Cold moderator scattering kernels

R. E. MacFarlane
Applied Nuclear Science Group
Los Alamos National Laboratory
Los Alamos, New Mexico 87545
USA

ABSTRACT: New thermal-scattering-law files in ENDF format have been developed for solid methane, liquid methane, liquid ortho- and para-hydrogen, and liquid ortho- and para-deuterium using up-to-date models that include such effects as incoherent elastic scattering in the solid, diffusion and hindered vibration and rotations in the liquids, and spin correlations for the hydrogen and deuterium. These files were generated with the new LEAPR module of the NJOY Nuclear Data Processing System. Other modules of this system were used to produce cross sections for these moderators in the correct format for the continuous-energy Monte Carlo code (MCNP) being used for cold-moderator-design calculations at the Los Alamos Neutron Scattering Center (LANSCE).

INTRODUCTION

When Gary Russell needed cold moderator cross sections to use with the MCNP continuous energy Monte Carlo code[1] during the design of the liquid hydrogen moderator for the Los Alamos Neutron Scattering Center (LANSCE), he naturally came to the Applied Nuclear Data group, because we provide the other cross sections for MCNP. As a starting point, he provided us with FORTRAN coding from Dr. Guy Robert at Grenoble that implemented the Young and Koppel model[2] for ortho and para hydrogen. We implemented the calculation in the THERMR module of the NJOY Nuclear Data Processing System[3] and results obtained using cross sections produced in this way were reported at the last ICANS conference.[4] Subsequently, a need developed for deuterium cross sections. A later version of the European coding for the Young and Koppel model was obtained from Dr. Rolf Neef at Julich, and the NJOY code was updated to be able to process para and ortho deuterium. Before this new capability was ever used, Gary became interested in liquid and solid methane as moderator materials. He obtained a version of the LEAP+ADDELT code that had been especially modified for cold methane calculations by Dr. Dave Picton.[5]

This part of the development was considerably more complex than the earlier steps. Instead of directly computing the differential cross section $\sigma(E \rightarrow E', \mu)$ from a (comparatively) simple formula, it became necessary to compute the scattering law $S(\alpha, \beta)$ in the Evaluated Nuclear Data Files (ENDF) format and feed it into the THERMR module of NJOY. Our initial results with the LEAP code were so encouraging, that we decided to use it as the basis for a new LEAPR module for the NJOY system. This involved modifying the code for consistency with NJOY standards, making some "improvements", and doing a careful study of the theory of the method. The result is a new general purpose code for producing scattering law files in ENDF-6 format[6] for both cold moderators and normal reactor moderators.

The final step in this long history was to make use of the knowledge gained from the liquid methane model and the LEAPR code to improve the data for liquid hydrogen and deuterium. The Young and Koppel model assumed that the molecular translations were free, but a number of experimental studies have shown the presence of quasi-elastic scattering that appears to obey a diffusive law. Following the procedures outlined by Keinert and Sax,[7] we replaced the free-gas law in the Young and Koppel formula with a new scattering law that attempts to represent the hindered motions of each hydrogen or deuterium molecule in its clump of local neighbors and the diffusive motions of these clumps through the liquid. Because of spin correlations, it was necessary to extend the ENDF-6 format and the NJOY code to handle asymmetric scattering laws, that is $S(\alpha, \beta) \neq S(\alpha, -\beta)$.

In the rest of this paper, we will give a short review of the theory of the LEAPR module of NJOY, and then describe the actual models used for solid methane, liquid methane, liquid hydrogen, and liquid deuterium.

LEAPR THEORY

The British code LEAP+ADDELT was originally written by McLatchie at Harwell,[8] then implemented by Butland at Winfrith, [9] and finally modified to work better for cold moderators as part of the Ph.D. thesis of D. J. Picton. The major modifications made while turning LEAP+ADDELT into LEAPR were extensive reworking of the coding and comments, the provision of output in ENDF-6 format, a capability to include either coherent or incoherent elastic scattering, a significant speedup for the diffusion calculation, and the liquid hydrogen/deuterium model.

In many practical moderator materials, the presence of some essential randomness (such as of position, spin orientation, isotopic content, or crystallite orienta-

tion) allows scattering of thermal neutrons to be described as "incoherent". It is shown in standard references[10] that the double differential scattering cross section of thermal neutrons by gases, liquids, or solids consisting of randomly ordered crystals can be written as

$$\sigma(E \to E', \mu) = \frac{\sigma_b}{2kT}\sqrt{\frac{E'}{E}}\, e^{-\beta/2}\, S(\alpha, \beta), \tag{1}$$

where E and E' are the incident and secondary neutron energies in the laboratory system, μ is the cosine of the scattering angle in the laboratory, σ_b is the characteristic bound scattering cross section for the material, kT is the thermal energy in eV, and S is the scattering law. The scattering law depends on only two variables: the momentum transfer

$$\alpha = \frac{E' + E - 2\sqrt{E'E}\mu}{AkT}, \tag{2}$$

where A is the ratio of scatterer mass to the neutron mass, and the energy transfer

$$\beta = \frac{E' - E}{kT}. \tag{3}$$

Note that β is positive for energy gain and negative for energy loss. Except in the case of the hydrogen molecule, S is symmetric in β and only the part for positive values is tabulated in the ENDF format.

