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SCATTERING OF SLOW NEUTRONS BY DIATOMIC MOLECULES

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We compute the cross sections for elastic and inelastic scattering of neutrons by molecules consisting of two identical or two different atoms. The general formulas are used to treat the scattering by T_2, HT and DT. Comparison of experimental data on the scattering cross sections of these molecules with our formulas makes it possible to determine the amplitudes for scattering of neutrons by tritium.

1. SCATTERING OF NEUTRONS BY MOLECULES CONSISTING OF TWO IDENTICAL ATOMS.

Schwinger and Teller[1] and Hamermesh and Schwinger[2] developed the theory of slow neutron scattering by molecules of ortho- and parahydrogen and deuterium. Using the Fermi quasipotential,[3] they expressed the neutron scattering cross sections of these molecules in terms of the amplitudes for neutron scattering by H and D nuclei.

In this section we shall treat molecules consisting of two arbitrary but identical atoms. (We shall refer to such molecules as "symmetric" molecules in contrast to "unsymmetric" molecules which contain different atoms.)

The interaction energy of the neutron and the symmetric diatomic molecule can be written as:[2]

$$\hat{U} = -\frac{2\pi\hbar^2}{M}\frac{A+1}{A}\frac{1}{2s_1+1}\left[(s_1+1)a_{s_1+1/2} + s_1 a_{s_1-1/2} + (\boldsymbol{\sigma}\cdot\mathbf{s}_1)(a_{s_1+1/2} - a_{s_1-1/2})\right]\delta^3(\mathbf{r}-\mathbf{r}_1) + \text{ similar terms with } 1\to 2$$

$$= -\frac{2\pi\hbar^2}{M}\frac{A+1}{A}\frac{1}{2s_1+1}\Big\{\Big[(s_1+1)a_{s_1+1/2} + s_1 a_{s_1-1/2} + \frac{1}{2}(\boldsymbol{\sigma}\cdot\mathbf{s})(a_{s_1+1/2} - a_{s_1-1/2})\Big]\left[\delta^3(\mathbf{r}-\mathbf{r}_1) + \delta^3(\mathbf{r}-\mathbf{r}_2)\right]$$

$$+ \frac{1}{2}\left[\boldsymbol{\sigma}\cdot(\mathbf{s}_1 - \mathbf{s}_2)\right](a_{s_1+1/2} - a_{s_1-1/2})\left[\delta^3(\mathbf{r}-\mathbf{r}_1) - \delta^3(\mathbf{r}-\mathbf{r}_2)\right]\Big\} \qquad (\mathbf{s} = \mathbf{s}_1 + \mathbf{s}_2). \tag{1}$$

The quantities $a_{s_1+1/2}$ and $a_{s_1-1/2}$ are the neutron scattering amplitudes for an atom with total spin $s_1 + 1/2$ and $s_1 - 1/2$, respectively; $1/2\ \sigma$, $\mathbf{s}_1$, $\mathbf{s}_2$ are the spin operators for the neutron, the first atom and the second atom; $\mathbf{r}$, $\mathbf{r}_1$, $\mathbf{r}_2$ are the respective radius vectors; A and s_1 are the atomic weight and spin of each of the atoms, and M is the mass of the nucleon.

The wave functions of the initial and final state of the system (if we treat the molecule as rigid rotator are

$$\Psi_1 = \exp\{i\mathbf{k}_0\cdot\mathbf{r} - i\mathbf{k}_0\cdot(\mathbf{r}_1+\mathbf{r}_2)/2\}\, Y_{j\mu}\left(\frac{\mathbf{l}}{l}\right)\frac{\sqrt{\delta(l-r_0)}}{r_0}\chi_\sigma\chi_{sM_s},$$

$$\Psi_2 = \exp\{i\mathbf{k}\mathbf{r} - i\mathbf{k}\cdot(\mathbf{r}_1+\mathbf{r}_2)/2\}\, Y_{j'\mu'}\left(\frac{\mathbf{l}}{l}\right)\frac{\sqrt{\delta(l-r_0)}}{r_0}\chi_{\sigma'}\chi_{s'M_s'} \qquad (\mathbf{l} = \mathbf{r}_1 - \mathbf{r}_2). \tag{2}$$

The factor $e^{i\mathbf{k}_0\cdot\mathbf{r}}$ describes the neutron incident on the molecule in the center of mass system; $e^{-i\mathbf{k}_0\cdot(\mathbf{r}_1+\mathbf{r}_2)/2}$ describes the motion of the center of mass of the molecule with momentum $-\mathbf{k}_0$; $Y_{j\mu}$ is the angular part of the wave function for a molecule with total angular momentum j and projection μ; $\sqrt{\delta(l-r_0)}/r_0$ is the radial part of the wave function, corresponding to internuclear distance r_0; χ_σ, χ_{sM_s} are the spin functions of the neutron (spin 1/2, projection σ), and the molecule (spin s, projection M_s). The notation for Ψ_2 is similar.

