THE
PHYSICAL REVIEW
A journal of experimental and theoretical physics established by E. L. Nichols in 1893

SECOND SERIES, VOL. 71, NO. 4 FEBRUARY 15, 1947

The Scattering of Slow Neutrons by Bound Protons

I. Methods of Calculation

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(Received November 29, 1946)

The mathematical problem of the scattering of slow neutrons by chemically bound protons is stated in terms of a boundary condition and its equivalent integral equation. By means of the latter it is possible to calculate corrections to the results of Fermi which can be considered as the first approximation to the more accurate equations. The method is applied to free protons, and it is shown how the well-known results for this case are obtained from the more general equations. This special case allows also an estimate (10^{-3}) of the order of the corrections in the case of chemically bound protons in agreement with general estimates in connection with Eq. (8.4) of Section 7 of the present paper and the application to harmonic oscillator binding made in the succeeding paper jointly with P. R. Zilsel. The corrections discussed are greater than the inaccuracies of the boundary condition formulation which are of the order 10^{-5}.

1. INTRODUCTION

FERMI[1] has given a theory of the effect of chemical binding of protons on their scattering cross section for slow neutrons. At the time of Fermi's work there was no necessity of great accuracy, and his answer was generally considered to be good enough. The advance in experimental methods that has taken place since makes it desirable to be able to estimate theoretical effects more accurately than previously. The whole effect dealt with is of the order of a factor 4, and it is natural, therefore, to inquire into the accuracy of its estimates. Its knowledge is needed in the interpretation of experimental material on neutron-proton scattering in terms of effective neutron proton potentials, and the comparison of such potentials with corresponding quantities for other pairs of nuclear particles. As is well known, such a comparison is essential for the field theories of nuclear particles, and it has indicated in the past that the specifically nuclear interactions are essentially independent of the charge. It appeared advisable to be reasonably sure of the accuracy of the Fermi correction factor in this connection on account of its bearing on the fundamental problem of forces between nuclear particles. An additional incentive has been the large accumulation[2] of experimental material on the scattering of slow neutrons by solids which presents very similar mathematical problems. In this case, just as in the scattering of neutrons by protons, the nuclear properties can be described by quantities a which have the significance of intercepts on the axis

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[1] Enrico Fermi, Ricerca Scient. VII–II, 13 (1936). See Eqs. (71)–(103).

[2] Herbert L. Anderson, Enrico Fermi, Leona Marschall, paper E 1, Proc. Amer. Phys. Soc. Meeting at Chicago, June 20–22 (1946); W. H. Zinn, *idem*, paper E 2, Phys. Rev. 70, 102 (1946).

referring to the neutron-scattering nucleus distance in a graph of the product of this distance by the radial wave function. The quantity a has the significance of the amplitude of the scattered wave per unit intensity of the incident wave in a suitable normalization. The interactions of the scattered neutron with individual nuclear particles, matter in the problem of scattering of slow neutrons only insofar as they affect the intercepts a which are therefore important nuclear parameters. The close relationship of the present paper to the mathematical problem of determining these parameters added to the desirability of finding a systematic way for the calculation presented below.

The method consists of two steps: (a) the replacement of the wave equation in the region of the nuclear potential by a boundary condition Eq. (3); (b) the formulation of the boundary condition in terms of an integral equation, Eq. (5). The physical justification for the boundary condition is made in Section 3, and it is found that the errors caused by this replacement are negligible in comparison with all effects considered here. The conversion of the problem to an integral equation is made in Section 4. Fermi's approximation is discussed in Sections 5 and 6, and the reasons for undertaking the present calculation are gone into in these sections. In Section 7 the expressions for the "background" are transformed into forms more suitable for applications than the original. In Section 8, the method is illustrated by considering free protons and seeing how the well-known answer is verified consistently with the approximations made.

2. NOTATION

$\mathbf{r}_\pi = (x_\pi, y_\pi, z_\pi)$ = proton coordinates.

$\mathbf{r}_\nu = (x_\nu, y_\nu, z_\nu)$ = neutron coordinates.

$U = U(x_\pi, y_\pi, z_\pi)$ = potential energy of proton caused by molecular binding.

$\mathbf{r} = \mathbf{r}_\nu - \mathbf{r}_\pi = (x, y, z)$ = relative coordinates.

E_n = energy of proton in a molecule in nth excited state.

$u_n(\mathbf{r}_\pi)$ = characteristic function of proton in state E_n.

