The Scattering of Slow Neutrons by Bound Protons
II. Harmonic Binding—Neutrons of Zero Energy

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The cross section for scattering of very slow neutrons by elastically bound protons is calculated by means of the method described in the preceding paper. The results are expressed in terms of a correction factor to be applied to Fermi's factor 4. According to Eq. (5) of the present paper this correction factor is $1+16aJ/\pi^{\frac{1}{2}}$ with J defined by Eq. (6) which is suitable for numerical work. The results of numerical calculations for the effects of anisotropy in molecules with axial symmetry are presented in Fig. 1 which has to be used with Eqs. (6.2), (6.3) of the text. For scattering by the H_2O molecule the correction to be applied to Fermi's result is only ~.3 percent of the final value. Fermi's method is very accurate in this case.

1. INTRODUCTION AND NOTATION

THE method of the preceding paper[1] is here applied to the calculation of the scattering cross section for neutrons having zero energy from protons bound in molecules by simple harmonic oscillator forces. The F transformation of the background term[1] is used to reduce the computation of the background to the evaluation of a definite integral by numerical quadrature. It is found, in agreement with order of magnitude considerations discussed in the preceding paper, that Fermi's factor 4, representing the increase in the scattering cross section caused by chemical binding, is accurate to within a few tenths of a percent, and the value of the correction factor is worked out in the last section of this paper. The notation is as in[1] with the addition of the following symbols:

a = constant having dimensions of length defined so that radial wave function is of the form const.$(1+a/r)$ for small proton-neutron distances r.

$\alpha_x, \alpha_y, \alpha_z$ = elastic binding constants of proton in molecule.

$\xi=x/\alpha_x;\ \eta=y/\alpha_y;\ \zeta=z/\alpha_z.$

$H_n(\xi)=(-)^n e^{\xi^2}(d/d\xi)^n e^{-\xi^2}$ = Hermite polynomial of degree n.

$q_x=\exp(-2\tau/\alpha_x^2);\ q_y=\exp(-2\tau/\alpha_y^2);\ q_z=\exp(-2\tau/\alpha_z^2).$

$4T_x=4\tau+\alpha_x^2(1-q_x^2)$; etc.

$Q=\frac{1}{2}+(1-e^{-\xi})/2\xi.$

The potential energy binding the proton in the molecule is taken as

$$U(\mathbf{r}_\pi)=\frac{\hbar^2}{2M}\left(\frac{x_\pi^2}{\alpha_x^4}+\frac{y_\pi^2}{\alpha_y^4}+\frac{z_\pi^2}{\alpha_z^4}\right), \tag{1}$$

for which the characteristic frequencies are

$$2\pi\nu_x=\hbar/M\alpha_x^2,\quad \text{etc.}, \tag{1.1}$$

so that the energy levels are given by

$$E_s=[(2n_x+1)/\alpha_x^2+(2n_y+1)/\alpha_y^2+(2n_z+1)/\alpha_z^2]\hbar^2/2M \tag{1.2}$$

and the proton eigenfunctions by[2]

$$u_s(\mathbf{r})=\prod[\alpha_x 2^{n_x} n_x!\pi^{\frac{1}{2}}]^{-\frac{1}{2}}H_{n_x}(x/\alpha_x)\exp(-x^2/2\alpha_x^2) \tag{1.3}$$

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[1] G. Breit, Phys Rev 71, 215 (1947). This will be referred to as I in the text. Formulas occurring in I will be referred to by prefixing the roman numeral I ahead of the number of the formula.

[2] In this paper the symbol Π always stands for the product over x, y, z.

with

$$H_n(\xi) = \text{Hermite polynomial.} \tag{1.4}$$

The following notation will be used

$$\xi = x/\alpha_x, \quad \eta = y/\alpha_y, \quad \zeta = z/\alpha_z. \tag{1.5}$$

The complete wave function of the system is given by Eq. (I, 6) with f given by (I, 5) and B by (I, 5′).

