Scattering of Neutrons by Deuterons*

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The elastic scattering of neutrons by deuterons is considered for energies small enough so that only the $l=0$ part of the incident wave is different from the corresponding part of a plane wave. The Breit-Feenberg Hamiltonian is used, assuming the same potential between all pairs of particles. Any possible polarization of the deuteron by the neutron is neglected, although the individual particles in the deuteron are taken into account by an approximate method. This method is capable of including exchange between the two neutrons. When the exchange term is included, the theory gives a cross section for thermal neutrons two to three times greater than observed; the cross section for 2.5 Mev neutrons is slightly greater than observed.

IN this paper we shall consider the elastic scattering of neutrons by deuterons at energies small enough so that only the $l=0$ part of the incident wave is different from the corresponding part of a plane wave. The interaction potential will be assumed to be the same for all pairs of particles[1] and to have the form used in previous researches;[2–4]

$$V(r)=J(r)[(1-g)P^M+gP^H]=J(r)[1-\tfrac{1}{2}g+2g\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2]P^M,$$
$$J(r)=De^{-2\epsilon r}-2De^{-\epsilon r},\quad \epsilon\equiv 2/r_0. \tag{1}$$

Here, P^M and P^H are the Majorana and Heisenberg operators, respectively, and the $\boldsymbol{\sigma}$'s are the Pauli spin matrices of amplitude $\frac{1}{2}$. Using nuclear units of length (8.97×10^{-13} cm) and of energy (0.506 Mev), we have $r_0=0.3$, $D=71.2$, and $g=0.3$.[5]

General Theory

Taking particle 1 to be the incident neutron and particle 3 to be the proton, we wish to find a solution of the wave equation (in nuclear units)

$$[-\tfrac{1}{2}(\Delta_1+\Delta_2+\Delta_3)+V(r_{12})+V(r_{13})+V(r_{23})-W_0-W]\Psi=0 \tag{2}$$

that has the asymptotic form (see Fig. 1a) as $r\rightarrow\infty$

$$\Psi\rightarrow[e^{ikr\cos\theta}+r^{-1}e^{ikr}f(\theta)]\phi_0(r_{23})S(123), \tag{3}$$

in the rest coordinate system (center of mass at rest). The beam of neutrons is directed along the negative z axis. S is a function involving only the spins (to be discussed in the next section), $\phi_0(r)$ is the wave function for the symmetric normal state of the deuteron with (negative) energy W_0, and W is the kinetic energy of the incident deuteron in the laboratory reference system (deuteron initially at rest).

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[1] Breit and Feenberg, Phys. Rev. **50**, 850 (1936).
[2] Morse, Fisk and Schiff, Phys. Rev. **50**, 748 (1936); **51**, 706 (1937). See also Ochiai, Phys. Rev. in press.
[3] Fisk, Schiff and Shockley, Phys. Rev. **50**, 1090 and 1191 (1936).
[4] Schiff, Phys. Rev. **51**, 783 (1937).
[5] The breadth used here ($r_0=2.7\times10^{-13}$ cm) is somewhat larger than the breadths used by other workers (Bethe and Bacher, Rev. Mod. Phys. **8**, 82 (1936), Feenberg and Share, Phys. Rev. **50**, 253 (1936), and Rarita and Present, Phys. Rev. **51**, 788 (1937)) even considering the difference in shape of the various potentials. The broader potential agrees (reference 2) with the older data (Harkins, Kamen, Newson, and Gans, Phys. Rev. **50**, 980 (1936), Kurie, Phys. Rev. **44**, 461 (1933)) on neutron-proton angle scattering. On the other hand, it seems to be incapable of explaining either the more recent data on this point (Bartlett, Phys. Rev. **51**, 889 (1937)), which is not yet certain, or the binding energy of H^3, if the variational method of Rarita and Present, Phys. Rev. **51**, 788 (1937) is as accurate as it appears to be. The calculations of the present paper were completed before the appearance of the paper of Rarita and Present. Since our calculations are essentially qualitative, it hardly seems worth while repeating them at this time. It does seem that the assumption of a narrower potential might bring the computed values closer to the experimental data on neutron-deuteron scattering.

