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The Scattering of Slow Neutrons by Ortho- and Paradeuterium*

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Information relating to the spin dependence of the neutron-deuteron interaction can be obtained from slow neutron scattering experiments in ortho- and paradeuterium. Theoretical formulae have been derived for the cross sections of the various transitions among the molecular rotational levels, which involve the scattering amplitudes $a_{3/2}$ and $a_{1/2}$ for the two spin states of the neutron-deuteron system. In particular, numerical results are given for the first few transitions originating from the ground levels of the ortho- and para-systems with neutron energies not exceeding 0.05 ev. The influence of the thermal motion of the molecule is described, and explicit formulae are given for the important transitions occurring at small neutron energies, on the assumption that the D_2 is in gaseous form at low temperature. The ratio of the ortho- and para-cross sections, under these conditions, is examined in its dependence upon the ratio of the scattering amplitudes. If the scattering amplitudes are of the same sign, the cross-section ratio is never greater than 1.31 and attains this magnitude only for small values of $a_{3/2}$ relative to $a_{1/2}$. If, however, the amplitudes are of opposite sign, this ratio can be as large as 1.75 and always exceeds 1.11. This experiment measures only the magnitudes of the amplitude combinations $(2a_{3/2}+a_{1/2})$ and $(a_{3/2}-a_{1/2})$, but not their signs, and thus leaves a fourfold ambiguity in interpretation. The possibility is discussed of determining the sign of $(2a_{3/2}+a_{1/2})$ by scattering experiments in HD. It is pointed out that the sign of $(a_{3/2}-a_{1/2})$ cannot be fixed by any experiment in which the deuteron spin is unoriented in space. An alternative experimental method, involving the depolarization of neutrons, is mentioned.

EXPERIMENTS on slow neutron scattering in ortho- and parahydrogen[1] have provided decisive information concerning the spin of the neutron[2] and the spin dependence of the neutron-proton interaction.[3] With improvements in technique, these experiments will yield data on the range of the neutron-proton interaction, and facilitate accurate measurements of the slow neutron cross sections for scattering and capture by protons.[4] It is evident that analogous investigations with ortho- and paradeuterium can be of value in supplying further information relating to the spin dependence and exchange character of the forces between elementary particles. It is the purpose of this note to analyze the scattering of slow neutrons by ortho- and paradeuterium in order that the values of the fundamental nuclear quantities may be readily extracted from the results of such an experiment. The basic ideas underlying the problem are essentially identical with those relating to ortho- and parahydrogen, and we shall therefore be content to indicate the necessary modifications in mathematical detail, together with some improvements in the treatment.[5]

The scattering of a slow neutron by a nucleus of mass number A and spin S can be described by an effective interaction operator to be employed in conjunction with the Born approximation:

$$U=-\frac{2\pi\hbar^2}{M}\frac{A+1}{A}\left[\frac{S+1}{2S+1}a_{S+\frac{1}{2}}+\frac{S}{2S+1}a_{S-\frac{1}{2}}+(a_{S+\frac{1}{2}}-a_{S-\frac{1}{2}})\frac{\boldsymbol{\sigma}\cdot\mathbf{S}}{2S+1}\right]\delta(\mathbf{r}-\mathbf{R}). \quad (1)$$

Here, M is the mass of the neutron; $\frac{1}{2}\boldsymbol{\sigma}$ and S are the spin operators of the neutron and nucleus,

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[1] J. Halpern, I. Estermann, O. C. Simpson, and O. Stern, Phys. Rev. **52**, 142 (1937); F. G. Brickwedde, J. R. Dunning, H. J. Hoge, and J. H. Manley, Phys. Rev. **54**, 266 (1938); W. F. Libby and E. A. Long, Phys. Rev. **55**, 339 (1939); L. W. Alvarez and K. S. Pitzer, Phys. Rev. **58**, 1003 (1940).

[2] J. Schwinger, Phys. Rev. **52**, 1250 (1937).

[3] J. Schwinger and E. Teller, Phys. Rev. **52**, 286 (1937).

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

[5] The notation used here conforms to that in reference 3. References to equations in that paper will be indicated by the prefix ST.

respectively; $\delta(\mathbf{r}-\mathbf{R})$ represents a delta-function of the distance between the position of the neutron, $\mathbf{r}$, and the position of the nucleus, $\mathbf{R}$; and $a_{S\pm\frac{1}{2}}$ are the amplitudes of the scattered waves for the two total spin states of the system. The amplitudes are related to the corresponding cross sections for each spin state by

$$\sigma_{S\pm\frac{1}{2}}=4\pi a^2{}_{S\pm\frac{1}{2}}. \tag{2}$$

The total scattering cross section for a free nucleus is an appropriately weighted average of the cross sections for the two states of spin:

$$\sigma=\frac{S+1}{2S+1}\sigma_{S+\frac{1}{2}}+\frac{S}{2S+1}\sigma_{S-\frac{1}{2}}. \tag{3}$$