2. CALCULATION OF THE BACKGROUND

Equation (I, 5′) can be evaluated by means of the transformation (I, 8.8). The first approximation to f is ψ_0, and the solution of Eq. (I, 5) by iteration leads, therefore, to an integral in which f is replaced by ψ_0 in (I, 5′). In the present case, with $E=E_0$ and u_0 given by (1.3), one can replace ψ_0 by

$$f = C\exp[-(\xi^2+\eta^2+\zeta^2)/2]. \tag{2}$$

Putting $H_n(\xi) = (-)^n \exp(\xi^2)(d^n/d\xi^n)\exp(-\xi^2)$ in (1.3) and substituting into Eq. (I, 8.6) one has

$$F(\mathbf{r}, \mathbf{r}') = \sum\nolimits_{n_x, n_y, n_z} \prod \left\{ \frac{\exp[(\xi^2+\xi'^2)/2]}{\alpha_x 2^{n_x} n_x! \pi^{\frac{1}{2}}} (\partial^{2n_x}/\partial\xi^{n_x}\partial\xi'^{n_x}) \cdot \exp[-\xi^2-\xi'^2-2n_x\tau/\alpha_x^2] \right\}. \tag{2.1}$$

The summations in (2.1) can be performed by expressing the exponentials containing $-\xi^2-\xi'^2$ by means of Fourier-integrals. One obtains

$$\exp(-\xi^2) = \frac{1}{2\pi^{\frac{1}{2}}} \int_{-\infty}^{\infty} \exp(i\omega\xi - \omega^2/4) d\omega,$$

and thus

$$\exp(-\xi^2-\xi'^2) = \frac{1}{4\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp[i(\omega\xi+\omega'\xi') - (\omega^2+\omega'^2)/4] d\omega d\omega'.$$

Putting

$$q_x = \exp(-2\tau/\alpha_x^2), \quad q_y = \exp(-2\tau/\alpha_y^2), \quad q_z = \exp(-2\tau/\alpha_z^2), \tag{2.2}$$

one obtains the auxiliary formula

$$\sum_{n=0}^{\infty} \exp(-2n\tau/\alpha^2)(\partial^2/\partial\xi\partial\xi')^n \exp(-\xi^2-\xi'^2)/2^n(n!) = F_x$$

$$= \frac{1}{4\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \sum_{n=0}^{\infty} \frac{(q/2)^n}{n!} (-\omega\omega')^n \exp[i(\omega\xi+\omega'\xi') - (\omega^2+\omega'^2)/4] d\omega d\omega' \tag{2.3}$$

$$= \frac{1}{4\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp\{i(\omega\xi+\omega'\xi') - \tfrac{1}{4}(\omega^2+\omega'^2+2q\omega\omega')\} d\omega d\omega'.$$

The subscript x has been dropped for α, n, and q so as to simplify the notation.

The integrations over ω, ω' can be carried out by transforming the homogeneous quadratic form in ω, ω' in the exponent of the last form of (2.3) to a diagonal form. It is thus found that

$$F_x = (1-q_x^2)^{-\frac{1}{2}} \exp\{-[\xi^2+\xi'^2-2q_x\xi\xi']/(1-q_x^2)\}. \tag{2.4}$$

Comparing (2.1) and (2.3) one sees that

$$F = \prod \exp[(\xi^2+\xi'^2)/2] F_x/(\pi^{\frac{1}{2}}\alpha_x),$$

so that

$$F(\mathbf{r}, \mathbf{r}') = \frac{1}{\pi^{\frac{3}{2}}} \prod \frac{\exp\{(\xi^2+\xi'^2)/2 - (\xi^2+\xi'^2-2q_x\xi\xi')/(1-q_x^2)\}}{\alpha_x(1-q_x^2)^{\frac{1}{2}}}. \tag{3}$$

