The Scattering of Slow Neutrons by Molecular Gases

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It has been shown by Fermi that the cross section for the scattering of slow neutrons by protons is four times greater for protons strongly bound to an infinite mass than it is for free protons initially at rest. A simple generalization of this factor of four can be given for the scattering of neutrons by molecular gases if the neutron energy is great as compared to the energy differences of the rotational levels of the scattering molecule but small compared to the quanta of molecular vibration. In this case, the proton may be replaced by a freely moving hypothetical mass point whose mass is a tensor depending on the mass and structure of the molecule. On this basis the total cross section for the scattering of slow neutrons by H_2 and by CH_4, NH_3 and H_2O at low temperatures has been calculated as a function of the ratio of the neutron energy to the thermal energy of the scattering gas. The possibility of applying the theory to a determination of the neutron-proton scattering cross section is discussed.

1. INTRODUCTION

THE problem of the scattering of slow neutrons by bound protons was first treated by Fermi[1] and then in somewhat more detail by Arley.[2] Fermi showed that for sufficiently slow neutrons the scattering cross section σ may be calculated by substituting a relatively wide and shallow neutron-proton interaction potential for the actual narrow and deep potential. Then the Born approximation may be applied to this shallow potential. The width of this potential must be small compared to the wave-length of the neutron (relative to the proton). The effect of the substitute potential is essentially the same as that of a delta-function interaction between neutron and proton since the neutron wave function varies but little over its width.

If the proton is elastically bound to an infinite mass the scattering cross section depends on the ratio of vibrational quantum to neutron energy. For neutrons of energy less than a vibrational quantum, only elastic collisions are possible and it has been shown[1,2] that the cross section is nearly independent of the vibrational proper functions. If such be the case, then according to perturbation theory the transition probability depends only on the density of energy states into which the neutron can be scattered. This density is proportional to p^2dp/dE, where p is the momentum of the neutron in the center of gravity coordinate system and E is the relative kinetic energy. In terms of E, $p^2dp/dE \sim \mu^{\frac{3}{2}}E^{\frac{1}{2}}$ where μ is the reduced mass of the neutron plus proton-system (i.e., the system of the proton and all the particles to which it is bound). If the proton is initially at rest, E is related to the initial kinetic energy, E_0, of the neutron in the laboratory system by $E=(\mu/m)E_0$. Thus the transition probability, and therefore the scattering cross section, is proportional to μ^2. Since we are considering a proton-system of infinite mass, μ is equal to the mass, m, of the neutron. The cross section for this case will be called σ_∞.

For the scattering by a free proton at rest the cross section is again proportional to μ^2, but in this case the reduced mass is $\mu=m/2$ and the cross section is $(\frac{1}{4})\sigma_\infty$. Thus we are led to the well-known factor of $\frac{1}{4}$ for the ratio of the cross section for a free proton to the cross section for a proton rigidly bound to an infinite mass.

In the case of the scattering of neutrons by hydrogen-containing molecules (in the gaseous state) the proton may be treated as free if the neutron energy is very great compared to both rotational and vibrational quanta (i.e., h times rotational and vibrational frequencies) of the molecule. When the neutron energy is much smaller than both of these energies, only the translational motion of the molecule as a whole is affected by the neutron impact so the cross section may be calculated as above with μ determined by $1/\mu=1/m+1/M$ where M is the

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total mass of the molecule. The cross section is then $(M/m+M)^2\sigma_\infty$ (as long as interference effects may be neglected).

In the intermediate case for which the neutron energy is great compared to a rotational quantum but too small to excite molecular vibrations, the situation is somewhat more complicated. For, if it is assumed that the rotational-translational motion of the molecule can be treated classically, the effective mass of a proton in the molecule during the collision depends on the direction of the initial and final momentum of the neutron. For example, a neutron in a head-on collision with one of the protons of the H_2 molecule will feel an effective proton mass of $2m$ if it is moving parallel to the H-H axis and a mass m if its path is perpendicular to this axis. In general, there will be a linear relation between the change in velocity of the proton and the change in momentum of the neutron due to the collision. Therefore we may associate with the proton a hypothetical mass point which moves with the velocity of the proton but whose mass is a tensor which depends on the mass and structure of the molecule.

In order to calculate the transition probability for the scattering of neutrons with energy that is great compared to the rotational quanta of the molecule, the rotational wave function in the final state can be replaced by a rotating wave packet which is a combination of neighboring rotational states since many rotational quanta will be excited by the collision. By making the packet sufficiently small the rotational wave function within it may be approximated by a plane wave. The molecular wave function is a product of the rotational and translational wave functions of the molecule multiplied by a vibrational wave function which in this case serves only to limit the position of the proton with respect to the other atoms in the molecule. Taking into account the fact that the translational wave function of the molecule is a plane wave, we see that the relevant part of the molecular wave function after collision may be treated as a plane wave which describes the properties of the wave packet under translation and infinitesimal rotation.

Insofar as the calculation of the matrix element for the transition is concerned, the initial rotational state may also be replaced by a plane wave since its only contribution to this matrix element is in the region of the wave packet. Therefore, just as in the case of free protons, the matrix element serves only to guarantee the conservation of momentum and angular momentum and the transition probability depends only on the density of final energy states into which the neutron can be scattered. By the conservation laws, the density of the neutron states is equal to the density of the permissible final states for the molecule. However this density will now depend on the reduced mass that is associated with the mass of the neutron and the mass tensor of the hypothetical mass point described above.