For the deuteron, the effective interaction operator becomes

$$U=-\frac{\pi\hbar^2}{M}[2a_{3/2}+a_{1/2}+(a_{3/2}-a_{1/2})\boldsymbol{\sigma}\cdot\mathbf{S}]\delta(\mathbf{r}-\mathbf{R}), \tag{4}$$

and the scattering cross section for a free deuteron is

$$\sigma=\tfrac{2}{3}\sigma_{3/2}+\tfrac{1}{3}\sigma_{1/2}. \tag{5}$$

The effective interaction between a neutron and the two deuterons in the D_2 molecule is conveniently expressed as

$$U=-\frac{\pi\hbar^2}{M}[2a_{3/2}+a_{1/2}+\tfrac{1}{2}(a_{3/2}-a_{1/2})\boldsymbol{\sigma}\cdot\mathbf{S}][\delta(\mathbf{r}_n-\mathbf{r}_1)+\delta(\mathbf{r}_n-\mathbf{r}_2)]$$
$$-\frac{\pi\hbar^2}{M}(a_{3/2}-a_{1/2})\boldsymbol{\sigma}\cdot\frac{\mathbf{S}_1-\mathbf{S}_2}{2}[\delta(\mathbf{r}_n-\mathbf{r}_1)-\delta(\mathbf{r}_n-\mathbf{r}_2)], \tag{6}$$

where now

$$\mathbf{S}=\mathbf{S}_1+\mathbf{S}_2 \tag{7}$$

represents the total spin of the molecule. The states of a deuterium molecule are divided into ortho-levels, those possessing even total spin and rotational angular momenta ($S=0,\ 2;\ J=0,\ 2,\ \cdots$), and para-levels, those with odd quantum numbers ($S=1;\ J=1,\ 3,\ \cdots$). The symmetrical part of the neutron-molecule interaction produces transitions in which the total molecular spin does not change, that is, ortho→ortho- and para→para-transitions. The antisymmetrical part of the interaction induces transitions accompanied by a spin change of unity; ortho→para- and para→ortho-transitions.

We wish to calculate the differential cross section for a scattering process in which a neutron with momentum $\mathbf{p}^0$ collides with a D_2 molecule with momentum $-\mathbf{p}^0$ in the internal state specified by the vibrational, rotational, and spin quantum numbers v, J, S, thereby producing a neutron with momentum $\mathbf{p}$ which has been scattered through the angle Θ into the solid angle $d\Omega$, leaving the molecule in the state characterized by $-\mathbf{p}$, v', J', S'. The differential cross section, as computed by the Born approximation, is

$$\sigma_{J',v',S';\,J,v,S}(\Theta)d\Omega=\frac{16}{25}\frac{p}{p^0}\frac{1}{2(2S+1)(2J+1)}\sum_{m',\,m_{J'},\,m_{S'}}\sum_{m,\,m_J,\,m_S}\left|\left(\Psi_f,\frac{MV}{2\pi\hbar^2}U\Psi_i\right)\right|^2 d\Omega, \tag{8}$$

which differs formally from the corresponding H_2 molecule cross section (ST (21)) only by the replacement of the numerical factor 4/9, the square of the reduced mass of the neutron $-H_2$ molecule system, by 16/25, the square of the reduced mass of the neutron $-D_2$ molecule system. These reduced mass factors arise in calculating the number of final neutron states per unit range of the total energy, and in the value of the neutron flux relative to the molecule. The differential cross section for those transitions in which the molecular spin is unchanged can be immediately obtained from the corresponding H_2 cross section (ST (28)) by suitable changes in the scattering amplitudes and the numerical replacement just discussed. The result is

$$\sigma_{J',v',S';\,J,v,S}(\Theta)d\Omega=\frac{16}{25}\frac{p}{p^0}[(2a_{3/2}+a_{1/2})^2+\tfrac{1}{4}(a_{3/2}-a_{1/2})^2S(S+1)]$$
$$\cdot\frac{1}{2J+1}\sum_{m_J,m_{J'}}\left|\int\cos\frac{\mathbf{p}^0-\mathbf{p}}{2\hbar}\cdot\mathbf{r}\phi^*_{v',J',m_{J'}}(\mathbf{r})\phi_{v,J,m_J}(\mathbf{r})d\tau\right|^2d\Omega. \quad (9)$$

The analog of (ST (30)), the cross section for transitions in which the molecular spin changes, is

$$\sum_{S'\neq S}\sigma_{J',v',S';\,J,v,S}(\Theta)d\Omega=\frac{16}{25}\frac{p}{p^0}(a_{3/2}-a_{1/2})^2\frac{8-S(S+1)}{4}$$
$$\cdot\frac{1}{2J+1}\sum_{m_J,m_{J'}}\left|\int\sin\frac{\mathbf{p}^0-\mathbf{p}}{2\hbar}\cdot\mathbf{r}\phi^*_{v',J',m_{J'}}(\mathbf{r})\phi_{v,J,m_J}(\mathbf{r})d\tau\right|^2d\Omega. \quad (10)$$

In these formulae, the magnitude of the neutron momentum after collision is obtained from energy conservation (cf. ST (17)):

$$\frac{5}{8M}p^{02}+E_{J,v}=\frac{5}{8M}p^2+E_{J',v'}, \quad (11)$$

and $\mathbf{p}^0$ is related to $\mathbf{p}_0$, the initial neutron momentum in a coordinate system in which the molecule is initially at rest, by

$$\mathbf{p}^0=\tfrac{4}{5}\mathbf{p}_0. \quad (12)$$

Further calculations will be restricted to molecules in the lowest vibrational state, $v=0$, and the rotational wave functions employed will be those of a rigid rotator with internuclear separation r_e:

$$\phi_{0,J,m_J}(\mathbf{r})=P_J^{m_J}(\mathbf{r})\frac{(\delta(r-r_e))^{\frac{1}{2}}}{r_e}. \quad (13)$$