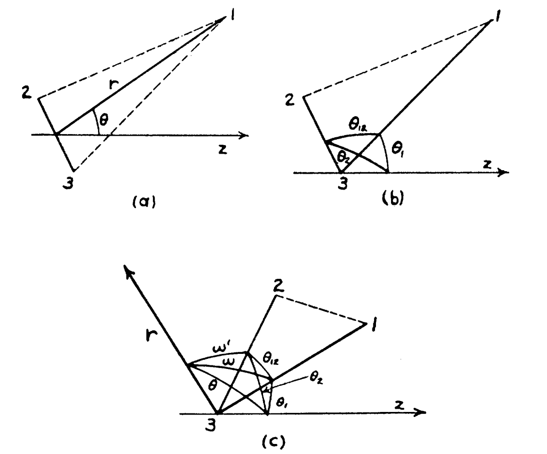

FIG. 1. The coordinate systems used in the theory. Particle 3 is the proton.

It soon becomes evident that in order to treat the problem in a reasonably simple manner, it is necessary to neglect any possible polarization of the deuteron by the incoming neutron, and to try to find a wave function which is the product of the normal deuteron function and a function for the scattered neutron. The coordinate system natural to the problem is that shown in Fig. 1a, in which the variables are r_{23} for the deuteron, and r and θ for the incoming neutron. The V's given by (1) involve space permutation operators, and will introduce functions of the medians of the (123) triangle other than r when they operate on a function of such coordinates. If a successive approximation method is used, this will make the resultant integrals exceedingly difficult to evaluate. This can be avoided by using the coordinate system of Fig. 1b, in which the incoming neutron is referred to the proton 3 rather than to the center of mass of the deuteron. The wave function then depends on the coordinates r_{23} of the deuteron and r_{13} and θ_1 of the incoming neutron; the space permutation operators introduce only the three sides of the (123) triangle into the successive approximation integrals. The Laplacian is no longer separable, but has the form

$$\tfrac{1}{2}(\Delta_1+\Delta_2+\Delta_3)\Psi(r_{23}, r_{13}, \theta_1)=\left\{\frac{1}{r_{23}^2}\frac{\partial}{\partial r_{23}}\left(r_{23}^2\frac{\partial}{\partial r_{23}}\right)+\frac{1}{r_{13}^2}\frac{\partial}{\partial r_{13}}\left(r_{13}^2\frac{\partial}{\partial r_{13}}\right)+\frac{1}{r_{13}^2\sin\theta_1}\frac{\partial}{\partial\theta_1}\left(\sin\theta_1\frac{\partial}{\partial\theta_1}\right)\right.$$
$$\left.+\cos\theta_{12}\frac{\partial^2}{\partial r_{13}\partial r_{23}}+\left(\frac{\cos\theta_2-\cos\theta_1\cos\theta_{12}}{r_{13}}\right)\frac{\partial^2}{\partial(\cos\theta_1)\partial r_{13}}\right\}\Psi(r_{23}, r_{13}, \theta_1). \quad (4)$$

Since we have decided to neglect polarization effects, (4) can be averaged over the orientation of the deuteron. Then the last two terms vanish, leaving

$$\tfrac{1}{2}(\Delta_1+\Delta_2+\Delta_3)\Psi(r_{23}, r_{13}, \theta_1)=(\Delta_{23}'+\Delta_1')\Psi(r_{23}, r_{13}, \theta_1), \quad (5)$$

where we adopt the definitions

$$\Delta_{23}'=\frac{1}{r_{23}^2}\frac{\partial}{\partial r_{23}}\left(r_{23}^2\frac{\partial}{\partial r_{23}}\right),\quad \Delta_1'=\frac{1}{r_{13}^2}\frac{\partial}{\partial r_{13}}\left(r_{13}^2\frac{\partial}{\partial r_{13}}\right)+\frac{1}{r_{13}^2\sin\theta_1}\frac{\partial}{\partial\theta_1}\left(\sin\theta_1\frac{\partial}{\partial\theta_1}\right). \quad (5')$$

Equation (3) gives the asymptotic form of the "ordinary" wave, in which the initially incident neutron is observed. There is also the "exchange" wave, in which the incident neutron changes places with the neutron initially bound in the deuteron, and the latter is observed. In the coordinate system of Fig. 1b, which we shall adopt throughout this paper, the asymptotic forms corresponding to the ordinary and exchange waves are

$$\Psi\rightarrow[e^{ikr_{13}\cos\theta_1}+r_{13}^{-1}e^{ikr_{13}}f(\theta_1)]\phi_0(r_{23})S(123), \quad \text{as } r_{13}\rightarrow\infty,$$

and

$$\Psi\rightarrow r_{23}^{-1}e^{ikr_{23}}g(\theta_2)\phi_0(r_{13})S'(123), \quad \text{as } r_{23}\rightarrow\infty. \quad (6)$$