$\Delta_\nu = \partial^2/\partial x_\nu^2 + \partial^2/\partial y_\nu^2 + \partial^2/\partial z_\nu^2$.

$\Delta_\pi = \partial^2/\partial x_\pi^2 + \partial^2/\partial y_\pi^2 + \partial^2/\partial z_\pi^2$.

$\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$.

ψ = wave function of proton and neutron.

$g(r)$ = potential energy of proton in the field of the neutron; assumed to be a function of the distance $r = |\mathbf{r}|$ only.

E = energy of system.

M = proton mass; the mass of the neutron is assumed to be equal to the mass of the proton.

∇ = vector operator (gradient) with components $\partial/\partial x$, $\partial/\partial y$, $\partial/\partial z$. This is distinguished by suffixes ν, π to indicate replacement of relative by neutron or proton coordinates.

ρ = distance of the order of 3×10^{-13} cm beyond which the function g may be assumed to be zero.

a = intercept of tangent to graph of r times radial function for proton-neutron motion plotted against an axis of r. The intercept is by definition positive if tangent cuts axis of r to the left of origin.

$d\mathbf{r} = dxdydz$ = volume element in space x, y, z.

$d\mathbf{r}_\pi = dx_\pi dy_\pi dz_\pi$.

$d\mathbf{r}_\nu = dx_\nu dy_\nu dz_\nu$.

$\mathbf{R} = (X, Y, Z) = (1/2)(x_\pi + x_\nu, y_\pi + y_\nu, z_\pi + z_\nu)$ = center of mass coordinates.

$\langle A \rangle$ = angular average of any quantity A over directions of the vector $\mathbf{r}$. Equal weights to all solid angles are given in the average.

3. THE BOUNDARY CONDITION REPLACING THE PROTON-NEUTRON INTERACTION

The wave equation will be taken to be

$$E\psi = [-(\hbar^2/2M)(\Delta_\nu + \Delta_\pi) + U + g(r)]\psi \quad (1)$$

in the notation just explained. It is assumed that it is good enough to use one function $g(r)$ so that the discussion is applicable only to slow neutrons since otherwise one would have to bring in phase shifts for p and d waves which may correspond in general to other interaction potentials. The wave function ψ in the above equation is supposed to correspond to a definite value of the total spin. Different values of $g(r)$ are supposed to be used for the triplet and singlet interactions. This means, of course, that the representation of an ordinary experimental situation involves an analysis into wave functions ψ such as those dealt with in Eq. (1) with different values of $g(r)$. Such an analysis is well known and is described in most books concerned with

the theory of nuclear physics. It will not be gone into, therefore, at this stage.

The eigenfunctions u_n describing the stable states of a proton in a molecule satisfy the equation

$$E_n u_n = (-(\hbar^2/2M)\Delta_\pi + U)u_n. \tag{1.1}$$

The wave function ψ can be analyzed into a linear combination of the functions $u_n(\mathbf{r}_\pi)$ with coefficients which are functions of the proton-neutron distance vector $\mathbf{r}$:

$$\psi = \sum_n a_n u_n(\mathbf{r}_\pi)\chi_n(\mathbf{r}). \tag{1.2}$$

The quantities a_n occurring in the above formula are taken to be constant while the functions χ_n depend only on the relative rather than the absolute position of the neutron with respect to the proton.

It will be shown next by means of a few estimates through substitution of this form of ψ into Eq. (1), that for small values of the proton-neutron distance r, the difference in the space character of different functions χ_n is negligible. This means that in a good approximation one will be able to describe the function ψ as a product of a function of $\mathbf{r}$ multiplied by a function of $\mathbf{r}_\pi$. This approximation will be used only for values of r of the order of nuclear dimensions. The argument for the separability of ψ into two factors in this range of values of r follows.

Substitution of (1.2) into (1) gives

$$\sum_n (E-E_n)a_n\chi_n u_n = \sum_m a_m\left[-\frac{\hbar^2}{M}u_m\Delta\chi_m + \frac{\hbar^2}{M}\nabla\chi_m\cdot\nabla_\pi u_m + g\chi_m u_m\right]. \tag{2}$$

