.861895-01	6.873347+00	7.000339+00
5	4.000000-03	2.000000-03	7.336000+00	-2.370291+00	7.305059+00	7.391140+00
6	4.000000-03	4.000000-03	1.476536+03	9.842528+01	3.500000+00	3.500000+00
7	6.500000-03	1.000000-03	4.808696+00	-9.674997-01	6.518227+00	6.937182+00
8	6.500000-03	2.000000-03	7.267707+00	-1.821479+00	6.814363+00	6.907477+00
9	6.500000-03	4.000000-03	1.194703+01	-3.588918+00	7.395952+00	7.403943+00
10	6.500000-03	6.500000-03	1.009918+03	1.000783+02	3.500000+00	3.500000+00
11	1.000000-02	1.000000-03	5.428241+00	-8.584685-01	5.352548+00	6.145860+00
12	1.000000-02	2.000000-03	8.192430+00	-1.677458+00	5.967003+00	6.349630+00
13	1.000000-02	4.000000-03	1.253430+01	-3.085014+00	6.740123+00	6.844626+00
14	1.000000-02	6.500000-03	1.860643+01	-4.369409+00	7.353467+00	7.327786+00
15	1.000000-02	1.000000-02	6.348065+02	8.874698+01	3.500000+00	3.500000+00
16	1.500000-02	1.000000-03	4.389151+00	-5.397718-01	6.362301+00	6.441021+00
17	1.500000-02	2.000000-03	7.005973+00	-1.133978+00	6.467294+00	6.350802+00
18	1.500000-02	4.000000-03	1.189739+01	-2.385916+00	6.116566+00	5.906199+00
19	1.500000-02	6.500000-03	1.725021+01	-3.798407+00	6.325623+00	6.722595+00
20	1.500000-02	1.000000-02	2.212759+01	-5.022631+00	7.262732+00	7.222202+00
21	1.500000-02	1.500000-02	4.887966+02	9.190406+01	3.500000+00	3.500000+00
22	2.000000-02	1.000000-03	2.471989+00	-2.760636-01	6.095736+00	5.546100+00
23	2.000000-02	2.000000-03	4.102006+00	-5.974706-01	6.193557+00	5.507208+00
24	2.000000-02	4.000000-03	7.783021+00	-1.378465+00	6.281290+00	4.952491+00
25	2.000000-02	6.500000-03	1.326381+01	-2.536606+00	6.412681+00	6.293617+00
26	2.000000-02	1.000000-02	2.091871+01	-4.064202+00	6.176524+00	6.750959+00
27	2.000000-02	1.500000-02	2.676579+01	-5.088156+00	7.412516+00	7.211847+00
28	2.000000-02	2.000000-02	3.819917+02	9.919978+01	3.500000+00	3.500000+00
29	2.530000-02	1.000000-03	1.589965+00	-1.707929-01	5.598008+00	5.819636+00
30	2.530000-02	2.000000-03	2.416783+00	-3.507191-01	5.484017+00	6.216157+00
31	2.530000-02	4.000000-03	4.176435+00	-7.590109-01	5.537087+00	6.098586+00
32	2.530000-02	6.500000-03	7.321504+00	-1.399633+00	5.940873+00	6.249902+00
33	2.530000-02	1.000000-02	1.396339+01	-2.522533+00	6.105231+00	6.635963+00
34	2.530000-02	1.500000-02	2.457634+01	-3.953745+00	6.574969+00	6.954801+00
35	2.530000-02	2.000000-02	2.627473+01	-4.378261+00	7.500126+00	7.200185+00
36	2.530000-02	2.530000-02	2.682490+02	8.151163+01	3.500000+00	3.500000+00
37	3.300000-02	1.000000-03	1.415937+00	-1.188206-01	6.013918+00	5.365636+00
38	3.300000-02	2.000000-03	2.105386+00	-2.400378-01	6.158755+00	5.602272+00
39	3.300000-02	4.000000-03	3.214773+00	-4.897981-01	5.986781+00	6.095770+00
40	3.300000-02	6.500000-03	4.403005+00	-8.168271-01	5.480921+00	6.252192+00
41	3.300000-02	1.000000-02	6.376237+00	-1.322641+00	5.860989+00	6.543679+00
42	3.300000-02	1.500000-02	1.251985+01	-2.151721+00	5.921672+00	6.839926+00
43	3.300000-02	2.000000-02	2.262694+01	-2.777237+00	6.510445+00	7.003404+00
44	3.300000-02	2.530000-02	2.994040+01	-2.822617+00	6.967840+00	6.230804+00
45	3.300000-02	3.300000-02	1.895128+02	6.853335+01	3.500000+00	3.500000+00

