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Scattering of Slow Neutrons by Water*†

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The motions of hydrogen atoms in water are considered in terms of the H_2O molecule at the basic dynamical unit. Vibrations, hindered rotations, and translations of the molecule are included. For the numerical calculations, the hindrance of the translations is neglected, and the hindered rotations are replaced by a torsional oscillation with a single energy, $h\nu = 0.06$ ev. When certain approximations are made in the average over molecular orientation, this model allows for the computation of differential and total slow-neutron cross sections. The computed cross sections are in good agreement with most of the available slow-neutron scattering data. The features of the high-resolution experiments directly associated with the hindrance of the molecular translations in the liquid are not reproduced.

I. INTRODUCTION

IT has been shown by Van Hove[1] that the differential energy-transfer cross-section $\sigma(E_0,E,\theta)$ for the incoherent scattering of slow neutrons by a chemically bound atom can be expressed in terms of a suitably defined time-dependent self-correlation function determined by the dynamics of the atomic motion. Because of the cancellation of the singlet and triplet neutron-proton scattering amplitudes, the scattering from chemically bound hydrogen is almost completely incoherent. A study of slow-neutron scattering in hydrogenous compounds therefore yields information primarily on the motion of individual protons as determined by the interatomic forces.

Brockhouse[2] has applied the approach of Van Hove to the analysis of his experimental determinations of $\sigma(E_0,E,\theta)$ for water and has developed a plausible description of the dynamics of proton motion in water. The general conclusions to be drawn from Brockhouse's work can be briefly summarized as follows:

(1) The frequencies of the internal motions of the H_2O molecule are all high in comparison with those of the translational motions.

(2) The hindered rotations of the molecule are of an essentially harmonic nature, with a broad distribution of energies centered about $h\nu \approx 0.06$ ev.

(3) There is definite evidence that the molecular translations are not harmonic in nature and that effects specific to the liquid state are observable.

Recent high-resolution measurements of $\sigma(E_0,E,\theta)$ in water[3,4] have yielded conflicting interpretations in terms of the atomic motions in the liquid. These measurements are sensitive to the details of the hindered molecular translation in the liquid and can therefore yield information of fundamental importance to an understanding of the liquid state. It should be possible, however, to describe most of the available data on slow-neutron scattering in water without including the hindrance of the molecular translations. Such a description helps to define the limits of sensitivity of the slow-neutron-scattering method for determination of effects specific to the liquid state. It also extends, to the region of thermal energies, our ability to describe quantitatively the slowing down and diffusion of neutrons in water.

The fundamental assumptions in the present description are that the H_2O molecule is the basic dynamical unit and that a classification of the atomic motions into vibrations, hindered rotations, and hindered translations of the molecule gives an adequate description of the proton motions in the liquid. We shall take as our starting point the approximation that the various degrees of freedom carry out simple harmonic oscillations. This permits an analytic expression to be written[5] for the differential energy-transfer cross-section, $\sigma(E_0,E,\theta)$. To evaluate this expression, we introduce simplifying approximations in the average over molecular orientations that are similar to approximations used earlier for calculating the scattering from free polyatomic molecules.[6] The internal vibrations of the molecule are assumed to be the same in liquid H_2O as in the vapor. The rotations of the molecule are replaced by a torsional oscillation of a single frequency. The energy of this oscillation is taken as $h\nu = 0.06$ ev.[2,4]

The assumption of harmonic motion for the molecular translations is quite poor. We will consider, however, only situations in which the characteristic potential energies associated with the translational motion are

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† A report on a portion of this work is contained in a combined experimental and theoretical paper by A. W. McReynolds, M. S. Nelkin, M. N. Rosenbluth, and W. L. Whittemore, *Proceedings of the Second United Nations International Conference on the Peaceful Uses of Atomic Energy* (United Nations, Geneva, 1958), Vol. 16, p. 297.

[1] L. Van Hove, Phys. Rev. **95**, 249 (1954).

[2] B. N. Brockhouse, *Proceedings of the Conference on the Condensed State of Simple Systems, Varenna, September, 1957* [Suppl. Nuovo cimento **9**, 45 (1958)].

[3] B. N. Brockhouse, Phys. Rev. Letters **2**, 287 (1959).

[4] D. J. Hughes, H. Palevsky, W. Kley, and E. Tunkelo, Phys. Rev. Letters **3**, 91 (1959).