It is understood here that the χ occur only with relative neutron-proton and the u only with proton coordinates. For a fixed value of $\mathbf{r}$, integration of the last equation over the proton coordinates after multiplication by u_n^* gives

$$\left[(E-E_n)\chi_n + \frac{\hbar^2}{M}\Delta\chi_n - g\chi_n\right]a_n = -\frac{1}{M}\sum_m(\mathbf{p}_{nm}^{(\pi)}\mathbf{p}\chi_m)a_m, \tag{2.1}$$

where the operators $\mathbf{p}$ stand for $(\hbar/i)\nabla$ and correspond to the usual representation of the momentum. It is now clear that if the right side of (2.1) were absent, then inside the range of action of the nuclear potential g, one would be dealing with separate equations for each χ_n, and that there would exist solutions in which only one of the a_n is distinct from zero. The states $u_n\chi_n$ can be considered as being uncoupled in this approximation. Further, it is readily seen that if one were to set all the E_n in these equations equal to zero, the results of calculations on scattering would be unaffected provided the left side of Eq. (2.1) is *never* used for values of r greater than the range of nuclear forces. Within these small distances the effect of the very slight change in the value of the effective kinetic energy $E-E_n-g$ is small, and the change in the logarithmic derivative of χ_n caused by E_n is negligible at $r=\rho$. The truth of this point of view may be seen by noting that the effective kinetic energy is affected by E_n to the extent of, say, 10 ev while its total magnitude is of the order of 10^7 ev. The effect on the logarithmic derivative $rd(r\chi)/(r\chi)dr$ at $r=\rho$ is[3] of the order

$$\frac{\partial}{\partial E}\left[\frac{\partial F}{F\partial r}\right]_{r=\rho}\cdot\delta E_{\text{kin}} = -\frac{M}{\hbar^2F^2}\int_0^\rho F^2dr\cdot\delta E_{\text{kin}}. \tag{2.2}$$

$$F = r\chi, \tag{2.3}$$

where δE_{kin} is the change in the effective kinetic energy. This change in the logarithmic derivative corresponds to a change in the intercept a in accordance with

$$\rho+a = \left[\frac{\partial F}{F\partial r}\right]^{-1}_{r=\rho};\quad \frac{\delta a}{\rho+a} = -(\rho+a)\delta\left[\frac{\partial F}{F\partial r}\right]_{r=\rho}.$$

[3] G. Breit and E. Wigner, Phys. Rev. 49, 519 (1936). See Eq. (29).

By means of (2.2) one can transform the right side of the above equation and obtain

$$\frac{\delta a}{\rho+a}=\frac{\rho+a}{\rho}\frac{\delta E}{E_{\text{kin}}}\cdot\frac{\rho^2p^2}{\hbar^2}\cdot\frac{1}{\rho F^2}\int_0^\rho F^2dr, \tag{2.4}$$

where

$$p^2/M=E_{\text{kin}}. \tag{2.5}$$

The factor $(1/\rho F^2)\int_0^s F^2dr$ in (2.4) is of the order of $\frac{1}{2}$ since this is the value of this factor for an interaction potential $g(r)$ in the form of a square well. The quantity $\rho^2p^2/\hbar^2$ is of the order $(2\pi)^2(\lambda/4)^2/\lambda^2=(\pi/2)^2=2.5$. Here λ is the wave-length of relative proton-neutron motion inside the potential well. With these approximate values one obtains by means of (2.4)

$$\frac{\delta a}{a}\cong 1.2\frac{(\rho+a)^2}{\rho a}\frac{\delta E}{E_{\text{kin}}}.$$

For $a=20\times10^{-13}$ cm, $\rho=3\times10^{-13}$ cm, this relation becomes

$$\delta a/a=10\delta E/E_{\text{kin}},$$

and for $\delta E=10$ ev, $E_{\text{kin}}=10$ Mev

$$\delta a/a\cong10^{-5}.$$

The corresponding change in the scattering cross section is 0.002 percent and is negligible in most problems. The magnitudes of the quantities used in the estimates just made have been such as to give a too large rather than a too small value for the effect of δE, and it may be considered justifiable, therefore, to neglect its effect.

So far it has been shown that one has a negligible error if one neglects the difference between E and $E-E_n$ on the left side of Eq. (2.1). It is seen also that the coupling between different a_n caused by the occurrence of non-vanishing right-hand members in this equation is similarly of little consequence. These terms are of the same order of magnitude as the terms just discussed and contribute approximately the same amount to $\Delta\chi_n$. They may usually be neglected, therefore. An exception to this general situation occurs if one of the a_n is very small compared with some other a_m, or with at least one of them. If this is the case, the right side of Eq. (2.1) cannot be neglected because it may contribute an important part of $\Delta\chi_n$. In order that this should take place the ratio a_n/a_m has to be of the order of 10^{-5}, and this means that one is dealing with an unimportant part of the wave function in the expansion (1.2). It is thus seen that for ranges of nuclear forces that are customarily assumed it is legitimate to neglect the coupling between the a_n as well as the differences between the χ_n, provided, of course, one stays in the part of configuration space $r<\rho$.