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46	4.100000-02	1.000000-03	1.244145+00	-9.225426-02	6.022025+00	4.744474+00
47	4.100000-02	2.000000-03	1.770868+00	-1.825565-01	6.025386+00	5.504803+00
48	4.100000-02	4.000000-03	2.587578+00	-3.592611-01	5.983146+00	5.940133+00
49	4.100000-02	6.500000-03	3.577424+00	-5.760057-01	5.908315+00	6.470355+00
50	4.100000-02	1.000000-02	5.099493+00	-8.855432-01	5.658737+00	6.429994+00
51	4.100000-02	1.500000-02	7.149409+00	-1.371956+00	6.103157+00	6.576300+00
52	4.100000-02	2.000000-02	1.057078+01	-1.840817+00	6.513324+00	6.817583+00
53	4.100000-02	2.500000-02	1.878710+01	-1.877515+00	6.954484+00	6.365621+00
54	4.100000-02	3.300000-02	2.970988+01	-1.022274+00	7.069414+00	5.812151+00
55	4.100000-02	4.100000-02	2.766679+02	1.344583+02	3.500000+00	3.500000+00

1 MOMENT MICROSCOPIC SCATTERING KERNEL

TO ENERGY FROM ENERGY	1.000-03	2.000-03	4.000-03	6.000-03	1.000-02	1.500-02	2.000-02	2.530-02	3.300-02	4.100-02
1.000-03	1.060+02	-2.416+01	-3.503+00	-5.058+00	-6.010+00	-4.650+00	-2.601+00	-1.650+00	-1.104+00	-7.757-01
2.000-03	-1.257+01	9.746+01	-4.330+00	-4.253+00	-6.109+00	-5.082+00	-2.929+00	-1.763+00	-1.160+00	-7.985-01
4.000-03	-9.862-01	-2.370+00	9.643+01	-5.282+00	-6.081+00	-5.787+00	-3.657+00	-2.065+00	-1.201+00	-8.504-01
6.000-03	-9.675-01	-1.821+00	-3.539+00	1.001+02	-5.852+00	-6.260+00	-4.572+00	-2.587+00	-1.452+00	-9.264-01
1.000-02	-8.535-01	-1.677+00	-3.085+00	-4.369+00	8.875+01	-6.180+00	-5.470+00	-3.481+00	-1.755+00	-1.063+00
1.500-02	-5.398-01	-1.134+00	-2.366+00	-3.798+00	-5.023+00	9.190+01	-5.565+00	-4.435+00	-2.320+00	-1.339+00
2.000-02	-2.751-01	-5.975-01	-1.378+00	-2.537+00	-4.064+00	-5.088+00	9.920+01	-4.490+00	-2.736+00	-1.643+00
2.530-02	-1.708-01	-3.507-01	-7.590-01	-1.400+00	-2.523+00	-3.954+00	-4.378+00	8.151+01	-2.714+00	-1.634+00
3.300-02	-1.188-01	-2.400-01	-4.698-01	-8.168-01	-1.323+00	-2.152+00	-2.777+00	-2.823+00	6.853+01	-9.252-01
4.100-02	-9.225-02	-1.826-01	-3.593-01	-5.760-01	-8.855-01	-1.372+00	-1.841+00	-1.878+00	-1.022+00	1.345+02

