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The Scattering of Neutrons by Ortho- and Parahydrogen

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Calculations have been performed which indicate that experiments on the scattering of neutrons by ortho- and parahydrogen would enable one to determine the sign of the singlet state binding energy and the range of the neutron-proton interaction, in addition to providing direct information concerning the spin dependence of the neutron-proton interaction. A dependence of the neutron-proton interaction upon the relative spin orientation of the particles will manifest itself in a marked difference between the slow neutron scattering cross sections of orthohydrogen (parallel proton spins) and parahydrogen (anti-parallel proton spins). Neutrons with energy less than 0.068 ev, incident upon *para*-H_2 in its ground state ($J=0$, $v=0$, $S=0$), may be either elastically scattered, or inelastically scattered with excitation of the molecule to the ground state of the *ortho* system ($J=1$, $v=0$, $S=1$). This latter process, requiring 0.023 ev, occurs only if the neutron-proton interaction is spin dependent. When the neutron energy is less than 0.045 ev, the cross section for the scattering of neutrons by *ortho*-H_2 in its ground state will be the sum of the elastic scattering cross section and the cross section for the inelastic process in which the molecule is converted to a *para*-H_2 molecule in its ground state, with the neutron taking up the excess energy. The cross sections of these four processes have been calculated, assuming an interaction range of 2×10^{-13} cm and a virtual singlet state of the deuteron. For liquid-air temperature neutrons ($3kT/2=0.012$ ev), σ_{para} $(0.012)=0.21\times 10^{-24}$ cm^2, while σ_{ortho} $(0.012)=65\times 10^{-24}$ cm^2. The cross sections for neutrons at ordinary temperatures ($3kT/2=0.037$ ev), however, are $\sigma_{\text{para}}(0.037)=19\times 10^{-24}$ cm^2, and $\sigma_{\text{ortho}}(0.037)=50\times 10^{-24}$ cm^2. Therefore, if the present concept of the neutron-proton interaction is valid, one would expect the following results: (a) The *ortho*-scattering cross section for liquid air neutrons should be about 300 times the corresponding *para*-scattering cross section. (b) The *para*-scattering cross section for ordinary thermal neutrons should be roughly 100 times the *para*-scattering cross section for liquid air neutrons. For a real singlet state, however, these ratios are of the order of one. The elastic *para*-scattering cross section is quite sensitive to the value of the range of interaction if the singlet state is virtual. For example, the value of this cross section at liquid air neutron temperatures with zero range of interaction is 1.75×10^{-24} cm^2, as compared with 0.26×10^{-24} cm^2 for an interaction range of 2×10^{-13} cm. Hence, from a measurement of the *para* elastic scattering cross section for homogeneous neutrons at some energy less than 0.023 ev, the range of interaction in the triplet state may be inferred with some degree of accuracy. A discussion of the influence of intermolecular forces on the previous results is given.

INTRODUCTION

WIGNER and Bethe and Peierls[1] have given a simple theory of the scattering of neutrons by protons, assuming a short range neutron-proton interaction. The resultant scattering cross section:

$$\sigma=\frac{4\pi\hbar^2}{M}\frac{1}{|E_0|+\frac{1}{2}E}, \tag{1}$$

depends only upon the binding energy $|E_0|$ of the deuteron, and the energy E of the neutron measured in the system in which the proton is initially at rest.

For small neutron energies ($E\ll|E_0|$), Eq. (1) predicts a scattering cross section of 2.40×10^{-24} cm^2, since $|E_0|=2.2\times 10^6$ ev. This is in complete disagreement with the experimental value of $\sigma=13\times 10^{-24}$ cm^2.[2] This discrepancy cannot be explained by using a finite value of r_0, the range of the neutron-proton force. Bethe and Bacher[3] have shown, for a rectangular potential hole, that the Bethe-Peierls formula must be multiplied by $1+\alpha_0 r_0$, i.e.,

$$\sigma=\frac{4\pi\hbar^2}{M}\frac{1+\alpha_0 r_0}{|E_0|+\frac{1}{2}E}, \tag{2}$$

where

$$\alpha_0=(M|E_0|/\hbar^2)^{\frac{1}{2}}=2.29\times 10^{12}\ \text{cm}^{-1}. \tag{3}$$

It is easily shown that this formula is practically

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[1] E. Wigner, Zeits. f. Physik **83**, 253 (1933); H. A. Bethe and R. Peierls, Proc. Roy. Soc. **A149**, 176 (1935).

[2] E. Amaldi and E. Fermi, Phys. Rev. **50**, 899 (1936).

[3] H. A. Bethe and R. F. Bacher, Rev. Mod. Phys. **8**, 82 (1936).

independent of the shape of the potential well. With a reasonable value of r_0 obtained from the theory of the light nuclei, namely $r_0 = 2\times 10^{-13}$ cm, this modified Bethe-Peierls formula gives a cross section of 3.50×10^{-24} cm^2, for slow neutrons.

To explain this marked lack of agreement, Wigner[4] advanced the suggestion that the neutron-proton interaction in the singlet state differs from that in the triplet state. From this assumption, it follows that

$$\sigma = \frac{4\pi\hbar^2}{M}\left(\frac{3}{4}\,\frac{1+\alpha_0 r_0}{|E_0|+\frac{1}{2}E} + \frac{1}{4}\,\frac{1+\alpha_1 r_0}{|E_1|+\frac{1}{2}E}\right), \quad (4)$$

where $|E_1|$ is the energy of the singlet state, and

$$\alpha_1 = \pm (M|E_1|/\hbar^2)^{\frac{1}{2}}, \quad (5)$$

the plus or minus sign obtaining according as the singlet state is real or virtual, respectively. Since the ground state of the deuteron gives no information about $|E_1|$, it can be chosen to give agreement with the experimental results. The large slow neutron scattering will be explained, therefore, if $|E_1| = 142{,}000$ ev for a real level, or $|E_1| = 114{,}000$ ev for a virtual level.

