

# Influence of the Rotational Levels on the Scattering of Slow Neutrons by Gaseous Methane\*

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The partial differential cross section for gaseous methane has been computed at incident neutron energies of 0.015 ev and 0.0252 ev at scattering angles of 16.3° and 26.0°. It is found that the quantum nature of the rotational levels has a marked effect on the scattering of neutrons. By comparing the results of these computations with the results of the experiments, it is demonstrated that this effect has also been observed in the experiments.

## I. INTRODUCTION

RECENTLY measurements of the partial differential cross section  $\sigma(E_0, \epsilon, \theta)$  for scattering slow neutrons of initial energy  $E_0$  with energy transfer  $\epsilon$  for a scattering angle  $\theta$  from methane<sup>1</sup> were made with the phased-chopper velocity selector at the Materials Testing Reactor. These experiments were compared with calculations which gave a classical description for the rotational energy states of the molecule. The agreement appeared satisfactory except for incident neutron energies of 0.015 and 0.0252 ev at scattering angles less than 30°. This latter disagreement was attributed to the inadequacy of the classical description of the molecular rotations.

In this paper results are presented which are obtained when a quantum description is given to the rotational energy states of the molecule. The quantum description is accomplished by making use of the theory of Zemach and Glauber<sup>2</sup> and explicitly summing over all the scattering processes that contribute to the cross sections. This summation procedure is practical for incident neutron energies below 0.0252 ev and scattering angles less than 30° that are considered. The calculations demonstrate that the quantum nature of the rotational levels affects the scattering of neutrons and this influence is clearly observed in the experiments. This is apparently the first time that the influence of the discrete nature of the rotational levels has been noted when neutrons are scattered by a gas.

## II. THEORY

If the neutron momentum changes from  $\mathbf{k}_0$  to  $\mathbf{k}$  during a collision with an energy transfer  $\epsilon$  while the molecule simultaneously undergoes a transition between an initial state  $\psi_i$  and a final state  $\psi_f$ , then the partial differential cross section in the laboratory system can be written<sup>2</sup> as

$$\sigma_{fi}(E_0, \epsilon, \theta) = (2\pi)^{-1} \sum_{\nu, \nu'} a_{\nu\nu'} \int (k/k_0) e^{-i\epsilon t} \langle f_i | \nu \nu' \rangle dt, \quad (1)$$

with

$$a_{\nu\nu'} = A_\nu A_{\nu'} + \delta_{\nu\nu'} C_\nu C_{\nu'},$$

$$\begin{aligned} \langle f_i | \nu \nu' \rangle &= e^{i(E_i - E_f)t} \langle \psi_i | \exp(i\mathbf{k} \cdot \mathbf{r}_\nu) | \psi_f \rangle \\ &\quad \times \langle \psi_f | \exp(-i\mathbf{k} \cdot \mathbf{r}_{\nu'}) | \psi_i \rangle, \end{aligned}$$

where  $A_\nu$  and  $C_\nu$  are the bound coherent and incoherent scattering lengths of the  $\nu$ th nucleus and  $\mathbf{r}_\nu$  its position vector. The neutron's gain of momentum and energy are denoted by  $\mathbf{k}$  and  $\epsilon$ . The total initial and final molecular energy are represented by  $E_i$  and  $E_f$ . The units are such that  $\hbar$  has unit magnitude. Since methane consists of four protons and one carbon nucleus, (1) can be written for methane as

$$\begin{aligned} \sigma_{fi}(E_0, \epsilon, \theta) &= 4\sigma(fi|pp) + 12\sigma(fi|pp') \\ &\quad + 8\sigma(fi|Cp) + \sigma(fi|CC), \end{aligned} \quad (2)$$

where

$$\sigma(fi|pp) = (2\pi)^{-1} a_{pp} \int (k/k_0) e^{-i\epsilon t} \langle fi|pp \rangle dt,$$

and the remaining terms are similarly defined. In (2),  $p$  denotes a proton,  $p'$  a different proton, and  $C$  the carbon nucleus. The partial differential cross section for the molecule is obtained by taking the thermal average over the initial states and summing over all possible final states in (2) and, as mentioned in the introduction, is designated by  $\sigma(E_0, \epsilon, \theta)$ .