[5] A. C. Zemach and R. J. Glauber, Phys. Rev. **101**, 118, 129 (1956).

[6] T. J. Krieger and M. S. Nelkin, Phys. Rev. **106**, 290 (1957).

sufficiently small that the translational motions can be considered as free. This avoids most of the problems of fundamental interest that involve the nature of the hydrogen-atom motions in the liquid, but it is useful in defining a model which can be used as a starting point for a more detailed study of these motions.

In Sec. II, the formulas to be used are derived, and the expected region of validity is discussed. In Sec. III, numerical calculations from these formulas are discussed. The results of these calculations are compared with experiment in Sec. IV. Comparisons are given for the total cross section as a function of energy, thermal diffusion parameters, angular distribution, and energy distribution. Agreement between theory and experiment is good in those situations where the theory can reasonably be expected to apply.

II. MATHEMATICAL FORMULATION

The scattering of slow neutrons by chemically bound hydrogen can be described accurately by the Fermi pseudopotential approximation.[7] Recent formulations[1,5] of this approximation have emphasized, in their formal development, the way in which the dynamics of the nuclear motion in the interatomic potential determine the neutron scattering. For the case of hydrogen, the theoretical treatment is greatly simplified by the predominantly incoherent nature of the scattering, which arises from the opposite signs of the singlet and triplet neutron-proton scattering amplitudes. We can, therefore, neglect interference scattering that involves the correlations in position among pairs of protons in the scattering system, provided that the temperature is not so low that nuclear spin correlations become important.[5]

We will begin with an expression for the differential cross section, $\sigma(E_0,E,\theta)$, for scattering of neutrons of incident energy E_0 into the energy interval dE at E and through an angle θ into the solid angle $d\Omega$. We will specialize to the case in which the motion of the scattering proton is a superposition of normal modes described by harmonic oscillator coordinates. For this case, an analytic solution of the slow-neutron scattering problem can be obtained[5] and gives

$$\sigma(E_0,E,\theta)=\left(\frac{\sigma_b}{8\pi^2}\right)\left(\frac{E}{E_0}\right)^{\frac{1}{2}}\int_{-\infty}^{\infty}dt\, e^{-i\epsilon t}\chi(\mathbf{K},T,t), \qquad (1)$$

where $\sigma_b=81.2$ barns is the bound-hydrogen cross section, $\epsilon=(E-E_0)$ is the energy transfer, $\mathbf{K}$ is the momentum transfer, T is the absolute temperature, and

$$\chi(\mathbf{K},T,t)=\left\langle \exp\left[\sum_{q=1}^{N}(\mathbf{K}\cdot\boldsymbol{\xi}_q)^2 f(\omega_q,T,t)\right]\right\rangle, \qquad (2)$$

where

$$f(\omega,T,t)=(2\omega)^{-1}[(n+1)(e^{-i\omega t}-1)+n(e^{i\omega t}-1)], \qquad (3)$$

and

$$n=[\exp(\omega/T)-1]^{-1}. \qquad (4)$$

We use a system of units in which $\hbar=1$, and the neutron mass is 1. Temperatures are measured in units of energy. The quantity $\boldsymbol{\xi}_q$ is the hydrogen-atom amplitude, and ω_q the angular frequency in the qth normal mode. The $\boldsymbol{\xi}_q$ will depend on the relative orientation of the molecule and incident neutron. The averaging indicated in Eq. (2) is done with respect to this orientation.

A normalization condition on the $\boldsymbol{\xi}_q$ can be obtained from the requirement that free-proton scattering be approached for incident neutron energies large compared with T and with the largest ω_q. This will be satisfied if

$$\chi(\mathbf{K},T,t)\rightarrow\exp(-\tfrac{1}{2}itK^2) \qquad (5)$$

as $t\rightarrow 0$. Since $f(\omega,T,t)\rightarrow -\frac{1}{2}it$ as $t\rightarrow 0$, we require that

$$\sum_{q=1}^{N}(\mathbf{K}\cdot\boldsymbol{\xi}_q)^2=K^2. \qquad (6)$$

We will approximate the normal modes of motion of the hydrogen atom in terms of the torsional oscillations and translational motions of rigid H_2O molecules, plus the internal vibrations of the molecule. The frequencies of the internal vibrations will be assumed to be the same as in H_2O vapor. Equation (2) gives χ as the average over orientation of a product of terms corresponding to different normal modes. We will approximate this by the product of the averages. This is difficult to justify quantitatively, but the method has been used previously[6] with some success for the angular distribution in CH_4 vapor.