Fermi[5] has shown that one can determine which of these two possibilities is realized by a measurement of the cross section for radiative capture of neutrons by protons. Such measurements have been performed,[2] and indicate the existence of a virtual singlet state of the deuteron It should be pointed out, however, that on the basis of the β-ray theory of magnetic moments, it is questionable whether Fermi's mechanism of magnetic dipole capture can be correctly treated by simply assuming the additivity of magnetic moments.

It is the purpose of this paper to point out that experiments on the scattering of neutrons by ortho- and parahydrogen would afford a direct means of testing Wigner's hypothesis of a spin-dependent interaction between neutrons and protons. Furthermore, it will be shown that, from the results of such experiments, one can deduce the energy of the singlet state and the range of the forces.

I

Neutrons of thermal energy have a wave-length which is of the same order as the distance between the protons in H_2. One should therefore observe interference between the neutron waves scattered from the two protons in the hydrogen molecule. If the neutron-proton interaction depends upon the relative spin orientation of the particles, this should manifest itself in a difference between the interference effects in ortho- and parahydrogen, i.e., parallel and antiparallel proton spins, respectively. In addition to demonstrating directly the existence or nonexistence of spin forces, an experimental determination of these scattering cross sections would give the amplitudes of the singlet and the triplet scattered waves, save for a possible common factor of (-1). It should be emphasized that these results can be obtained without a detailed theory of the mechanism of interaction. Making the usual assumptions about the interaction, one can then determine the energy of the singlet level, and the range of the neutron-proton force.

The problem of calculating scattering cross sections is complicated by the presence of inelastic scattering processes. In general, all possible transitions consistent with conservation of energy and momentum will occur. However, a neutron-proton interaction which is independent of spin will only induce transitions between states of the molecule with the same total spin angular momentum, that is, *ortho-ortho* and *para-para* transitions, while spin-dependent interactions will also cause *ortho-para* and *para-ortho* transitions.

It is interesting to note that, for neutrons with energy comparable to the excitation energy of the first few rotational levels, the *ortho*-scattering cross section differs from the *para*-scattering cross section, even if no spin-dependent forces act between neutrons and protons. This is a consequence of the different rotational energy levels of ortho- and parahydrogen. Neutrons with energies large compared with the lowest rotational levels, however, will have the same scattering cross sections in ortho- and parahydrogen. If, on the other hand, the neutron wave-length is large compared with the internuclear separation in hydrogen, the elastic

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[4] E. Feenberg and J. K. Knipp, Phys. Rev. **48**, 906 (1935).

[5] E. Fermi, Phys. Rev. **48**, 570 (1935); Ricerca Scient. VII–II, 13 (1936).

scattering in ortho- and parahydrogen will differ if spin-dependent forces are present, but will be the same if no such spin forces are operative.

At sufficiently low temperatures, the molecules of H_2 are in their respective ground states, namely $J=0$, $v=0$ for *para*-molecules and $J=1$, $v=0$ for *ortho*-molecules. In the absence of spin-dependent neutron-proton forces, slow neutrons will suffer only elastic collisions. The scattering cross sections of slow neutrons in ortho- and parahydrogen will, therefore, be the same.

If, however, the neutron-proton interaction involves the relative spin orientation of the particles, the cross section corresponding to the conversion of an *ortho*-molecule into a *para*-molecule will also contribute to the *ortho*-scattering cross section, whereas the *para* cross section will still consist of only the elastic cross section. Therefore, at sufficiently low neutron energies, a difference between the scattering of ortho- and parahydrogen should manifest itself.

II

The mathematical treatment of the scattering of neutrons by hydrogen molecules may be given with the aid of a theorem which Fermi[6] utilized in his considerations on the effect of molecular binding forces on the neutron-proton scattering cross section. With neglect of the dependence of the neutron-proton interaction upon the relative spin orientation of the particles, this theorem states that the scattering of a neutron by a bound proton may be calculated with the Born approximation, by using

$$-(4\pi\hbar^2/M)a\delta(\mathbf{r}_n-\mathbf{r}_p) \tag{6}$$

as the effective neutron-proton interaction. Here $\delta(\mathbf{r})$ is the three-dimensional Dirac δ-function, and a is defined by the solution corresponding to zero energy of the wave equation for the relative motion of the particles, namely:

$$1+a/r \quad \text{for} \quad r>r_0. \tag{7}$$

The condition of validity of this result is that there exist a quantity R which is large compared with r_0 and a, but small compared with the de Broglie wave-lengths of the neutron and the proton. This condition is easily satisfied for slow neutrons and the protons in the hydrogen molecule.

The extension of this theorem to an interaction which differs in the singlet state from that in the triplet state is made without difficulty. We need merely replace a in formula (6) by an operator whose eigenvalue for a triplet state is a_1, the value of a calculated for the triplet interaction, and whose eigenvalue for a singlet state is a_0, the value of a calculated for the singlet interaction. Such an operator can be written:

$$\tfrac{1}{2}a_1(1+Q)+\tfrac{1}{2}a_0(1-Q), \tag{8}$$

where Q is an operator with the eigenvalues $+1$ and -1 for triplet and singlet states, respectively. It has been shown by Dirac[7] that Q can be expressed algebraically in terms of $\boldsymbol{\sigma}_n$ and $\boldsymbol{\sigma}_p$, the Pauli matrices of the neutron and the proton, *viz.:*

$$Q=\tfrac{1}{2}(1+\boldsymbol{\sigma}_n\cdot\boldsymbol{\sigma}_p). \tag{9}$$

Therefore, (6) must be replaced by

$$\begin{aligned}-(\pi\hbar^2/M)(3a_1+a_0&\\ +(a_1-a_0)\boldsymbol{\sigma}_n\cdot\boldsymbol{\sigma}_p)&\delta(\mathbf{r}_n-\mathbf{r}_p).\end{aligned} \tag{10}$$