When Ψ is made antisymmetric in the two neutrons (particles 1 and 2) as required by the Pauli principle, it has the asymptotic form when r_{13} (say) is large

$$\Psi(123)-\Psi(213)\rightarrow\phi_0(r_{23})\{e^{ikr_{13}\cos\theta_1}S(123)+r_{13}^{-1}e^{ikr_{13}}[f(\theta_1)S(123)-g(\theta_1)S'(213)]\}. \tag{7}$$

The forms (7) and (3) must of course involve the same k. On noting that the kinetic energy in the rest coordinate system is $2W/3$ and the reduced mass is $\frac{2}{3}$ of the neutron mass, it is readily seen that $k^2=8W/9$.

Since we are neglecting polarization and want Ψ to have the asymptotic forms (6), we write it as

$$\Psi=\phi_0(r_{23})F(r_{13},\theta_1)S(123)+\phi_0(r_{13})G(r_{23},\theta_2)S'(123)+\Phi, \tag{8}$$

where Φ involves a sum over excited and unbound states of the deuteron and will be neglected hereafter. We assume that in the zero-order approximation G vanishes and F is a solution of the equation

$$[\Delta_1'+k^2-U(r_{13})]F_0(r_{13},\theta_1)=0, \tag{9}$$

where U is the average field of the deuteron for the incoming neutron and can be written approximately as

$$U(r)=D_0e^{-2\epsilon_0 r}-2D_0e^{-\epsilon_0 r}. \tag{10}$$

It is clear that U must not contain a Majorana operator.

It has been shown by Morse[6] that the solution of (9) is given quite closely by a function of the form[7]

$$F_0(r,\theta)=(kr)^{-1}e^{i\delta}[\sin(kr+\delta)-e^{-\epsilon' r}\sin\delta\cos kr]+\sum_{l>0}(2l+1)i^lP_l(\cos\theta)j_l(kr) \tag{11}$$

whenever U has the general shape of a potential hole. For the potential (10), Morse[6] has found that when ϵ' is set equal to ϵ_0, and δ is obtained by setting $\int F_0(\Delta_1'+k^2-U)F_0d\tau$ equal to zero, the $l=0$ phase shift δ obtained in this way is never more than 7° from the phase shift obtained by exact solution of (9), and is generally less than 3° off, for a range of values of k, D_0 and ϵ_0. The depth D_0 of U depends strongly on spin orientation and on the manner in which the omission of the Majorana operator in U is corrected for; the mean breadth $(2/\epsilon_0)$ of U, however, depends principally on the mean breadth $(2/\epsilon)$ of the two-body potential (1). We take for the normal state deuteron function the normalized variational form[3]

$$\phi_0(r)=(a^3/\pi)^{\frac{1}{2}}e^{-ar},\quad a=3.236, \tag{12}$$

which gives within five percent of the deuteron binding energy (4.35 nuclear units) obtained from an exact solution of the deuteron equation

$$[\Delta_{23}'+W_0-V(r_{23})]\phi_0(r_{23})=0. \tag{12'}$$

Then we can fix r_{13} and average the potential $[J(r_{12})+J(r_{13})]$ over r_{23} and θ_{12}. The resulting estimate $\epsilon_0=5.701$ is relatively insensitive to D and g. This ϵ_0 is somewhat smaller than the corresponding quantity $\epsilon=6.667$ appearing in (1), as would be expected.

Morse's method for finding the $l=0$ phase shift using the potential (10) would serve to give the scattering for energies up to the point where the $l=1$ phase shift becomes appreciable, if we had some knowledge of the depth D_0 of the equivalent field U which best accounts for the operator nature of the V's. D_0 can be estimated by writing (2) in a form which can be used to calculate the next approximation to F. Neglecting the G and Φ terms in (8), we obtain on substitution into (2), using (5) and (12') and subtracting $U\phi_0FS$ from each side

$$[\Delta_1'+k^2-U(r_{13})]\phi_0(r_{23})F(r_{13},\theta_1)S(123)=[V(r_{12})+V(r_{13})-U(r_{13})]\phi_0(r_{23})F(r_{13},\theta_1)S(123). \tag{13}$$

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[6] Morse, abstract 26 at the Washington meeting, April 28, 1937.