It turns out that the scattering law depends on the frequency spectrum of excitations in the system. In general, this spectrum can be expressed as a weighted sum of a number of simple spectra,

$$\rho(\beta) = \sum_{j=1}^{K} w_j \rho_j(\beta), \tag{4}$$

where some of the possibilities are:

$$\rho_j(\beta) = \delta(\beta_j) \text{ discrete oscillator} \tag{5}$$

$$\rho_j(\beta) = \rho_f(\beta) \text{ free translation} \tag{6}$$

$$\rho_j(\beta) = \rho_s(\beta) \text{ solid-type spectrum} \tag{7}$$

$$\rho_j(\beta) = \rho_d(\beta) \text{ diffusion-type spectrum} \tag{8}$$

The weights sum to one, and all the individual distributions are normalized. The net scattering law for this sum of spectra can be expressed as a recursion based

on convolutions:

$$S(\alpha,\beta) = S^{(K)}(\alpha,\beta), \tag{9}$$

where

$$S^{(J)}(\alpha,\beta) = \int_{-\infty}^{\infty} S_J(\alpha,\beta')\, S^{(J-1)}(\alpha,\beta-\beta')\, d\beta'. \tag{10}$$

where S_J is the scattering law for partial spectrum J, and $S^{(J-1)}$ is the composite scattering law including all partial distributions with $j<J$. As an example of the use of this recursive procedure, consider a case like solid methane where the desired spectrum is a combination of ρ_s and several discrete oscillators. First calculate $S^{(1)}=S_1$ using ρ_s. Then calculate S_2 using $\rho(\beta_1)$, the distribution for the first discrete oscillator, and convolve S_2 with $S^{(1)}$ to obtain $S^{(2)}$, the composite scattering law for the first two partial distributions. Repeat the process with the rest of the discrete oscillators, one at a time, to obtain the full distribution.

The Phonon Expansion

The two main methods available for computing the scattering law for solid-type spectra are the time integration of the intermediate scattering function used by GASKET[11] and the phonon expansion used by LEAP. Our tests indicate that the LEAP method is faster and more stable, especially for the very high values of α and β found in low-temperature problems. Therefore, we decided to use the phonon expansion for our new thermal module. The resulting formula for $S_s(\alpha,\beta)$ is

$$S_s(\alpha,\beta) = \mathrm{e}^{-\alpha\lambda} \sum_{n=0}^{\infty} \frac{1}{n!} [\alpha B]^n\, T_n(\beta), \tag{11}$$

where

$$\lambda = \int_{-\infty}^{\infty} P_s(\beta)\, \mathrm{e}^{-\beta/2}\, d\beta \tag{12}$$

is the Debye-Waller factor,

$$B = \int_{-\infty}^{\infty} P_s(\beta)\, d\beta, \tag{13}$$

is a constant,

$$T_0(\beta) = \delta(\beta), \tag{14}$$

$$T_1(\beta) = \frac{1}{B} P_s(\beta), \tag{15}$$

and in general,

$$T_n(\beta) = \int_{-\infty}^{\infty} T_{n-1}(\beta')\, T_1(\beta-\beta')\, d\beta'. \tag{16}$$

In these formulas,

$$P_s(\beta) = \frac{\rho_s(\beta)\,e^{-\beta/2}}{2\beta\sinh(\beta/2)}. \tag{17}$$

The coefficients are precomputed using this convolution process for n up through 20. It is then a simple process to compute S for any desired value of α or β using eq.(11). For high values of α and β the sum may not converge adequately with only 20 terms. It is then possible to extend the sum to higher values of n using an approximation for the T_n, or the code can choose to use the "Short Collision Time" (SCT) approximation. We are still exploring the various strategies for making use of these approximations.

Diffusion

The neutron scattering from many important liquids, including water and liquid methane, can be represented using a solid-type spectrum of rotational and vibrational modes combined with a diffusion term. Egelstaff and Schofield have proposed an especially simple model for diffusion called the "effective width model." It has the advantage of having analytic forms for both $S_d(\alpha,\beta)$ and the associated spectrum $\rho_d(\beta)$:

$$S_d(\alpha,\beta) = \frac{2d\alpha}{\pi}\,e^{2dc\alpha}\frac{\sqrt{c^2+.25}}{\sqrt{\beta^2+4d^2\alpha^2}}K_1\left\{\sqrt{c^2+.25}\sqrt{\beta^2+4d^2\alpha^2}\right\}, \tag{18}$$

and

$$\rho_d(\beta) = \frac{4d}{\pi\beta}\sqrt{c^2+.25}\,\sinh(\beta/2)\,K_1\left\{\sqrt{c^2+.25}\,\beta\right\}. \tag{19}$$

In these equations, $K_1(x)$ is a modified Bessel function of the second kind, and the diffusion constant c and parameter d (usually $w_d c$) are provided as inputs.

In LEAPR, $S_s(\alpha,\beta)$, the scattering law for the solid-type modes, is calculated using the phonon expansion as described above. The diffusive contribution $S_d(\alpha,\beta)$ is then calculated using the formula above on a β grid chosen to represent its shape fairly well. The combined scattering law is then obtained by convolution as follows:

$$S(\alpha,\beta) = S_d(\alpha,\beta) + \int_{-\infty}^{\infty} S_d(\alpha,\beta')\,S_s(\alpha,\beta-\beta')\,d\beta'. \tag{20}$$

The first term arises from the delta function in eq.(11), which isn't included in the numerical results for the phonon series calculation. The values for $S_d(\beta)$ and $S_s(\beta-\beta')$ are obtained from the precomputed functions by interpolation. This makes LEAPR run much faster than LEAP+ADDELT for diffusive cases, because the original code did direct recalculations of the solid-type scattering law for all the desired values of $\beta-\beta'$. It also had to take pains to compute S_d on a β grid that was commensurate with the input grid. This often resulted in more points for S_d than were necessary to obtain useful accuracy for the convolutions.