It follows from Eq. (I, 8.8), on noting that $E=E_0$, and thus setting $\sigma=0$, that

$$\sum_0^\infty u_s(\mathbf{r}_\pi)u_s^*(\mathbf{r}')\frac{2\exp(i\kappa_s|\mathbf{r}_\nu-\mathbf{r}'|)-1}{|\mathbf{r}_\nu-\mathbf{r}'|}=\frac{1}{\pi^{\frac{1}{2}}}\int_0^\infty \exp(-|\mathbf{r}_\nu-\mathbf{r}'|^2/4\tau)F(\mathbf{r}_\pi,\mathbf{r}')d\tau-\delta(\mathbf{r}_\pi-\mathbf{r}')/|\mathbf{r}_\nu-\mathbf{r}'|$$

$$=(1/\pi^{\frac{1}{2}})\int_0^\infty\left[\prod\frac{\exp\{-(\xi_\pi^2+\xi'^2)(1+q_x^2)/2(1-q_x^2)+2q_x\xi_\pi\xi'/(1-q_x^2)\}}{\pi^{\frac{1}{2}}\alpha_x(1-q_x^2)^{\frac{1}{2}}}-\frac{\delta(\mathbf{r}_\pi-\mathbf{r}')}{2}\right]$$

$$\times\frac{\exp(-|\mathbf{r}_\nu-\mathbf{r}'|^2/4\tau)}{\tau^{\frac{1}{2}}}d\tau. \quad (3.1)$$

where $1/|\mathbf{r}_\nu-\mathbf{r}'|$ is represented as

$$(1/2\pi^{\frac{1}{2}})\int_0^\infty[\exp(-|\mathbf{r}_\nu-\mathbf{r}'|^2/4\tau)/\tau^{\frac{1}{2}}]d\tau.$$

Putting (3.1) and (2) into (I, 5′) and performing the integration over $\mathbf{r}'$ it is found that

$$B(\mathbf{r}_\pi,\mathbf{r}_\nu)=(8/\pi^{\frac{1}{2}})f(\mathbf{r}_\pi)\int_0^\infty\{\prod(4T_x)^{-\frac{1}{2}}\exp\{-(x_\nu-q_xx_\pi)^2/4T_x\}-\exp(-|\mathbf{r}_\nu-\mathbf{r}_\pi|^2/8\tau)/(8\tau)^{\frac{3}{2}}\}d\tau \quad (3.2)$$

with

$$4T_x=4\tau+\alpha_x^2(1-q_x^2). \quad (3.25)$$

The limit of (3.2) as $\mathbf{r}_\nu\rightarrow\mathbf{r}_\pi$ is independent of the angle $(\mathbf{r}_\nu, \mathbf{r}_\pi)$ so that the averaging process required for Eq. (I, 5) reduces to

$$B(\mathbf{r}_\pi,\mathbf{r}_\pi)=(8/\pi^{\frac{1}{2}})f(\mathbf{r}_\pi)\int_0^\infty\{\prod(4T_x)^{-\frac{1}{2}}\exp\{-(1-q_x^2)x_\pi^2/4T_x\}-(8\tau)^{-\frac{3}{2}}\}d\tau. \quad (4)$$

In the calculation leading to this equation it was assumed that f can be replaced by a constant multiple of u_0. This is justifiable only if the molecule is originally in its lowest state, if the neutrons have a very low energy and if a is sufficiently small to make aB small compared with f. The latter assumption is justified *a posteriori* by the smallenss of the effect of B.

3. THE SCATTERING CROSS SECTION

For zero energy neutrons the amplitude of the scattered wave is proportional to

$$\int u_0^*(\mathbf{r}')f(\mathbf{r}')d\mathbf{r}'.$$

f is given by (I, 5) with B from (4), in which f is taken as $f=\psi_0=u_0$.

Thus,

$$\int u_0^*(\mathbf{r}')f(\mathbf{r}')d\mathbf{r}'=\int|u_0(\mathbf{r}')|^2\left(1+8a/\pi^{\frac{1}{2}}\int_{\tau=0}^\infty\{\quad\}d\tau\right)d\mathbf{r}'=1+(8a/\pi^{\frac{1}{2}})J(\alpha_x,\alpha_y,\alpha_z). \quad (5)$$

The square of this factor, *i.e.*, the quantity $1+16aJ/\pi^{\frac{1}{2}}$, is the correction factor for the cross section. The quantity J occurring in this formula is given by

$$J(\alpha_x,\alpha_y,\alpha_z)=\int_0^\infty\{\prod[4\tau+2\alpha_x^2(1-q_x)]^{-\frac{1}{2}}-8\tau^{-\frac{3}{2}}\}d\tau \quad (6)$$

as is found by performing the integration over $\mathbf{r}'$.