The effective interaction between a neutron and the protons in the hydrogen molecule will then be

$$\begin{aligned}&-(\pi\hbar^2/M)(3a_1+a_0\\ &\qquad+(a_1-a_0)\boldsymbol{\sigma}_n\cdot\boldsymbol{\sigma}_1)\delta(\mathbf{r}_n-\mathbf{r}_1)\\ &-(\pi\hbar^2/M)(3a_1+a_0\\ &\qquad+(a_1-a_0)\boldsymbol{\sigma}_n\cdot\boldsymbol{\sigma}_2)\delta(\mathbf{r}_n-\mathbf{r}_2),\end{aligned} \tag{11}$$

in consequence of the small probability that the protons approach within a distance of the order of R.

It is convenient to separate (11) into two parts which are, respectively, symmetrical and antisymmetrical in the proton spins, namely:

$$\begin{aligned}&-(\pi\hbar^2/M)(3a_1+a_0+(a_1-a_0)\boldsymbol{\sigma}_n\cdot\mathbf{S})\\ &\qquad\times(\delta(\mathbf{r}_n-\mathbf{r}_1)+\delta(\mathbf{r}_n-\mathbf{r}_2))\\ &-(\pi\hbar^2/2M)(a_1-a_0)\boldsymbol{\sigma}_n\cdot(\boldsymbol{\sigma}_1-\boldsymbol{\sigma}_2)\\ &\qquad\times(\delta(\mathbf{r}_n-\mathbf{r}_1)-\delta(\mathbf{r}_n-\mathbf{r}_2)),\end{aligned} \tag{12}$$

where

$$\mathbf{S}=\tfrac{1}{2}(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2) \tag{13}$$

represents the total spin angular momentum of the molecule. It is evident that the symmetrical part of the interaction will be responsible for

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[6] E. Fermi, Ricerca Scient. VII–II, 13 (1936).

[7] P. A. M. Dirac, *Quantum Mechanics*, second edition (Oxford, 1935).

those transitions in which the spin symmetry of the molecule does not change, that is, *ortho-ortho* and *para-para* transitions. The antisymmetrical part of the interaction, however, will induce *ortho-para* and *para-ortho* transitions.

Consider a scattering process in which a neutron with momentum $\mathbf{p}^0$ collides with a hydrogen molecule with the momentum $-\mathbf{p}^0$, the vibrational quantum number v, the rotational quantum number J, and the quantum number S of the resultant proton spin. We wish to calculate the probability that the neutron is scattered with the momentum $\mathbf{p}$, leaving the molecule in a state described by the set of quantum numbers $-\mathbf{p}$, v', J', S'. The wave function of the initial state, normalized in a volume V, is:

$$\Psi_i = V^{-\frac{1}{2}} \exp\left((i/\hbar)\mathbf{p}^0\cdot\mathbf{r}_n\right)\chi_m V^{-\frac{1}{2}} \exp\left(-(i/\hbar)\mathbf{p}^0\cdot(\mathbf{r}_1+\mathbf{r}_2)/2\right)\phi_{v,\,J,\,m_J}(\mathbf{r}_1-\mathbf{r}_2)\chi_{S,\,m_S}, \tag{14}$$

where $V^{-\frac{1}{2}} \exp((i/\hbar)\mathbf{p}^0\cdot\mathbf{r}_n)$ is the wave function of a free neutron with momentum $\mathbf{p}^0$, χ_m is the eigenfunction of the z-component of the neutron spin corresponding to the eigenvalue m, $V^{-\frac{1}{2}} \exp(-(i/\hbar)\mathbf{p}^0\cdot(\mathbf{r}_1+\mathbf{r}_2)/2)$ is the wave function which describes the motion of the center of gravity of the hydrogen molecule with momentum $-\mathbf{p}^0$, $\phi_{v,\,J,\,m_J}(\mathbf{r}_1-\mathbf{r}_2)$ is the wave function of the relative motion of the two protons in a state with vibrational quantum number v, rotational quantum number J and magnetic quantum number m_J, and, finally, $\chi_{S,\,m_S}$ is the eigenfunction of the proton spins corresponding to a resultant spin angular momentum S and an eigenvalue of the z-component of the total spin equal to m_S. Similarly, the wave function of the final state is:

$$\Psi_f = V^{-\frac{1}{2}} \exp\left((i/\hbar)\mathbf{p}\cdot\mathbf{r}_n\right)\chi_{m'} V^{-\frac{1}{2}} \exp\left(-(i/\hbar)\mathbf{p}\cdot(\mathbf{r}_1+\mathbf{r}_2)/2\right)\phi_{v',\,J',\,m'_J}(\mathbf{r}_1-\mathbf{r}_2)\chi_{S',\,m'_S}. \tag{15}$$

According to the well-known Born formula, the probability of the transition per unit time is given by:

$$(2\pi/\hbar)\left|(\Psi_f,\ U\Psi_i)\right|^2\rho_E, \tag{16}$$

where U denotes the expression (12) for the interaction, and ρ_E represents the number of neutron momentum states per unit range of the total final energy. Writing $E_{J,\,v}$ for the internal energy of the molecule in a state characterized by the quantum numbers v and J, we have

$$E = (3/4M)p^{0\,2} + E_{J,\,v} = (3/4M)p^2 + E_{J',\,v'}, \tag{17}$$

by the law of conservation of energy. Therefore, if we consider a process in which the neutron is scattered through an angle Θ into a solid angle $d\Omega$, the number of final states per unit range of the total final energy is

$$\rho_E = \frac{Vp^2}{8\pi^3\hbar^3}\frac{dp}{dE}d\Omega = V\frac{Mp}{12\pi^3\hbar^3}d\Omega. \tag{18}$$