[7] Morse, *Vibration and Sound* (McGraw-Hill, 1936), p. 246, defines the functions: $j_m(z)=(\pi/2z)^{\frac{1}{2}}\cdot J_{m+\frac{1}{2}}(z)$, and gives several of their properties.

Multiplying both sides of (13) by $\phi_0^*(r_{23})S(123)$, integrating over r_{23}, and putting the approximate form F_0 for F on the right side, we obtain

$$[\Delta_1'+k^2-U(r_{13})]F_1(r_{13},\theta_1)$$
$$=\int \phi_0^*(r_{23})S(123)[V(r_{12})+V(r_{13})-U(r_{13})]\phi_0(r_{23})F_0(r_{13},\theta_1)S(123)d\tau_{23}. \quad (14)$$

Remembering that F_0 is a solution of (9), the asymptotic form of the solution of (14) is (see Fig. 1c)

$$F_1(r,\theta)\rightarrow F_0(r,\theta)-(4\pi r)^{-1}e^{ikr}\int F_0(r_{13},\pi-\omega)\phi_0^*(r_{23})S(123)[V(r_{12})+V(r_{13})-U(r_{13})]$$
$$\times\phi_0(r_{23})F_0(r_{13},\theta_1)S(123)d\tau_{123}, \quad \text{as } r\rightarrow\infty. \quad (15)$$

We now have an expression for the first approximation F_1 which involves the difference between the true potential $[V(r_{12})+V(r_{13})]$ and the average potential $U(r_{13})$. Then the best approximation to U from our point of view is that which makes the integral on the right side of (15) vanish, so that $F_1=F_0$.

A form like (15) for the first approximation to G can be obtained by similar methods. Neglecting the Φ term in (8), we obtain on substitution into (2), using the equations obtained from (5) and (12′) by nterchange of 1 and 2

$$[\Delta_2'+k^2-V(r_{12})-V(r_{23})]\phi_0(r_{13})G(r_{13},\theta_2)S'(123)$$
$$=[V(r_{12})+V(r_{13})-\Delta_1'-k^2]\phi_0(r_{23})F(r_{13},\theta_1)\ S(123). \quad (16)$$

Putting approximately $V(r_{12})+V(r_{23})=U(r_{23})$ on the left side of (16), and F_0 for F and

$$(\Delta_1'+k^2)F_0(r_{13},\theta_1)=U(r_{13})F_0(r_{13},\theta_1)$$

on the right side, we obtain

$$[\Delta_2'+k^2-U(r_{23})]\phi_0(r_{13})G(r_{23},\theta_2)S'(123)=[V(r_{12})+V(r_{13})-U(r_{13})]\phi_0(r_{23})F_0(r_{13},\theta_1)S(123). \quad (17)$$

Multiplying both sides of (17) by $\phi_0^*(r_{13})S'(123)$ and integrating over r_{13}, we obtain an equation analogous to (14); the asymptotic form of its solution is (see Fig. 1c)

$$G_1(r,\theta)\rightarrow -(4\pi r)^{-1}e^{ikr}\int F_0(r_{23},\pi-\omega')\phi_0^*(r_{13})S'(123)[V(r_{12})+V(r_{13})-U(r_{13})]$$
$$\times\phi_0(r_{23})F_0(r_{13},\theta_1)S(123)d\tau_{123}, \quad \text{as } r\rightarrow\infty. \quad (18)$$

Spin Functions[8]

The spin function $S(123)$ must represent a neutron (particle 1) and a deuteron (particles 2 and 3) far apart, when the deuteron is known to be in a triplet state; it must also be an eigenfunction of the operator $\boldsymbol{\sigma}_1\cdot(\boldsymbol{\sigma}_2+\boldsymbol{\sigma}_3)$ in order to remove off-diagonal matrix components which would prevent convergence of the successive approximations. The spin states divide into quartets (S_q) and doublets (S_d)

$$\begin{aligned}
S_q^1&=(+++),\\
S_q^2&=(1/\sqrt{3})[(++-)+(+-+)+(-++)],\\
S_q^3&=(1/\sqrt{3})[(--+)\\
&\qquad+(-+-)+(+--)], \quad (19)\\
S_q^4&=(---),\\
S_d^1&=(1/\sqrt{6})[(++-)+(+-+)-2(-++)],\\
S_d^2&=(1/\sqrt{6})[(--+)+(-+-)-2(+--)].
\end{aligned}$$