In an actual crystal lattice there will be a purely elastic scattering which falls off with increasing momentum transfer as $\exp(-K^2u^2)$, where u^2 is the mean-square displacement of the vibrating atom from its equilibrium position. An approximately Gaussian dependence of the "quasi-elastic" scattering as a function of K^2 has been measured for water by Brockhouse.[2] It gives a value for u of about 0.4×10^{-8} cm at room temperature. Because the contribution to u^2 from the vibrations and hindered rotations is only 0.02×10^{-6} cm², the measured value of u can be used to give a crude measure of an effective Debye temperature for the translational motions.

The value of u^2 for a Debye frequency distribution is given by

$$u^2=(3/2M\Theta^3)\int_0^{\Theta}\omega d\omega\coth(\omega/2T),$$

where Θ is the Debye temperature. For $u^2=0.14\times10^{-16}$ cm^2$=33$ (ev)$^{-1}$, we obtain a Debye temperature of 0.011 ev. This characteristic energy associated with the hindrance of the translational motions is sufficiently small that we are justified in considering the trans-

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[7] E. Fermi, Ricerca sci. 1, 13 (1936).

lational motions to be free for many applications. This approximation will be applicable for K^2u^2 much greater than 1. It yields a χ function for the translations corresponding to an ideal monatomic gas at temperature T with a mass of 18:

$$\chi_t \approx \exp[-(K^2/2M)(it+Tt^2)]. \tag{7}$$

The hindered molecular rotations will be replaced by a torsional oscillation with a single frequency, ω_r. The expression for χ_r describing the neutron scattering from such a torsional oscillator has been shown by Krieger[5,8] to be

$$\chi_r = \langle \exp[(\mathbf{K}\cdot\mathfrak{K}\cdot\mathbf{K})f(\omega_r,T,t)]\rangle, \tag{8}$$

where

$$\mathfrak{K} = \mathfrak{M}^{-1} - M^{-1}\mathbf{1}, \tag{9}$$

and $\mathfrak{M}$ is the Sachs-Teller[9] mass tensor. This result, which is rigorous only for small torsional oscillations, goes over into the Sachs-Teller approximation in the limit of free rotation where

$$f(\omega_r,T,t) \rightarrow -\tfrac{1}{2}(it+Tt^2). \tag{10}$$

In the intermediate range of hindered rotation with motions of large angular amplitude, the form given by Eq. (8) will be less accurate.

We will make the further approximation of averaging over molecular orientations in the same manner that was used previously for the scattering by freely rotating molecules.[6] This gives as our final approximation

$$\chi_r \approx \exp[(K^2/m_r)f(\omega_r,T,t)]. \tag{11}$$

This is just the χ that would apply to an isotropic harmonic oscillator of frequency ω_r and mass m_r.

The choice of m_r for a freely rotating molecule has been discussed previously.[6,10] It was shown in this earlier work that the replacement of the mass tensor by an equivalent scalar was quite accurate for the total cross section, and that the angular distribution in CH_4 was not seriously affected by this approximation. The best value of m_r for the free molecule is very nearly the same as would be obtained from averaging Eq. (8) over orientation by averaging in the exponent. For H_2O, the best fit to the free-molecule cross section calculated from the full mass-tensor approximation is obtained using $m_r = 2.32$.[10] We will use this value for the torsional oscillations in the liquid. This corresponds to assuming that the bond angle of the H_2O molecule is the same in liquid water as in water vapor.

Recent measurements of the energy distribution after scattering through 90 deg of initially cold neutrons show a pronounced peak corresponding to an energy gain of 0.06 ev. This peak almost certainly corresponds to a characteristic excitation of the hindered rotation of the molecule. We will therefore choose $\hbar\omega_r = 0.06$ ev. This is the only parameter in the present model which will be taken directly from neutron scattering data. The observed peak is broader than that which would correspond to a single torsional frequency. Considering the crudity of the present model, however, we did not feel it was worthwhile to add the complication of including a distribution of torsional frequencies.