Formula (16) gives the transition probability for definite values of m, m_J, m_S and m', m_J', m_S'. Since we are not interested in the transition probabilites between particular degenerate states, we must sum over all values of m', m_J', m_S' and average with respect to m, m_J, m_S. Therefore, the total transition probability per unit time will be

$$\frac{1}{2(2S+1)(2J+1)}\sum_{m',\,m'_J,\,m'_S}\ \sum_{m,\,m_J,\,m_S}\left|(\Psi_f,\ U\Psi_i)\right|^2\frac{VMp}{6\pi^2\hbar^4}d\Omega. \tag{19}$$

Dividing by the neutron flux relative to the hydrogen molecule, namely

$$3p^0/2MV, \tag{20}$$

we obtain the differential cross section $\sigma_{J',\,v',\,S';\,J,\,v,\,S}(\Theta)d\Omega$ for scattering of a neutron through an angle Θ into the solid angle $d\Omega$ with excitation of the molecule from the state J, v, S to the state

J', v', S', referred to the system in which the center of gravity of the neutron and the molecule is at rest, *viz.:*

$$\sigma_{J',\,v',\,S';\,J,\,v,\,S}(\Theta)d\Omega=\frac{4}{9}\frac{p}{p^0}\frac{1}{2(2S+1)(2J+1)}\sum_{m',\,m'_J,\,m'_S}\ \sum_{m,\,m_J,\,m_S}\left|\left(\Psi_f,\frac{MV}{2\pi\hbar^2}U\Psi_i\right)\right|^2 d\Omega. \tag{21}$$

The summation with respect to m, m_S and m', $m_S{}'$ may be performed without difficulty. We consider first those transitions in which the total spin of the molecule remains unchanged, i.e., $S'=S$. Utilizing the expressions (14) and (15) for the initial and final wave functions, we obtain:

$$\left(\Psi_f,\frac{MV}{2\pi\hbar^2}U\Psi_i\right)=-\frac{1}{2V}(m';S,m_S{}'\,|\,3a_1+a_0+(a_1-a_0)\boldsymbol{\sigma}_n\cdot\mathbf{S}\,|\,m;S,m_S)$$
$$\cdot\int\exp\left[(i/\hbar)(\mathbf{p}^0-\mathbf{p})\cdot(\mathbf{r}_n-(\mathbf{r}_1+\mathbf{r}_2)/2)\right]\phi^*_{v',\,J',\,m'_J}(\mathbf{r}_1-\mathbf{r}_2)\phi_{v,\,J,\,m_J}(\mathbf{r}_1-\mathbf{r}_2)$$
$$\times(\delta(\mathbf{r}_n-\mathbf{r}_1)+\delta(\mathbf{r}_n-\mathbf{r}_2))d\tau_n d\tau_1 d\tau_2=-(m';S,m_S{}'\,|\,3a_1+a_0+(a_1-a_0)\boldsymbol{\sigma}_n\cdot\mathbf{S}\,|\,m;S,m_S)$$
$$\cdot\int\cos\frac{(\mathbf{p}^0-\mathbf{p})\cdot\mathbf{r}}{2\hbar}\phi^*_{v',\,J',\,m'_J}(\mathbf{r})\phi_{v,\,J,\,m_J}(\mathbf{r})d\tau. \tag{22}$$

Therefore,

$$\sum_{m,\,m_S}\ \sum_{m',\,m'_S}\left|\left(\Psi_f,\frac{MV}{2\pi\hbar^2}U\Psi_i\right)\right|^2=\left|\int\cos\frac{(\mathbf{p}^0-\mathbf{p})\cdot\mathbf{r}}{2\hbar}\phi^*_{v',\,J',\,m'_J}(\mathbf{r})\phi_{v,\,J,\,m_J}(\mathbf{r})d\tau\right|^2$$
$$\cdot\sum_{m,\,m_S}\ \sum_{m',\,m'_S}|(m';S,m_S{}'\,|\,3a_1+a_0+(a_1-a_0)\boldsymbol{\sigma}_n\cdot\mathbf{S}\,|\,m;S,m_S)|^2. \tag{23}$$

Since $3a_1+a_0+(a_1-a_0)\boldsymbol{\sigma}_n\cdot\mathbf{S}$ is diagonal with respect to the total spin of the molecule, the second factor of this expression may be written:

$$\sum_{m,\,m_S}\ \sum_{m',\,S',\,m'_S}|(m';S',m_S{}'\,|\,3a_1+a_0+(a_1-a_0)\boldsymbol{\sigma}_n\cdot\mathbf{S}\,|\,m;S,m_S)|^2, \tag{24}$$

which becomes

$$\sum_{m,\,m_S}(m;S,m_S\,|\,(3a_1+a_0+(a_1-a_0)\boldsymbol{\sigma}_n\cdot\mathbf{S})^2\,|\,m;S,m_S) \tag{25}$$

by the matrix law of multiplication. Now

$$(3a_1+a_0+(a_1-a_0)\boldsymbol{\sigma}_n\cdot\mathbf{S})^2=(3a_1+a_0)^2+(a_1-a_0)^2\mathbf{S}^2+2(3a_1+a_0)(a_1-a_0)\boldsymbol{\sigma}_n\cdot\mathbf{S}-(a_1-a_0)^2\boldsymbol{\sigma}_n\cdot\mathbf{S}, \tag{26}$$

from which we obtain

$$2(2S+1)((3a_1+a_0)^2+S(S+1)(a_1-a_0)^2) \tag{27}$$

for the sum (25), using the fact that the diagonal sum of an angular momentum matrix is zero.