This situation suggests a reformulation of the problem in terms of a boundary condition at $r=0$. The quantity ρ is made to approach zero. Simultaneously $g(r)$ is varied in such a way as to keep a at its experimental value. As the limit of $\rho=0$ is approached, the errors in the cross section assume values much smaller than the above estimate of 0.002 percent and finally approach zero. In view of the fact that the difference between this idealized and the more realistic original picture is negligible for most practical purposes, the limit of very deep and narrow potential wells will be used in what follows. This means that as $r\to0$ the limiting form of any χ will be taken to be

$$(1+a/r)b,$$

where b is a constant. Accordingly the limiting form of $\psi(\mathbf{r}_p, \mathbf{r}_n)$ for $|\mathbf{r}_p-\mathbf{r}_n|=r\to0$ will be taken to be

$$\lim_{r\to0}\psi(\mathbf{r}_p, \mathbf{r}_n)=(1+a/r)f(\mathbf{r}_n). \tag{3}$$

In this equation, the function f is a three-dimensional function of the proton coordinates. It is so far an unknown function and has to be determined through the requirement that ψ behave properly in other regions than those corresponding to near coincidence of the proton and neutron.

4. CONVERSION TO AN INTEGRAL EQUATION

By means of the boundary condition (3) the problem is simplified through the fact that through all of the configuration space with the exception of the three-dimensional region $r=0$, one may require instead of (1) the more manageable equation

$$H_0\psi = E\psi, \tag{4}$$

where

$$H_0 = -(\hbar^2/2M)(\Delta_\pi+\Delta_\nu)+U(\mathbf{r}_\pi). \tag{4.1}$$

One has to find solutions of this equation subject to the following requirements:

(a) Validity of boundary condition (3).

(b) The correct behavior of ψ in regions of configuration space corresponding to large values of $|\mathbf{r}_\nu|$. In these regions one should require that the wave function be representable as the sum of a plane neutron wave with a proton in a definite bound state plus diverging neutron waves with the proton in different bound states.

An explicit construction of such a wave function can be made by means of the quantity

$$K(\mathbf{r}_\pi, \mathbf{r}_\nu; \mathbf{r}_\pi', \mathbf{r}_\nu') = \frac{2\pi M}{h^2}\sum_s u_s(\mathbf{r}_\pi)u_s^*(\mathbf{r}_\pi')\frac{e^{i\kappa_s|\mathbf{r}_\nu-\mathbf{r}_\nu'|}}{|\mathbf{r}_\nu-\mathbf{r}_\nu'|}, \tag{4.2}$$

where

$$\kappa_s^2 = (2M/\hbar^2)(E-E_s) \tag{4.3}$$

with the understanding that for real κ_s one makes $\kappa_s>0$, and for pure imaginary κ_s, $i\kappa_s$ is negative. This choice of the signs for κ_s has as a consequence that, in Eq. (4.2), the separate terms contributing to K are either diverging waves as is the case for real κ_s, or else they are attenuated waves which vanish exponentially as $|\mathbf{r}_\nu-\mathbf{r}_\nu'|\to\infty$. The construction of the kernel K is very similar to that employed[4] in the discussion of resonances in nuclear reactions. The especially useful property of K is expressed by the equation

$$(H_0-E)\int K(\mathbf{r}_\pi, \mathbf{r}_\nu; \mathbf{r}_\pi', \mathbf{r}_\nu')D(\mathbf{r}_\pi', \mathbf{r}_\nu')d\mathbf{r}_\pi'd\mathbf{r}_\nu' = D(\mathbf{r}_\pi, \mathbf{r}_\nu), \tag{4.4}$$

where D is a so far arbitrary density function. It will be convenient from now on to employ the abbreviation

$$K(\mathbf{r}_\pi, \mathbf{r}_\nu; \mathbf{r}_\pi', \mathbf{r}_\nu') = K(\ ,\ ') \tag{4.5}$$

and to express the wave function ψ as

$$\psi = \psi_0(\mathbf{r}_\pi, \mathbf{r}_\nu)+\int K(\ ,\ ')D(\mathbf{r}_\pi', \mathbf{r}_\nu')d\mathbf{r}_\pi'd\mathbf{r}_\nu' \tag{4.6}$$

where $\psi_0(\mathbf{r}_\pi, \mathbf{r}_\nu)$ is the incident wave

$$\psi_0 = u_i(\mathbf{r}_\pi)e^{i(\mathbf{p}_i\mathbf{r}_\nu)/\hbar}. \tag{4.6'}$$