Here, a term such as $(+-+)$ signifies that spin state in which particles 1 and 3 have spin components whose eigenvalues are $+\frac{1}{2}$ along some arbitrary axis, and particle 2 has a spin component whose eigenvalue is $-\frac{1}{2}$ along the same axis. When neutron 2 is free, and particles

[8] The treatment given here is similar to that given in reference 4 in the section labeled "symmetry properties."

1 and 3 are bound in the deuteron (exchange wave), the spin states are given by (19) except that positions 1 and 2 are interchanged; thus $S'(123)=S(213)$.

If an energy M has the general form $A_0+B_0\sigma_1\cdot\sigma_2+C_0\sigma_1\cdot\sigma_3+D_0\sigma_2\cdot\sigma_3$, where A_0 ,etc., may be permuting functions of the space coordinates, it is readily shown that all matrix elements of this energy of the form SMS or $S'MS$ vanish unless the two spin functions correspond both to quartet states or both to doublet states. Thus only quartet-quartet and doublet-doublet transitions are possible. Since the final quartet and doublet states are orthogonal, we can compute the quartet and doublet scattering separately, and later combine the cross sections in the ratio 2 : 1 of their statistical weights. With the help of (7), we have the result that the whole differential cross section in the rest coordinate system is

$$\sigma(\theta)d\omega=\tfrac{1}{3}[2|f_q(\theta)-g_q(\theta)|^2+|f_d(\theta)-g_d(\theta)|^2]d\omega. \quad (20)$$

The subscripts refer to the use of quartet and doublet spin functions in calculating f from (15) and g from (18).

Results

The integrals (15) and (18) can be evaluated analytically for all energies (k values) with the help of the relation[3]

$$\int_v \frac{e^{-\alpha r_{12}-\beta r_{13}-\gamma r_{23}}}{r_{12}r_{13}r_{23}}d\tau_{123}=\frac{16\pi^2 v}{(\alpha+\beta)(\beta+\gamma)(\gamma+\alpha)}, \quad (21)$$

although the computations become exceedingly complicated for $k>0$. When $k=0$, (11) becomes

$$F_0(r,\theta)=1+(\Delta/r)(1-e^{-\epsilon' r}), \quad (22)$$

and the integrations are readily carried through. The f and g in (20) are then independent of θ, and the scattering is spherically symmetric in the rest coordinate system. In (22), $\Delta=\pm\lim(\sin\delta/k)$ as $k\to 0$, according as δ approaches an even or odd multiple of π. The criterion for determining whether $\delta\to 0, \pi, 2\pi, \cdots$ as $k\to 0$ is whether the potential hole U contains 0, 1, 2, $\cdots$ negative energy levels;[2] these levels may not correspond to physical reality. It turns out that the U's obtained below for both the quartet and doublet cases each contain one level, so that δ approaches π.

To determine D_0, we set $k=0$, $\epsilon'=\epsilon_0=5.701$, and find by trial and error a pair of values of D_0 and Δ that will make the integral on the right

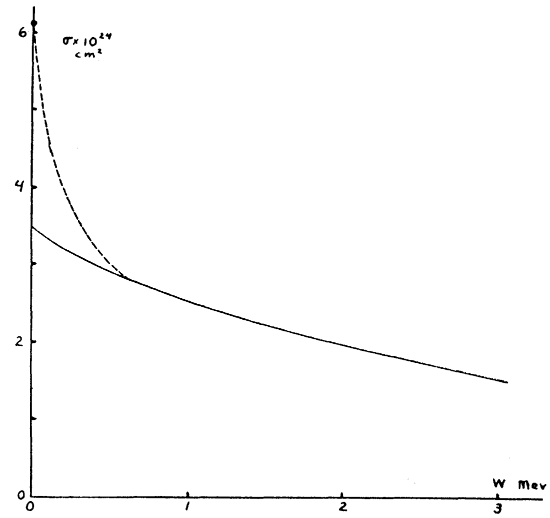

Fig. 2. Elastic scattering cross section of deuterons for neutrons as a function of incident neutron energy; without exchange (solid line), and with exchange (dotted line).