We first treat scattering processes in which $Y_{j\mu}$ and $Y_{j'\mu'}$ have the same parity. In this case the parities of χ_{sM_s} and $\chi_{s'M_s'}$ also coincide. We may therefore limit ourselves to terms in (1) whose spin parts are 1 or $\boldsymbol{\sigma}\cdot\mathbf{s}$. Since both these operators commute with $\mathbf{s}^2$, $s = s'$.

For this case the space integral which occurs when we calculate the matrix element of $\hat{U}$ between

Ψ_2 and Ψ_1 is

$$I^{(1)}_{\mu\mu'} = 2\int Y^*_{j'\mu'}\left(\frac{1}{l}\right) Y_{j\mu}\left(\frac{1}{l}\right)\frac{\delta(l-r_0)}{r_0^2}\cos\left(\frac{\mathbf{q}\cdot\mathbf{l}}{2}\right) d\mathbf{r}_1 d\mathbf{r}_2 \qquad (\mathbf{q}=\mathbf{k}_0-\mathbf{k}).$$

Expanding the product of the spherical harmonics in a Clebsch—Gordan series and writing cos $(\mathbf{q}\cdot\ell/2)$ as a sum of Legendre polynomials, we easily find

$$I^{(1)}_{\mu\mu'} = 2\sqrt{(2j+1)(2j'+1)}\sum_{\text{even } l}(-1)^{\mu'} C^{l0}_{j0j'0}\, i^l f_l\left(\frac{qr_0}{2}\right) C^{l\mu-\mu'}_{j\mu j'\mu'} P_{l\mu-\mu'}\left(\frac{\mathbf{q}}{q}\right)$$

($C^{\ell 0}_{j0j'0}$ and $C^{\ell\mu-\mu'}_{j\mu j'\mu'}$ are Clebsch—Gordan coefficients, $P_{\ell\mu-\mu'}$ are spherical harmonics normalized to the value $4\pi/(2\ell+1)$, $f_\ell(qr_0/2)$ are spherical Bessel functions).

We want the square modulus of this expression, summed over μ' and averaged over μ:

$$\frac{1}{(2j+1)}\sum_{\mu'\mu}|I^{(1)}_{\substack{jj'\\ \mu\mu'}}|^2 = 4(2j'+1)\sum_{\text{even } l}(C^{l0}_{j0j'0})^2 f_l^2\left(\frac{qr_0}{2}\right).$$

The calculation of the various spin sums and the summation over σ, σ', M_S and M'_S is done by the standard methods; we give the final result for the differential cross section for scattering with j → j′ (where j and j′ have the same parity)

$$\frac{d\sigma^{(1)}{}_{jj'}}{d\Omega} = \frac{k}{k_0}\frac{(A+1)^2}{(2A+1)^2}\frac{16}{(2s_1+1)^2}\left[((s_1+1)a_{s_1+1/2}+s_1 a_{s_1-1/2})^2+\frac{s(s+1)}{4}(a_{s_1+1/2}-a_{s_1-1/2})^2\right](2j'+1)\sum_{\text{even } l}(C^{l0}_{j0j'0})^2 f_l^2\left(\frac{qr_0}{2}\right). \qquad (3)$$

For transitions j → j′ with change of parity, we must use only the term proportional to $\sigma\cdot(\mathbf{s}_1-\mathbf{s}_2)$ in (1). In this case, the expression for the cross section will depend on the spin s′ of the final state. Obviously, we want to sum the cross section over those values of s′ for which the given j′ can occur (for even j′ and half-integer s_1, these are s′ = 0, 2, ... $2s_1-1$; for odd j′ and half-integer s_1, s′ = 1, 3, ... $2s_1$; etc.). In carrying out the summation, we can formally sum over all s′, since the values of s′ which don't match give null terms.

This remark enables us to simplify the calculation of the spin sum

$$\frac{1}{2(2s+1)}\sum|\chi^*_{\sigma'}\chi^*_{s'M'_s}[\sigma\cdot(\mathbf{s}_1-\mathbf{s}_2)]\chi_\sigma\chi_{sM_s}|^2$$

$$=\frac{1}{2(2s+1)}\sum_{\sigma M_s}(\chi^*_\sigma\chi^*_{sMs}[\sigma\cdot(\mathbf{s}_1-\mathbf{s}_2)]^2\chi_\sigma\chi_{sM_s}) = 4s_1(s_1+1)-s(s+1).$$