Collecting our formulae, we obtain finally

$$\sigma_{J',\,v',\,S;\,J,\,v,\,S}(\Theta)d\Omega=(4p/9p^0)((3a_1+a_0)^2+S(S+1)(a_1-a_0)^2)$$
$$\cdot\frac{1}{2J+1}\sum_{m_J,\,m'_J}\left|\int\cos\frac{(\mathbf{p}^0-\mathbf{p})\cdot\mathbf{r}}{2\hbar}\phi^*_{v',\,J',\,m_J{}'}(\mathbf{r})\phi_{v,\,J,\,m_J}(\mathbf{r})d\tau\right|^2 d\Omega. \tag{28}$$

We may note that Eq. (28) gives a nonvanishing transition probability only if J and J' are both even or both odd, since $\phi_{v,\,J,\,m_J}(-\mathbf{r})=(-1)^J\phi_{v,\,J,\,m_J}(\mathbf{r})$. Indeed, this is required by the well-known condition

$$(-1)^J=(-1)^S, \tag{29}$$

imposed by the Pauli exclusion principle. Therefore *ortho-ortho* transitions are associated with transitions between states of odd rotational quantum number, while *para-para* transitions are associated with transitions between states of even J.

A similar calculation shows that the scattering cross sections for transitions in which the total spin of the molecule changes, i.e., $S'=1-S$, are given by:

$$\sigma_{J',\,v',\,1-S;\;J,\,v,\,S}(\Theta)d\Omega=(4p/9p^0)(a_1-a_0)^2(3-2S) \cdot\frac{1}{2J+1}\sum_{m_J,\,m'_J}\left|\int \sin\frac{(\mathbf{p}^0-\mathbf{p})\cdot\mathbf{r}}{2\hbar}\phi^*_{v',\,J',\,m'_J}(\mathbf{r})\phi_{v,\,J,\,m_J}(\mathbf{r})d\tau\right|^2 d\Omega. \tag{30}$$

It is evident from (29) that *ortho-para* and *para-ortho* transitions are accompanied by odd-even and even-odd transitions in the rotational quantum number J, respectively.

III

The minimum energy necessary to excite the molecule from the state J, v to the state J', v' is $(2/3)(E_{J',\,v'}-E_{J,\,v})$, if the neutron energy is measured in a system moving with the center of gravity of the neutron and the molecule. Measured in the system in which the molecule is initially at rest, the requisite energy is $(3/2)(E_{J',\,v'}-E_{J,\,v})$ since $\mathbf{p}_0$, the initial momentum of the neutron in the latter system of reference, is given by

$$\mathbf{p}_0=3\mathbf{p}^0/2. \tag{31}$$

For small rotational and vibrational quantum numbers, the energy levels of the molecule, in volts, are:[8]

$$E_{J,\,v}=0.015\tfrac{1}{2}J(J+1)+0.533v. \tag{32}$$

Therefore, if the neutron energy is less than 0.045 ev, the energy necessary to excite the J transition 1→2, the only excitation process which may take place is the J transition 0→1, requiring 0.023 ev.

The most interesting effects are obtained at low temperatures which are such that practically all the hydrogen molecules will be in their respective ground states, namely $v=0$, $J=0$ for *para*-molecules, and $v=0$, $J=1$ for *ortho*-molecules. With these restrictions upon the neutron energy and the initial states of the molecule, the only processes which can occur are those in which the vibrational states remain unexcited and J undergoes any of the four possible transitions: 0→0, 0→1, 1→0, 1→1.

To a sufficient approximation, the probability of these transitions may be calculated by treating the H_2 molecule as a rigid rotator. The wave function appropriate to this model is:

$$\phi_{0,\,J,\,m_J}(\mathbf{r})=\left(\frac{2J+1}{4\pi}\,\frac{(J-|m_J|)!}{(J+|m_J|)!}\right)^{\frac{1}{2}}\sin^{|m_J|}\vartheta\left(\frac{d}{d\cos\vartheta}\right)^{J+|m_J|}\frac{(\cos^2\vartheta-1)^J}{2^J J!}e^{im_J\varphi}(\delta(r-r_e))^{\frac{1}{2}}/r_e, \tag{33}$$

where r_e, the equilibrium nuclear separation, has the numerical value[8]

$$r_e=0.75\times 10^{-8}\text{ cm}. \tag{34}$$

According to the principle of spectroscopic stability, the sums which occur in Eqs. (28) and (30) have a value which is independent of the direction of quantization. It is evident from (33) that, if the direction of quantization is taken to be the direction of the vector $\mathbf{p}^0-\mathbf{p}$, the only nonvanishing terms in these sums are those for which $m_J=m_J'$. Therefore, the number of terms is equal to the rotational multiplicity of the state with smaller rotational quantum number.

The only matrix element which need be evaluated to calculate the elastic scattering from parahydrogen (0→0), is

$$\int\cos\left(\frac{|\mathbf{p}^0-\mathbf{p}|r\cos\vartheta}{2\hbar}\right)|\phi_{0,\,0,\,0}(r)|^2 2\pi r^2 dr\sin\vartheta d\vartheta=\frac{\sin(|\mathbf{p}^0-\mathbf{p}|r_e/2\hbar)}{|\mathbf{p}^0-\mathbf{p}|r_e/2\hbar}. \tag{35}$$

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[8] W. Jevons, *Report on Band-Spectra of Diatomic Molecules* (Cambridge, 1932).