Since the quantum calculations are essentially concerned with small wave packets moving under the influence of constant or slowly varying potentials and since the only quickly varying interaction—that between the neutron and proton—leads to matrix elements that merely represent conservation laws, the entire calculation can be carried out according to classical mechanics. The meaning of the mass tensor as the linear relation between velocity and momentum vectors is the same in the classical and quantum treatment. Instead of the density of energy levels the volume of momentum space per unit energy interval will enter into the classical theory.

The condition that the energy of the neutron be greater than the separation between rotational states is roughly $\lambda < r_0$, where λ is the neutron wave-length and r_0 is a measure of the linear dimensions of the molecule. Therefore, under this condition, interference between the scattering from two different protons in the molecule may be neglected.

2. The Mass Tensor

Since the hypothetical mass point has only three degrees of freedom and the molecule (treated as rigid) has five or six, the motion of the molecule cannot be described completely by the motion of the mass point.

We separate the infinitesimal displacements of the molecule into the set of two or three displacements for which the proton remains fixed

and the set for which the angular momentum about the proton is zero. In a collision with a thermal (S) neutron the angular momentum around the proton is unchanged. Therefore the change in motion suffered by the molecule involves only displacements of the latter type. The velocities associated with these displacements are uniquely determined by the velocity components of the proton so the behavior of these displacements can be equivalently described by the motion of the mass point to be associated with the proton.

It will be shown below that the two sets of displacements described above are orthogonal in the sense that the kinetic energy of the molecule can be written as the sum of two terms depending on the first and second types of displacement, respectively.

The molecular motion is usually described by means of its angular velocity $\mathbf{w}$ about the center of gravity, and the velocity $\mathbf{V}_c$ of the center of gravity. In order to obtain for the displacements per unit time the two types described above we write $\mathbf{w}$ and $\mathbf{V}_c$ as the sum of two terms:

$$\mathbf{w}=\mathbf{w}'+\mathbf{w}'', \quad \mathbf{V}_c=\mathbf{V}_c'+\mathbf{V}_c'',$$

where the set $(\mathbf{w}', \mathbf{V}_c')$ satisfies

$$[\mathbf{w}'\times\mathbf{r}]+\mathbf{V}_c'=0 \tag{1}$$

and the set $(\mathbf{w}'', \mathbf{V}_c'')$ satisfies

$$\mathbf{I}\mathbf{w}''-M_0[\mathbf{r}\times\mathbf{V}_c'']=0, \tag{2}$$

if $\mathbf{r}$ is the vector drawn from the center of gravity of the molecule to the proton, M_0 is the mass of the molecule, and $\mathbf{I}$ is the moment of inertia tensor of the molecule. Equation (1) corresponds to the condition that the proton be at rest and (2) to the condition that the angular momentum about the proton be zero. Thus we have written the original displacement described by $\mathbf{w}$ and $\mathbf{V}_c$ as the sum of two displacements $(\mathbf{w}', \mathbf{V}_c')$ and $(\mathbf{w}'', \mathbf{V}_c'')$ which satisfy the conditions for the displacements of the first and second type.

The kinetic energy of the molecule is

$$\begin{aligned}2E_M&=(\mathbf{w}\cdot\mathbf{I}\mathbf{w})+M_0V_c^2\\&=(\mathbf{w}'\cdot\mathbf{I}\mathbf{w}')+M_0V_c'^2+(\mathbf{w}''\cdot\mathbf{I}\mathbf{w}'')+M_0V_c''^2\\&\quad+2[(\mathbf{w}'\cdot\mathbf{I}\mathbf{w}'')+M_0(\mathbf{V}_c'\cdot\mathbf{V}_c'')]\end{aligned}$$

and the condition for orthogonality,

$$(\mathbf{w}'\cdot\mathbf{I}\mathbf{w}'')+M_0(\mathbf{V}_c'\cdot\mathbf{V}_c'')=0. \tag{3}$$

To verify Eq. (3) we make use of Eq. (2) and find that

$$\begin{aligned}(\mathbf{w}'\cdot\mathbf{I}\mathbf{w}'')&=M_0(\mathbf{w}'\cdot[\mathbf{r}\times\mathbf{V}_c''])\\&=M_0([\mathbf{w}'\times\mathbf{r}]\cdot\mathbf{V}_c'').\end{aligned}$$

Then by Eq. (1) the condition (3) is satisfied.

We now wish to describe the part of the motion corresponding to $(\mathbf{w}'', \mathbf{V}_c'')$ by the motion of the hypothetical mass point. Assume that the momentum of the mass point is equal to the momentum of the molecule,

$$\mathbf{P}=M_0\mathbf{V}_c''. \tag{4}$$

Conservation of momentum will then be satisfied for the molecule if it is satisfied for the mass point since the motion $(\mathbf{w}', \mathbf{V}_c')$ is unaffected by the collision; and, for the same reason, the angular momentum around the proton will be conserved.

Since the mass point is defined as having a velocity $\mathbf{V}$ equal to the velocity of the proton, the inverse mass tensor is defined by $\mathbf{V}=\mathbf{M}^{-1}\mathbf{P}$. Now $\mathbf{V}=[\mathbf{w}''\times\mathbf{r}]+\mathbf{V}_c''$, so Eqs. (2) and (4) give

$$\mathbf{V}=[\mathbf{I}^{-1}[\mathbf{r}\times\mathbf{P}]\times\mathbf{r}]+M_0^{-1}\mathbf{P}, \tag{5}$$

which is the desired linear relation between $\mathbf{V}$ and $\mathbf{P}$.