A crude estimate of the validity of assuming small torsional oscillations can be obtained by calculating the mean-square angular displacement of a hydrogen atom from its equilibrium position. This is given approximately by (u_r^2/r^2); here $m_r r^2$ is an average moment of inertia for the rotating molecule, and

$$u_r^2 = [2m_r\omega_r \tanh(\omega_r/2T)]^{-1}.$$

For the present parameters this gives a root-mean-square angular displacement of 8 deg. The assumption of small torsional oscillations is therefore likely to be quite good at least for elastic transitions and for one-quantum transitions involving the hindered rotations. For the higher excited states of the hindered rotational motion, the approximation of small oscillations will be much less satisfactory.

The neutron scattering will not, in any case, be sensitive to the details of the rotational wave functions in the higher excited states. For sufficiently large energy transfers, only small collision times will be important, and we can expand $f(\omega_r,T,t)$ in Eq. (11) in powers of t. A convenient approximate form for χ_r in the high-energy limit is thus obtained:

$$\chi_r \approx \exp\left[-\frac{K^2}{2m_r}(it+\bar{E}_r t^2)\right], \tag{12}$$

where

$$\bar{E}_r = [n(\omega_r/T)+\tfrac{1}{2}]\omega_r = 0.036 \text{ ev}.$$

This free-atom approximation conveniently expresses the condition that the asymptotic behavior of the cross section at high neutron energies is determined by the average kinetic energy of the target particles.[11,12] This approximation is applicable when the collision time t is short compared with the characteristic period for the degree of freedom under study.[13] Its use enables

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[8] T. J. Krieger (private communication).

[9] R. G. Sachs and E. Teller, Phys. Rev. **60**, 18 (1941).

[10] T. J. Krieger and M. S. Nelkin, Knolls Atomic Power Laboratory Report KAPL-1597, August, 1956, and Addendum, April, 1957 (Office of Technical Services, U. S. Department of Commerce, Washington, D. C.).

[11] G. Placzek, Phys. Rev. **86**, 377 (1952).

[12] G. C. Wick, Phys. Rev. **94**, 1228 (1954).

[13] The asymptotic expansion for short collision times introduced by Wick in reference 12 yields a series of singular functions for $\sigma(E_0,E,\theta)$. If one also retains the t^2 term in the exponent, and then expands χ in powers of t, an expansion in nonsingular functions will be obtained. For a harmonic system, this can be shown to be exactly the asymptotic expansion associated with the central limit theorem of probability theory. The approximate form in Eq. (12) is then the first term in an asymptotic expansion with corrections of the order of $(m_r/\bar{E}_r K^2)^{\frac{1}{2}}$. This expansion is discussed in detail in the General Atomic report GA-1258, by Donald Parks and the present author. This report which has been submitted to the *Physical Review* for publication, is available on request from the authors.

a considerable simplification of the numerical work in Sec. III.

The energies of the molecular vibrations will be assumed to be the same in liquid water as in water vapor. These have been measured[14] to be 0.205, 0.474, and 0.488 ev. The average over molecular orientation will be carried out once more according to the same approximation procedure. We will further assume that the two higher-frequency vibrational modes are degenerate and that the vibrations are not thermally excited. This gives as our final expression

$$\chi_v=\chi_1\chi_2=\exp\left[\frac{K^2}{6m_v\omega_1}(e^{-i\omega_1 t}-1)\right]\times\exp\left[\frac{K^2}{3m_v\omega_2}(e^{-i\omega_2 t}-1)\right], \quad (13)$$

where $\hbar\omega_1=0.205$ ev and $\hbar\omega_2=0.481$ ev. The effective mass for vibration $m_v=1.95$ is determined from the condition (6) that the scattering approach the free-atom scattering at high incident neutron energy. In terms of our approximate average over orientation this condition becomes

$$\frac{1}{M}+\frac{1}{m_r}+\frac{1}{m_v}=1. \quad (14)$$

III. CALCULATION OF CROSS SECTIONS

The differential energy-transfer cross-section

$$\sigma(E_0,E,\theta)$$

will be calculated from Eq. (1) with χ approximated by

$$\chi\approx\chi_t\chi_r\chi_v,$$

where χ_t is defined by Eq. (7), χ_r by Eq. (11), and χ_v by Eq. (13). For convenience in numerical calculation we will make the further approximation that the excitation of only one of the modes has to be treated properly for a given range of incident and final neutron energies.