To bring out some features in the present work which are different from that of Zemach and Glauber, their treatment will be outlined briefly. It is clear that in general it would be convenient to sum first over the final molecular states. Introducing the molecular Hamiltonian  $H$  and writing

$$\begin{aligned} \langle f_i | \nu \nu' \rangle &= \langle \psi_i | e^{iHt} \exp(i\mathbf{k} \cdot \mathbf{r}_\nu) e^{-iHt} | \psi_f \rangle \\ &\quad \times \langle \psi_f | \exp(-i\mathbf{k} \cdot \mathbf{r}_{\nu'}) | \psi_i \rangle, \end{aligned} \quad (4)$$

the final states may be summed over provided the final states of the molecule form a complete set. The position vector  $\mathbf{r}_\nu$  is then written as the sum of the position vector  $\mathbf{R}$  of the molecular center of mass, the displace-

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<sup>1</sup> P. D. Randolph, R. M. Brugger, K. A. Strong, and R. E. Schmunk, *Phys. Rev.* **124**, 460 (1961).

<sup>2</sup> A. C. Zemach and R. J. Glauber, *Phys. Rev.* **101**, 118, 119 (1956).

ment vector  $\mathbf{b}_\nu$  of the  $\nu$ th nucleus from the center of mass, and the displacement vector  $\mathbf{V}_\nu$  of the  $\nu$ th nucleus from its equilibrium position due to vibration. The Hamiltonian operator  $H$  is expressed as a sum of the operators  $H_v$ ,  $H_r$ , and  $H_t$  representing the operators for the vibrational, rotational, and translational modes of the molecule. Assuming that there is no rotation-vibration interaction, the initial molecular wave function  $\psi_i$  is written as a product

$$\psi_i = (\psi_v)_i (\psi_r)_i (\psi_t)_i,$$

of the initial wave functions for the vibrational, rotational, and translational modes. If it is supposed that the rotational and vibrational coordinates commute at all times, it would then be possible to express (4)

$$\begin{aligned} \langle f i | \nu \nu' \rangle = & \exp\{it[(E_r)_i - (E_r)_f]\} \langle (\psi_r)_i | \exp(i\mathbf{k} \cdot \mathbf{b}_\nu) | (\psi_r)_f \rangle \langle (\psi_r)_f | \exp(-i\mathbf{k} \cdot \mathbf{b}_{\nu'}) | (\psi_r)_i \rangle \\ & \times \exp\{it[(E_t)_i - (E_t)_f]\} \langle (\psi_t)_i | \exp(i\mathbf{k} \cdot \mathbf{R}) | (\psi_t)_f \rangle \langle (\psi_t)_f | \exp(-i\mathbf{k} \cdot \mathbf{R}) | (\psi_t)_i \rangle \\ & \times \exp\{it[(E_v)_i - (E_v)_f]\} \langle (\psi_v)_i | \exp(i\mathbf{k} \cdot \mathbf{V}_\nu) | (\psi_v)_f \rangle \langle (\psi_v)_f | \exp(-i\mathbf{k} \cdot \mathbf{V}_{\nu'}) | (\psi_v)_i \rangle. \quad (5) \end{aligned}$$

Introducing the Hamiltonian operators  $H_t$  and  $H_v$  corresponding to the energies of translation and vibration and making the assumption that the final states of each of these modes form a complete set, then the summation over the final states of each of these modes is taken. The summation over the final rotational states is considered later. With the understanding that  $f'$  now represents the final rotational states, (5) reduces to

$$\begin{aligned} \langle f' i | \nu \nu' \rangle = & \exp\{it[(E_r)_i - (E_r)_f]\} \langle (\psi_r)_i | \exp(i\mathbf{k} \cdot \mathbf{b}_\nu) | (\psi_r)_f \rangle \langle (\psi_r)_f | \exp(-i\mathbf{k} \cdot \mathbf{b}_{\nu'}) | (\psi_r)_i \rangle \\ & \times \langle (\psi_t)_i | e^{itH_t} \exp(i\mathbf{k} \cdot \mathbf{R}) e^{-itH_t} \exp(-i\mathbf{k} \cdot \mathbf{R}) | (\psi_t)_i \rangle \langle (\psi_v)_i | e^{itH_v} \exp(i\mathbf{k} \cdot \mathbf{V}_\nu) e^{-itH_v} \exp(-i\mathbf{k} \cdot \mathbf{V}_{\nu'}) | (\psi_v)_i \rangle. \quad (6) \end{aligned}$$

The terms corresponding to the various modes will now be discussed separately.