In terms of Θ, the angle of scattering in the system of the center of gravity, this may be written

$$\frac{\sin\left[(p^0r_e/\hbar)\sin\frac{1}{2}\Theta\right]}{(p^0r_e/\hbar)\sin\frac{1}{2}\Theta}. \tag{36}$$

Therefore,

$$\sigma_{0,\,0,\,0;\,0,\,0,\,0}(\Theta)2\pi\sin\Theta d\Theta=\frac{4}{9}(3a_1+a_0)^2\left(\frac{\sin\left[(p^0r_e/\hbar)\sin\frac{1}{2}\Theta\right]}{(p^0r_e/\hbar)\sin\frac{1}{2}\Theta}\right)^2 2\pi\sin\Theta d\Theta. \tag{37}$$

The total elastic scattering cross section is

$$\begin{aligned}\sigma_{0,\,0,\,0;\,0,\,0,\,0}&=\frac{32\pi}{9}(3a_1+a_0)^2\left(\frac{\hbar}{p^0r_e}\right)^2\int_0^{p^0r_e/\hbar}\frac{\sin^2 x}{x}dx\\ &=\frac{16\pi}{9}(3a_1+a_0)^2\left(\frac{\hbar}{p^0r_e}\right)^2\left[\log\frac{2p^0r_e}{\hbar}-Ci\frac{2p^0r_e}{\hbar}+0.5772\right],\end{aligned} \tag{38}$$

where

$$Cix=-\int_x^\infty\frac{\cos t}{t}dt. \tag{39}$$

A similar calculation yields the following cross sections for the 0→1, 1→0, 1→1 transitions, respectively:

$$\sigma_{1,\,0,\,1;\,0,\,0,\,0}=32\pi(a_1-a_0)^2\left(\frac{\hbar}{p^0r_e}\right)^2\left[\frac{\sin x}{x}+\frac{\cos x-1}{x^2}+\frac{1}{2}\log x-\frac{1}{2}Cix\right]_{(p^0-p)r_e/\hbar}^{(p^0+p)r_e/\hbar},\quad p=\left(p^{0^2}-\frac{4M}{3}E_{1,\,0}\right)^{\frac{1}{2}};$$

$$\sigma_{0,\,0,\,0;\,1,\,0,\,1}=\frac{32\pi}{3}(a_1-a_0)^2\left(\frac{\hbar}{p^0r_e}\right)^2\left[\frac{\sin x}{x}+\frac{\cos x-1}{x^2}+\frac{1}{2}\log x-\frac{1}{2}Cix\right]_{(p-p^0)r_e/\hbar}^{(p+p^0)r_e/\hbar},\quad p=\left(p^{0^2}+\frac{4M}{3}E_{1,\,0}\right)^{\frac{1}{2}};$$

$$\sigma_{1,\,0,\,1;\,1,\,0,\,1}=\frac{16\pi}{3}((3a_1+a_0)^2+2(a_1-a_0)^2)\frac{1}{\xi^2}\left[-\frac{3}{\xi^2}\left(\frac{\sin\xi}{\xi}-\cos\xi\right)^2+\frac{\sin^2\xi}{\xi^2}+\log 2\xi-Ci2\xi-0.4228\right],$$

$$\xi=\frac{p^0r_e}{\hbar}. \tag{40}$$

These four cross sections, calculated for a virtual singlet state of the deuteron and a range $r_0=2\times10^{-13}$ cm, are plotted in Figs. 1, 2 as a function of the neutron energy.[9] The curves for any other choice of the range of interaction and the sign of the binding energy of the singlet state[10] may be obtained by an appropriate change of scale since only the values of a_1 and a_0 need be changed. Thus, if the singlet state is taken as real rather than virtual, the cross sections for the elastic scattering by parahydrogen should be multiplied by 244.

It is evident from these graphs that the present concept of the neutron-proton interaction as a spin-dependent force leading to a virtual state of the deuteron, and of range $r_0=2\times10^{-13}$ cm, implies the following qualitative predictions:

(a) The scattering cross section of parahydrogen for ordinary thermal neutrons ($E=0.037$ ev) should be about 100 times the scattering cross section of parahydrogen for liquid-air neutrons ($E=0.012$ ev);

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[9] The quantities a_1 and a_0 are obtained from the free proton triplet and singlet scattering cross sections with the aid of the relations: $\sigma_{\text{triplet}}=4\pi a_1^2$, $\sigma_{\text{singlet}}=4\pi a_0^2$. The sign of a_0/a_1 is positive if the singlet state is real, negative if the singlet state is virtual.

[10] We speak of a positive binding energy if the state is real, a negative binding energy if it is virtual.

(b) The scattering cross section of orthohydrogen for liquid-air neutrons should be roughly 300 times the scattering cross section of parahydrogen for liquid-air neutrons;

(c) The scattering cross section of orthohydrogen for ordinary thermal neutrons should be only 2 or 3 times larger than the scattering cross section of parahydrogen for these neutrons;

(d) The *ortho*-scattering cross section for ordinary thermal neutrons should be about three-fourths of the *ortho*-scattering cross section for liquid-air neutrons.

If, however, the singlet state is real, the parahydrogen scattering cross section for ordinary thermal neutrons should be about $\frac{3}{4}$ of the parahydrogen scattering cross section for liquid-air neutrons, and the orthohydrogen cross section should be approximately 7/5 of the *para*-scattering cross section for liquid-air neutrons. A comparison of these two predictions shows clearly that this, rather than the capture of neutrons by protons, is the ideal method for determining the sign of the deuteron singlet state binding energy.