If the incident neutron energy is between 0.01 and 0.15 ev, we will assume free translations and only elastic vibrational transitions. The appropriate expression for χ_v becomes

$$\chi_v\approx\exp\left[-\frac{K^2}{2m_v}\left(\frac{1}{3\omega_1}+\frac{2}{3\omega_2}\right)\right]\equiv\exp(-\tfrac{1}{2}K^2\alpha_v). \quad (15)$$

The cross section corresponding to this choice of χ can be evaluated by using a result of Zemach and Glauber,[5] which gives

$$\sigma(E_0,E,\theta)=\frac{\sigma_b}{4\pi}\left(\frac{E}{E_0}\right)^{\frac{1}{2}}\left(\frac{m}{2\pi\bar{E}K^2}\right)^{\frac{1}{2}}\exp\left(-\frac{K^2}{2A}\right)\times\sum_{n=-\infty}^{\infty}\exp\left(\frac{-n\omega}{2T}\right)I_n\left(\frac{K^2}{2B}\right)\times\exp\left[-\frac{m}{2\bar{E}K^2}\left(E-E_0-n\omega+\frac{K^2}{2m}\right)^2\right], \quad (16)$$

where $I_n(x)$ is the usual Bessel function of imaginary argument, and

$$\begin{aligned}
m&=M=18,\\
\bar{E}&=T=0.0255 \text{ ev},\\
A^{-1}&=\alpha_v^{-1}+[m_r\omega_r\tanh(\omega_r/2T)]^{-1},\\
A&=0.0971 \text{ ev},\\
B&=m_r\omega_r\sinh(\omega_r/2T)=0.206 \text{ ev},\\
\omega&=\omega_r=0.06 \text{ ev}.
\end{aligned} \quad (17)$$

An expression of this form is suitable for repeated calculation on a large digital computer, and it has been programmed for calculation on the IBM 704 by Brown and Sprague.[15]

For incident neutron energies between 0.20 ev and 0.48 ev, we treat the excitations of the 0.2-ev vibrational level properly and use the approximate form (12) for the rotations. Only elastic transitions for the high-frequency vibrations are considered. The cross section is again given by an expression of the form of Eq. (16) with

$$\begin{aligned}
m^{-1}&=M^{-1}+m_r^{-1},\\
m&=2.06,\\
\bar{E}&=[(Tm_r+\bar{E}_rM)/(m_r+M)]=0.0350 \text{ ev},\\
T&=0.0255 \text{ ev},\\
A&=\alpha_v=0.65 \text{ ev},\\
B&=3m_v\omega_1\sinh(\omega_1/2T)=33.31 \text{ ev},\\
\omega&=\omega_1=0.205 \text{ ev}.
\end{aligned} \quad (18)$$

Between 0.15 and 0.20 ev, we use the parameters of (17) for energy transfers less than 0.1 ev and the parameters of (18) for energy transfers greater than 0.1 ev.

Finally, for incident neutron energies above 0.48 ev, we also treat χ_1 as free-atom motion with the appropriate average kinetic energy, and we consider the excitation of the 0.48-ev vibrations. This again leads to an expression of the form of (16), with a choice of

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[14] G. Herzberg, *Molecular Spectra and Molecular Structure* (D. Van Nostrand Company, Inc., Princeton, New Jersey, 1950), 2nd ed., Vol. II.

[15] A FORTRAN statement of this program is attached to the unpublished General Atomic Report GAMD-754 (Rev.), July 1, 1959 (available on request).

TABLE I. Theoretical and experimental values for the thermal neutron diffusion properties of water.

	Diffusion coefficient, D_0 (cm^2/sec)	Diffusion cooling, c (cm^4/sec)	$d(\ln D_0)/dT$ (per °C)
Experiment	35 000±1000	4000±1000	0.0045±0.0005
Theory	37 900	3000	0.0034

parameters given by

$$
\begin{aligned}
m^{-1}&=M^{-1}+m_r^{-1}+\tfrac{1}{3}m_v^{-1},\\
m&=1.522,\\
\bar{E}&=[(T/M)+(\bar{E}_r/m_r)+(\bar{E}_1/3m_v)]\\
&\qquad\times[M^{-1}+m_r^{-1}+\tfrac{1}{3}m_v^{-1}]^{-1},\\
\bar{E}&=0.0525\text{ ev},\\
T&=0.0255\text{ ev},\\
A&=(3m_v\omega_2/2)=1.402\text{ ev},\\
B&=\tfrac{2}{3}m_v\omega_2\sinh(\omega_2/2T)=8744\text{ ev},\\
\omega&=\omega_2=0.481\text{ ev}.
\end{aligned}
\tag{19}
$$