Considering the expectation value of the translational mode and assuming the momenta of the molecule to be distributed according to a Boltzmann distribution, the thermal average of the translational expectation value as given by Zemach and Glauber is

$$\begin{aligned} \langle (\psi_t)_i | e^{itH_t} \exp(i\mathbf{k} \cdot \mathbf{R}) e^{-itH_t} \exp(-i\mathbf{k} \cdot \mathbf{R}) | (\psi_t)_i \rangle_T \\ = \exp[-k^2(it + \ell^2 T)/(2M)], \quad (7) \end{aligned}$$

in which the temperature  $T$  of the gas is expressed in units of Boltzmann's constant and  $M$  is the mass of the molecule.

Zemach and Glauber have also evaluated the expectation value of the vibration mode. This expectation value will be assumed to be independent of time. This requires that all of the molecules are in their ground vibrational state and that the incident neutrons do not have sufficient energy to excite a vibrational state. Since the molecule with which the neutron collides can have any given orientation, it is also necessary to average the expectation value over the molecular orientations with respect to the incoming neutrons. Krieger and Nelkin<sup>3</sup> have done this in an approximate manner.<sup>4</sup> Their result is

$$\begin{aligned} \langle (\psi_v)_i | e^{itH_v} \exp(i\mathbf{k} \cdot \mathbf{V}_\nu) e^{-itH_v} \exp(-i\mathbf{k} \cdot \mathbf{V}_{\nu'}) | (\psi_v)_i \rangle_{T,\Omega} \\ = \exp(-k^2 \gamma_{\nu\nu'}), \quad (8) \end{aligned}$$

<sup>3</sup> T. J. Krieger and M. S. Nelkin, Phys. Rev. **106**, 290 (1957).

<sup>4</sup> In an Atomic Energy Commission Report IDO-16692 (un-

published) by H. L. McMurry, G. W. Griffing, W. A. Hestir, and L. J. Gannon it was found that a precise average over molecular orientations gives results in the energy range under consideration which are not significantly different.

In this work it is assumed that the initial total energy of the molecule is given by

$$E_i = (E_t)_i + (E_r)_i + (E_v)_i,$$

where  $(E_t)_i$ ,  $(E_r)_i$ , and  $(E_v)_i$  are the initial energies of translation, rotation, and vibration. A similar assumption is made for the final total energy of the molecule. If the position vector  $\mathbf{r}_\nu$  is expressed as above and in addition the same assumption regarding the initial and final molecular wave functions is made, then one can write

where

$$\gamma_{\nu\nu'} = \sum_{\lambda} \{ (12\omega_{\lambda})^{-1} [ (C_{\nu}^{(\lambda)})^2 + (C_{\nu'}^{(\lambda)})^2 ] \},$$

with  $C_{\nu}^{(\lambda)}$  being the magnitude of the amplitude vector corresponding to the  $\nu$ th nucleus and the  $\lambda$ th vibrational mode, and  $\omega_{\lambda}$  the angular frequency of the  $\lambda$ th vibrational mode.

Finally consideration is given to the rotational factor. Taking the rotational wave function of methane to be represented by that for a spherical top, one obtains for a transition from an initial state  $j$  to a final state  $J$  and the case<sup>5</sup> of  $\nu = \nu'$

$$\begin{aligned} \langle (\psi_r)_i | \exp(i\mathbf{k} \cdot \mathbf{b}_\nu) | (\psi_r)_f \rangle \langle (\psi_r)_f | \exp(-i\mathbf{k} \cdot \mathbf{b}_\nu) | (\psi_r)_i \rangle \\ = [(2J+1)/(2j+1)] \sum_{n=|j-J|}^{j+J} j_n^2(\kappa b_\nu), \quad (9) \end{aligned}$$

where  $j_n(x)$  is the spherical Bessel function of order  $n$  and argument  $x$ . The case of  $\nu \neq \nu'$  has been given by Rahman<sup>6</sup> and the above case can be inferred from his work. The initial molecular states must be weighted by the Boltzmann thermal distribution function for a

<sup>5</sup>  $\nu$  refers to the proton. Collisions with the carbon atom will not produce rotations since it is located at the center of mass of the molecule.