It immediately follows from Eqs. (2), (4), and (5) that the kinetic energy of the mass point is equal to that part of the molecular kinetic energy due to $(\mathbf{w}'', \mathbf{V}_c'')$; that is,

$$\tfrac{1}{2}(\mathbf{P}\cdot\mathbf{V})=\tfrac{1}{2}(\mathbf{w}''\cdot\mathbf{I}\mathbf{w}'')+\tfrac{1}{2}M_0\mathbf{V}_c''^2.$$

Finally, the expression (5) written in terms of components is

$$V_i=\left(\frac{r_j^2}{I_k}+\frac{r_k^2}{I_j}+\frac{1}{M_0}\right)P_i-\frac{r_ir_j}{I_k}P_j-\frac{r_ir_k}{I_j}P_k,$$

where the subscripts i, j, k refer to the directions of the principal axes of inertia and r_1, r_2, r_3 are the coordinates of the proton under consideration with respect to the center of gravity. Therefore, the inverse mass tensor is

$$(M^{-1})_{ii}=\left(\frac{r_j^2}{I_k}+\frac{r_k^2}{I_j}+\frac{1}{M_0}\right), \quad (M^{-1})_{ij}=-\frac{r_ir_j}{I_k}. \tag{6}$$

It is seen that the tensor is symmetric, a fact which can be proved directly from Eq. (5); thus it can be transformed to diagonal form.

It will be convenient to introduce the dimensionless tensor $\mathbf{n}=m\mathbf{M}^{-1}$. In the following paragraphs we shall calculate the characteristic values n_1, n_2, n_3 of $\mathbf{n}$ for a few cases.

H_2

For the hydrogen molecule, the principal axes of inertia and mass coincide. As stated in Section 1, the mass perpendicular to the H-H axis is m and that parallel to the axis is $2m$. Thus $n_1=n_2=1$, $n_3=\frac{1}{2}$ for both protons.

CH_4

In methane the moment of inertia ellipsoid is a sphere so the axes of inertia may be chosen in such a way that one of them passes through the proton under consideration. These axes are then the principal axes of mass for this proton. The mass along the axis that passes through the proton and the center of gravity of the molecule is the total mass of the molecule; thus the corresponding component of $\mathbf{n}$ is $n_1=\frac{1}{16}$. The other two components of $\mathbf{n}$ are $n_2=n_3=\frac{7}{16}$.

NH_3

The principal axes of mass do not coincide with those of the moment of inertia for ammonia, but one of them is the line joining the given proton with the center of gravity; another is perpendicular to this and in the plane determined by the proton, the nitrogen atom, and the center of gravity; and the third is perpendicular to these two. The mass for the first of these directions is again the total mass of the molecule so $n_1=\frac{1}{17}(=0.0589)$. In sufficient approximation one can set the HNH angle in ammonia equal to the HCH angle in methane (109° 28′). Under this assumption, the other two characteristic values of $\mathbf{n}$ are given by $n_2=0.604$ and $n_3=0.439$.

H_2O

One principal axis of the mass tensor for water is, as usual, the line joining the proton with the center of gravity. The other two are perpendicular to this (and to each other) and one of them lies in the plane of the molecule. If the HOH angle is taken to be 106°, the results for the components of $\mathbf{n}$ are $n_1=\frac{1}{18}(=0.0555)$, $n_2=0.535$, $n_3=1$.

3. Scattering Cross Section

The collision of a slow neutron with a proton in the molecule gives rise to changes in $\mathbf{w}$ and $\mathbf{V}_c$ which are represented by vectors of the type $(\mathbf{w}'', \mathbf{V}_c'')$. The density of final neutron states, and therefore the transition probability, is then independent of motions of the molecule of the type $(\mathbf{w}', \mathbf{V}_c')$ and depends only on the motion of the mass point.

If the mass $\mathbf{M}$ of the hypothetical mass point has the characteristic values M_1, M_2, M_3, the position of the center of gravity of the neutron-mass point system is defined by $(m+M_i)\bar{x}_i = mx_i+M_i\xi_i$, $i=1, 2, 3$. Here, x_i are the coordinates of the neutron and ξ_i those of the mass point. The velocity, momentum and kinetic energy of the two particles in the center of gravity system may now be calculated in the usual way. The total kinetic energy E_0 separates into the sum of the kinetic energy of the center of gravity $\bar{E}$, and the relative kinetic energy E.

The density of final states for the neutron is proportional to $d\tau/dE$, where τ is the volume in momentum space contained within a surface of constant relative energy (E). That is,

$$\tau=\int\int\int_{E=\text{const.}} dp_1dp_2dp_3$$

where (p_1, p_2, p_3) is the final momentum of the neutron in the center of gravity coordinate system. E is the sum of the kinetic energy of the neutron and the kinetic energy of the mass point (both taken in the center of gravity system). The former energy is $(\mathbf{p}\cdot\mathbf{p})/2m$ and the latter is $(\frac{1}{2})(\mathbf{p}\cdot\mathbf{M}^{-1}\mathbf{p})$ since $\mathbf{p}=(p_1, p_2, p_3)$ is also the negative momentum of the mass point in the C.G. system. Therefore the surface of constant energy is given by

$$2mE=(\mathbf{p}\cdot\mathbf{p})+(\mathbf{p}\cdot\mathbf{np})=(\mathbf{p}\cdot\boldsymbol{\mu}^{-1}\mathbf{p})=\text{const.},$$

where $\boldsymbol{\mu}^{-1}=\mathbf{1}+\mathbf{n}$. The tensor $\boldsymbol{\mu}$ can be considered as the reduced mass tensor measured in units of the mass of the neutron. When $\boldsymbol{\mu}$ is in diagonal form, the energy surface is the ellipsoid

$$2mE=\mu_1^{-1}p_1^2+\mu_2^{-1}p_2^2+\mu_3^{-1}p_3^2$$

TABLE I. *The limits of validity of Eq. (7) are given by* $E_n > E_{\text{rot}}$, $E_n > (E_{\text{rot}}kT)^{\frac{1}{2}}$, *and* $E_n < E_{\text{vib}}$ *where* E_n *is the neutron energy and* T *is the temperature of the scattering gas.*