In order to minimize the amount of computation, the cross sections are computed only for $E<E_0$. The cross sections for energy gain are determined from the detailed balance condition

$$\sigma(E,E_0,\theta)=\sigma(E_0,E,\theta)(E_0/E)\exp[(E-E_0)/T]. \tag{20}$$

This condition is satisfied by an exact calculation, as well as by the approximate models employed in this work.

The most important numerical errors in the present calculation arise from the use of the free-atom approximation (12) for the hindered rotations for incident neutron energies as low as 0.15 ev. The accuracy can be improved either by including the multiple excitations of the 0.06-ev level properly, in combination with single excitation of the 0.20-ev level, or by making use of the asymptotic expansion in $(m_r/\bar{E}_rK^2)^{\frac{1}{2}}$, discussed in reference 13. The use of the free-atom approximation does not appreciably affect the computed total cross section, but it gives an average energy loss per collision that is somewhat too large.

IV. COMPARISON WITH EXPERIMENT

We expect the model outlined in the previous sections to describe well the low-resolution data on slow-neutron scattering but to become less applicable as the energy and momentum transfers become small enough that the hindrance of translational motion becomes important. We will consider first the total cross section as a function of energy. The cross section is computed by first determining the differential energy-transfer cross-section $\sigma(E_0,E,\theta)$ from the equations given in Sec. III. This cross section is then integrated numerically over final energy and scattering angle. The total cross section so computed is compared with experiment in Fig. 1. The experimental points are those of Melkonian,[16] as read from the cross-section compilation BNL-325.[17] The agreement between theory and experiment in the range from 0.01 to 1.0 ev is good. The deviation in the neighborhood of 0.05 ev is probably due to the assumption of a single torsional frequency in the calculation. A small wiggle in the calculated cross section between 0.15 and 0.20 ev has been smoothed out in drawing Fig. 1 since the origin of this wiggle is almost certainly in the numerical approximation used in this region, and not in the physical model employed.

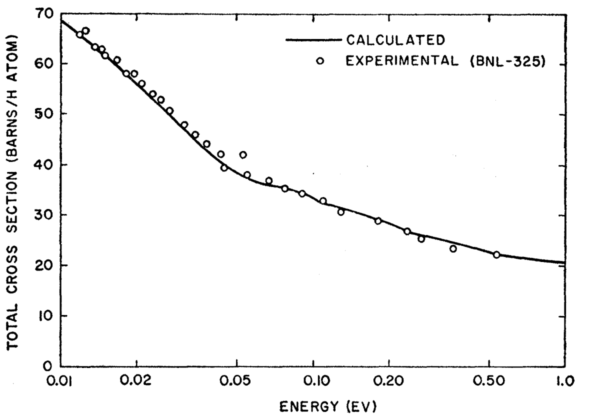

FIG. 1. The total cross section of water in barns per hydrogen atom as a function of incident neutron energy.

A second integral measurement of interest is the determination of the diffusion parameters for thermal neutrons. This information is usually obtained by measuring the mean lifetime of the thermal-neutron distribution following a pulse of fast neutrons.[18] The dependence of the lifetime on the size of the sample determines the thermal-neutron leakage rate and thus the diffusion coefficient. For smaller samples, there will be transport corrections, and the equilibrium spectrum will be cooled with respect to the moderator temperature because of the preferential leakage of fast neutrons. Both of these effects contribute to a second measurable quantity, the diffusion cooling coefficient. An essentially rigorous formulation for determining these coefficients from $\sigma(E_0,E,\theta)$ has been given by the present author.[19] A comparison of theory and experiment is given in Table I. The temperature dependence of the diffusion coefficient was obtained under the assumption that $\hbar\omega_r$ remains equal to 0.06 ev independently of temperature.

The experimental numbers are a subjectively weighted average by the author of the values summar-

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[16] E. Melkonian, Phys. Rev. **76**, 1750 (1949).