Discrete Oscillators

The scattering law for a discrete oscillator term $w_i\delta(\beta_i)$ is known to be

$$S_i(\alpha,\beta) = \mathrm{e}^{-\alpha\lambda_i} \sum_{n=-\infty}^{\infty} I_n\Big(\frac{w_i\alpha}{\beta_i \sinh(\beta_i/2)}\Big)\, \delta(\beta-n\beta_i), \tag{21}$$

where

$$\lambda_i = w_i \frac{\coth(\beta_i/2)}{\beta_i}, \tag{22}$$

and $I_n(x)$ is a modified Bessel function of the first kind and n-th order. As discussed in connection with eq.(10), the net $S(\alpha,\beta)$ for a complex distribution consisting of a smooth part and several discrete oscillators is obtained by convolving each oscillator in turn with the $S(\alpha,\beta)$ resulting from all the previous parts of the distribution. The δ-function makes the convolution trivial.

A variation of this procedure used for liquid hydrogen and deuterium will be discussed below.

ENDF-6 Output

The Evaluated Nuclear Data Files (ENDF) format originated in the U. S., but it is now being used throughout the world. Thermal data is recorded in "File 7", and the new ENDF-6 version of the File 7 format is capable of representing the following types of data.

- *Incoherent Inelastic.* This type is important for all materials, and it requires $S(\alpha,\beta)$ vs T and some auxiliary information such as bound scattering cross section and effective temperatures.

- *Coherent Elastic.* This type is important for crystalline materials like graphite and beryllium, and it requires information on the position and strengths of

the Bragg edges, a characteristic coherent cross section, and a Debye-Waller function.

- *Incoherent Elastic.* This type is important for hydrogenous solids like polyethylene, zirconium hydride, and solid methane, and it requires a characteristic cross section plus a Debye-Waller function.

The calculation of $S(\alpha,\beta)$ was described above. The ENDF output subroutine of LEAPR simply stores it in the correct format. Effective temperatures for the ENDF Short-Collision-Time approximation can be determined from integrals performed by LEAPR, and they are also added to the file.

Coherent elastic parameters can be computed for the three materials graphite, beryllium, and beryllium oxide using methods based on the HEXSCAT code.[12] The Debye-Waller function needed to determine the temperature dependence of coherent elastic scattering is obtained from the LEAPR calculation of $S(\alpha,\beta)$ for the material. Similarly, the Debye-Waller function for incoherent elastic scattering in hydrogenous materials is obtained from the LEAPR calculation of the inelastic scattering law for that material.

The speed and simplicity of the LEAP method for computing $S(\alpha,\beta)$ combined with the comprehensive capabilities of the ENDF output routine make LEAPR a very useful module for all problems involving thermal neutron scattering.

SOLID METHANE

The methane molecule consists of an atom of carbon surrounded by four atoms of hydrogen placed on the corners of a tetrahedron. The carbon atom is at the center of mass of the system; because of its symmetry, the methane molecule is often called a "spherical top". Optical measurements of methane in the gas phase show four fairly well defined vibrational modes at 162, 190, 361, and 374 meV. Following the lead of Picton, they have been included in this model as discrete oscillators with weights equal to .308, .186, .042, and .144, respectively.

Specific heat measurements in solid methane near one atmosphere show three phases with transitions at 8K and 20.4K. The melting point is about 89K. X-ray measurements show that the carbon atoms are arranged on an fcc lattice for both of the higher two phases; it has been speculated that the phase transition is due to a change in the degree of rotational order, or perhaps due to the onset of a self-diffusion behavior. Because of this interesting question, a series of slow

neutron inelastic scattering experiments were carried out with samples in each of the phases.[13] Because hydrogen is an incoherent scatterer, it was possible to analyze the data to obtain a frequency spectrum for hydrogen in solid methane. The results didn't really explain what was happening in the 20K phase transition, but they did provide us with just the data needed for our calculation.

Again following Picton, we chose the spectrum for 22.1K for our model. Instead of using Picton's numbers directly, we digitized the curve from the graph in the reference, plotted it on a large scale, and then smoothed it by hand. Care was taken to use an ω^2 variation for low energies. The resulting spectrum is shown in Figure 1. As discussed by Harker and Brugger, the appropriate normalization for this curve is 0.32.

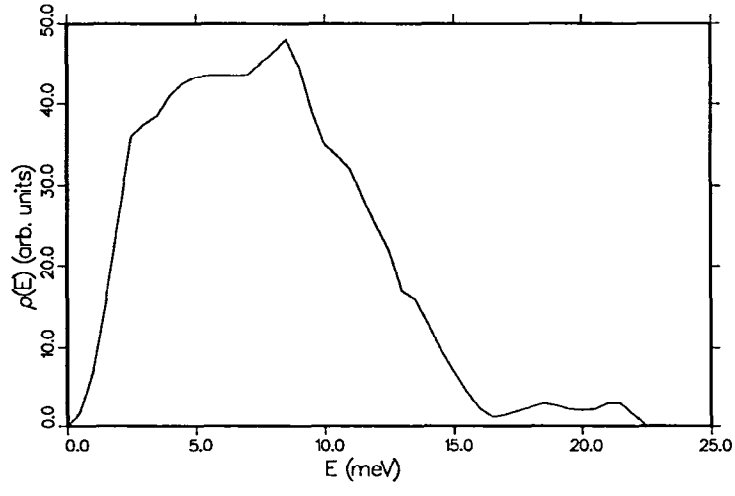

Figure 1: The Harker-Brugger frequency spectrum used for solid methane. Note the quadratic shape at low energies.

This spectrum and the four discrete oscillators were then used to calculate $S(\alpha,\beta)$ with LEAPR using the α and β grids of Picton. During this calculation, the moments of T_n and $S(\alpha,\beta)$ were checked and the errors were modest. The output listing was examined carefully to see that the α and β ranges were sufficient, and no obvious problems were found. LEAPR automatically prepared an output file in ENDF-6 format, including both incoherent elastic and incoherent inelastic representations, and complete with descriptive comments on the resulting evaluation. Plots of $S(\alpha,\beta)$ versus α for several values of β are give in Figure 2.