<sup>6</sup> A. Rahman, J. Nucl. Energy, Part A: Reactor Sciences **13**, 128 (1961).

spherical top which is given by<sup>7</sup>

$$B_T(j) = \{ (2j+1)^2 \exp[-j(j+1)/(2IT)] \} / \{ \sum_j (2j+1)^2 \exp[-j(j+1)/(2IT)] \}, \quad (10)$$

where  $I$  is the moment of inertia of the molecule. Using (9) and (10), the thermal average of the rotational factor is

$$\begin{aligned} & \langle \exp\{i[\langle (E_r)_i - (E_r)_f \rangle] \langle (\psi_r)_i | \exp(i\mathbf{k} \cdot \mathbf{b}_p) | (\psi_r)_f \rangle \} \rangle_T \\ &= \sum_j \exp\{i[j(j+1) - J(J+1)]/2I\} B_T(j) \\ & \quad \times [(2J+1)/(2j+1)] \sum_{n=|j-J|}^{j+J} j_n^2(\kappa b_p). \quad (11) \end{aligned}$$

Using (7), (8), and (11) in (2) and designating  $\sigma_{pp}(E_0, \epsilon, \theta)$  as the result of averaging  $\sigma(fi|pp)$  over the initial states and summing over the final states, the result is obtained that

$$\sigma_{pp}(E_0, \epsilon, \theta) = \sum_{j,J} \sigma_{JJ}(E_0, \epsilon, \theta | pp), \quad (12)$$

where

$$\begin{aligned} & \sigma_{JJ}(E_0, \epsilon, \theta | pp) \\ &= a_{pp}(2\pi)^{-1} (k/k_0) [(2\pi M)/(T\kappa^2)]^{\frac{1}{2}} \\ & \quad \times \exp[-(\epsilon + \alpha)^2/(2T\kappa^2/M)] [(2J+1)/(2j+1)] \\ & \quad \times B_T(j) \exp(-\kappa^2 \gamma_{pp}) \sum_{n=|j-J|}^{j+J} j_n^2(\kappa b_p), \end{aligned}$$

and

$$\alpha = \left[ \frac{\kappa^2}{2M} - \frac{j(j+1)}{2I} + \frac{J(J+1)}{2I} \right].$$

The contributions from the other terms which will contribute to the partial differential cross section will now be written down. They are obtained in a similar manner as that used to obtain  $\sigma_{pp}(E_0, \epsilon, \theta)$ .

$$\sigma_{pp'}(E_0, \epsilon, \theta) = \sum_{j,J} \sigma_{JJ}(E_0, \epsilon, \theta | pp'), \quad (13)$$

where

$$\begin{aligned} & \sigma_{JJ}(E_0, \epsilon, \theta | pp') \\ &= a_{pp'}(2\pi)^{-1} (k/k_0) [(2\pi M)/(T\kappa^2)]^{\frac{1}{2}} \\ & \quad \times \exp[-(\epsilon + \alpha)^2/(2T\kappa^2/M)] [2(2J+1)/(2j+1)] \\ & \quad \times B_T(j) \exp(-\kappa^2 \gamma_{pp'}) \sum_{n=|j-J|}^{j+J} \{ j_0^2(\kappa b_p) \\ & \quad - \frac{1}{3} j_1^2(\kappa b_p) - \frac{1}{3} j_2^2(\kappa b_p) \dots \}, \end{aligned}$$

and the choice of terms in the summation is from  $|j-J|$  to  $(j+J)$ .

$$\sigma_{Cp}(E_0, \epsilon, \theta) = \sum_j \sigma_{jj}(E_0, \epsilon, \theta | Cp), \quad (14)$$

where

$$\begin{aligned} & \sigma_{jj}(E_0, \epsilon, \theta | Cp) = 2a_{Cp}(2\pi)^{-1} (k/k_0) [2\pi M/(T\kappa^2)]^{\frac{1}{2}} \\ & \quad \times \exp[-(\epsilon + \alpha)^2/(2T\kappa^2/M)] \\ & \quad \times \exp(-\kappa^2 \gamma_{Cp}) B_T(j) j_0(\kappa b_p). \\ & \sigma_{CC}(E_0, \epsilon, \theta) = \sum_j \sigma_{jj}(E_0, \epsilon, \theta | CC), \quad (15) \end{aligned}$$

where

$$\begin{aligned} & \sigma_{jj}(E_0, \epsilon, \theta | CC) = a_{CC}(2\pi)^{-1} (k/k_0) [2\pi M/T\kappa^2]^{\frac{1}{2}} \\ & \quad \times \exp[-(\epsilon + \alpha)^2/(2T\kappa^2/M)] \\ & \quad \times \exp(-\kappa^2 \gamma_{CC}) B_T(j). \quad (16) \end{aligned}$$