The integral occurring in Eq. (6) has been evaluated numerically in a few cases, and the results

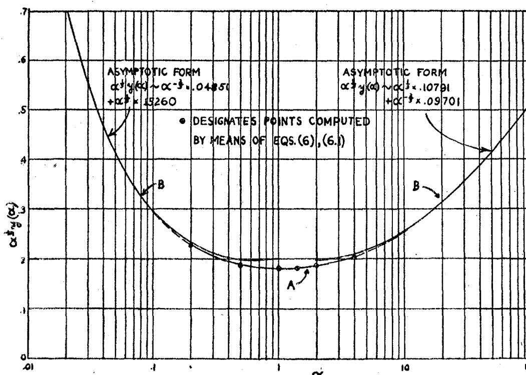

FIG. 1. Plot of $\alpha^{\frac{1}{3}}I(\alpha)$ *vs.* α. Curve A is drawn through points computed by means of Eqs. (6), (6.1). Curves B are the asymptotic forms given by Eqs. (6.3), (6.4). The ordinate of the graph can be used for the computation of the correction factor of Eq. (5) by means of Eqs. (6.1), (6.2) with α defined by Eq. (6.3).

are plotted in Fig. 1. In this figure the ordinate is the quantity

$$\alpha^{\frac{1}{3}}I(\alpha)=\alpha^{\frac{1}{3}}J(1,\,1,\,\alpha). \tag{6.1}$$

The asymptotic forms of this quantity for large and for small α are indicated on the graph, and their derivation is described in the Appendix. By means of the graph one can evaluate J for any harmonic oscillator with axial symmetry by means of the following formula

$$J(\alpha_x,\,\alpha_x,\,\alpha_z)=I(\alpha_z/\alpha_x)/\alpha_x. \tag{6.2}$$

The ordinate plotted is

$$\alpha^{\frac{1}{3}}I(\alpha)=\alpha_x^{\frac{2}{3}}\alpha_z^{\frac{1}{3}}J(\alpha_x,\,\alpha_x,\,\alpha_z);\quad \alpha=\alpha_z/\alpha_x. \tag{6.3}$$

The asymptotic forms of J are

$$\begin{aligned} J(\alpha_x,\,\alpha_x,\,\alpha_z)&\sim I_1/\alpha_z+2^{\frac{1}{3}}I_2/\alpha_x=0.0485/\alpha_z+0.1526/\alpha_x;\quad (\alpha\ll 1);\\ J(\alpha_x,\,\alpha_x,\,\alpha_z)&\sim I_2/\alpha_x+2I_1/\alpha_z=0.1079/\alpha_x+0.0970/\alpha_z;\quad (\alpha\gg 1), \end{aligned} \tag{6.4}$$

where

$$I_1=(1/16)\int_0^\infty (Q^{-\frac{1}{2}}-1)\,\xi^{-\frac{4}{3}}d\xi; \tag{6.5}$$

$$I_2=(1/16)\int_0^\infty (Q^{-1}-1)\,\xi^{-\frac{4}{3}}d\xi; \tag{6.6}$$

$$Q=\tfrac{1}{2}+(1-e^{-\xi})/2\xi. \tag{6.7}$$

The two asymptotic branches extrapolate to nearly the same value for an harmonic oscillator with spherical symmetry and agree rather well with values computed directly by means of Eqs. (6), (6.1).