The parahydrogen elastic scattering cross section varies sensitively with the range of the neutron-proton interaction. This is illustrated in Fig. 3 for a virtual singlet state. It is seen, for example, that the scattering cross section for zero range is 7 times the scattering cross section for a range of $r_0 = 2 \times 10^{-13}$ cm. An experimental determination of the parahydrogen scattering cross section for neutrons of some definite energy less than 0.023 ev would, therefore, permit one to calculate the range of the neutron-proton interaction with some degree of accuracy. Neutron beams with a sufficient energy homogeneity can be obtained with a mechanical velocity selector[11] or with the aid of Bragg reflection from crystals.[12]

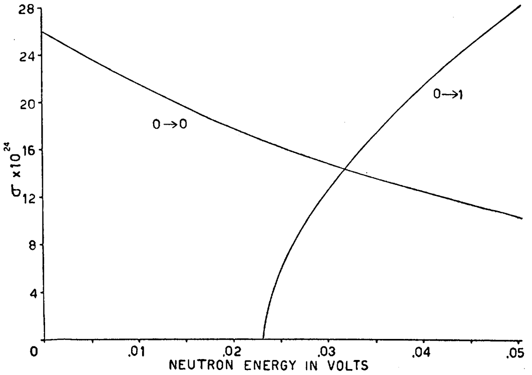

FIG. 1. The elastic (0→0) and inelastic (0→1) scattering cross sections of parahydrogen, calculated for a virtual singlet state of the deuteron and a range of interaction in the triplet state equal to 2×10^{-13} cm. The ordinates of the elastic scattering curve are enlarged 100 fold.

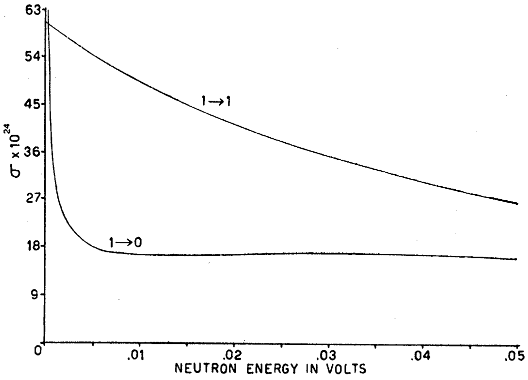

FIG. 2. The elastic (1→1) and inelastic (1→0) scattering cross sections of orthohydrogen, calculated under the same assumptions as Fig. 1.

Unfortunately, this scattering cross section is of the same order as the capture cross section if the singlet state is virtual. This necessitates a theoretical knowledge of the capture cross section if one performs absorption measurements. Since the deuteron formed in a capture process has a recoil energy (~1000 ev) which is very large compared with the molecular binding energy of a proton, the cross section for this process can be calculated by assuming the protons to be free.[13] The capture cross section per molecule, therefore, is twice the free proton capture cross section, and thus has the numerical magnitude[5] 0.6×10^{-24} cm^2 at liquid-air temperatures ($E = 0.012$ ev), provided the singlet state is virtual.

IV

The neglect of intermolecular forces in the preceding discussion limits its applicability to the scattering by H_2 in its gaseous state. However, experiments are most easily carried out with liquid or solid hydrogen where intermolecular

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[11] G. A. Fink, Phys. Rev. **50**, 738 (1936).

[12] D. P. Mitchell and P. N. Powers, Phys. Rev. **50**, 486 (1936).

[13] An analytical proof has been given by W. E. Lamb, Jr., Phys. Rev. **51**, 187 (1937).

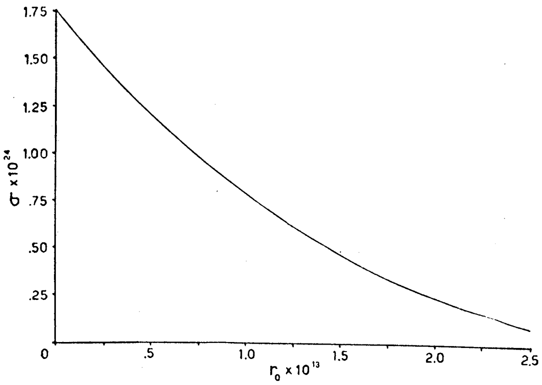

FIG. 3. The elastic scattering cross section of parahydrogen for neutrons of zero energy, as a function of the range of interaction in the triplet state. The singlet state of the deuteron is assumed to be virtual.

forces may have an appreciable effect. The discussion of this effect may be simplified by supposing the molecules to vibrate independently about positions of equilibrium with a frequency ν, given by

$$h\nu = k\Theta_E, \tag{41}$$

where Θ_E, the characteristic Einstein temperature, is related to the characteristic Debye temperature Θ_D by[14]

$$\Theta_E = 3\Theta_D/4. \tag{42}$$

Experimentally,[15] $\Theta_D = 105°\text{K}$, from which we obtain

$$h\nu = 0.007 \text{ ev}. \tag{43}$$

Consequently, if the neutron energy is large compared with 0.007 ev, the molecules may be treated as if they were free and the preceding results are applicable.

The heat of evaporation and the heat of fusion of normal and parahydrogen agree to within 1 percent,[16] which is good evidence for the free rotation of hydrogen molecules in the liquid and solid phase.[17] This is supported by experiments upon the Raman effect in liquid H_2.[18] We may conclude that intermolecular forces act only upon the center of gravity of a hydrogen molecule, and do not affect its internal motion. Therefore, the appropriate description of the effect of intermolecular forces upon the *elastic* scattering cross sections is obtained by multiplying our previous results by a function $F(E/h\nu)$ which approaches 1 rapidly as E becomes greater than $h\nu$. The limiting value of this function for $E/h\nu \ll 1$ may be obtained by an elementary consideration. When E is small compared with $h\nu$, the effective mass of a molecule is the same as the mass of the whole liquid or solid. Now the scattering cross section is proportional to the square of the reduced mass of the system, that is, $4M^2/9$ for a free molecule, and M^2 for a strongly bound molecule. Therefore $F(0) = 9/4$ so that the elastic scattering cross sections we have obtained should be multiplied by a function which decreases rapidly from 9/4 to 1 with increasing neutron energy.[19] The effect of intermolecular forces upon the $1 \rightarrow 0$ transition will be much less important, for even with $E = 0$ the molecule has a recoil energy of the order of $h\nu$.