The partial differential cross section for the methane molecule is given by

$$\begin{aligned} \sigma(E_0, \epsilon, \theta) &= 4\sigma_{pp}(E_0, \epsilon, \theta) + 12\sigma_{pp'}(E_0, \epsilon, \theta) \\ & \quad + 8\sigma_{Cp}(E_0, \epsilon, \theta) + \sigma_{CC}(E_0, \epsilon, \theta). \end{aligned}$$

### III. RESULTS

The value of the parameters<sup>3,7,8</sup> used in the computations were  $C_C=0$ ,  $A_C=0.64 \times 10^{-12}$  cm,  $C_p=2.52 \times 10^{-12}$  cm,  $A_p=-0.42 \times 10^{-12}$  cm,  $b_p=1.093 \times 10^{-8}$  cm,  $\gamma_{pp}=6.266 \times 10^{-19}$  cm<sup>2</sup>,  $\gamma_{CC}=2.1375 \times 10^{-20}$  cm<sup>2</sup>,  $M=26.757 \times 10^{-24}$  g,  $I=5.330 \times 10^{-40}$  g cm<sup>2</sup>. In the restricted neutron energy range and scattering angles considered, the argument of the spherical Bessel function is always less than two so that only spherical Bessel functions of order 0, 1, and 2 need be used in the computations. The initial and final rotational quantum numbers run from 0 to 20. This range of quantum numbers was determined by inspecting the relative population of the initial levels of the molecule for the given temperature. By inspection of (12) through (16) and using the above parameters, it may be seen that  $\sigma_{pp'}(E_0, \epsilon, \theta)$  and  $\sigma_{Cp}(E_0, \epsilon, \theta)$  are small compared to  $\sigma_{pp}(E_0, \epsilon, \theta)$  and can be neglected. It will also be noted that  $\sigma_{CC}(E_0, \epsilon, \theta)$  contributes the same order of magnitude to  $\sigma(E_0, \epsilon, \theta)$  as these terms. However this term was retained and thus the results are for the computations of

$$\sigma(E_0, \epsilon, \theta) = 4\sigma_{pp}(E_0, \epsilon, \theta) + \sigma_{CC}(E_0, \epsilon, \theta). \quad (17)$$

If (16) or (17) is multiplied by  $(k_0/k) \exp(\epsilon/2T)$  then, after some rearrangement, it may be verified that the resulting expression is an even function of  $\epsilon$  for a fixed value of  $\kappa^2$ . This expresses the fact that the cross section must satisfy the condition of detailed balance<sup>9</sup> and serves as a check on the numerical calculations.

Before comparing the computed with the experimental partial differential cross section a few remarks are in order. It should be noted that the experimental results<sup>1</sup> for a quoted scattering angle represents the

<sup>7</sup> G. Herzberg, *Molecular Spectra and Molecular Structure* (D. Van Nostrand Company, Inc., Princeton, New Jersey, 1945), Vol. II, p. 40.

<sup>8</sup> N. K. Pope, Can. J. Phys. **30**, 597 (1952).

<sup>9</sup> P. Schofield, Phys. Rev. Letters **4**, 239 (1960).

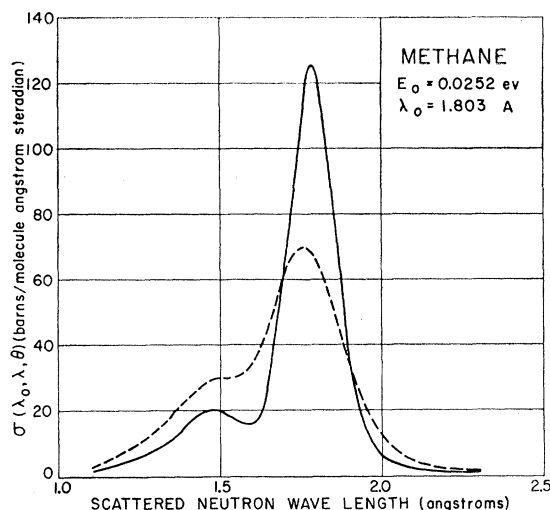


FIG. 1. Computed partial differential cross section shown as a function of the outgoing neutron wavelength. The solid line curve was computed for a scattering angle of  $12.8^\circ$  and the broken line curve for a scattering angle of  $19.8^\circ$ . The temperature of the gas is  $21^\circ\text{C}$ .

