Neutron Scattering in Ortho- and Parahydrogen

MORTON HAMERMESH
New York University, University Heights, New York, New York

AND

JULIAN SCHWINGER
Harvard University, Cambridge, Massachusetts

The cross section for the scattering of cold neutrons by parahydrogen is sensitive to the range of the forces in the triplet state. To facilitate the determination of the range from such measurements, expressions have been obtained for the dependence of the ortho and para cross sections on neutron energy and hydrogen temperature. The interpretation of transmission measurements is complicated by the existence of radiative capture, which is comparable in importance to scattering in parahydrogen. The different energy dependence of the two processes should permit an accurate determination of the individual cross sections.

SEVERAL papers[1] have emphasized the importance of measurements of neutron scattering in gaseous ortho- and parahydrogen, as a means for obtaining accurate information concerning the range of nuclear forces. Preliminary experiments were performed by Alvarez and Pitzer,[2] but with insufficient precision for this purpose.* In anticipation of more accurate experiments, a letter to *The Physical Review*[3] presents curves showing the dependence of the ortho- and parahydrogen cross sections on the range of the nuclear forces and the free-proton cross section. These curves must be corrected for three reasons:

1. The calculation of the triplet amplitude, a_1, was based on the formula: $a_1 = -(1+\alpha r_0)^{\frac{1}{2}}/\alpha$, where $\alpha = [ME_0/\hbar^2]^{\frac{1}{2}}$, E_0 is the binding energy of the deuteron, and r_0 is the range of a rectangular potential well interaction. This expression is an approximate one, whose validity is restricted to ranges that are small in comparison with $1/\alpha = 4.35\times 10^{-13}$ cm. This approximation may lead to errors of as much as 1×10^{-13} cm in the range deduced from the observed para scattering cross section.

2. The curves are based on equations given by Schwinger[4] for the cross sections at a hydrogen gas temperature $T = 20°$K, and neutron energy $E = kT$. The constants in these equations were obtained by an approximate procedure and are in error by a few percent.

3. The underlying theory has been based on a rigid-rotator model for the H_2 molecule. This approximation introduces small but not negligible errors.**

Accurate calculations of σ_{para} and σ_{ortho} have been made using essentially the same procedure as for D_2,[5] but modified to include the effect of zero-point oscillations. The only change in the theory is the replacement of $j_L(kr_e)$ by $\langle j_L(kr)\rangle_{\text{Av}}$, the mean value of $j_L(kr)$ in the lowest vibrational state. In the calculation of this average we have performed an expansion in powers of $y = r - r_e/r_e$ and dropped terms beyond $\bar{y}$ and $\langle y^2\rangle_{\text{Av}}$. It should be noted that $\bar{y}$ must be included since the zero-point vibrations are anharmonic. $\langle y^2\rangle_{\text{Av}}$ is obtained directly from the harmonic oscillator model which gives $\langle y^2\rangle_{\text{Av}} = \frac{1}{2}E_1/\hbar\omega$ where $\hbar\omega(=0.513$ ev) is the excitation energy of the first vibrational state, and $E_1(=0.0147$ ev) is the energy of the $J=1$ rotational level of H_2. A numerical value of $\bar{y}$ can be obtained by considering the dependence of the rotational energy levels on the vibration quantum number. One need only compare $r_e = 0.7414\times 10^{-8}$ cm, the equilibrium separation, with $r_0 = 0.7506$

[1] J. Schwinger and E. Teller, Phys. Rev. **52**, 286 (1937); J. Schwinger, Phys. Rev. **58**, 1004 (1940).
[2] L. W. Alvarez and K. S. Pitzer, Phys. Rev. **58**, 1003 (1940).
* Recent experiments at Los Alamos have shown that ortho-para conversion during the course of the experiments is a serious source of error. The data of these investigators, which differs considerably from that of Alvarez and Pitzer, will be published shortly.
[3] C. S. Wu, L. J. Rainwater, W. W. Havens, Jr., and J. R. Dunning, Phys. Rev. **69**, 236 (1946).
[4] J. Schwinger, Phys. Rev. **58**, 1004 (1940).
** We are indebted to E. Teller for discussions of this point.
[5] M. Hamermesh and J. Schwinger, Phys. Rev. **69**, 145 (1946).