MOLECULE	H_2	CH_4	NH_3	H_2O
E_{rot}(ev)	0.015	0.001	0.002	0.006
E_{vib}(ev)	0.5	0.15	0.1	0.2

and the volume, τ, is $\tau = 4\pi/3(2mE)^{\frac{3}{2}}(\mu_1\mu_2\mu_3)^{\frac{1}{2}}$ so that

$$d\tau/dE = 2\pi(2m)^{\frac{3}{2}}(\mu_1\mu_2\mu_3)^{\frac{1}{2}}E^{\frac{1}{2}}.$$

The transition probability is therefore proportional to $(\mu_1\mu_2\mu_3)^{\frac{1}{2}}E^{\frac{1}{2}}$. Now, by conservation of energy, $E = E_0 - \bar{E}$, where E_0 and $\bar{E}$ are the total energy and the energy of the center of gravity before collision. If $\mathbf{P}_n$ and $\mathbf{P}$ are the momenta of the neutron and mass point in the laboratory system before collision,

$$2mE_0 = P_n^2 + (\mathbf{P}\cdot\mathbf{nP})$$

and

$$2m\bar{E} = (\bar{\mathbf{P}}\cdot\mathbf{n}\mathfrak{y}\bar{\mathbf{P}}),$$

where $\bar{\mathbf{P}} = \mathbf{P} + \mathbf{P}_n$ is the total momentum. Taking the difference between these equations we obtain

$$2mE = [\mathfrak{y}^{\frac{1}{2}}(\mathbf{P}_n - \mathbf{nP})]^2.$$

Thus in terms of the components of momentum along the principal axes of mass of the molecule the transition probability is proportional to

$$(\mu_1\mu_2\mu_3)^{\frac{1}{2}}\{\textstyle\sum_i \mu_i(P_{ni} - n_iP_i)^2\}^{\frac{1}{2}}.$$

The scattering cross section is given by the transition probability divided by the initial velocity of the neutron in the laboratory system. Consequently

$$\sigma = c(\mu_1\mu_2\mu_3)^{\frac{1}{2}}\left\{\frac{1}{P_n^2}\sum_i \mu_i(P_{ni} - n_iP_i)^2\right\}^{\frac{1}{2}},$$

where c is the constant of proportionality. When the proton is rigidly bound to an infinite mass, $n_1 = n_2 = n_3 = 0$ and $\mu_1 = \mu_2 = \mu_3 = 1$, so the cross section is $\sigma_\infty = c$.

If the vector with components $n_i^{\frac{1}{2}}P_i$ has the magnitude ρ and the direction cosines β_i, then the energy of the mass point is given by $2mE_p = \sum_i n_iP_i^2 = \rho^2$. The cross section σ may be expressed in terms of ρ and β_i, and in terms of the magnitude P_n, and the direction cosines α_i of the initial momentum of the neutron by the equation

TABLE II. *Scattering cross sections per proton in the given molecules as a function of neutron energy* E_n *and the temperature* T *of the molecular gas. The last column gives the region over which the formulae are valid. In addition* E_n *must satisfy the conditions given in Table I. The total cross section per molecule is obtained by multiplying* $\bar{\sigma}$ *by the number of protons in the molecule and adding* $\bar{\sigma}_h$ *(Eq. (14)).*

MOLECULE	CROSS SECTION PER PROTON	LIMITS OF VALIDITY
CH_4	$\bar{\sigma}/\sigma_H = 2.7 + 0.42kT/E_n$	$0 \leq kT/E_n < 0.1$
NH_3	$\bar{\sigma}/\sigma_H = 2.18 + 0.39kT/E_n$	$0 \leq kT/E_n < 0.1$
H_2O	$\bar{\sigma}/\sigma_H = 1.855 + 0.46kT/E_n$	$0 \leq kT/E_n < 0.05$

$$\sigma = \sigma_\infty(\mu_1\mu_2\mu_3)^{\frac{1}{2}}\left\{\sum_i \mu_i\left(\alpha_i - \frac{\rho}{P_n}n_i^{\frac{1}{2}}\beta_i\right)^2\right\}^{\frac{1}{2}}. \quad (7)$$

This equation is then the generalization of the proportionality of the cross section to the square of the reduced mass. For use in specific problems such as the calculation of the mean scattering cross section or the mean free path, expressions obtained from (7) have to be averaged over the angles α_i and β_i, over the velocity distribution of the molecules, and often over the neutron velocities. In order to carry out these calculations, it is necessary to know the experimental conditions. We shall first calculate the mean cross section for the scattering of monochromatic neutrons. This quantity is connected with the diminution in intensity of a neutron beam in passing through a sufficiently small amount of gas. The effective cross section will also be calculated for a neutron current distribution of the form $P_n^2\exp(-P_n^2/2mkT_n)dP_n$. Although this distribution is difficult to realize experimentally, we will make use of it since it leads to relatively simple results.