The calculation of the space integral is just like the one done previously, and the final result for the scattering cross section with j → j′ and change of parity is

$$\frac{d\sigma^{(2)}_{jj'}}{d\Omega} = \frac{k}{k_0}\frac{(A+1)^2}{(2A+1)^2}\frac{16}{(2s_1+1)^2}\left[s_1(s_1+1)-\frac{s(s+1)}{4}\right](a_{s_1+1/2}-a_{s_1-1/2})^2(2j'+1)\sum_{\text{odd } l}(C^{l0}_{j0j'0})^2 f_l^2\left(\frac{qr_0}{2}\right). \qquad (4)$$

To get the total cross sections, (3) and (4) must be integrated over all solid angle. The procedure is the same as that of Hamermesh and Schwinger.[2] The result is

$$\sigma^{(1)}_{jj'} = \frac{(A+1)^2}{(2A+1)^2}\frac{1}{(2s_1+1)^2}\frac{64\pi}{(k_0r_0)^2}\left[((s_1+1)a_{s_1+1/2}+s_1a_{s_1-1/2})^2+\frac{s(s+1)}{4}(a_{s_1+1/2}-a_{s_1-1/2})^2\right](2j'+1)A_{jj'};$$

$$\sigma^{(2)}_{jj'} = \frac{(A+1)^2}{(2A+1)^2}\frac{1}{(2s_1+1)^2}\frac{64\pi}{(k_0r_0)^2}\left[\left(s_1(s_1+1)-\frac{s(s+1)}{4}\right)(a_{s_1+1/2}-a_{s_1-1/2})^2\right](2j'+1)A_{jj'};\quad A_{jj'}=\left[\operatorname{Cin}2x-\sum_l(C^{l0}_{j0j'0})^2\,F_l(x)\right]_{x_1}^{x_2};$$

$$x_1=\frac{|k-k_0|r_0}{2};\qquad x_2=\frac{(k+k_0)r_0}{2};\qquad F_l(x)=0,\quad l=0;\qquad F_l(x)=x^2(f_0^2+f_1^2),\quad l=1;$$

$$F_l(x)=x^2\left(f_0^2+\frac{1}{l}f_l^2+\sum_{k=1}^{l-1}\frac{2k+1}{k(k+1)}f_k^2\right),\quad l>1;\qquad \operatorname{Cin}x=\ln x+C-\operatorname{Ci}x; \qquad (5)$$

where Ci is the integral cosine, and C the Euler constant.

The next problem is the averaging of the cross sections $\sigma^{(1)}_{jj'}$ and $\sigma^{(2)}_{jj'}$ over those values of s which are present in a gas for a given value of j. For example, for half integer s_1 and even j the gas is a mixture of molecules with s = 0, 2, ..., $2s_1-1$. Then the total number of initial states is

$$1+(2\cdot 2+1)+\ldots+[2(2s_1-1)+1]=s_1(2s_1+1).$$

The statistical weights of the individual states are

$$\begin{array}{llll} s=0, & 2\ , & \ldots & 2s_1-1 \\ g=1/s_1(2s_1+1), & (2\cdot 2+1)/s_1(2s_1+1),\ldots, & & (4s_1-1)/s_1(2s_1+1). \end{array}$$

In this case, after averaging, $s(s + 1)$ should be replaced by

$$s(s+1)\to\sum_{(\text{even})\,s=0}^{2s_1-1} s(s+1)\frac{2s+1}{s_1(2s_1+1)}=(s_1+1)(2s_1-1).$$

If s_1 is integral and j odd, the replacement is

$$s(s+1)\to(s_1+1)(2s_1-1).$$

Similarly, for s_1 half integral, j odd, or s_1 integral and j even,

$$s(s+1)\to(s_1+1)(2s_1+3).$$

We give the cross sections for the following three processes: (1) elastic scattering, j = 0 → j′ = 0; (2) elastic scattering, j = 1 → j′ = 1; and (3) collision of the second kind, j = 1 → j′ = 0. We assume that the incident neutron energy E is below the threshold E_1 for excitation of the first rotational level of the molecule (cf. Refs. 1, 2).