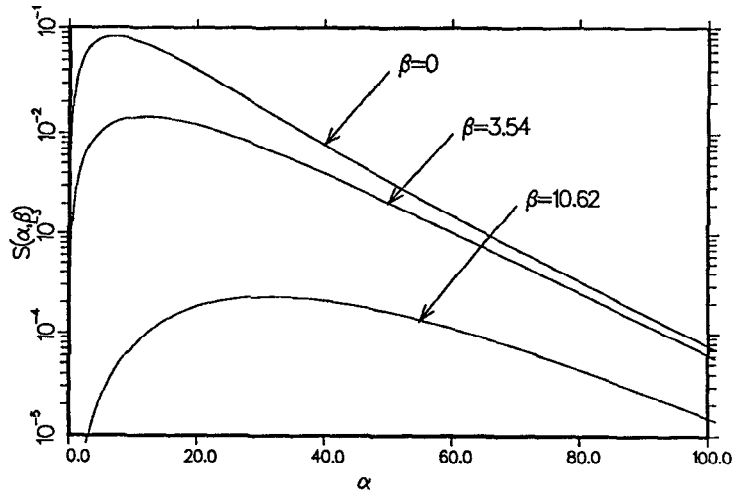

Figure 2: $S(\alpha,\beta)$ for solid methane shown as a function of α for several values of β.

Next, the new evaluation for $S(\alpha,\beta)$ was processed into integrated cross sections and double differential cross sections using the THERMR module of NJOY. It was necessary to slightly modify the code to allow for the very large values of β appropriate to these low temperatures (note that β is inversely proportional to kT for a given energy transfer); it is necessary to keep values of S as small as $1\text{x}10^{-80}$ for this evaluation. This is quite a dynamic range! Plots of the integrated cross sections for the elastic and inelastic processes are given in Figure 3, and plots of the outgoing neutron spectrum integrated over angle at several incident energies are given in Figure 4.

Finally, the output of THERMR was passed to the ACER module of NJOY for conversion to ACE format for the MCNP Continuous-Energy Monte-Carlo code. The result of this step was made available to Group X-6 for addition to the standard MCNP thermal library.

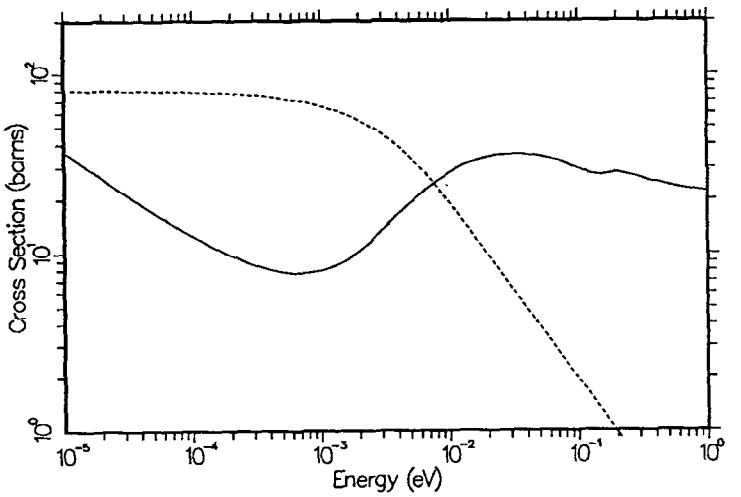

Figure 3: Incoherent inelastic cross section (solid) and incoherent elastic cross section (dashed) for solid methane.

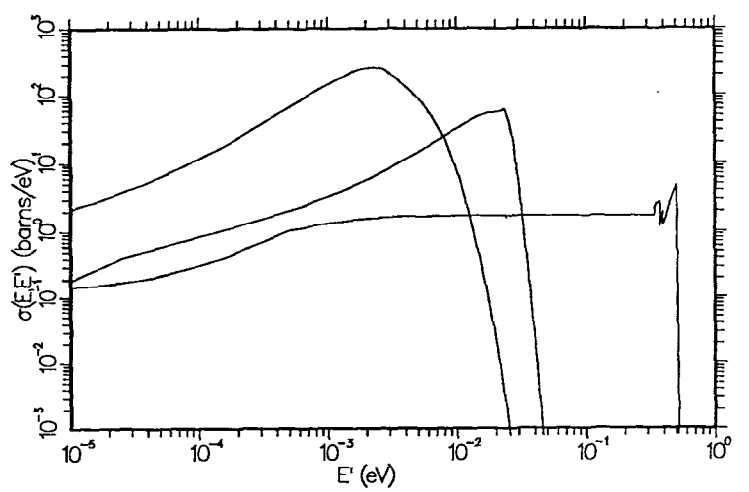

Figure 4: Neutron spectra $\sigma(E \rightarrow E')$ for solid methane shown for E =0.0001, .0253, and .503 eV.

LIQUID METHANE

The preparation of a model for liquid methane at 90K was a little more difficult. Once again, we use the four discrete oscillators to represent the the molecular vibrations. In addition, we need a continuous frequency distribution to represent the molecular rotations, and a pair of parameters d and c to represent diffusion. This latter component was omitted from Picton's model, but we felt that it might be needed to obtain a reasonable quasi-elastic peak in the spectrum of scattered neutrons. Therefore, we couldn't use the Picton input directly, and we had to refer to his source.[14] Agrawal and Yip divided the problem into two parts: translations and rotations.