It has been pointed out in the introduction that the formula (7) can be expected to hold only if the neutron energy is large compared to the separation between rotational states and small compared to any vibrational quantum. In Table I are given the values of $E_{\text{rot}} = \hbar^2/I_{\min}$ and $E_{\text{vib}} = h\nu_{\min}$ for those molecules which will be considered below. $I_{\min}$ is the smallest moment of inertia of the molecule and $\nu_{\min}$ the smallest vibrational frequency. The condition that the neutron energy be large compared to the separation between rotational states is then: $E_n > E_{\text{rot}}$, $E_n > (E_{\text{rot}}kT)^{\frac{1}{2}}$, where T is the temperature of the molecular gas under consideration. In order that E_n be small compared to a vibrational quantum we have $E_n < E_{\text{vib}}$.

4. Mean Cross Section for Monochromatic Neutrons

The direction cosines α_i, β_i are given with respect to axes fixed in the molecule. Therefore, in order to obtain the mean cross section, the expression (7) must be averaged over all possible orientations α_i, β_i of the molecule. For the purpose of carrying out this average, let

$$\gamma_i=\left\langle\left(\alpha_i-\frac{\rho}{P_n}n_i^{\frac{1}{2}}\beta_i\right)^2\right\rangle_{\text{Av}}$$

and

$$X_i=\left(\alpha_i-\frac{\rho}{P_n}n_i^{\frac{1}{2}}\beta_i\right)^2-\gamma_i,$$

where the average is taken over α_i, β_i. Then σ is given by

$$\sigma=\sigma_\infty(\mu_1\mu_2\mu_3)^{\frac{1}{2}}(\textstyle\sum_i\gamma_i\mu_i)^{\frac{1}{2}}\{1+\sum_j\mu_jX_j/\sum_i\gamma_i\mu_i\}^{\frac{1}{2}}.$$

If the quantity $X=\sum_j\mu_jX_j/\sum_i\gamma_i\mu_i$ is less than one, the square root may be expanded in powers of X and then averaged. Thus

$$\sigma_{\text{Av}}=\sigma_\infty(\mu_1\mu_2\mu_3)^{\frac{1}{2}}(\textstyle\sum_i\gamma_i\mu_i)^{\frac{1}{2}}\{1-\frac{1}{2}\langle X\rangle_{\text{Av}}-\frac{1}{8}\langle X^2\rangle_{\text{Av}}+\frac{1}{16}\langle X^3\rangle_{\text{Av}}+\cdots\}. \tag{8}$$

The conditions under which this expansion is valid will be discussed below. The ranges of values of kT/E_n for which it holds are given in the last column of Table II.

Now making use of the averages

$$\langle\alpha_i^{2n}\rangle_{\text{Av}}=\frac{1}{2n+1},\quad \langle\alpha_i^2\alpha_j^{2n}\rangle_{\text{Av}}=\frac{1}{(2n+1)(2n+3)},\quad \langle\alpha_1^2\alpha_2^2\alpha_3^2\rangle_{\text{Av}}=\frac{1}{105},$$

we find

$$\textstyle\sum_i\gamma_i\mu_i=\mu+(1-\mu)\rho^2/P_n^2,\quad X_{\text{Av}}=0,$$

$$(\textstyle\sum_i\gamma_i\mu_i)^2\langle X^2\rangle_{\text{Av}}=\frac{4}{45}\{a_1(1+\rho^4/P_n^4)+a_2\rho^2/P_n^2\},$$

$$(\textstyle\sum_i\gamma_i\mu_i)^3\langle X^3\rangle_{\text{Av}}=\frac{8}{45}\{b_1(1-\rho^6/P_n^6)+b_2(1-\rho^2/P_n^2)\rho^2/P_n^2\},$$

where

$$\begin{aligned}
&\mu=\tfrac{1}{3}\textstyle\sum_i\mu_i,\\
&a_1=\tfrac{1}{2}\textstyle\sum_{i>j}(\mu_i=\mu_j)^2,\\
&a_2=5\textstyle\sum_i n_i\mu_i^2,\\
&b_1=\tfrac{1}{21}(2\textstyle\sum_j\mu_j^3-3\sum_{i\neq j}\mu_j^2\mu_i+12\mu_1\mu_2\mu_3),\\
&b_2=2\textstyle\sum_j\mu_j^3n_j-\sum_{i\neq j}\mu_i^2\mu_jn_i.
\end{aligned} \tag{9}$$

In obtaining these expressions, use has been made of the relation $1/\mu_i=n_i+1$. With $a=1/\mu-1$, the average of the cross section over α_i, β_i becomes

$$\sigma_{\text{Av}}=\sigma_\infty(\mu_1\mu_2\mu_3\mu)^{\frac{1}{2}}(1+a\rho^2/P_n^2)^{\frac{1}{2}}\left\{1-\frac{a_1(1+\rho^4/P_n^4)+a_2\rho^2/P_n^2}{90\mu^2(1+a\rho^2/P_n^2)^2}+\frac{b_1(1-\rho^6/P_n^6)+b_2(1-\rho^2/P_n^2)(\rho^2/P_n^2)}{90\mu^3(1+a\rho^2/P_n^2)^3}+\cdots\right\}. \tag{10}$$

If the scattering molecules are at a temperature[3] T, their energy distribution is proportional to $\exp(-E_M/kT)$ times the element of volume in momentum space. The kinetic energy E_M of the

[3] It is assumed throughout the paper that the temperature T is not high enough to excite molecular vibrations.