Here, $P_J^{m_J}$ is a spherical harmonic of the angular coordinates associated with the vector $\mathbf{r}$, normalized in accordance with

$$\int|P_J^{m_J}(\mathbf{r})|^2d\omega=1. \quad (14)$$

The cross-section formulae for both types of spin transitions ($S'=S$, $S'\neq S$) involve summations of the type

$$\frac{1}{2J+1}\sum_{m_J,m_{J'}}\left|\int\exp(i\mathbf{k}\cdot\mathbf{r})\phi^*_{0,J',m_{J'}}(\mathbf{r})\phi_{0,J,m_J}(\mathbf{r})d\tau\right|^2$$
$$=\frac{1}{2J+1}\sum_{m_J,m_{J'}}\left|\int\exp(i\mathbf{k}\cdot\mathbf{r})P_{J'}^{m_{J'}*}(\mathbf{r})P_J^{m_J}(\mathbf{r})d\omega\right|^2\equiv\sum, \quad (15)$$

with

$$\mathbf{k}=(\mathbf{p}^0-\mathbf{p})/2\hbar \quad (16)$$

for the symmetry properties of the rotational functions will automatically select the real or imaginary part of $\exp(i\mathbf{k}\cdot\mathbf{r})$. To evaluate this sum, we regard the square of the absolute value of the integral as a double integral and perform the summations with respect to m_J and $m_{J'}$, employing the spherical harmonic addition theorem:

$$\sum_{m_J}P_J^{m_J*}(\mathbf{r})P_J^{m_J}(\mathbf{r}')=\frac{2J+1}{4\pi}P_J(\cos\theta), \quad (17)$$

where $P_J(\cos\theta)$ is a Legendre polynomial of the cosine of the angle between the vectors $\mathbf{r}$ and $\mathbf{r}'$.

Hence

$$\sum=(2J'+1)\int \exp\left[i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')\right]P_J(\cos\theta)P_{J'}(\cos\theta)\frac{d\omega}{4\pi}\frac{d\omega'}{4\pi}. \tag{18}$$

Now it is evident that the scattering cross section cannot depend upon the absolute direction of the initial neutron momentum, but involves only the angle Θ between $\mathbf{p}^0$ and $\mathbf{p}$. Hence the above integral is unaffected on replacing $\exp[i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')]$ by its average over all directions of the vector $\mathbf{k}$, namely $\sin k|\mathbf{r}-\mathbf{r}'|/k|\mathbf{r}-\mathbf{r}'|$. With the aid of the expansion[6]

$$\frac{\sin k|\mathbf{r}-\mathbf{r}'|}{k|\mathbf{r}-\mathbf{r}'|}=\frac{\sin(2kr_e\sin\frac{1}{2}\theta)}{2kr_e\sin\frac{1}{2}\theta}=\sum_{L=0}^{\infty}(2L+1)j_L^2(kr_e)P_L(\cos\theta), \tag{19}$$

where

$$j_L(x)=\left(\frac{\pi}{2x}\right)^{\frac{1}{2}}J_{L+\frac{1}{2}}(x) \tag{20}$$

the quantity $\sum$ can be cast into the form

$$\sum=(2J'+1)\sum\nolimits_L(2L+1)C_{LJJ'}j_L^2(kr_e), \tag{21}$$

with

$$C_{LJJ'}=\int_0^{\pi}P_L(\cos\theta)P_J(\cos\theta)P_{J'}(\cos\theta)\frac{\sin\theta d\theta}{2}. \tag{22}$$

Hence, the various differential cross sections can be expressed as

$$\sigma_{J',S;J,S}(\Theta)d\Omega=\frac{16}{25}\frac{p}{p^0}\left[(2a_{3/2}+a_{1/2})^2+\tfrac{1}{4}(a_{3/2}-a_{1/2})^2S(S+1)\right]$$
$$\cdot(2J'+1)\sum\nolimits_L(2L+1)C_{LJJ'}j_L^2\left[\frac{r_e}{2\hbar}(p^{02}+p^2-2p^0p\cos\Theta)^{\frac{1}{2}}\right]d\Omega, \tag{23}$$

$$\sum_{S'\neq S}\sigma_{J',S';J,S}(\Theta)d\Omega=\frac{16}{25}\frac{p}{p^0}(a_{3/2}-a_{1/2})^2\frac{8-S(S+1)}{4}$$
$$\cdot(2J'+1)\sum\nolimits_L(2L+1)C_{LJJ'}j_L^2\left[\frac{r_e}{2\hbar}(p^{02}+p^2-2p^0p\cos\Theta)^{\frac{1}{2}}\right]d\Omega.$$

The constants $C_{LJJ'}$ are zero unless L has one of the values

$$L=J+J',\ J+J'-2,\ \cdots|J-J'|. \tag{24}$$

Some important and useful properties can be obtained from the defining Eq. (22), rewritten as

$$\sum\nolimits_L(2L+1)C_{LJJ'}P_L(z)=P_J(z)P_{J'}(z). \tag{25}$$

On placing $z=1$, and recalling that $P_J(1)=1$, we obtain the sum formula

$$\sum\nolimits_L(2L+1)C_{LJJ'}=1. \tag{26}$$

If Eq. (25) is multiplied by z, and use is made of the relation

$$zP_L(z)=\frac{L+1}{2L+1}P_{L+1}(z)+\frac{L}{2L+1}P_{L-1}(z), \tag{27}$$

a recurrence relation is obtained for the $C_{LJJ'}$ as a function of L

$$\frac{L+1}{2L+1}C_{L+1,J,J'}+\frac{L}{2L+1}C_{L-1,J,J'}=\frac{J+1}{2J+1}C_{L,J+1,J'}+\frac{J}{2J+1}C_{L,J-1,J'}. \tag{28}$$

[6] J. A. Stratton, *Electromagnetic Theory* (McGraw-Hill Book Company, Inc., New York, 1941), p. 413.