$$\sigma_{\substack{0\leftarrow 0\\ 1\leftarrow 1}}(E)=\left[\left((s_1+1)a_{s_1+{}^1\!/_2}+s_1a_{s_1-{}^1\!/_2}\right)^2+\left\{\begin{matrix}(s_1+1)(2s_1-1)/4\\ s_1(2s_1+3)/4\end{matrix}\right\}\left(a_{s_1+{}^1\!/_2}-a_{s_1-{}^1\!/_2}\right)^2\right]F_{\substack{0\leftarrow 0\\ 1\leftarrow 1}}(E),$$

$$\sigma_{0\leftarrow 1}(E)=\left(a_{s_1+{}^1\!/_2}-a_{s_1-{}^1\!/_2}\right)^2F_{0\leftarrow 1}(E);\quad F_{0\leftarrow 0}(E)=\frac{64\pi}{(2s_1+1)^2}\frac{(A+1)^2}{(2A+1)^2}\frac{1}{\xi^2}\operatorname{Cin}2\xi, \tag{6}$$

$$F_{1\leftarrow 1}(E)=\frac{64\pi}{(2s_1+1)^2}\frac{(A+1)^2}{(2A+1)^2}\frac{3}{\xi^2}\left[\operatorname{Cin}2\xi-\xi^2\left(\frac{2}{3}f_0^2(\xi)+f_1^2(\xi)+\frac{1}{3}f_2^2(\xi)\right)\right],$$

$$F_{0\leftarrow 1}(E)=\frac{64\pi}{(2s_1+1)^2}\frac{(A+1)^2}{(2A+1)^2}\left\{\begin{matrix}s_1(2s_1+1)/4\\ (s_1+1)(2s_1+1)/4\end{matrix}\right\}\frac{1}{\xi^2}\left[\operatorname{Cin}2x-x^2(f_0^2+f_1^2)\right]_{\xi_1}^{\xi_2} \tag{7}$$

$$\xi=k_0r_0,\quad \xi_{1.2}={}^1\!/_2\,(kr_0\mp k_0r_0).$$

In the formula for $\sigma_{\substack{0\leftarrow 0\\ 1\leftarrow 0}}$, the upper expression in the curly brackets is taken for half integral s_1 in $\sigma_{0\leftarrow 0}$ and for integral s_1 in $\sigma_{1\leftarrow 1}$; the lower expression applies when s_1 is half integral in $\sigma_{1\leftarrow 1}$ and when s_1 is integral in $\sigma_{0\leftarrow 0}$.

In $F_{0\leftarrow 1}(E)$, the upper expression should be used for half integral s_1 and the lower for integral S_1.

Following the procedure of Ref. 2, we express ξ, ξ_1 and ξ_2 in terms of E and E_1

$$\xi=\frac{4}{2A+1}\sqrt{\frac{AE}{E_1}};\quad \xi_{1,2}=\frac{1}{2}\left[\sqrt{\xi^2+\frac{8}{2A+1}}\mp\xi\right]. \tag{8}$$

We give the expressions for $\sigma_{0\leftarrow 0}$, $\sigma_{1\leftarrow 1}$ and $\sigma_{0\leftarrow 1}$, which are obtained when $F_{0\leftarrow 0}(E)$, $F_{1\leftarrow 1}(E)$ and $F_{0\leftarrow 1}(E)$ are expanded in powers of E/E_1 up to first order terms, for the T_2 molecule:

$$\sigma_{0\leftarrow 0}={}^1\!/_4\,(3a_1+a_0)^2F_{0\leftarrow 0}(E),\quad \sigma_{1\leftarrow 1}={}^1\!/_4\,[(3a_1+a_0)^2+2(a_1-a_0)^2]\,F_{1\leftarrow 1}(E),\quad \sigma_{0\leftarrow 1}=(a_1-a_0)^2F_{0\leftarrow 1}(E),$$

$$F_{0\leftarrow 0}(E)\approx F_{1\leftarrow 1}(E)\approx\frac{256\pi}{49}\left(1-\frac{8}{49}\frac{E}{E_1}\right),\quad F_{0\leftarrow 1}(E)\approx\frac{64\pi}{49}\left(0.03201\sqrt{\frac{E_1}{E}}+0.06413\sqrt{\frac{E}{E_1}}\right). \tag{9}$$

The results for H_2 and D_2 were given in Refs. 1 and 2.

Finally, we can tackle the problem of averaging the cross section over the thermal motion of the gas molecules. The calculations are exactly like those of Hamermesh and Schwinger.[2] For the case of T_2, the functions $F_{0\leftarrow 0}$, $F_{1\leftarrow 1}$ and $F_{0\leftarrow 1}$ are replaced by $G_{0\leftarrow 0}$, $G_{1\leftarrow 1}$ and $G_{0\leftarrow 1}$. For $kT < 6E$,

$$G_{0\leftarrow 0}(E)\approx G_{1\leftarrow 1}(E)=\frac{256\pi}{49}\left[1+\frac{1}{12}\frac{kT}{E}-\frac{8}{49}\frac{E}{E_1}\left(1+\frac{1}{2}\frac{kT}{E}+\frac{1}{48}\left(\frac{kT}{E}\right)^2\right)\right],$$

$$G_{0\leftarrow 1}(E)\approx\frac{64\pi}{49}\left[0.03201\sqrt{\frac{E_1}{E}}+0.06413\sqrt{\frac{E}{E_1}}\left(1+\frac{1}{4}\frac{kT}{E}\right)\right]. \tag{10}$$

2. SCATTERING OF NEUTRONS BY MOLECULES CONSISTING OF TWO DIFFERENT ATOMS

In this section, we treat neutron scattering by non-symmetric molecules. The ground state of a non-symmetric molecule always has rotational quantum number j = 0, so that when the energy E of the incident neutron is insufficient for excitation of rotation, of three processes treated above the only one which remains is the elastic scattering with j = 0 → j′ = 0.