For translations, they proposed a model that matches the expected diffusive behavior at long times and provides an oscillatory behavior at short times. Each methane molecule is assumed to move in a "cage" formed by its neighbors, and the cage itself is allowed to relax with time. As Agrawal and Yip point out, the molecule will oscillate initially, but gradually as the restoring forces decay into a frictional background, it will go over into diffusive motions. The resulting analytic expression for the frequency spectrum is

$$f_t(\omega) = \frac{2}{\pi} \frac{\omega_0^2/\tau_0}{\omega^2 - \omega_0^2)^2 + (\omega/\tau_0)^2} . \tag{23}$$

The fact that $f(\omega)$ is nonzero at ω=0 indicates that the molecules are capable of diffusion.

For rotations, they establish that the rotational excitations are related to the "dipole correlation function". The same function appears in the classical limit of the theory of optical line shapes for infrared absorption as presented by Gordon,[15] and he has used this method to compute the correlation function for liquid methane at 98K based on the infrared data of Ewing.[16] The desired spectrum of rotational excitations, $\rho_r(\omega)$ can be obtained by transforming the function graphed by Gordon.

The net result is shown in Figure 5, together with the translational frequency distribution discussed above. These numbers were generated by digitizing the curve from Agrawal and Yip. The fact that the distribution is nonzero at zero energy transfer indicates that diffusion is present. Agrawal and Yip compared

their model with both double-differential and integrated cross sections, with very good agreement.

Unfortunately, this model does not match the requirements of LEAPR. The only type of frequency distribution that is nonzero at ω=0 that can be used by the code is the diffusive law of Egelstaff and Schofield, which does not have the short-time oscillatory behavior of eq.(23). Our main reason for using the diffusion term in our model for liquid methane was to improve the "quasi-elastic" peak, which depends mostly on the small-ω part of the frequency distribution. Therefore, it seemed reasonable to select diffusion parameters d and c that gave a reasonable representation for the full width at half maximum of the quasi-elastic peak, to subtract the result f_d from the sum of the two curves shown in Figure 5, and to use the difference to represent both the translational oscillatory modes and the rotational modes. Figure 6 shows this breakdown. Once again, there has been some hand smoothing, and the low energy part of the distribution was forced to follow an ω^2 law. The final breakdown was 1.5% diffusion, 30.5% rotation, and 68% molecular vibrations.

LEAPR was run with this input taking advantage of the much accelerated diffusion calculation discussed above. Once again the moments of T_n and $S(\beta)$ were checked, and no great problems were seen. These checks help to prove that the ω grid for the input frequency spectrum and the β grid for calculating S are reasonable. We also checked the range of α and β to be sure that no significant cross section contributions were being cut off. The results seem to be good for all energy transfers possible with incident neutron energies up to 1 eV. Once again, LEAPR produced an output file in ENDF-6 format. This time, there was no elastic contribution at all. Plots of $S(\alpha,\beta)$ versus α for several values of β are shown in Figure 7. Note that the behavior of the curves for small β is quite different than in Figure 2. This reflects the presence of the diffusive component.

The new evaluation for liquid methane was run through the THERMR module of NJOY to produce integrated and differential cross sections. Sample results are given in Figures 8 and 9. The integrated cross section is compared with experimental data at 110K that was quoted in the Agrawal and Yip paper. The THERMR output was then processed by ACER to obtain the final MCNP library for Group X-6.

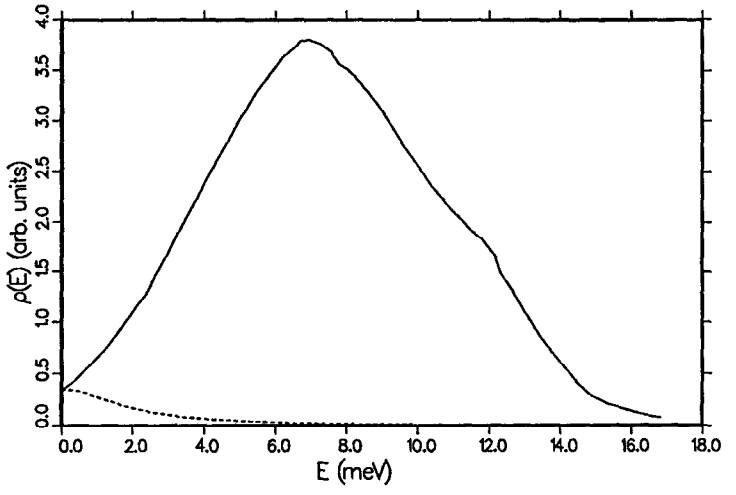

Figure 5: Frequency spectrum for liquid methane (solid) as given by Agrawal and Yip, including an analytic translational part (dashed) and a rotational part based on Gordon's analysis of the optical measurements of Ewing.

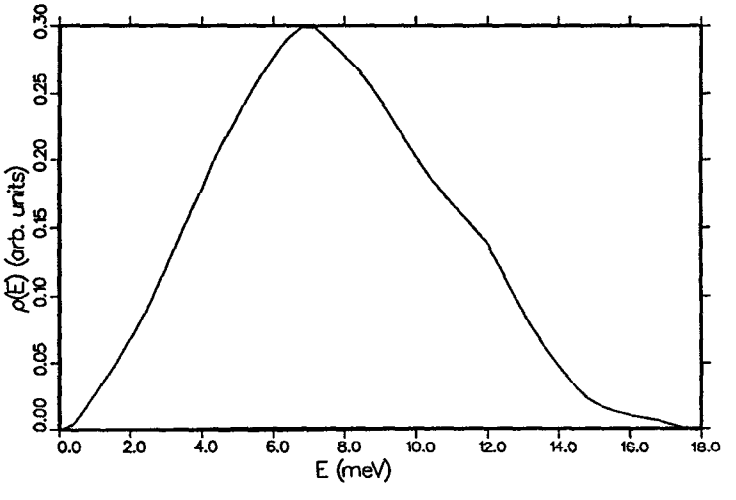

Figure 6: Effective frequency spectrum for methane including both translational and rotational modes, but not including diffusive modes.