Thus, starting with the orthogonality integral

$$C_{0JJ'}=\frac{\delta_{JJ'}}{2J+1}, \tag{29}$$

where $\delta_{JJ'}$ is the customary Kronecker symbol, one obtains, successively

$$\begin{aligned} C_{1JJ'}&=\frac{1}{(2J+1)(2J'+1)}[J\delta_{J,\,J'+1}+J'\delta_{J',\,J+1}],\\ C_{2JJ'}&=\frac{J(J+1)}{(2J-1)(2J+1)(2J+3)}\delta_{JJ'}+\frac{3}{2}\frac{1}{(2J+1)(2J'+1)}\left[\frac{J(J'+1)}{2J-1}\delta_{J,\,J'+2}+\frac{J'(J+1)}{2J'-1}\delta_{J',\,J+2}\right] \end{aligned} \tag{30}$$

and so on. The recurrence relation combined with the sum formula and the symmetry of $C_{LJJ'}$, enables one to obtain the required values with little effort. Alternatively, the values of $C_{LJJ'}$ can be computed directly from the explicit formula:[7]

$$C_{LJJ'}=\frac{(J+L-J')!(J'+L-J)!(J+J'-L)!}{(J+J'+L+1)!}\left[\left(\frac{J+J'+L}{2}\right)!\Big/\left(\frac{J+L-J'}{2}\right)!\left(\frac{J'+L-J}{2}\right)!\left(\frac{J+J'-L}{2}\right)!\right]^2. \tag{31}$$

To evaluate the total scattering cross section for a given transition, we integrate Eq. (23) with respect to the scattering angle Θ and obtain:

$$\sigma_{J'S;\,JS}=\frac{16}{25}\pi\left[(2a_{3/2}+a_{1/2})^2+\frac{1}{4}(a_{3/2}-a_{1/2})^2S(S+1)\right](2J'+1)\left(\frac{2\hbar}{p^0r_e}\right)^2A_{JJ'}, \tag{32}$$

$$\sum_{S'\neq S}\sigma_{J'S';\,JS}=\frac{16}{25}\pi(a_{3/2}-a_{1/2})^2\frac{8-S(S+1)}{4}(2J'+1)\left(\frac{2\hbar}{p^0r_e}\right)^2A_{JJ'},$$

where

$$A_{JJ'}=2\sum\nolimits_L(2L+1)C_{LJJ'}\int_{(r_e/2\hbar)|p^0-p|}^{(r_e/2\hbar)(p^0+p)}j^2{}_L(x)xdx. \tag{33}$$

A relation between the Bessel function integrals for successive values of L can be established with the aid of the recurrence formulae:[8]

$$j_{L-1}(x)=\frac{d}{dx}j_L(x)+\frac{L+1}{x}j_L(x),\quad j_L(x)=-\frac{d}{dx}j_{L-1}(x)+\frac{L-1}{x}j_{L-1}(x). \tag{34}$$

On multiplying the first equation by $x^2j_L(x)$, the second equation by $x^2j_{L-1}(x)$, and comparing the resultant expressions, we find that

$$xj^2{}_L-xj^2{}_{L-1}=-\frac{1}{2L}\frac{d}{dx}[x^2(j^2{}_{L-1}+j^2{}_L)], \tag{35}$$

or

$$\int_0^x xj^2{}_Ldx-\int_0^x xj^2{}_{L-1}dx=-\frac{1}{2L}x^2(j^2{}_{L-1}(x)+j^2{}_L(x)). \tag{36}$$

Hence

$$\int_0^x xj^2{}_1dx=\int_0^x xj^2{}_0dx-\tfrac{1}{2}x^2(j^2{}_0(x)+j^2{}_1(x)), \tag{37}$$

and, in general,

$$\int_0^x xj^2{}_Ldx=\int_0^x xj^2{}_0dx-\tfrac{1}{2}x^2\left[j^2{}_0(x)+\sum_{K=1}^{L-1}\frac{2K+1}{K(K+1)}j^2{}_K(x)+\frac{1}{L}j^2{}_L(x)\right]. \tag{38}$$

[7] E. T. Whittaker and G. N. Watson, *Modern Analysis* (The MacMillan Company, New York, 1944), p. 331.
[8] Reference 6, p. 406.

Thus, all such Bessel function integrals are reduced to that for $L=0$:

$$\int_0^x x j^2{}_0 dx=\int_0^x \frac{\sin^2 x}{x}dx=\tfrac{1}{2}\int_0^{2x}\frac{1-\cos t}{t}dt=\tfrac{1}{2}Cin2x. \tag{39}$$

The function *Cinx* is related to the more customary cosine integral

$$Cix=-\int_x^\infty \frac{\cos t}{t}dt, \tag{40}$$

by

$$Cinx=\log x+C-Cix, \tag{41}$$

where $C=0.5772$ is the Eulerian constant. Finally, then, the quantity $A_{JJ'}$ can be expressed as

$$A_{JJ'}=\left[Cin2x-\textstyle\sum_L (2L+1)C_{LJJ'}f_L(x)\right]_{(r_e/2\hbar)|p^0-p|}^{(r_e/2\hbar)(p^0+p)}, \tag{42}$$

where use has been made of the sum formula (26), and

$$\begin{aligned} f_L(x)&=0, \quad L=0\\ &=x^2(j^2{}_0+j^2{}_1), \quad L=1,\\ &=x^2\left(j^2{}_0+\sum_{K=1}^{L-1}\frac{2K+1}{K(K+1)}j^2{}_K+\frac{1}{L}j^2{}_L\right), \quad L>1. \end{aligned} \tag{43}$$