If the *ortho*-scattering cross section consisted only of the elastic cross section, the ratio of the *ortho*- to the *para*-scattering would be independent of intermolecular forces, since the interaction between *ortho*-molecules is practically identical with the interaction between *para*-molecules.[20] It is clear, therefore, that the effect of intermolecular forces will not be such as to alter our qualitative comparison between the *ortho*- and *para*-scattering cross sections. Unfortunately, however, the $1 \rightarrow 0$ cross section, with its different dependence upon the intermolecular forces, is added to the elastic orthoscattering cross section. It is necessary, therefore, to perform measurements at energies which are large compared with $h\nu$, so that intermolecular forces may be neglected, but yet are less than 0.023 ev. A measurement of the scattering cross sections of both ortho- and parahydrogen at some such energy would enable one to calculate the amplitudes a_1 and a_0, from which we may obtain r_0 and the free proton scattering cross

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[14] N. F. Mott and H. Jones, *The Theory of the Properties of Metals and Alloys* (Oxford, 1936).

[15] G. Bartholomé, Zeits. f. physik. Chemie **33**, 387 (1936).

[16] A. Farkas, *Orthohydrogen, Parahydrogen and Heavy Hydrogen* (Cambridge, 1935).

[17] The anomalous specific heat of solid orthohydrogen at very low temperatures indicates that, at these temperatures, rotation ceases to be free.

[18] J. C. McLennan and J. H. McLeod, Nature **123**, 160 (1929).

[19] A similar argument enables one to deduce Fermi's result of an increase in the scattering cross section of a proton bound to a heavy molecule by a factor of 4 over the corresponding value for a free proton, in the limiting case of zero neutron velocity.

[20] R. B. Scott and F. G. Brickwedde, Phys. Rev. **51**, 684 (1937).

section, thus permitting a check of the consistency of the whole theory.

Note added in proof: Recently published experiments by J. Halpern, I. Estermann, O. C. Simpson and O. Stern, Phys. Rev. **52**, 142 (1937) indicate that the scattering cross section of *ortho*-H_2 for liquid-air neutrons is much larger than the corresponding *para*-H_2 scattering cross section. This proves conclusively that the singlet state of the deuteron is virtual.

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Statistics and Nuclear Reactions

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It is possible to apply statistical methods to the calculation of nuclear processes provided that the energies involved are large in comparison with the lowest excitation energies of nuclei. Expressions are obtained for the emission probability of neutrons or charged particles by highly excited heavy nuclei. These expressions are built up in a similar way to the formula for the probability of evaporation of a particle from a body at low temperatures. In applying it to the impact of high energy neutrons on heavy nuclei, the mean energy loss per impact turns out to be $E[1-2(a/E)^{\frac{1}{2}}]$ where E is the energy of the incident neutrons and a is dependent on the nuclear structure; we can put approximately $a \sim 0.05$–0.2 MV. The energy distribution of the scattered neutrons is approximately a Maxwellian one with a mean energy of $2(aE)^{\frac{1}{2}}$.

I

The application of quantum mechanics to the calculation of nuclear reactions in heavy nuclei gives rise to extremely complicated expressions which cannot be treated by ordinary methods, since there is no approximate solution for this complex many-body problem on account of the intense interaction between the constituents of atomic nuclei. On the other hand Bohr[1] has pointed out that just the extreme facility of energy exchange gives rise to a characteristic simplification of the course of every nuclear process initiated by a collision between a particle or a light quantum and a nucleus. It consists in the possibility of dividing the process into two well-separated stages. The first is the formation of a compound nucleus in a well-defined state in which the incident energy is shared among all the constituents, the second is the disintegration of that compound system, which can be treated as quite independent of the first stage of the process. This conception has been extremely fruitful in the treatment of all kinds of nuclear reactions.[2] Qualitative statistical conclusions about the energy exchange between the nuclear constituents in the compound state have led to simple explanations of many characteristic features of nuclear reactions. In particular the use of thermodynamical analogies has proved very convenient for describing the general trend of nuclear processes. The energy stored in the compound nucleus can in fact be compared with the heat energy of a solid body or a liquid, and, as first emphasized by Frenkel,[3] the subsequent expulsion of particles is analogous to an evaporation process.[4]

In this note an attempt is made to apply statistical methods in a more quantitative way to nuclear processes in which heavy nuclei are involved and become highly excited as, for example, in the case of the collision of very fast neutrons with heavy nuclei. The individual properties of the separate nuclear quantum states are then of no interest, on account of the extremely small distance between the energy levels of highly excited heavy nuclei; it is thus possible to obtain statistical information on the behavior of these nuclei by averaging over many quantum states

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[1] N. Bohr, Nature **137**, 344 (1936); N. Bohr, Science (1937), in print.

[2] A comprehensive account of the application of the ideas in question to nuclear phenomena will be given in a paper by Bohr and Kalckar to appear shortly in the Proceedings of the Danish Academy.

[3] I. Frenkel, Sov. Phys. **9**, 533 (1936).

[4] A general discussion of the application of thermodynamical conceptions to nuclear processes can be found in the paper by Bohr, Science, reference 1.