4. APPLICATION TO THE WATER MOLECULE

In order to apply the present theory, the mass of the proton will be considered to be small in comparison with the mass of the molecule. One has then

$$\alpha=\frac{6.39\times 10^{-10}\text{ cm}}{[(h\nu)_{\text{ev}}]^{\frac{1}{2}}},$$

where the subscript ev indicates that the electron volt is the unit of energy. For H_2O Slater[3] lists the following frequencies:

$h\nu$ (ev) = 0.443 0.462 0.248

[3] J. C. Slater, *Introduction to Chemical Physics* (McGraw-Hill Book Company, Inc., New York, 1939), p. 146.

which correspond to

$$\alpha \quad (\text{cm}) = 9.6\times10^{-10} \qquad 9.4\times10^{-10} \qquad 1.28\times10^{-9}.$$

The values given by Herzberg[4] are in essential agreement with the above. The lower frequency and, therefore, the higher α corresponds to a vibration roughly at right angles to the other two. The value of α_z/α_x is 1.35. According to Fig. 1 the anisotropy has no important effect in this case. The values of a for singlet and triplet scattering are $a_1 = 1.92\times10^{-12}$ cm; $a_3 = -0.584\times10^{-12}$ cm. For singlet scattering the correction factor is

$$1+0.82\frac{1.92\times10^{-12}}{1.06\times10^{-9}}=1.0015.$$

The square of this factor matters for the scattered intensity. There is thus a correction of about 0.3 percent for the expected scattered intensity in the singlet state. Since slow neutrons are mostly scattered in the singlet state, this is the approximate magnitude of the correction for very slow neutrons.

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APPENDIX

Asymptotic Forms for $I(\alpha)$

The consideration will be carried out for $\alpha \ll 1$. It follows from Eqs. (6), (6.1) that

$$I(\alpha)=J(1,1,\alpha)=\int_0^\infty \{[\tfrac{1}{2}+(1/4\tau)(1-e^{-2\tau})]^{-1}[\tfrac{1}{2}+(\alpha^2/4\tau)(1-\exp(-2\tau/\alpha^2))]^{-\frac{1}{2}}-1\}(8\tau)^{-\frac{1}{2}}d\tau. \quad (\text{A, }1)$$

The integral will be represented as

$$I(\alpha)=A(\alpha)+B(\alpha), \quad (\text{A, }1.1)$$

with

$$A(\alpha)=\int_0^{N\alpha^2}\cdots d\tau, \quad B(\alpha)=\int_{N\alpha^2}^\infty\cdots d\tau, \quad (\text{A, }1.2)$$

where the integrand is the same as in (A, 1). The number N is chosen so as to satisfy the requirement

$$N\gg1, \quad N\alpha^2\ll1. \quad (\text{A, }1.3)$$

In the limit $\alpha=0$ both of these requirements can be satisfied perfectly in the sense that N can be made to approach ∞ while $N\alpha^2$ approaches zero. Integral $A(\alpha)$ can be transformed through the introduction of the variable

$$\xi=2\tau/\alpha. \quad (\text{A, }1.4)$$

On account of the second condition (A, 1.3) the quantity $e^{-2\tau}$ can be expanded by Taylor's series, and the contributions to the integral form a rapidly converging series. Keeping the first two terms of the expansion one has

$$A(\alpha)=\int_0^{2N}(1/16\alpha)\{(1+\alpha^2\xi/4)[\tfrac{1}{2}+(1-e^{-\xi})/2\xi]^{-\frac{1}{2}}-1\}\xi^{-\frac{1}{2}}d\xi. \quad (\text{A, }2)$$

The discussion of the contribution of the term in $\alpha^2\xi/4$ will be postponed. It will be shown later that its contribution to A approaches zero as α approaches zero. Only terms that do not approach

[4] G. Herzberg, *Infrared and Raman Spectra* (D. Van Nostrand Company, Inc., New York, 1945), p. 161.

zero with α will be kept. One has thus

$$A(\alpha)\sim\frac{1}{16\alpha}\left(\int_0^{\infty}-\int_{2N}^{\infty}\right)\left\{\left[\frac{1}{2}+\frac{1-e^{-\xi}}{2\xi}\right]^{-\frac{1}{2}}-1\right\}\xi^{-\frac{3}{2}}d\xi. \qquad \text{(A, 2.1)}$$