side of (15) zero and will also satisfy (9) according to Morse's criterion (vanishing of the average $H-k^2$). This must be done twice, using quartet and doublet spin functions. For the quartet case, $D_0=70.0$ and $\Delta=-0.564$; for the doublet case, $D_0=62.0$ and $\Delta=-0.629$. We can then say that the U's given by (10) with the above D_0's and $\epsilon_0=5.701$ in both cases are the best representations of the average field of a deuteron for an incoming neutron, when the coordinate system of Fig. 1b is used. For $k\doteq 0$, $f=\Delta$; for $k>0$, the $l=0$ phase shift can be found by Morse's method, in which case $f=\sin\delta/k$. The higher l phase shifts cannot be found by this method, so that our calculations are good only up to energies where the $l=1$ phase shift becomes appreciable. The total cross section computed in this way (neglecting exchange) is plotted as the solid line in Fig. 2. The effect of the exchange wave can be computed at zero energy by using (18) and (22). It is found that g is $+0.352$ for the quartet case, and -0.248 for the doublet case. The total elastic cross section at zero energy (including exchange) is, from (20), $(4\pi/3)[2\times(0.916)^2+(0.381)^2]=7.64$ square nuclear units or 6.11×10^{-24} cm^2. This is plotted as the solid circle in Fig. 2. The evaluation of (18) is very difficult for $k>0$; however, it is reasonable to assume that the exchange effect drops off fairly rapidly with increasing energy. Although further calculations should be made on this point, the dotted curve shows roughly the expected behavior of the total cross section, including exchange. A further improvement in the theory could be effected by evaluating (15) as well as (18) for $k>0$ instead of using Morse's more approximate method; at the present time the increased accuracy does not seem to warrant the considerable computational labor that would be required.

It is interesting to note that the cross section at zero energy due to the initial quartet spin state is almost six times that due to the initial doublet spin state, even omitting the effect of the different statistical weights (see preceding paragraph). It seems likely that this arises principally from the short-range repulsion between neutrons with parallel spins due to the Pauli principle.

The only published experimental values for the neutron-deuteron collision are those of Dunning *et al.*,[9] which include capture as well as elastic scattering cross section. However there is good reason[10] to believe that the capture cross section is negligibly small compared to the elastic scattering cross section even at thermal energies. The experimental cross sections using D_2O are 4.0×10^{-24} cm^2 for thermal neutrons, and 1.6×10^{-24} cm^2 for neutrons of about 2.5 Mev energy. The effect of chemical binding of the deuteron in the D_2O molecule is negligible at the higher energy, but will serve to reduce the experimental value for thermal energy neutrons[11] by an uncertain factor that is probably between 1.5 and 2.0. Thus the theoretical value is two to three times too large at zero (thermal) energy, and about 25 percent too large at 2.5 Mev (see Fig. 2). The theory would give worse agreement than indicated at the higher energy if the $l=1$ phase shift were appreciable, but it seems unlikely that it will be large at this energy.

In conclusion, we can say that the agreement between theory and experiment is at least qualitatively satisfactory, and that it seems likely that a more accurate theory (taking polarization into account, for example) will be capable of explaining the experiments quantitatively. The assumption of a narrower and deeper potential between pairs of particles[5] would probably make the cross sections calculated here somewhat smaller, improving the agreement with experiment.

It is a pleasure to thank Professor Philip M. Morse for helpful discussions of many points of the theory, particularly in connection with the positive energy wave function.

[9] Dunning, Pegram, Fink and Mitchell, Phys. Rev. **48**, 265 (1935). I am indebted to Professor Dunning for confirming these values recently.

[10] Kikuchi, Aoki and Takeda, Tokyo Inst. Phys. and Chem. Research **31**, 195 (1937).

[11] Fermi, Ricerca Scient. **2**, 13 (1936). The ratio 4 : 1 given by Fermi between the cross sections of slow neutrons on rigidly bound protons and on free protons, becomes 2.25 : 1 for the neutron-deuteron collision. The precise value of the ratio of the observed cross section to that for a free deuteron depends on the molecular energy levels and on the neutron energy; it is probably between 1.5 and 2.0