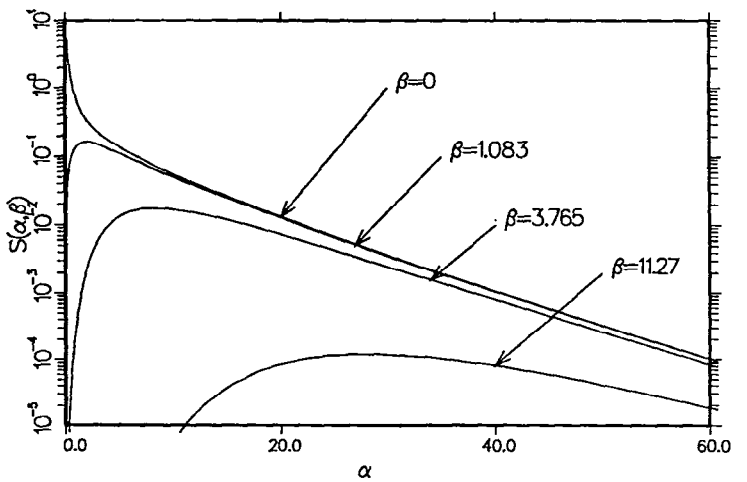

Figure 7: $S(\alpha, \beta)$ curves for liquid methane. Note the diffusive behavior at low α and β.

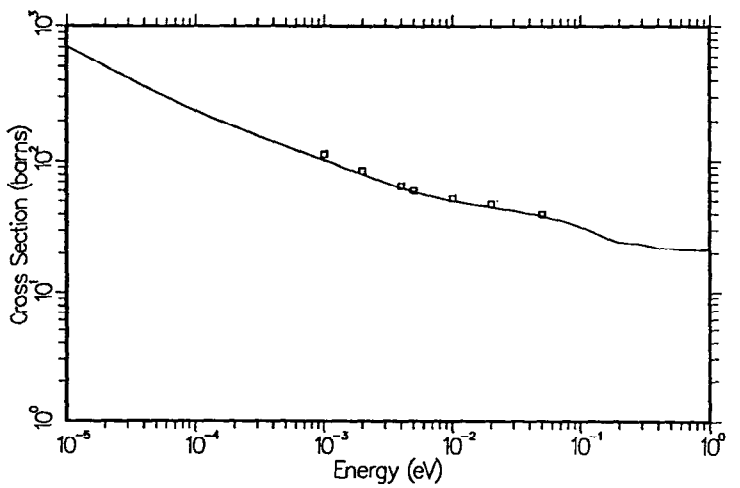

Figure 8: The computed cross section for liquid methane at 100K (solid) is compared to experimental data (squares) by Whittemore and by Rogalska as quoted by Agrawal and Yip.

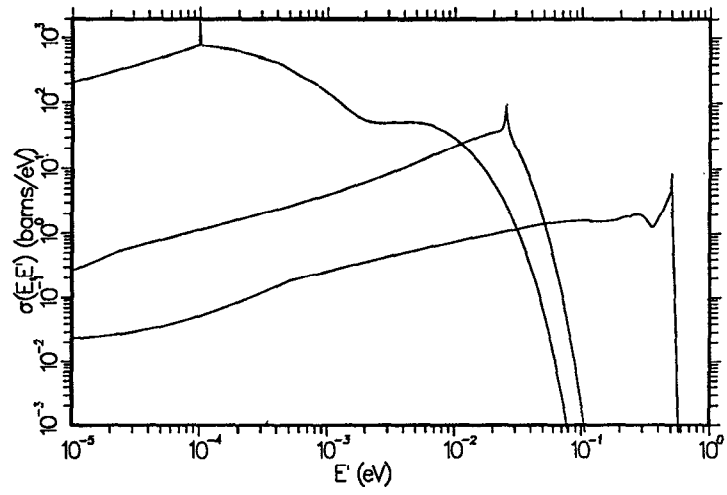

Figure 9: Neutron spectra $\sigma(E \to E')$ are shown for E =.0001, .0253, and .503 meV. Note the sharp quasi-elastic peak that results from the diffusive term in the theory used here.

LIQUID HYDROGEN AND DEUTERIUM

Materials containing hydrogen or deuterium molecules violate the assumption that spins are distributed randomly that underlies the incoherent approximation used for eq.(11), and an explicitly quantum-mechanical formula is required to take account of the correlations between the spins of two atoms in the same molecule. This problem was considered by Young and Koppel, who gave the formulas for that were incorporated into the European coding that we originally received from Robert and Neef. Changing to our notation, the formulas for the hydrogen molecule (neglecting vibrations) become

$$S_{\rm para}(\alpha,\beta) = \sum_{J=0,2,4,\ldots} P_J \tag{24}$$

$$\times \frac{4\pi}{\sigma_b}\Big[a_c^2 \sum_{J'=0,2,4,\ldots} + a_i^2 \sum_{J'=1,3,5,\ldots}\Big](2J'+1) \tag{25}$$

$$\times S_f(\alpha/2, \beta+\beta_{JJ'})\, e^{-\beta_{JJ'}/2} \tag{26}$$

$$\times \sum_{\ell=|J'-J|}^{J'+J} 4j_\ell^2(y) C^2(JJ'\ell;00), \tag{27}$$

and

$$S_{\text{ortho}}(\alpha,\beta) = \sum_{J=1,3,5,\ldots} P_J \tag{28}$$

$$\times \frac{4\pi}{\sigma_b}\Big[\frac{a_i^2}{3}\sum_{J'=0,2,4,\ldots} + \frac{3a_c^2+2a_i^2}{3}\sum_{J'=1,3,5,\ldots}\Big](2J'+1) \tag{29}$$