In addition, since the assignment of j now imposes no limitations on the molecular spin s, the averaging of the cross section over s and s′ can be done very simply. In fact, in the present case we need only calculate the sum

$$\frac{1}{(2j+1)\,2\,(2s_1+1)\,(2s_2+1)}\sum_{(ss'M_sM'_s\sigma\sigma'\mu\mu')}\sigma_{jj'}\,(ss'M_sM'_s\sigma\sigma'\mu\mu')$$

over all values of $ss'M_SM'_S\sigma\sigma'\mu\mu'$ ($\sigma_{jj'}$ is the cross section for the transition from $j\mu sM_S\sigma$ to $j'\mu's'M'_S\sigma'$.

The interaction energy of the neutron and molecule is now

$$\hat{U} = -\frac{2\pi\hbar^2}{M}\left\{\frac{A_1+1}{A_1}\,\frac{1}{2s_1+1}\left[(s_1+1)\,a_{s_1+{}^1/_2}+s_1a_{s_1-{}^1/_2}\right]\delta^3(\mathbf{r}-\mathbf{r}_1)+\frac{A_2+1}{A_2}\,\frac{1}{2s_2+1}\left[(s_2+1)\,a_{s_2+{}^1/_2}+s_2a_{s_2-{}^1/_2}\right]\delta^3(\mathbf{r}-\mathbf{r}_2)\right.$$

$$+\frac{1}{2}(\boldsymbol{\sigma}\cdot\mathbf{s})\left[\frac{A_1+1}{A_1}\,\frac{1}{2s_1+1}\,(a_{s_1+{}^1/_2}-a_{s_1-{}^1/_2})\,\delta^3(\mathbf{r}-\mathbf{r}_1)+\frac{A_2+1}{A_2}\,\frac{1}{2s_2+1}\,(a_{s_2+{}^1/_2}-a_{s_2-{}^1/_2})\,\delta^3(\mathbf{r}-\mathbf{r}_2)\right]$$

$$\left.+\frac{1}{2}\left[\boldsymbol{\sigma}\cdot(\mathbf{s}_1-\mathbf{s}_2)\right]\left[\frac{A_1+1}{A_1}\,\frac{1}{2s_1+1}\,(a_{s_1+{}^1/_2}-a_{s_1-{}^1/_2})\,\delta^3(\mathbf{r}-\mathbf{r}_1)-\frac{A_2+1}{A_2}\,\frac{1}{2s_2+1}\,(a_{s_2+{}^1/_2}-a_{s_2-{}^1/_2})\,\delta^3(\mathbf{r}-\mathbf{r}_2)\right]\right\} \qquad (11)$$

[the notation is the same as in Eq. (1)]. The wave functions of the initial and final states are:

$$\Psi_1=\exp\{i\mathbf{k}_0\cdot(\mathbf{r}-\mathbf{r}_c)\}\,Y_{j\mu}\left(\frac{1}{l}\right)\frac{\sqrt{\delta(l-r_0)}}{r_0}\,\chi_\sigma\chi_{sM_s},\quad \Psi_2=\exp\{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}_c)\}\,Y_{j'\mu'}\left(\frac{1}{l}\right)\frac{\sqrt{\delta(l-r_0)}}{r_0}\,\chi_{\sigma'}\chi_{s'M'_s}, \qquad (12)$$

where now

$$\mathbf{r}_c=(A_1\mathbf{r}_1+A_2\mathbf{r}_2)/(A_1+A_2).$$

The calculation of the spin sums is somewhat lengthy, but entirely trivial. The expression for the j → j′ cross section now does not depend on the relative parity of j and j′, and has the form

$$\frac{d\sigma_{jj'}}{d\Omega}=\frac{k}{k_0}\,\frac{(A_1+A_2)^2}{(A_1+A_2+1)^2}\sum_{\mu\mu'}\frac{1}{(2j+1)}\left\{|B|^2+(|C|^2+|D|^2)\left[s_1(s_1+1)+s_2(s_2+1)\right]\right.$$