integrated contributions from a counter bank that produces a spread in the scattering angles of  $\pm 3.5^\circ$  in the horizontal about the quoted scattering angle. In addition it may be computed that, for a counter bank whose center is located at  $16.3^\circ$ , the scattering angle of a counter located at  $12.8^\circ$  varies from  $12.8^\circ$  at the center of the counter to  $14.3^\circ$  at the end of the counter. At the other extreme of the counter bank the scattering angle for a counter located at  $19.8^\circ$  varies from  $19.8^\circ$  to  $20.8^\circ$ . To make a quantitative comparison of the theoretical and experimental results the theoretical results should be averaged over the counter bank. In addition there are other effects such as the size of the neutron beam that should be considered. Since the primary purpose of this paper is to examine the effect that the discrete rotational states have on the scattering and to point out that such an influence is observed in the experiments, it was not felt justified to make an extensive investigation of the above effects.<sup>10</sup> To illustrate that the qualitative aspects of the partial differential cross section are not likely to be changed if an average was taken over a counter bank, a computation for a neutron energy of 0.0252 eV was made at scattering angles of  $12.8^\circ$  and  $19.8^\circ$ . The results are shown in Fig. 1. In this figure the partial differential cross section is shown as a function of the incident and scattered neutron wavelengths and is plotted against the scattered neutron wavelength. Of particular concern is the feature on the left-hand side of the curves whose qualitative aspects would not be changed by an

<sup>10</sup> In Figs. 2 and 3 the theoretical curves at the main peak are approximately a factor 1.4 higher than those displayed experimentally. In a partial analysis of the various effects that are necessary for a proper comparison it was concluded that there is no real disagreement.

average over the counter bank. This feature will be discussed more fully.

The computed partial differential cross sections are shown and compared with experiments in Figs. 2 and 3. For clarity a small arrow indicates the peak of that portion of the computed curve that has been influenced by the rotational structure of the molecule. This feature is most clearly observed in the experiments at a scattering angle of  $16.3^\circ$  in both figures. As a point of interest the partial differential cross section shown by a dashed curve is presented in Fig. 2 which was computed on the assumption that the rotations could be treated classically. This curve is the same that would be obtained if it were computed according to the method of Krieger and Nelkin. Even if it were considered that the feature on the left side of the experimental curve was due to some unknown spurious effect and that the peak of the experimental curve was too high there is serious disagreement in that the width at half maximum of the computed curve is greater than that observed experimentally. Due to various resolution effects the opposite result would be expected. The curve obtained when discrete rotational levels are considered does not suffer

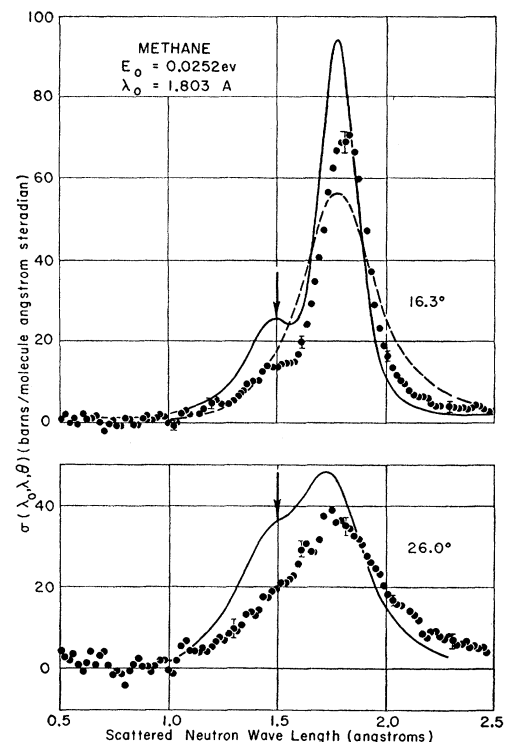


FIG. 2. The experimental and computed partial differential cross sections shown as a function of the outgoing neutron wavelength. The dashed curve for a scattering angle of  $16.3^\circ$  presents an example for the case when the rotations are treated classically. The solid line curve presents the results when the quantum nature of the rotational levels are considered. The arrow indicates the maximum of that portion of the curve that is due to rotations. Its position is at 1.47 Å. The temperature of the gas is  $21^\circ\text{C}$ .