Here u_i is the eigenfunction of the proton in its "initial" state, and $\mathbf{p}_i$ is the momentum of the neutron in its incident condition. The form (4.6) assures the correct behavior of ψ for large $|\mathbf{r}_\nu|$. The density function D has to be determined next so as to satisfy the requirements at small r. Substitution into (1) with the aid of (4.4) shows that

$$g\psi = -D(\mathbf{r}_\pi, \mathbf{r}_\nu). \tag{4.7}$$

One obtains on substitution into (4.6)

$$\psi(\mathbf{r}_\pi, \mathbf{r}_\nu) = \psi_0-\int K(\ ,\ ')g(r')\psi(\mathbf{r}_\pi', \mathbf{r}_\nu')d\mathbf{r}_\pi'd\mathbf{r}_\nu'. \tag{4.8}$$

[4] G. Breit, Phys. Rev. **58**, 506 (1940). See Eq. (13.4).

This integral equation has been obtained without approximations from the original differential equation. It does not involve the approximations of the shortness of the range of nuclear forces or any of the specializations made in connection with the introduction of the boundary condition for small r of the preceding paragraph. One could employ this integral equation if it were necessary to take into account a finite range of nuclear forces. Since the arguments of the preceding paragraph have shown that the error caused by neglecting the finite range is negligible for ordinary problems, the integral equation (4.8) will now be modified so as to eliminate $g(r)$ and to bring in instead the intercept a.

The transformations involved in this process are described in Appendix I. It is shown there that in the limit of a very short range of nuclear forces

$$\int K(\ ,\ ')g(r')\psi(\ ')d\mathbf{r}_\pi' d\mathbf{r}_\nu' = -2a\sum_s u_s(\mathbf{r}_\pi)\int u_s^*(\mathbf{r}_\pi')f(\mathbf{r}_\pi')\frac{e^{i\kappa_s|\mathbf{r}_\pi'-\mathbf{r}_\nu|}}{|\mathbf{r}_\pi'-\mathbf{r}_\nu|}d\mathbf{r}_\pi', \tag{4.9}$$

where f is that of Eq. (3). Substitution into (4.8) gives now

$$(1+a/r)f(\mathbf{r}_\pi)=\psi_0(\mathbf{r}_\pi,\mathbf{r}_\nu)+2a\left\langle\sum_s u_s(\mathbf{r}_\pi)\int u_s^*(\mathbf{r}_\pi')f(\mathbf{r}_\pi')\frac{e^{i\kappa_s|\mathbf{r}_\pi'-\mathbf{r}_\nu|}}{|\mathbf{r}_\pi'-\mathbf{r}_\nu|}\right\rangle d\mathbf{r}_\pi', \quad (r\to 0). \tag{4.95}$$

This equation has been averaged over the directions of the small vector $\mathbf{r}$ because otherwise one does not obtain a limit independent of the direction in which the point $r=0$ is approached. The reason for averaging over directions is apparent also in the discussion of Eqs. (5.3) to (5.7). The boundary condition at $r\to 0$ is expressed directly by Eq. (4.95). It is inconvenient to leave the condition in this form, however, because for $r=0$, the left and the right sides become infinite. Substitution for $f(\mathbf{r}_\pi)/|\mathbf{r}_\pi-\mathbf{r}_\nu|$ of its expansion in terms of the $u_s(\mathbf{r}_\pi)$ gives a neater result, *viz.*

$$f(\mathbf{r}_\pi)-a\langle B(\mathbf{r}_\pi,\mathbf{r}_\pi)\rangle=\psi_0(\mathbf{r}_\pi,\mathbf{r}_\pi) \tag{5}$$

with

$$B(\mathbf{r}_\pi,\mathbf{r}_\nu)=\sum u_s(\mathbf{r}_\pi)\int u_s^*(\mathbf{r}')\frac{2e^{i\kappa_s|\mathbf{r}'-\mathbf{r}_\nu|}-1}{|\mathbf{r}'-\mathbf{r}_\nu|}f(\mathbf{r}')d\mathbf{r}'. \tag{5'}$$

In this form every term approaches a finite limit as $r=|\mathbf{r}_\pi-\mathbf{r}_\nu|\to 0$. Equations (4.95), (5) amount to three-dimensional integral equations on the function $f(\mathbf{r}_\pi)$, and the problem is now reduced to the solution of an integral equation.