$$\left.+(C^*D+CD^*)\left[s_1(s_1+1)-s_2(s_2+1)\right]\right\},\quad B=\alpha_1I_1+\alpha_2I_2,\quad \alpha_i=\frac{A_i+1}{A_i}\,\frac{1}{2s_i+1}\left[(s_i+1)\,a_{s_i+{}^1/_2}+s_ia_{s_i-{}^1/_2}\right],$$

$$C=\frac{1}{2}(\beta_1I_1+\beta_2I_2),\quad \beta_i=\frac{A_i+1}{A_i}\,\frac{1}{2s_i+1}\left[a_{s_i+{}^1/_2}-a_{s_i-{}^1/_2}\right],\quad D=\frac{1}{2}(\beta_1I_1-\beta_2I_2),\quad I_i=\int\varphi_2^*\delta^3(\mathbf{r}-\mathbf{r}_i)\,\varphi_1\,d\mathbf{r}\,d\mathbf{r}_1\,d\mathbf{r}_2,$$

where φ_1 and φ_2 are the coordinate parts of the wave functions (12).

The calculation of the integrals is completely analogous to those in the first section. The result is

$$\frac{1}{(2j+1)}\sum_{\mu\mu'}|I_1|^2=(2j'+1)\sum_l(C^{l0}_{j0j'0})^2f_l^2\left(\frac{q_1r_0}{2}\right),\quad \frac{1}{(2j+1)}\sum_{\mu\mu'}|I_2|^2=(2j'+1)\sum_l(C^{l0}_{j0j''0})^2f_l^2\left(\frac{q_2r_0}{2}\right),$$

$$\frac{1}{(2j+1)}\sum_{\mu\mu'}I_1^*I_2=\frac{1}{(2j+1)}\sum_{\mu\mu'}I_1I_2^*=(2j'+1)\sum_l(-1)^l(C^{l0}_{j0j'0})^2f_l\left(\frac{q_1r_0}{2}\right)f_l\left(\frac{q_2r_0}{2}\right),\quad q_1=\frac{2A_2}{A_1+A_2}(\mathbf{k}_0-\mathbf{k}),$$

$$q_2=\frac{2A_1}{A_1+A_2}(\mathbf{k}_0-\mathbf{k}).$$

The expression for the differential cross section is

$$\frac{d\sigma_{jj'}}{d\Omega}=\frac{k}{k_0}\,\frac{(A_1+A_2)^2}{(A_1+A_2+1)^2}\left[G_{jj'}+s_1(s_1+1)\,Q^{(1)}_{jj'}+s_2(s_2+1)\,Q^{(2)}_{jj'}\right],$$

$$G_{jj'}=(2j'+1)\sum_l(C^{l0}_{j0j'0})^2\left[\alpha_1f_l\left(\frac{q_1r_0}{2}\right)+(-1)^l\alpha_2f_l\left(\frac{q_2r_0}{2}\right)\right]^2,\quad Q^{(i)}_{jj'}=(2j'+1)\sum_l(C^{l0}_{j0j'0})^2\beta_i^2f_l^2\left(\frac{q_ir_0}{2}\right)\quad (i=1,2). \qquad (15)$$

The total cross section for elastic scattering, j = 0 → j′ = 0, is

$$\sigma = \pi \frac{(A_1+A_2)^4}{A_1^2A_2^2(A_1+A_2+1)^2}\left\{\frac{(A_1+1)^2}{(2s_1+1)^2}\left[((s_1+1)a_{s_1+{}^1/_2}+s_1a_{s_1-{}^1/_2})^2+s_1(s_1+1)(a_{s_1+{}^1/_2}-a_{s_1-{}^1/_2})^2\right]\frac{1}{\xi^2}\operatorname{Cin}2\lambda_1\xi\right.$$

$$+\text{ similar terms with } 1\to 2+4\frac{(A_1+1)(A_2+1)}{(2s_1+1)(2s_2+1)}((s_1+1)a_{s_1+{}^1/_2}+s_1a_{s_1-{}^1/_2})((s_2+1)a_{s_2+{}^1/_2}+s_2a_{s_2-{}^1/_2})\frac{1}{\xi^2}R(\xi,\lambda_1,\lambda_2), \tag{16}$$

where

$$\lambda_1=\frac{2A_2}{A_1+A_2},\quad \lambda_2=\frac{2A_1}{A_1+A_2},\ \xi=k_0r_0=\frac{A_1+A_2}{A_1+A_2+1}\sqrt{\frac{2(A_1+A_2)}{A_1A_1}}\sqrt{\frac{E}{E_1}},\ R(\xi,\lambda_1,\lambda_2)=\int_0^\xi\frac{\sin\lambda_1t\sin\lambda_2t}{t}\,dt$$

$$=\frac{1}{2}\left[\ln\frac{\lambda_1+\lambda_2}{|\lambda_1-\lambda_2|}+\operatorname{Ci}[|\lambda_1-\lambda_2|\xi]-\operatorname{Ci}[(\lambda_1+\lambda_2)\xi]\right].$$