The cross section for any transition originating from an ortho-level must be averaged over the two ortho-spin states, $S=0, 2$ with the statistical weights $\frac{1}{6}$ and $\frac{5}{6}$, respectively. Therefore, the final cross-section formulae for ortho→ortho- and ortho→para-transitions are:

$$\begin{aligned} &\text{ortho→ortho:}\quad \sigma_{J'\leftarrow J}=\frac{16}{25}\pi\left[(2a_{3/2}+a_{1/2})^2+\frac{5}{4}(a_{3/2}-a_{1/2})^2\right]\left(\frac{2\hbar}{p^0r_e}\right)^2(2J'+1)A_{JJ'},\\ &\text{ortho→para:}\quad \sigma_{J'\leftarrow J}=\frac{12}{25}\pi(a_{3/2}-a_{1/2})^2\left(\frac{2\hbar}{p^0r_e}\right)^2(2J'+1)A_{JJ'}. \end{aligned} \tag{44}$$

To obtain the cross sections for transitions originating in a para-level, we need merely place $S=1$, whence

$$\begin{aligned} &\text{para→para:}\quad \sigma_{J'\leftarrow J}=\frac{16}{25}\pi[(2a_{3/2}+a_{1/2})^2+\tfrac{1}{2}(a_{3/2}-a_{1/2})^2]\left(\frac{2\hbar}{p^0r_e}\right)^2(2J'+1)A_{JJ'},\\ &\text{para→ortho:}\quad \sigma_{J'\leftarrow J}=\frac{24}{25}\pi(a_{3/2}-a_{1/2})^2\left(\frac{2\hbar}{p^0r_e}\right)^2(2J'+1)A_{JJ'}. \end{aligned} \tag{45}$$

The energy levels of the deuterium molecule, considered as a rigid rotator, are

$$E_J=\frac{\hbar^2}{2Mr_e^2}J(J+1), \tag{46}$$

and, in particular,

$$E_1=\hbar^2/Mr_e^2. \tag{47}$$

The initial neutron momentum p^0, expressed in terms of the neutron energy in the rest system of the molecule before collision, is

$$p^0=\tfrac{4}{5}(2ME)^{\frac{1}{2}} \tag{48}$$

whence

$$\frac{p^0r_e}{\hbar}=\frac{4}{5}\left(\frac{2E}{E_1}\right)^{\frac{1}{2}}\equiv\xi. \tag{49}$$

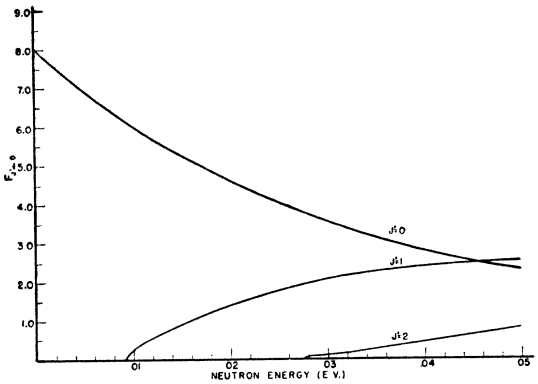

FIG. 1. Cross sections for transitions originating from the orthodeuterium ground state, omitting amplitude factors (cf. Eq. (52)).

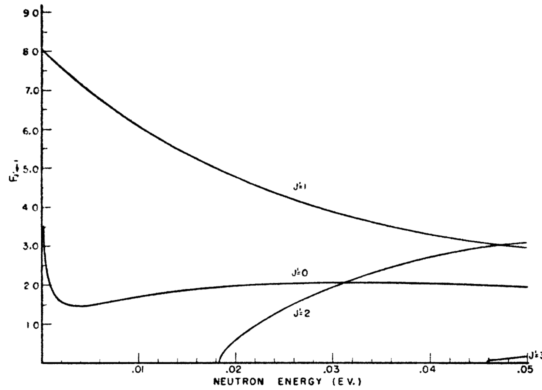

FIG. 2. Cross sections for transitions originating from the paradeuterium ground state, omitting amplitude factors (cf. Eq. (52)).

The neutron momentum p after a rotational transition $J\rightarrow J'$ is determined by (cf. Eq. (11))

$$p^2=p^{0^2}+\frac{4}{5}\frac{\hbar^2}{r_e^2}[J(J+1)-J'(J'+1)], \tag{50}$$

or

$$\frac{pr_e}{\hbar}=\{\xi^2+\tfrac{4}{5}[J(J+1)-J'(J'+1)]\}^{\frac{1}{2}}. \tag{51}$$

Hence the neutron energy is effectively measured in units of the energy of the first rotational level, $E_1=0.0074$ ev.[9]