0 MOMENT MICROSCOPIC SCATTERING KERNEL

TO ENERGY FROM ENERGY	1.000-03	2.000-03	4.000-03	6.500-03	1.000-02	1.500-02	2.000-02	2.530-02	3.300-02	4.100-02
1.000-03	3.703+03	5.924+01	1.407+01	2.514+01	3.800+01	3.781+01	2.329+01	1.536+01	1.315+01	1.046+01
2.000-03	3.082+01	2.385+03	1.355+01	1.070+01	2.984+01	3.140+01	2.011+01	1.215+01	1.018+01	7.746+00
4.000-03	3.962+00	7.336+00	1.477+03	1.750+01	2.471+01	2.826+01	2.065+01	1.136+01	8.409+00	6.125+00
6.500-03	4.809+00	7.268+00	1.195+01	1.010+03	2.224+01	2.043+01	2.394+01	1.353+01	7.825+00	5.754+00
1.000-02	5.428+00	8.192+00	1.253+01	1.061+01	6.348+02	2.723+01	2.815+01	1.927+01	8.461+00	6.124+00
1.500-02	4.389+00	7.006+00	1.190+01	1.725+01	2.213+01	4.588+02	2.928+01	2.757+01	1.350+01	6.978+00
2.000-02	2.472+00	4.102+00	7.783+00	1.328+01	2.092+01	2.677+01	3.820+02	3.002+01	2.231+01	9.432+00
2.530-02	1.590+00	2.417+00	4.176+00	7.322+00	1.396+01	2.458+01	2.927+01	2.682+02	2.679+01	1.635+01
3.300-02	1.416+00	2.105+00	3.215+00	4.403+00	6.376+00	1.252+01	2.263+01	2.994+01	1.895+02	2.689+01
4.100-02	1.244+00	1.771+00	2.589+00	3.577+00	5.099+00	7.149+00	1.057+01	1.879+01	2.971+01	2.767+02

PROGRAM TSKSIG

TISK, WATER 293K 6RES FIT TO RHO(BETA)

PAGE

5

TOTAL SCATTERING CROSS SECTIONS

ENERGY	RESULT
9.999999-04	4.6146818+00
2.000000-03	4.2750169+00
4.000000-03	3.9099178+00
6.499999-03	3.6047354+00
9.999999-03	3.2909795+00
1.500000-02	2.9452839+00
2.000000-02	2.6639631+00
2.530000-02	2.4045560+00
3.300000-02	2.0210816+00
4.100000-02	1.5943245+00

ENERGY	RESULT
--------	--------

ENERGY	RESULT
--------	--------

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PROGRAM TSKSIG

TISK, WATE. 293K 6RES FIT TO RHO(BETA)

PAGE 6

TOTAL P1 SCATTERING CROSS SECTIONS

ENERGY	RESULT
9.9999999-04	0.0000000
2.0000000-03	1.8683366-02
4.0000000-03	1.0057407-01
6.4999999-03	1.7682503-01
9.9999999-03	2.5401780-01
1.5000000-02	3.3811253-01
2.0000000-02	3.9903326-01
2.5300000-02	4.4234593-01
3.3000000-02	4.8122511-01
4.1000000-02	4.9459869-01

ENERGY	RESULT
--------	--------

ENERGY	RESULT
--------	--------

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PROGRAM TSKSIG

TISK, WATER, 293K 6RES FIT TO RHO(BETA)

PAGE 7

TRANSPORT CROSS SECTIONS

ENERGY	RESULT
9.999999-04	4.614681e+00
2.000000-03	4.256333e+00
4.000000-03	3.809343e+00
6.499999-03	3.427910e+00
9.999999-03	3.036961e+00
1.500000-02	2.607171e+00
2.000000-02	2.264929e+00
2.530000-02	1.962210e+00
3.300000-02	1.539856e+00
4.100000-02	1.099725e+00

ENERGY	RESULT
--------	--------

ENERGY	RESULT
--------	--------

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PROGRAM TSKSIG

TASK DATE 293K 6RES FIT TO RHO(BETA)

PAGE 8

AVERAGE SCATTERING COSINE

ENERGY	RESULT
9.999999-04	0.000000
2.000000-03	4.3703609-03
4.000000-03	2.5722810-02
6.499999-03	4.9053539-02
9.999999-03	7.7186079-02
1.500000-02	1.1479794-01
2.000000-02	1.4978933-01
2.530000-02	1.8396156-01
3.300000-02	2.3810274-01
4.100000-02	3.1022460-01

ENERGY	RESULT
--------	--------

ENERGY	RESULT
--------	--------

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BML-1675

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