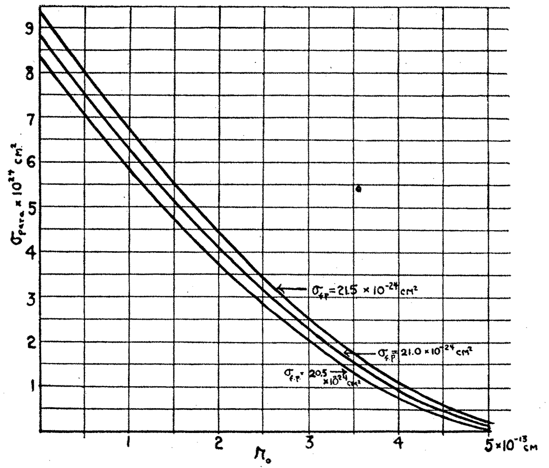

FIG. 1. Dependence of parahydrogen cross section on the range of nuclear forces. (Gas temperature $T=20°$K, neutron energy $E=kT$.)

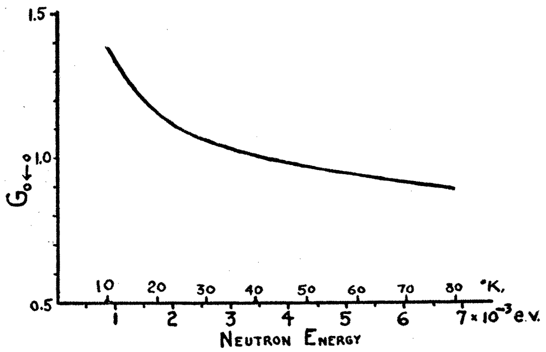

FIG. 3. Parahydrogen cross section as a function of neutron energy, omitting amplitude factors (cf. Eq. (1)). (Gas temperature = 20°K.)

$\times10^{-8}$ cm, which is defined by $1/r_0^2=\langle 1/r^2\rangle_{Av}\simeq 1/r_e^2(1-2\bar{y}+3\langle y^2\rangle_{Av})$. This procedure gives $\bar{y}=0.0337$, $\langle y^2\rangle_{Av}=0.0143$.

The cross sections for the various transitions have been expanded in powers of E/E_1, where E is the neutron energy. The thermal averages of the cross sections for the various transitions are:

$$\sigma_{0\leftarrow0}=\frac{16\pi}{9}(3a_1+a_0)^2G_{0\leftarrow0},$$

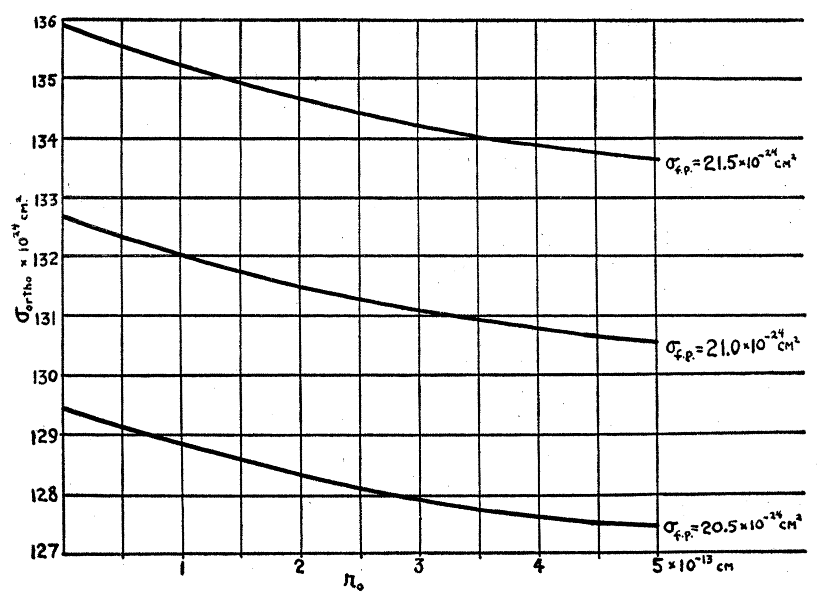

FIG. 2. Dependence of orthohydrogen cross section on the range of nuclear forces. (Gas temperature $T=20°$K, neutron energy $E=kT$.)