Explicit expressions for the cross sections describing the first few transitions originating from the ground levels of the ortho- and para-systems are:

$$\sigma_{0\leftarrow 0}=[(2a_{3/2}+a_{1/2})^2+(5/4)(a_{3/2}-a_{1/2})^2]F_{0\leftarrow 0}(E),$$

$$F_{0\leftarrow 0}(E)=\frac{64}{25}\pi\frac{1}{\xi^2}Cin2\xi,$$

$$\sigma_{1\leftarrow 0}=(a_{3/2}-a_{1/2})^2F_{1\leftarrow 0}(E),$$

$$F_{1\leftarrow 0}(E)=\frac{144}{25}\pi\frac{1}{\xi^2}[Cin2x-x^2(j^2{}_0(x)+j^2{}_1(x))]_{\frac{1}{2}[\xi-(\xi^2-(8/5))^{\frac{1}{2}}]}^{\frac{1}{2}[\xi+(\xi^2-(8/5))^{\frac{1}{2}}]},$$

$$\sigma_{2\leftarrow 0}=[(2a_{3/2}+a_{1/2})^2+(5/4)(a_{3/2}-a_{1/2})^2]F_{2\leftarrow 0}(E),$$

$$F_{2\leftarrow 0}(E)=\frac{64}{5}\pi\frac{1}{\xi^2}[Cin2x-x^2(j^2{}_0(x)+\tfrac{3}{2}j^2{}_1(x)+\tfrac{1}{2}j^2{}_2(x))]_{\frac{1}{2}[\xi-(\xi^2-(24/5))^{\frac{1}{2}}]}^{\frac{1}{2}[\xi+(\xi^2-(24/5))^{\frac{1}{2}}]},$$

$$\sigma_{0\leftarrow 1}=(a_{3/2}-a_{1/2})^2F_{0\leftarrow 1}(E),$$

$$F_{0\leftarrow 1}(E)=\frac{96}{25}\pi\frac{1}{\xi^2}[Cin2x-x^2(j^2{}_0(x)+j^2{}_1(x))]_{\frac{1}{2}[(\xi^2+(8/5))^{\frac{1}{2}}-\xi]}^{\frac{1}{2}[(\xi^2+(8/5))^{\frac{1}{2}}+\xi]}, \tag{52}$$

$$\sigma_{1\leftarrow 1}=[(2a_{3/2}+a_{1/2})^2+\tfrac{1}{2}(a_{3/2}-a_{1/2})^2]F_{1\leftarrow 1}(E),$$

$$F_{1\leftarrow 1}(E)=\frac{192}{25}\pi\frac{1}{\xi^2}[Cin2\xi-\xi^2(\tfrac{2}{3}j^2{}_0(\xi)+j^2{}_1(\xi)+\tfrac{1}{3}j^2{}_2(\xi))],$$

$$\sigma_{2\leftarrow 1}=(a_{3/2}-a_{1/2})^2F_{2\leftarrow 1}(E),$$

$$F_{2\leftarrow 1}(E)=\frac{96}{5}\pi\frac{1}{\xi^2}\left[Cin2x-x^2\left(j^2{}_0(x)+\frac{13}{10}j^2{}_1(x)+\frac{1}{2}j^2{}_2(x)+\frac{1}{5}j^2{}_3(x)\right)\right]_{\frac{1}{2}[\xi-(\xi^2-(16/5))^{\frac{1}{2}}]}^{\frac{1}{2}[\xi+(\xi^2-(16/5))^{\frac{1}{2}}]},$$

[9] A. Farkas, *Orthohydrogen, Parahydrogen, and Heavy Hydrogen* (Cambridge University Press, New York, 1935).

$$\sigma_{3\leftarrow1}=[(2a_{3/2}+a_{1/2})^2+\tfrac{1}{2}(a_{3/2}-a_{1/2})^2]F_{3\leftarrow1}(E),$$

$$F_{3\leftarrow1}(E)=\frac{448}{25}\pi\frac{1}{\xi^2}\left[Cin2x-x^2\left(j^2_0(x)+\frac{3}{2}j^2_1(x)+\frac{29}{42}j^2_2(x)+\frac{1}{3}j^2_3(x)+\frac{1}{7}j^2_4(x)\right)\right]_{\frac{1}{2}[\xi-(\xi^2-8)^{\frac{1}{2}}]}^{\frac{1}{2}[\xi+(\xi^2-8)^{\frac{1}{2}}]}$$

The functions $F_{J'\rightarrow J}(E)$ for these seven transitions are plotted in Figs. 1 and 2 over the neutron energy range: $E=0-0.05$ ev.

The minimum neutron energy required for an excitation process is $E=(5/4)E_1=0.0093$ ev, corresponding to the $0\rightarrow1$ transition. If the neutron energy does not exceed this threshold, and the deuterium temperature is sufficiently low, insuring that the $J=0$ and 1 rotational levels alone are occupied, the only transitions that can occur are $0\rightarrow0$, $1\rightarrow1$, $1\rightarrow0$. Approximate expressions for the energy dependence of these cross sections, accurate to within a few percent for $E\lesssim E_1$, are

$$F_{0\leftarrow0}(E)=F_{1\leftarrow1}(E)=\frac{64}{25}\pi\left(1-\frac{16}{75}\frac{E}{E_1}\right),\quad F_{0\leftarrow1}(E)=\frac{24}{25}\pi\left(\frac{E_1}{E}\right)^{\frac{1}{2}}\left(0.1833+0.3276\frac{E}{E_1}\right). \tag{53}$$

Under the conditions thus contemplated—neutron and molecular velocities of comparable magnitudes—the thermal agitation of the molecules must be considered before a comparison with experiment is possible.