[17] *Neutron Cross Sections*, compiled by D. J. Hughes and R. B. Schwartz, Brookhaven National Laboratory Report BNL-325 (Superintendent of Documents, U. S. Government Printing Office, Washington, D. C., 1958), 2nd ed.

[18] G. von Dardel and N. G. Sjöstrand, Phys. Rev. **96**, 1245 (1954). See also the review article by these authors in *Progress in Nuclear Energy* (Pergamon Press, New York, 1958), Ser. I, Vol. II.

[19] M. Nelkin, Nuclear Sci. and Eng. **7**, 210 (1960).

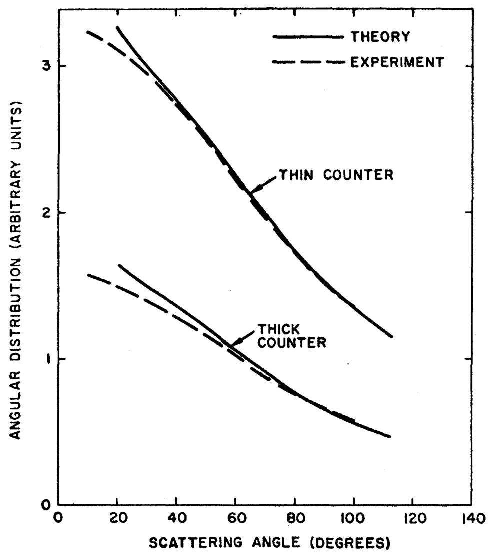

FIG. 2. The angular distribution for 0.065-ev neutrons scattered from water for two counters with different energy-dependent sensitivities. The normalization is arbitrary.

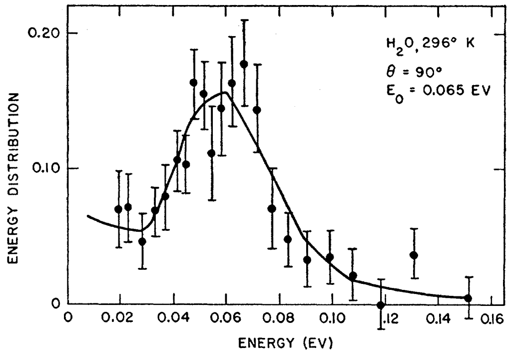

FIG. 3. The energy distribution of neutrons of incident energy 0.065 ev after scattering through 90 deg by water.

ized in the review article by Von Dardel and Sjöstrand.[18] Since the calculated total cross section is in good agreement with experiment, the disagreement in D_0 indicates that the present model gives an angular distribution that is somewhat too steep.

In Fig. 2 the calculated and measured angular distributions are compared for an incident neutron energy of 0.065 ev. The calculated distributions were obtained by integrating $\sigma(E_0,E,\theta)$ over the energy-dependent sensitivity of the thick and thin counters. The experimental angular distribution and the counter sensitivity vs energy are taken from Brockhouse.[2] The thin counter is very nearly $1/v$ so that the uncertainties in its sensitivity do not appreciably affect the calculated angular distribution. For the thick counter, this is probably not the case. In addition, the calculations are not very accurate for angles less than 30 deg since the energy distribution of the scattered neutrons is too narrow for the energy mesh used in the computations.

The agreement between calculation and experiment for the angular distribution is fairly good. Because of the uncertainties mentioned, it is not possible to derive any physical information from the deviation between the experimental and calculated curves in Fig. 2.

Finally, we consider a direct comparison of theory and experiment for $\sigma(E_0,E,\theta)$. We consider the measurement of Brockhouse[2] for $E_0=0.065$ ev and $\theta=90$ deg. The comparison is shown in Fig. 3. The agreement is well within the large experimental error. We note that for this choice of incident energy and scattering angle, the present model should be applicable with good accuracy.

There are also a considerable number of measurements[2–4] which show direct evidence, in their structure for small energy transfer, for the hindrance of the translational motions in the liquid. The present model does not show this structure because of the assumption of free translations. The agreement obtained with the low-resolution experimental data using this model is, however, quite good. It is therefore likely that the present work forms an adequate basis for the treatment of the hydrogen-atom motion at short times. It remains to study more carefully the nature of the hindered translations in the liquid, as well as the sensitivity of the high-resolution data for low-energy neutrons to these motions. The present model does give, however, an adequate basis for the quantitative calculation of neutron thermalization in water, a subject of considerable practical significance in the design of water-moderated reactors.

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