$$\times S_f(\alpha/2,\beta+\beta_{JJ'})\,\mathrm{e}^{-\beta_{JJ'}/2} \tag{30}$$

$$\times \sum_{\ell=|J'-J|}^{J'+J} 4j_\ell^2(y)C^2(JJ'\ell;00), \tag{31}$$

where a_c and a_i are the coherent and incoherent scattering lengths (note that the characteristic bound cross section $\sigma_b{=}4\pi[a_c^2{+}a_i^2]$), P_J is the statistical weight factor, $\beta_{JJ'}{=}(E'_J{-}E_J)/kT$ is the energy transfer for a rotational transition, $j_\ell(x)$ is a spherical Bessel function of order ℓ, and $C(JJ'\ell;00)$ is a Clebsch-Gordan coefficient. The parameter y is given by $\kappa a/2{=}(a/2)\sqrt{4MkT\alpha/2}$, where a is the interatomic distance in the molecule. The sums over J' are treated as operators into order to keep the notation compact.

Young and Koppel assumed that the molecular translations were free, so the equations contain

$$S_f(\alpha,\beta) = \frac{1}{\sqrt{4\pi\alpha}}\exp\Big[-\frac{\alpha^2+\beta^2}{4\alpha}\Big], \tag{32}$$

the free-atom scattering function. Note that α is divided by two when this equation is used to make the formula apply to a molecule containing two atoms. That is, the normalization of the translational part is 0.5.

These formulas as stated are appropriate for a gas of hydrogen molecules. In a liquid, there are two additional effects to be considered: interference between the neutron waves scattered from different molecules, and the fact that the recoil of the hydrogen molecule is not really free. So far, we have only considered the latter effect. Experiments by Egelstaff, Haywood, and Webb at Harwell[17] and Schott at Karlsruhe[18] showed appreciable broadening of the quasi-elastic scattering peak for liquid hydrogen, and both groups ascribed this to diffusive effects. Later, Utsuro of Kyoto University constructed a simple analytic model[19] that included both diffusion and intermolecular vibrations and showed good agreement with experiment. More recently, Keinert and Sax of the University of Stuttgart proposed the model[7] that we follow here.

They suggested that the free translation term in the Young and Koppel formu-

las be replaced by the superposition of a solid-state like motion and a diffusive law. One can picture a hydrogen molecule bound in a cluster of about 20 molecules and undergoing vibrations similar to those of a hydrogen molecule in a solid. These clumps then diffuse through the liquid (hindered translations) according to the Egelstaff-Schofield effective width model discussed above. The Keinert-Sax distribution function is shown in Figure 10. They assumed a weight of 0.025 for the hindered translation, leaving a value of 0.475 for the solid-like distribution.

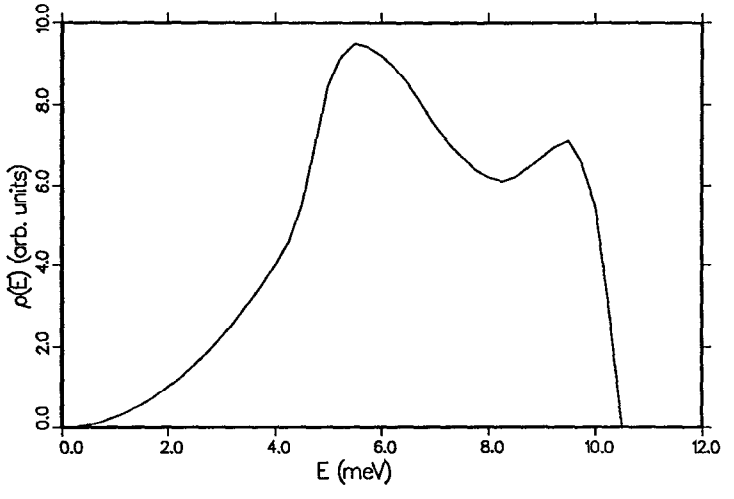

Figure 10: The Keinert-Sax frequency distribution for the effective translational modes of liquid hydrogen.

This model was then used in LEAPR. Some results for the effective translational $S(\alpha,\beta)$ to be used in the Young and Koppel formulas are shown in Figure 11 along with the corresponding free translation curves. A new subroutine was added to LEAPR to carry out the rest of operations in the Young and Koppel formulas. Because of the spin correlations, $S(\alpha,\beta)\neq S(\alpha,-\beta)$, and it is necessary to calculate both sides of the function. These results were then passed to the ENDF output subroutine. Here again, it was necessary to make a slight modification to allow for asymmetric scattering functions. A new parameter called "LASYM" was added to the File 7 format (it is in the "L1" position of the head card for MF=7, MT=4). When LASYM=1, the β grid in File 7 starts with $-\beta_{\max}$ and increases through zero to $+\beta_{\max}$. Of course, it was also necessary to modify the THERMR module of NJOY to recognize the LASYM=1 option. This turned out to be very easy, and

some examples of cross sections and energy distributions computed by THERMR are shown in Figures 12 and 13.