The effective scattering cross section for a neutron of velocity $\mathbf{v}$, $\bar{\sigma}(v)$, is related to the true cross section, $\sigma(v)$, by

$$v\bar{\sigma}(v)=\int|\mathbf{v}-\mathbf{u}|\sigma(|\mathbf{v}-\mathbf{u}|)N(\mathbf{u})(d\mathbf{u})=\int w\sigma(w)N(\mathbf{v}+\mathbf{w})(d\mathbf{w}), \tag{54}$$

where $N(\mathbf{u})$ is the velocity distribution function of the target molecules, which is subject to the normalization condition

$$\int N(\mathbf{u})(d\mathbf{u})=1. \tag{55}$$

In order that the effect of thermal agitation be analyzable with precision, we shall suppose the deuterium to be in the gaseous phase at the temperature T, whence

$$N(\mathbf{u})=\left(\frac{2M}{\pi kT}\right)^{\frac{3}{2}}\exp\left(-2Mu^2/kT\right) \tag{56}$$

and

$$\bar{\sigma}(v)=\frac{2}{v^2}\left(\frac{2M}{\pi kT}\right)^{\frac{1}{2}}\exp\left(-2Mv^2/kT\right)\int_0^\infty\exp\left(-2Mw^2/kT\right)\sinh\frac{4Mvw}{kT}w^2\sigma(w)dw. \tag{57}$$

The effective cross sections for the three transitions under consideration, as described by Eq. (53), can be written as:

$$\begin{aligned}
\bar{\sigma}_{0\leftarrow0}(E)&=\frac{64}{25}\pi[(2a_{3/2}+a_{1/2})^2+(5/4)(a_{3/2}-a_{1/2})^2]G_{0\leftarrow0}(E),\\
\bar{\sigma}_{1\leftarrow1}(E)&=\frac{64}{25}\pi[(2a_{3/2}+a_{1/2})^2+\tfrac{1}{2}(a_{3/2}-a_{1/2})^2]G_{1\leftarrow1}(E),\\
\bar{\sigma}_{0\leftarrow1}(E)&=\frac{24}{25}\pi(a_{3/2}-a_{1/2})^2G_{0\leftarrow1}(E),
\end{aligned} \tag{58}$$

with

$$\begin{aligned}
G_{0\leftarrow0}(E)=G_{1\leftarrow1}(E)&=\left[\frac{1}{(\pi)^{\frac{1}{2}}}\frac{\exp(-x^2)}{x}+\left(1+\frac{1}{2x^2}\right)\Phi(x)\right]\\
&\quad-\frac{16}{75}\frac{E}{E_1}\left[\frac{1}{(\pi)^{\frac{1}{2}}}\left(1+\frac{5}{2x^2}\right)\frac{\exp(-x^2)}{x}+\left(1+\frac{3}{x^2}+\frac{3}{4x^4}\right)\Phi(x)\right],
\end{aligned} \tag{59}$$

$$G_{0\leftarrow1}(E)=0.1833\left(\frac{E_1}{E}\right)^{\frac{1}{2}}+0.3276\left(\frac{E}{E_1}\right)^{\frac{1}{2}}\left(1+\frac{3}{8}\frac{kT}{E}\right).$$

Here,

$$x^2=\frac{2Mv^2}{kT}=\frac{4E}{kT},\tag{60}$$

and

$$\Phi(x)=\frac{2}{(\pi)^{\frac{1}{2}}}\int_0^x \exp\,(-t^2)dt.\tag{61}$$

An approximate expression for $G_{0\leftarrow 0}(E)$, which is accurate within one percent for $x>1$, or $E>\frac{1}{4}kT$, is

$$G_{0\leftarrow 0}(E)=1+\frac{kT}{E}-\frac{16}{75}\frac{E}{E_1}\left(1+\frac{3}{4}\frac{kT}{E}+\frac{3}{64}\left(\frac{kT}{E}\right)^2\right).\tag{62}$$

As a numerical illustration of these results, we shall assume that $E=kT=0.233E_1$, corresponding to a temperature $T=20°\mathrm{K}$. Under these conditions,

$$G_{0\leftarrow 0}=G_{1\leftarrow 1}=1.036,\quad G_{0\leftarrow 1}=0.5971,\tag{63}$$

and

$$\begin{aligned}\bar{\sigma}_{0\leftarrow 0}&=8.33[(2a_{3/2}+a_{1/2})^2+(5/4)(a_{3/2}-a_{1/2})^2],\\ \bar{\sigma}_{1\leftarrow 1}&=8.33[(2a_{3/2}+a_{1/2})^2+\tfrac{1}{2}(a_{3/2}-a_{1/2})^2],\\ \bar{\sigma}_{0\leftarrow 1}&=1.80(a_{3/2}-a_{1/2})^2.\end{aligned}\tag{64}$$

Hence

$$\begin{aligned}\bar{\sigma}_{\mathrm{para}}&=\bar{\sigma}_{1\leftarrow 1}+\bar{\sigma}_{0\leftarrow 1}=8.33(2a_{3/2}+a_{1/2})^2+5.97(a_{3/2}-a_{1/2})^2,\\ \bar{\sigma}_{\mathrm{ortho}}&=\bar{\sigma}_{0\leftarrow 0}=8.33(2a_{3/2}+a_{1/2})^2+10.42(a_{3/2}-a_{1/2})^2.\end{aligned}\tag{65}$$

The cross section for neutron scattering by free deuterons

$$\sigma_0=\frac{4\pi}{9}[(2a_{3/2}+a_{1/2})^2+2(a_{3/2}-a_{1/2})^2]\tag{66}$$

is related to the ortho- and para-cross sections by

$$\sigma_0=0.403\bar{\sigma}_{\mathrm{ortho}}-0.235\bar{\sigma}_{\mathrm{para}}\tag{67}$$

which provides a useful check on the measurements.