this defect. Messiah<sup>11</sup> and also Krieger and Nelkin have estimated that the mass-tensor approximation should hold for methane when the neutron energy is greater than about 0.01 ev. In view of our calculations it appears that this estimate is too optimistic, especially at small scattering angles.

At a scattering angle of 26.0° in Fig. 2 the theoretical results indicate that the main peak is overlapping the peak due to the rotations so that it would be difficult to detect. Although the experimental results tend to be in harmony with the theoretical prediction, admittedly it would be difficult to state with certainty that the rotational feature appears in the experiments. There also appears to be some measure of qualitative agreement at a scattering angle of 26.0° in Fig. 3 but the experimental data have considerable fluctuation and any attempt at comparison is probably not very meaningful.

The theoretical computations predict that the peak of the rotational feature occurs at an energy gain by the neutron of about 0.013 ev in each case considered in Figs. 2 and 3. Consideration of the energy and the relative population of the rotational levels of methane makes it appear quite reasonable that the peak should occur at an energy gain of 0.013 ev. The width of the rotational feature is due mainly to the fact that it is a composite of contributions of transitions from various initial to various lower final rotational states of the molecule. These are broadened by the translational motion of the molecule and thus the resulting structure appears as a smooth curve.

The neutron will also lose energy to the rotational states. The computations and apparently the experiments do not indicate an influence due to the neutron losing energy similar to that for its gaining energy. The reason for this can be argued as follows: Let us consider the most favorable case for observing an influence due to the neutron losing energy, namely that for which the neutron has an incident energy of 0.0252 ev. The greatest relative population of the rotational levels occurs at  $j=6$  corresponding to an energy of approximately 0.027 ev. Physically it would be expected that in a collision with the molecule in this state, it would be much more probable for the neutron to gain energy rather than lose energy since the energy of the state is greater than the energy of the neutron. If

<sup>11</sup> A. M. L. Messiah, Phys. Rev. 84, 204 (1951).

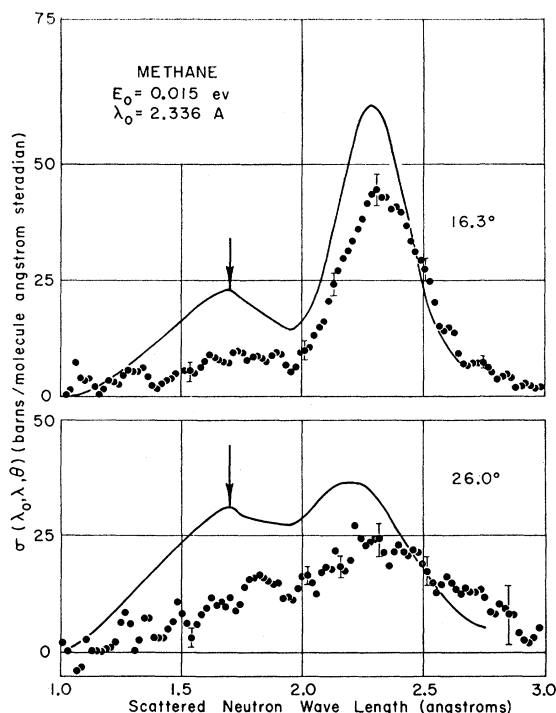


FIG. 3. The experimental and computed partial differential cross section shown as a function of the outgoing neutron wavelength. The solid line curve presents the results when the quantum nature of the rotational levels are considered. The arrow indicates the maximum of the profile feature that is due to rotations. Its position is at 1.7 Å. The temperature of the gas is 21°C.

consideration is given to the lower energy states for which the probability of the neutron giving up energy to the molecule has increased, then the relative population for the molecule to be in such a state has decreased and also the energy changes are such that the contribution from such a transition would be obscured by the main peak.

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