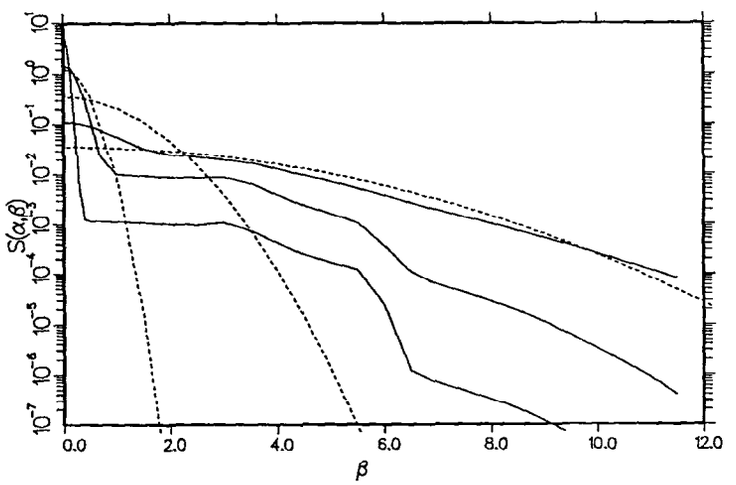

Figure 11: The effective translational $S(\alpha,\beta)$ for liquid hydrogen (solid) compared with the corresponding free translation curves (dashed). The α values shown are 0.1, 1, and 10 (broadest).

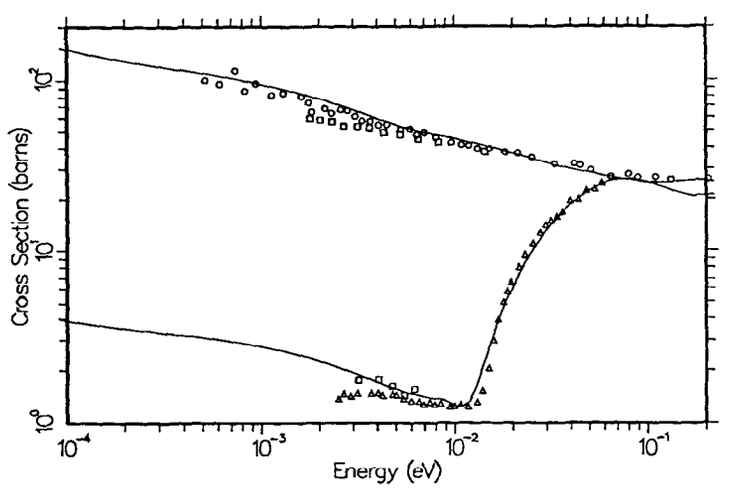

Figure 12: The cross sections for liquid ortho hydrogen (upper curve) and liquid para hydrogen (lower curve) at 20 K are compared with experimental data[20] due to Squires (gas) at 20K (squares), Whittemore at 20K (circles), and Seiffert at 14K (triangles).

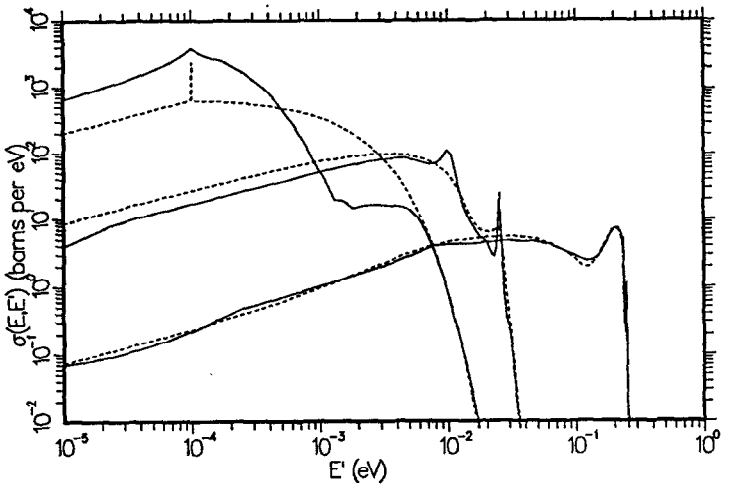

Figure 13: The spectra $\sigma(E \rightarrow E')$ for liquid para hydrogen are shown for E=.0001, .0253, and .251 eV. Note the sharp quasi-elastic peak arising from the diffusion treatment. The dashed lines show the free translation results from the original Young and Koppel formulas.

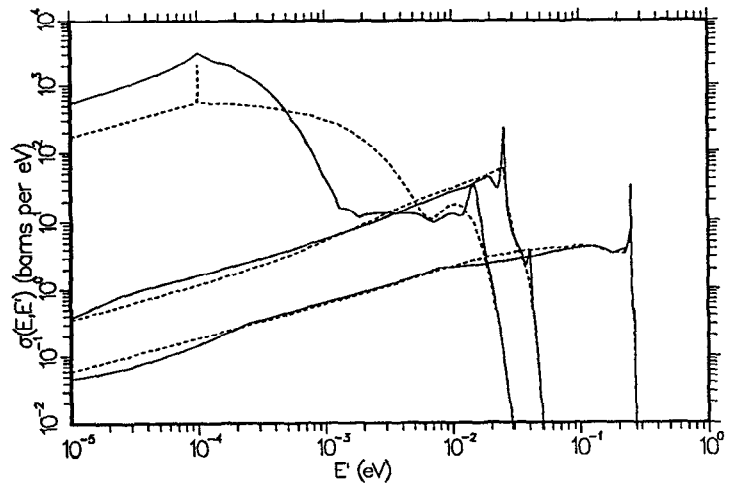

Figure 14: The spectra $\sigma(E \rightarrow E')$ for liquid ortho hydrogen are shown for E=.0001, .0253, and .251 eV. Again note the sharp quasi-elastic peak arising from the diffusion treatment. The dashed lines show the free translation result.

CONCLUSIONS

The result of this work is set of state-of-the-art scattering law files for ortho and para liquid hydrogen, ortho and para liquid deuterium, liquid methane, and solid methane that can be used with the NJOY Nuclear Data Processing System to produce thermal scattering data for both continuous-energy Monte Carlo and multigroup applications. As a very useful spin-off, we have the LEAPR module, which can be used to produce new scattering law files for the traditional reactor moderators for the upcoming ENDF/B-VI library of evaluated nuclear data.

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