molecule is the sum of E_p (kinetic energy of the mass point) and a kinetic energy that is independent of the motion of the mass point. The element of volume in the molecular momentum space is the product of an element of volume in the momentum space of the mass point and a second volume element that is independent of the momentum of the mass point. Therefore the number of molecules for which $(2mE_p)^{\frac{1}{2}}$ lies between the values ρ and $\rho+d\rho$ is proportional to $\exp(-\rho^2/2mkT)\rho^2 d\rho$. The expression (10) must now be averaged over this distribution. If we let $\eta=\rho/P_n$, this average is

$$\bar{\sigma}=\sigma_\infty(\mu_1\mu_2\mu_3\mu)^{\frac{1}{2}}(T_0+T_1+T_2+\cdots), \tag{11}$$

where

$$T_0=\int_0^\infty (1+a\eta^2)^{\frac{1}{2}}\exp[-(E_n/kT)\eta^2]\eta^2 d\eta \Big/ \int_0^\infty \exp[-(E_n/kT)\eta^2]\eta^2 d\eta,$$

$$T_1=-\frac{1}{90\mu^2}\int_0^\infty (1+a\eta^2)^{-\frac{3}{2}}\exp[-(E_n/kT)\eta^2](a_1\eta^2+a_2\eta^4+a_1\eta^6)d\eta \Big/ \int_0^\infty \exp[-(E_n/kT)\eta^2]\eta^2 d\eta,$$

$$T_2=\frac{1}{90\mu^3}\int_0^\infty (1+a\eta^2)^{-5/2}\exp[-(E_n/kT)\eta^2] \times(b_1\eta^2+b_2\eta^4-b_2\eta^6-b_1\eta^8)d\eta \Big/ \int_0^\infty \exp[-(E_n/kT)\eta^2]\eta^2 d\eta.$$

These integrals may be put into a convenient form by writing

$$I_0=\frac{4\vartheta^{\frac{3}{2}}}{\sqrt{\pi}}\int_0^\infty (1+x^2)^{\frac{1}{2}}x^2\exp[-\vartheta x^2]dx$$

and

$$I_{pq}=\frac{4\vartheta^{\frac{3}{2}}}{\sqrt{\pi}}\int_0^\infty (1+x^2)^{-(p+\frac{1}{2})}x^{2q}\exp[-\vartheta x^2]dx,$$

where

$$\vartheta=E_n/akT.$$

Then the terms T_0, T_1, T_2 become

$$\begin{aligned} T_0&=I_0,\\ T_1&=-(a_1I_{11}+a_2I_{12}/a+a_1I_{13}/a^2)/90\mu^2,\\ T_2&=(b_1I_{21}+b_2I_{22}/a-b_2I_{23}/a^2-b_1I_{24}/a^3)/90\mu^3. \end{aligned} \tag{12}$$

Unfortunately, the integrals I_0, I_{pq} could not be carried out explicitly so that it has been necessary to evaluate them numerically. A rough evaluation of I_0 has been carried out as follows: In the range $0\leq x\leq 0.5$, the expression $(1+x^2)^{\frac{1}{2}}$ may be expanded in power series and the resulting expression integrated. Similarly, from $x=2$ to ∞, $(1+1/x^2)^{\frac{1}{2}}$ may be expanded and the direct integration carried out. Then in the range from 0.5 to 2 the integration has been done numerically.

The integrals I_{1q} have been treated similarly, except that in this case the ranges chosen were $0\leq x\leq 0.1$ and $10\leq x\leq\infty$, because of the slower convergence of $(1+x^2)^{-\frac{3}{2}}$. Only upper limits have been obtained for I_{2q} in order to check the convergence of the expression for the scattering cross section.

The values of n_i may be taken from Section 2 and the corresponding values of μ_i, μ, a, a_1, a_2, b_1, b_2 may be calculated from them by Eqs. (9). The results for the T_i are then given by Eq. (12) and $\bar{\sigma}$ may finally be obtained from Eq. (11).

The final result for the scattering of slow neutrons with energy E_n by one of the protons in H_2 is given in Fig. 1 for $0.1 \leq E_n/kT \leq 10$. The ordinate in this figure is $\bar{\sigma}$ divided by the cross section, σ_H, of a free proton at rest ($\sigma_H = \frac{1}{4}\sigma_\infty$). The abscissa is $\log_{10} E_n/kT$ where T is the temperature of the molecules. In computing these curves T_2 and all higher terms have been neglected, which is a rather good approximation for H_2. The broken part of the curve was interpolated with the help of rough integrations of I_0 and I_{pq}.

The validity of this curve depends upon the convergence of the expansion (8). In the case of H_2, it turns out that for all values of E_p/E_n (E_p is the energy of the mass point), the quantity X in Eq. (8) is less than one in absolute value so the expansion can be expected to converge in this case. However, for other molecules such as CH_4, NH_3, and H_2O, X is less than one only for a restricted range of values of E_p/E_n. In these regions, the quantities $\bar{\sigma}/\sigma_H$ are, to a very good approximation, linear functions of kT/E_n. Formulae for the scattering cross sections per proton in the molecules CH_4, NH_3 and H_2O and their limits of validity are given in Table II. It is to be noted that the conditions given in the last column of Table II indicate that these results may only be applied to gases at low temperatures if the limits on E_n given in Table I are taken into account.