The first integral will be kept in the above form. The second can be estimated as follows

$$-\frac{1}{16\alpha}\int_{2N}^{\infty}(2^{\frac{1}{2}}-1-2^{-\frac{1}{2}}\xi^{-1})\xi^{-\frac{3}{2}}d\xi\cong-\frac{2^{\frac{1}{2}}-1}{8\alpha(2N)^{\frac{1}{2}}}. \qquad \text{(A, 2.2)}$$

The right side of (A, 2.2) becomes infinite for $\alpha=0$ on account of the second condition (A, 1.3). The omitted terms, however, are of order $N^{-\frac{3}{2}}\alpha^{-1}$. They can be made to approach zero by requiring

$$N^3\alpha^2\gg 1. \qquad \text{(A, 2.3)}$$

This means that N should be made to approach ∞ more strongly than $\alpha^{-\frac{2}{3}}$ which can be done consistently with the second condition (A, 1.3). Any dependence between α^{-2} and $\alpha^{-\frac{2}{3}}$ is satisfactory. With this additional restriction on N it suffices to consider only the right side of (A, 2.2).

In the evaluation of B one makes use of the smallness of $\alpha^2/\tau\ll 1/N$. At the lower limit of integration

$$\left[\frac{1}{2}+\frac{\alpha^2}{4\tau}(1-\exp(-2\tau/\alpha^2))\right]^{-\frac{1}{2}}_{\tau=N\alpha^2}\cong 2^{\frac{1}{2}}\left(1-\frac{1}{4N}+\cdots\right)\cong 2^{\frac{1}{2}}. \qquad \text{(A, 3)}$$

The omission of further terms here is justifiable because B turns out to be of the order $1/(N\alpha^2)^{\frac{1}{2}}$ so that (A, 2.3) will make negligible the term in $1/(4N)$ which has just been omitted. One obtains by means of (A, 3)

$$B(\alpha)\sim\frac{1}{16}\left(\int_0^{\infty}-\int_0^{N\alpha^2}\right)\left\{\left[\frac{1}{2}+\frac{1}{4\tau}(1-e^{-2\tau})-1\right]^{-1}-1\right\}\tau^{-\frac{3}{2}}d\tau+\frac{2-2^{\frac{1}{2}}}{16(N\alpha^2)^{\frac{1}{2}}}. \qquad \text{(A, 3.1)}$$

The right side of the above relation contains $\int_0^{N\alpha^2}$. Its contribution is estimated by expanding the brace in a Taylor series. It is found to be $-(N\alpha^2)^{\frac{1}{2}}/16$ which vanishes on account of the second condition (A, 1.3).

Adding B to A the last term in (A, 3.1) is canceled by (A, 2.2). The integral I_1 of Eq. (6.5) of the text arises from (A, 2.1), the integral I_2 of Eq. (6.6) from (A, 3.1) and one obtains

$$I(\alpha)\sim\frac{I_1(\alpha)}{\alpha}+2^{\frac{1}{2}}I_2(\alpha),$$

which is equivalent to

$$J(\alpha_x,\,\alpha_x\alpha_z)\sim I_1/\alpha_z+2^{\frac{1}{2}}I_2/\alpha_x$$

on account of Eq. (6.2). This, together with numerical evaluations of I_1, I_2 gives the first line of Eq. (6.4).

It remains to explain the legitimacy of neglecting the term in $\alpha^2\xi/4$ in Eq. (A, 2). This term contributes to $I(\alpha)$ the amount

$$\frac{\alpha}{64}\int_0^{2N}\xi^{-\frac{1}{2}}\left[\frac{1}{2}+\frac{1-e^{-\xi}}{2\xi}\right]^{-\frac{1}{2}}d\xi.$$

The integral converges near $\xi=0$. The [ ] has the value 1 for $\xi=0$, and its value decreases to about $\frac{1}{2}$ for large ξ. The contribution is, therefore, less than

$$(2^{\frac{1}{2}}\alpha/64)\int_0^{2N}\xi^{-\frac{1}{2}}d\xi=(2^{\frac{1}{2}}\alpha/64)(2N)^{\frac{1}{2}}$$

which vanishes as $N\alpha^2$. The explanation of the first line of Eq. (6.4) has now been completed. The second line is obtained by very similar reasoning.