It is apparent that the ortho-cross section always exceeds the para-cross section. A consideration of the ratio of the cross sections in its dependence upon the ratio of the unknown scattering amplitudes is of importance in indicating the degree of precision with which the experiment must be performed in order to yield useful information. The ratio

$$\frac{\bar{\sigma}_{\mathrm{ortho}}}{\bar{\sigma}_{\mathrm{para}}}=\frac{1+1.25\rho}{1+0.716\rho},\quad \rho=\left(\frac{a_{3/2}-a_{1/2}}{2a_{3/2}+a_{1/2}}\right)^2\tag{68}$$

is plotted as a function of $a_{3/2}/a_{1/2}$ in Fig. 3. If the scattering amplitudes possess the same sign, the cross-section ratio never exceeds 1.31 and attains this order of magnitude only for very small values of $a_{3/2}$ relative to $a_{1/2}$. If, however, the amplitudes are of opposite sign, the cross-section ratio is always greater than 1.11, but never exceeds 1.75. The latter value corresponds to $a_{3/2}/a_{1/2}=-\frac{1}{2}$. It is clear that if the experiment is to provide significant data, one must be prepared to measure the ortho- and para-cross

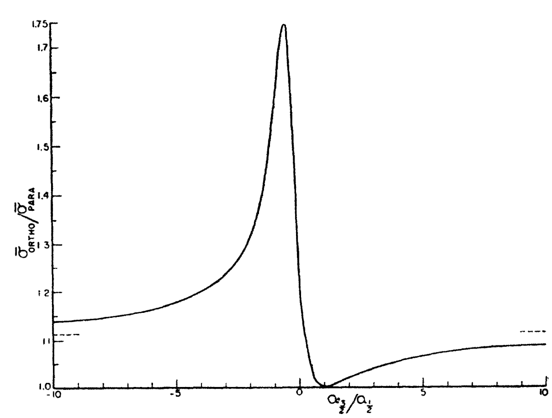

FIG. 3. Ratio of ortho- to para-scattering cross section as a function of $a_{3/2}/a_{1/2}$ (cf. Eq. (68)).

sections with an accuracy of a few percent.[10] It should also be noted that a given ortho-para-scattering ratio may correspond to either of two amplitude ratios, and the experiment can in no way distinguish between them. The amplitudes are further undetermined to the extent of a common sign factor. This fourfold ambiguity obviously stems from the fact that the ortho- and para-cross sections fix only the magnitudes of the amplitude factors $2a_{3/2}+a_{1/2}$ and $a_{3/2}-a_{1/2}$, but not their signs. The same situation arises, of course, in ortho-para-H_2 experiments, but with hydrogen our theoretical knowledge of the sign and order of magnitude of the triplet amplitude permits a unique determination.

In order to reduce this ambiguity in the interpretation of the ortho-para-measurements, it is necessary to measure the deuterium scattering amplitudes relative to the known values of some other nucleus. Since hydrogen is the only substance with well-known scattering properties, this suggests a consideration of scattering by the HD molecule. We give, without derivation, the total cross section for neutron scattering by HD molecules in the $J=0$ rotational level, in the limit of zero neutron energy:

$$\begin{aligned}\sigma_{\mathrm{HD}}&=\frac{9\pi}{16}[(3a_1+a_0+2a_{3/2}+a_{1/2})^2\\&\qquad+3(a_1-a_0)^2+2(a_{3/2}-a_{1/2})^2],\\&=\frac{9}{4}\sigma_{\mathrm{H}}+\frac{81}{64}\sigma_{\mathrm{D}}+\frac{9\pi}{8}(3a_1+a_0)(2a_{3/2}+a_{1/2}).\end{aligned}\tag{69}$$

In this formula, a_1 and a_0 are the hydrogen scattering amplitudes for the triplet and singlet spin states; σ_{H} and σ_{D} are the total cross sections for scattering by a free proton and deuteron, respectively. It is clear that an absolute measurement of the HD cross section, combined with the information supplied by ortho-parahydrogen and deuterium experiments, namely the numerical magnitudes of all the quantities appearing in Eq. (69), together with the theoretically known sign of a_1, in principle determines the sign of the amplitude combination $2a_{3/2}+a_{1/2}$. Unfortunately, the influence of the interference term on σ_{HD} is slight, since the hydrogen amplitude factor $3a_1+a_0$ is small, as evidenced by the very low parahydrogen elastic cross section. If one inserts the theoretically known hydrogen amplitudes and a free deuteron cross section $\sigma_{\mathrm{D}}=4\times10^{-24}$ cm^2, the contribution of the interference term to σ_{HD} is found to be less than 7 percent, and attains this magnitude only if $a_{3/2}\cong a_{1/2}$. Thus, in order that this experiment be successful, the large cross sections σ_{H} and σ_{HD} must be measured with high precision, and the corrections for the finite neutron energy and molecular motion must be accurately incorporated into the theory.

It may be remarked that the sign of the amplitude combination $a_{3/2}-a_{1/2}$ can never be determined by any experiment in which the deuteron spin remains arbitrarily oriented in space.

In the event that the scattering amplitudes $a_{3/2}$ and $a_{1/2}$ are not such as to produce an observable difference between the ortho- and para-D_2 cross sections, information may still be obtained by studies on the depolarization of polarized neutrons diffusing through substances containing deuterium. The cumulative effect of a large number of slightly depolarizing collisions can produce easily measurable effects in much the same way that diffusion experiments allow the determination of small capture cross sections. A paper dealing with this subject is being prepared for publication.

[10] From the experimental viewpoint, it would be desirable to use liquid, rather than gaseous, deuterium. If the scattering cross sections are to be unaffected by the intermolecular forces in the liquid phase, the neutron energy must exceed, say, 0.01 ev. An inspection of the data contained in Figs. 1 and 2, which are now directly applicable to the experimental results, indicates that effects comparable with those discussed in the text are obtained if the neutron energy is insufficient to excite the $1\rightarrow2$ transition, that is, $E<0.018$ ev.