Using the well-known expansion of the integral cosine, we find, for $E \ll E_1$, to terms of order $\sim E/E_1$:

$$\sigma=\frac{(A_1+A_2)^2}{(A_1+A_2+1)^2}\left\{\sigma_1\left(\frac{A_1+1}{A_1}\right)^2\left[1-\frac{4}{3}\frac{A_2}{A_1}\frac{A_1+A_2}{(A_1+A_2+1)^2}\frac{E}{E_1}\right]+\sigma_2\left(\frac{A_2+1}{A_2}\right)^2\left[1-\frac{4}{3}\frac{A_1}{A_2}\frac{A_1+A_2}{(A_1+A_2+1)^2}\frac{E}{E_1}\right]\right. \tag{17}$$

$$\left.+8\pi\frac{A_1+1}{A_1}\frac{A_2+1}{A_2}\left[\frac{s_1+1}{2s_1+1}a_{s_1+{}^1/_2}+\frac{s_1}{2s_1+1}a_{s_1-{}^1/_2}\right]\left[\frac{s_2+1}{2s_2+1}a_{s_2+{}^1/_2}+\frac{s_2}{2s_2+1}a_{s_2-{}^1/_2}\right]\left[1-\frac{2}{3}\frac{A_1^2+A_2^2}{A_1A_2}\frac{A_1+A_2}{(A_1+A_2+1)^2}\frac{E}{E_1}\right]\right\}$$

We have introduced the scattering cross section for the i-th atom

$$\frac{1}{4\pi}\sigma_i=\frac{s_i+1}{2s_i+1}|a_{s_i+{}^1/_2}|^2+\frac{s_i}{2s_i+1}|a_{s_i-{}^1/_2}|^2\qquad(i=1,2). \tag{18}$$

We apply formula (17) to HD, HT, and DT. (We give the cross sections averaged over the thermal motion of the molecules.)

For the HD molecule (a_0 and a_1 are the scattering amplitudes for H, $a_{1/2}$ and $a_{3/2}$ are the amplitudes for D)

$$\sigma_{\mathrm{HD}}=\left[\frac{9}{4}\sigma_{\mathrm{H}}+\frac{81}{64}\sigma_{\mathrm{D}}+\frac{9\pi}{8}(3a_1+a_0)(2a_{{}^3/_2}+a_{{}^1/_2})\right]\left(1+\frac{1}{6}\frac{kT}{E}\right)$$

$$-\left[\frac{9}{8}\sigma_{\mathrm{H}}+\frac{81}{512}\sigma_{\mathrm{D}}+\frac{45\pi}{128}(3a_1+a_0)(2a_{{}^3/_2}+a_{{}^1/_2})\right]\frac{E}{E_1}\left(1+\frac{kT}{E}+\frac{1}{12}\left(\frac{kT}{E}\right)^2\right) \tag{19}$$

For the HT molecule (a_0 and a_1 are the H scattering amplitudes, b_0 and b_1 are the T scattering amplitudes)

$$\sigma_{\mathrm{HT}}=\left[\frac{64}{25}\sigma_{\mathrm{H}}+\frac{256}{225}\sigma_{\mathrm{T}}+\frac{64\pi}{75}(3a_1+a_0)(3b_1+b_0)\right]\left(1+\frac{1}{8}\frac{kT}{E}\right)-\left[\frac{1024}{625}\sigma_{\mathrm{H}}+\frac{4096}{50625}\sigma_{\mathrm{T}}+\frac{1024\pi}{3375}(3a_1+a_0)(3b_1+b_0)\right]$$

$$\times\frac{E}{E_1}\left(1+\frac{3}{4}\frac{kT}{E}+\frac{3}{64}\left(\frac{kT}{E}\right)^2\right). \tag{19'}$$

For the DT molecule

$$\sigma_{\mathrm{DT}}=\left[\frac{25}{16}\sigma_{\mathrm{D}}+\frac{1100}{81}\sigma_{\mathrm{T}}+\frac{25\pi}{27}(2a_{{}^3/_2}+a_{{}^1/_2})(3b_1+b_0)\right]\left(1+\frac{1}{10}\frac{kT}{E}\right)-\left[\frac{125}{288}\sigma_{\mathrm{D}}+\frac{1000}{6561}\sigma_{\mathrm{T}}+\frac{1625\pi}{8748}(2a_{{}^3/_2}+a_{{}^1/_2})(3b_1+b_0)\right]$$

$$\times\frac{E}{E_1}\left(1+\frac{3}{5}\frac{kT}{E}+\frac{3}{100}\left(\frac{kT}{E}\right)^2\right). \tag{19''}$$