The scattering cross section per proton for H_2 in the range $0 \leq kT/E_n \leq 0.1$ is also an approximately linear function of kT/E_n. It may be expressed by the equation

$$\bar{\sigma}/\sigma_H = 1.22 + 0.86 kT/E_n. \tag{13}$$

The total cross section per molecule is given by $\bar{\sigma}$ multiplied by the number of protons in the molecule plus the cross section for the heavy nucleus in the molecule. This latter cross section may again be computed by associating a mass tensor with the motion of the heavy nucleus. The characteristic values of the mass tensor will lie between the mass of the molecule and the mass of the heavy nucleus. In CH_4, the symmetry of the molecule causes the mass tensor to be spherically symmetrical and to be equal to the molecular mass. For H_2O and NH_3 the mass tensors are still nearly spherical and they may be sufficiently approximated by using a spherical mass tensor the characteristic values of which are chosen equal to the average of the characteristic values of the correct mass tensor. This gives an effective mass of 16 m for the nucleus C^{12} in CH_4, an effective mass 16.6 m for the nucleus N^{14} in NH_3, and an effective mass of 17.06 m for the nucleus O^{16} in H_2O. If we designate the actual mass of the nucleus by M and its effective mass by M_e, then integration over the motion of the mass point representing the heavy nucleus yields[4]

$$\bar{\sigma}_h = \sigma_X \left(\frac{M+m}{M_e+m}\right)^2 \left(\frac{M_e}{M}\right)^2 \left[\left(1+\frac{1}{2\xi^2}\right)\Phi(\xi) + \frac{\pi^{-\frac{1}{2}}}{\xi^{\frac{1}{2}}} \exp[-\xi^2]\right], \tag{14}$$

where

$$\xi^2 = \frac{M_e E_n}{mkT} \quad \text{and} \quad \frac{\sqrt{\pi}}{2}\Phi(\xi) = \int_0^\xi \exp[-x^2]dx.$$

σ_X is the scattering cross section for the heavy nucleus when it is initially at rest.

The total cross sections (σ_T) per molecule are given in Table III for very low temperatures, that is, for $kT/E_n \approx 0$.

5. Effective Cross Section for Neutrons with a Maxwell-Like Distribution

We now assume that the number of neutrons with momentum between P_n and $P_n + dP_n$ passing through unit surface per unit time is proportional to $P_n^2 \exp(-P_n^2/2mkT_n)dP_n$, where the effective temperature T_n is not in general equal to the temperature T of the scattering gas. Then the expression (10) for σ_{Av} must be averaged over this distribution as well as the velocity distribution of the mass point. When the expansion (8) is valid (cf. Table II) the average cross section may again be written

[4] Compare J. Schwinger, Phys. Rev. **58**, 1004 (1940).

in the form

$$\bar{\sigma}=\sigma_\infty(\mu_1\mu_2\mu_3\mu)^{\frac{1}{2}}(T_0'+T_1'+T_2'+\cdots) \tag{11'}$$

with

$$T_0'=\int_0^\infty\int_0^\infty(1+a\rho^2/P_n^2)^{\frac{1}{2}}\exp\left[-\frac{1}{2mk}\left(\frac{P_n^2}{T_n}+\frac{\rho^2}{T}\right)\right]P_n^2\rho^2dP_nd\rho\Big/$$

$$\int_0^\infty\int_0^\infty\exp\left[-\frac{1}{2mk}\left(\frac{P_n^2}{T_n}+\frac{\rho^2}{T}\right)\right]P_n^2\rho^2dP_nd\rho, \tag{12'}$$

$$T_1'=-\frac{1}{90\mu^2}(a_1J_1+a_2J_2+a_1J_3),$$

etc., where J_1, J_2, J_3 are integrals of the form

$$J_q=\frac{16}{\pi}\lambda^{\frac{3}{2}}(2mkT_n)^{-3}\int_0^\infty\int_0^\infty(P_n^2+a^2\rho^2)^{-\frac{3}{2}}\exp\left[-\frac{1}{2mkT_n}(P_n^2+\lambda\rho^2)\right]P_n^{7-2q}\rho^{2q}dP_nd\rho \quad\text{and}\quad \lambda=T_n/T.$$

These integrals can be evaluated explicitly and the result[5] for $\lambda>a^2$ is

$$T_0'=\frac{2\lambda^{\frac{3}{2}}}{\pi(\lambda-a^2)}\left\{\frac{a}{\lambda^2}(\lambda-2a^2)+(\lambda-a^2)^{-\frac{1}{2}}\operatorname{arccot}(\lambda/a^2-1)^{\frac{1}{2}}\right\},$$

$$J_1+J_3=\frac{2\lambda^{\frac{3}{2}}}{\pi(\lambda-a^2)^3}\left\{(\lambda^2-8\lambda a^2-8a^4-15)(\lambda-a^2)^{-\frac{1}{2}}\operatorname{arccot}(\lambda/a^2-1)^{\frac{1}{2}}\right.$$

$$\left.+\frac{1}{a\lambda^2}(a^2\lambda^3+14a^4\lambda^2+8\lambda^2+9\lambda a\quad 2a^4)\right\},$$

$$J_2=\frac{2\lambda^{\frac{3}{2}}}{\pi(\lambda-a^2)^3}\left\{3(\lambda+4a^2)(\lambda-a^2)^{-\frac{1}{2}}\operatorname{arccot}(\lambda/a^2-1)^{\frac{1}{2}}-\frac{a}{\lambda}(13\lambda+2a^2)\right\}.$$

For $\lambda<a^2$ all of the terms $(\lambda-a^2)^{-\frac{1}{2}}\operatorname{arccot}(\lambda/a^2-1)^{-\frac{1}{2}}$ are to be replaced by

$$(a^2-\lambda)^{-\frac{1}{2}}\operatorname{arccoth}(1-\lambda/a^2)^{-\frac{1}{2}}.$$

6. Application to Experiment

In applying the foregoing calculations to experiments a number of limitations, most of which have been previously mentioned, must be borne in mind. First, the entire theory is limited to neutron energies satisfying the conditions $E_n>E_{\text{rot}}$, $E_n>(E_{\text{rot}}kT)^{\frac{1}{2}}$, and $E_n<E_{\text{vib}}$ where E_{rot} and E_{vib} are given in Table I. In addition, the particular approximate methods applied in Sections 4 and 5 are limited in every case except that of H_2 by the conditions given in the last column of Table II. In the particular case of H_2 the cross sections have been roughly interpolated in the part of Fig. 1 which is indicated by a broken curve.