$$G_{0\leftarrow 0}=\frac{1}{\pi^{\frac{1}{2}}}\frac{\exp(-x^2)}{x}+\left(1+\frac{1}{2x^2}\right)\Phi(x)-\frac{8}{27}(1+2\bar{y}+\langle y^2\rangle_{\mathrm{Av}})\frac{E}{E_1}\left[\frac{1}{\pi^{\frac{1}{2}}}\left(1+\frac{5}{2x^2}\right)\frac{\exp(-x^2)}{x}+\left(1+\frac{3}{x^2}+\frac{3}{4x^4}\right)\Phi(x)\right]+\frac{512}{(81)(135)}\left(1+4\bar{y}+\frac{5}{2}\{\bar{y}\}^2+\frac{7}{2}\langle y^2\rangle_{\mathrm{Av}}\right)\left(\frac{E}{E_1}\right)^2$$
$$\times\left[\frac{1}{\pi^{\frac{1}{2}}}\left(1+\frac{7}{x^2}+\frac{33}{4x^4}\right)\frac{\exp(-x^2)}{x}+\left(1+\frac{15}{2x^2}+\frac{54}{4x^4}+\frac{15}{8x^6}\right)\Phi(x)\right],$$

$$\sigma_{1\leftarrow 1}=\frac{16\pi}{9}[(3a_1+a_0)^2+2(a_1-a_0)^2]G_{1\leftarrow 1},$$

where $G_{1\leftarrow 1}$ is identical with $G_{0\leftarrow 0}$, except that the factor preceding $(E/E_1)^2$ is replaced by

$$\frac{1024}{(81)(225)}\left(1+4\bar{y}+\frac{11}{4}\{\bar{y}\}^2+\frac{13}{4}\langle y^2\rangle_{\mathrm{Av}}\right);$$

$$\sigma_{0\leftarrow 1}=\frac{64\pi}{9}(a_1-a_0)^2\left(\frac{E_1}{E}\right)^{\frac{1}{2}}\left[0.01982(1+1.73\bar{y}-0.15\langle y^2\rangle_{\mathrm{Av}})+0.02719(1+1.23\bar{y}-0.664\langle y^2\rangle_{\mathrm{Av}})\frac{E}{E_1}\left(1+\frac{3kT}{4E}\right)+0.000264\left(\frac{E}{E_1}\right)^2\left\{1+\frac{5}{2}\frac{kT}{E}+\frac{15}{16}\left(\frac{kT}{E}\right)^2\right\}\right], \quad (1)$$

$a_{1,0}$ are the triplet and singlet amplitudes, T is the temperature of the gas in °K, $x^2=2E/kT$ and

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

For $T=20$°K and $E=kT$ we obtain:

$$\sigma_{0\leftarrow 0}=6.444(3a_1+a_0)^2,\quad \sigma_{1\leftarrow 1}=6.450[(3a_1+a_0)^2+2(a_1-a_0)^2],\quad \sigma_{0\leftarrow 1}=1.753(a_1-a_0)^2,$$

so that

$$\sigma_{\mathrm{para}}=6.444(3a_1+a_0)^2,\quad \sigma_{\mathrm{ortho}}=6.450(3a_1+a_0)^2+14.653(a_1-a_0)^2.$$

The dependence of a_1 on r_0 was computed for a rectangular potential well, using the expansion given by Kittel and Breit.[6] Then a_0 was calculated for several values of the free-proton cross section, $\sigma_{\mathrm{f.p.}}$ The results are shown in Figs. 1 and 2.

The parahydrogen scattering cross section is obtained from transmission measurements which determine only the total cross section of the molecule including the radiative capture cross section. From the measured value of the mean lifetime of slow neutrons in water,[7] the capture cross section of the hydrogen molecule for 20° neutrons is calculated to be 2.5×10^{-24} cm², which is approximately equal to the parahydrogen scattering cross section corresponding to the range of nuclear forces customarily assumed in current theory, ($r_0=2.8\times 10^{-13}$ cm). Transmission experiments at several neutron energies will enable a separate determination of the scattering and capture cross sections since they differ in their energy dependence. The capture cross section follows a $1/v$ law, whereas the scattering cross section varies with energy as shown in Fig. 3. Thus, for example, the capture cross section for 80° neutrons is one-half of that for 20° neutrons, whereas the scattering cross section at the higher neutron temperature is only 25 percent less than that at 20°.

---

[6] C. Kittel and G. Breit, Phys. Rev. 56, 744 (1939).
[7] J. H. Manley, L. J. Haworth, and E. A. Luebke, Phys. Rev. 61, 152 (1942).