3. INCLUSION OF ZERO-POINT VIBRATIONS OF THE MOLECULE

All the computations done in the previous sections were based on the rigid rotator model for the molecule, i.e., on a molecule having a fixed internuclear distance r_0. This was expressed mathematically in the use of $\sqrt{\delta(\ell-r_0)}/r_0$ as the radial part of the wave function, in place of the appropriate oscillator functions. Our next problem is to examine the validity of this approximation, and to include the normal vibrations of the molecule at least to first approximation. The analogous problem for the hydrogen molecule was considered recently by Drozdov.[4]

We shall restrict ourselves to treating the zero point vibrations, since the excitation of higher vibrational levels is much more difficult than rotational excitation. In addition, we shall treat only elastic scattering with $j = 0 \to j' = 0$ and $j = 1 \to j' = 1$ for symmetric molecules.

Carrying out the calculations, which are exactly the same as those in Sec. 1, we easily verify that the only change from our previous results is that, in formulas (3) and (4), the quantities $f_\ell^2(qr_0/2)$ are replaced by the integral:

$$I_l = \sqrt{\frac{\alpha}{\pi}} \int_0^{\infty} f_l\left(\frac{ql}{2}\right) e^{-\alpha(l-r_0)^2} dl \approx \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{+\infty} f_l\left(\frac{q}{2}(r_0+r)\right) e^{-\alpha r^2} dr,$$

where $\alpha = 1/x_0^2 = \mu\omega/\hbar$, μ is the reduced mass of the molecule, and ω the frequency of zero point vibration of the molecule.

To calculate the integral I_ℓ approximately, we expand the slowly varying Bessel function f_ℓ in series around the point $qr_0/2$, and integrate term by term. Then $A_{jj'}$ in formula (5) is changed to

$$A_{jj'} = \sum_l (C_{j0j'0}^{l0})^2 \left[2 \int_{x_1}^{x_2} f_l^2(x)\, x dx + \left(\frac{x_0}{r_0}\right)^2 \int_{x_1}^{x_2} f_l(x) f_l''(x)\, x^3 dx \right].$$

We note that $x_0 = (\hbar/\mu\omega)^{1/2} = (2\hbar/AM\omega)^{1/2}$, $r_0 = (2\hbar^2/AME_1)^{1/2}$, so that

$$(x_0/r_0)^2 = E_1/\hbar\omega.$$

Our computation corresponds to the first approximation with respect to $E/\hbar\omega$; in order to avoid dropping terms of this same order, we must also keep quadratic terms in E/E_1.

After expanding in series, we get the following final result for T_2 [cf. Eq. (19)]:

$$F_{0\leftarrow 0}(E) = \frac{256\pi}{49}\left[1 - \frac{8}{49}\left(\frac{E}{E_1} + \frac{E}{2\hbar\omega}\right) + \frac{512}{15\cdot 7^4}\left(\frac{E}{E_1}\right)^2\right], \quad F_{1\leftarrow 1}(E) = \frac{256\pi}{49}\left[1 - \frac{8}{49}\left(\frac{E}{E_1} + \frac{E}{2\hbar\omega}\right) + \frac{1024}{25\cdot 7^4}\left(\frac{E}{E_1}\right)^2\right].$$

The correction may be 2 — 3% of the leading term which gives the dependence on the energy E/E_1.

DISCUSSION OF RESULTS

The results obtained can be used for the solution of an important experimental problem: the determination of the amplitudes a_0 and a_1 for scattering of slow neutrons by tritium.

According to formulas (9) and (10), if we know the elastic scattering cross section for paratritium ($\sigma_{0\leftarrow 0}$), orthotritium ($\sigma_{1\leftarrow 1}$) or the cross section for scattering with transition of the molecule from the ortho to the para state ($\sigma_{0\leftarrow 1}$), we can determine the absolute values and relative sign of the amplitudes a_0 and a_1. The common sign of the amplitudes cannot be determined from the values of these cross sections. (A change in sign of both amplitudes produces no change in the values of $\sigma_{0\leftarrow 0}$, $\sigma_{1\leftarrow 1}$ and $\sigma_{0\leftarrow 1}$.)

One possibility for determining this common sign is to investigate the scattering of neutrons by molecules consisting of T and any other atom whose neutron scattering amplitudes are known. The formulas (19) show how the interference term depends on the common sign of the amplitudes. Unfortunately, this term is usually smaller than the other terms appearing in the formula.

A final decision on the question of determining the common sign of the amplitudes can be made only by examining the experimental accuracy attainable.

In conclusion, I express my profound gratitude to K. A. Ter-Martirosian for proposing this topic and for continual interest in the work.

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Translated by M. Hamermesh
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