The greatest difficulty arises from the fact that the neutron current distribution is not known. It has been assumed in Section 5 that it is of the form $P_n^2\exp(-E_n/kT_n)dP_n$. This is the distribution that one might expect if the neutrons leave the free surface of a slowing down material in which the time required for the neutrons to reach the Maxwell distribution is small compared to the lifetime of the neutrons in the material. On the other hand, a distribution of the form $P_n^3\exp(-E_n/kT_n)$ would be expected if the neutrons behave like a gas at thermal equilibrium escaping through an opening of linear dimensions small compared to the mean free path. It is probable that the usual experimental situation corresponds to a condition that is between the two. However only the first case

[5] Cf. N. Arley, reference 2 (note 6), for a discussion of one of the integrals of this type.

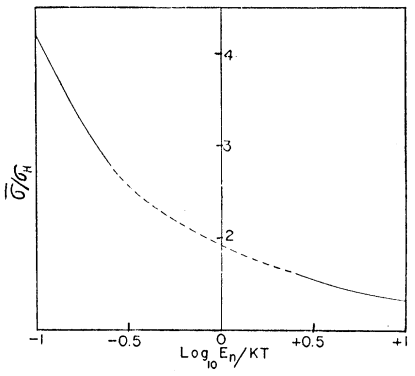

FIG. 1. Cross section for the scattering of neutrons with energy E_n by one of the protons in H_2 gas at temperature T. σ_H is the cross section for a free proton initially at rest. The broken part of the curve was interpolated with the help of rough calculations. In the range $0 \leq kT/E_n \leq 0.1$ the cross section is given by Eq. (13).

was treated here because the second apparently involves a double numerical integration.

Preliminary experiments on the scattering of 300°K neutrons by H_2 and CH_4 at room temperature have been carried out by Carroll and Dunning.[6] According to Table II, we see that the present theory cannot be applied to the experiments on CH_4 since $E_n/kT \approx 1$. In the case of H_2, the neutron energy, $\frac{3}{2}kT_n$, is approximately equal to the limiting energy E_{rot} given in Table I, so we can only expect a rough agreement.

This experimental value of the cross section per proton for scattering by H_2 is given in the first column of Table IV. In the second column the theoretical value of $\bar{\sigma}/\sigma_H$ is given on the assumption that the neutrons have a Maxwell-like distribution (Section 5). The third column contains the value of σ_H obtained from the first two columns. In the fourth column is the experimental value of σ_H found by Cohen, Goldsmith and Schwinger[7] and by Hanstein,[8]

[6] H. Carroll and J. R. Dunning, Phys. Rev. **54**, 541 (1938).

[7] V. W. Cohen, H. H. Goldsmith and J. Schwinger, Phys. Rev. **55**, 106 (1939).

[8] H. B. Hanstein, Phys. Rev. **57**, 1045 (1940); **59**, 489 (1941).

TABLE III. *σ_T is the total cross section per molecule for the scattering of monochromatic neutrons if the thermal energy of the molecules is much smaller than the energy of the neutrons ($kT/E_n \approx 0$). σ_H, σ_C, σ_N, and σ_O are the scattering cross sections for the free nuclei* H, C, N and O *when they are initially at rest.*

MOLECULE	σ_T	MOLECULE	σ_T
H_2	$2.44\sigma_H$	NH_3	$6.55\sigma_H+1.02\sigma_N$
CH_4	$10.8\sigma_H+1.04\sigma_C$	H_2O	$3.72\sigma_H+1.01\sigma_O$

TABLE IV. *The first column contains the experimental values of $\bar{\sigma}$ obtained by Carroll and Dunning,[6] the second gives the theoretical value of $\bar{\sigma}/\sigma_H$ assuming a neutron current distribution of the form $P_n^2\, exp(-P_n^2/2mkT_n)dP_n$. σ_H has been calculated from these two. $\sigma_H^{(1)}$ is the value given by Cohen, Goldsmith and Schwinger[7] and by Hanstein,[8] and $\sigma_H^{(2)}$ is the value given by Schwinger.[4,9]*

EXPERIMENTAL $\bar{\sigma}$	THEORETICAL $\bar{\sigma}/\sigma_H$	σ_H	EXPERIMENTAL $\sigma_H^{(1)}$	EXPERIMENTAL $\sigma_H^{(2)}$
32×10^{-24} cm^2	1.69	18.9×10^{-24}	21×10^{-24}	16.6×10^{-24}

and the last column gives the value obtained by Schwinger[4] from the experiments of Alvarez and Pitzer[9] with very slow (20°K) neutrons.

If it had been assumed that the neutron current distribution was of the form $P_n^3 \exp(E_n/kT)dP_n$ rather than $P_n^2 \exp(E_n/kT)dP_n$, then greater weight would have been given to higher values of E_n in calculating the theoretical cross section. It can be seen from Fig. 1 that this would tend to decrease the theoretical value of $\bar{\sigma}/\sigma_H$ and thus increase the value of σ_H given in Table IV.

It would be particularly interesting to measure the cross section for the scattering by H_2 of monochromatic neutrons with an energy somewhat greater than E_{rot} (Table I). If this measurement were carried out at different temperatures of the H_2 gas it would be a means of checking the theory and should yield a fairly accurate value of σ_H.

The authors take pleasure in thanking Professor Placzek for valuable discussions.

[9] L. W. Alvarez and K. S. Pitzer, Phys. Rev. **58**, 1003 (1940).