It follows from the way in which Eq. (5) has been derived that the coefficient of a on its left side should be finite. Otherwise the equation could not hold because all other terms in it are obviously finite. This fact may be verified as follows. One finds by direct calculation

$$(H_0-E)\sum_s u_s(\mathbf{r}_\pi)\int u_s^*(\mathbf{r}')f(\mathbf{r}')\frac{e^{i\kappa_s|\mathbf{r}'-\mathbf{r}_\nu|}}{|\mathbf{r}'-\mathbf{r}_\nu|}d\mathbf{r}'=\frac{h^2}{2\pi M}f(\mathbf{r}_\nu)\delta(\mathbf{r}_\pi-\mathbf{r}_\nu). \tag{5.1}$$

It will now be noted that the multiplication by U which is contained in H_0-E on $\sum_s$ on the left side of Eq. (5.1) cannot introduce a δ function unless the δ function should be a part of the $\sum_s$. It is clear, however, that for a regular f the δ function is not a factor in f. The δ function on the right side of Eq. (5.1) has to arise therefore through the application of the Laplacian operators in H_0. The combination of these that occurs is

$$-\frac{h^2}{2M}(\Delta_\pi+\Delta_\nu)=-\frac{h^2}{M}\Delta-\frac{h^2}{4M}\Delta_{\pi+\nu} \tag{5.2}$$

where the last term represents the Laplacian with respect to the center of mass coordinates of the proton and neutron. Only the first term on the right side of Eq. (5.2) has anything to do with the

right side of Eq. (5.1) so that the coefficient of $1/r$ in $\sum_s$ can be readily ascertained. It is thus found that

$$\sum_s \text{ of } (5.1) = 1/2r + \cdots,$$

where the remaining terms indicated by dots do not give rise to the singularity. Comparison with Eqs. (4.95), (5), (5.1) shows now that the coefficient 2 in the numerator under the integral sign in Eq. (5′) is just right to cancel the singularity in $1/r$. That this is the case will also be verified in the course of applications of the integral equation.

The integral equation (5) will now be derived without the use of the contraction of range procedure. The employment of the interaction potential $g(r)$ will be replaced by the requirement that the s part of the wave function is of the form $(1+a/r)f$ everywhere except at $r=0$. The wave function ψ can be analyzed in spherical harmonics Y_L of the angular coordinates of $\mathbf{r}$ as follows:

$$\psi(\mathbf{r}_\pi, \mathbf{r}_\nu) = \Phi_0(\mathbf{R}, r) + \sum_{L=1}^{\infty} \varphi_L(\mathbf{R}, r)\, Y_L. \tag{5.3}$$

Here $\mathbf{r}$, $\mathbf{R}$ are the relative coordinates and the coordinates of the center of mass, the functions φ_L are regular everywhere, while Φ_0 is not regular at $r=0$. There is no assumption involved in expressing ψ in the form (5.3). For any fixed $\mathbf{R}$, ψ is a function of $\mathbf{r}$ only, and if r is fixed in addition, then one has a function of the angular coordinates of $\mathbf{r}$ which can be expanded in terms of the spherical harmonics Y_L. Averaging Eq. (5.3) over angles one finds, of course,

$$\langle \psi(\mathbf{R}-\mathbf{r}/2, \mathbf{R}+\mathbf{r}/2)\rangle = \Phi_0(\mathbf{R}, r). \tag{5.31}$$

It has been assumed that the functions φ_L ($L=1, 2, \cdots$) are regular everywhere so that as $\mathbf{r}$ is made to go to zero, the limit of any φ_L is the same independently of the direction from which the point $r=0$ is approached. The function Φ_0, on the other hand, is assumed to be such that

$$\lim_{r=0}[\Phi_0(\mathbf{R}, r) - \Phi(\mathbf{R})(1+a/r)] = 0. \tag{5.32}$$

The assumptions just made about Φ_0 and φ are what replaces the employment of $g(r)$ in the original wave equation (1). In Eq. (5.32) the function $\Phi(R)$ is independent of r as is indicated by the notation used.

It must now be explained that to a sufficient approximation for small values of r,

$$\langle \psi(\mathbf{R}-\mathbf{r}/2, \mathbf{R}+\mathbf{r}/2)\rangle = \langle \psi(\mathbf{r}_\nu-\mathbf{r}, \mathbf{r}_\nu)\rangle = \langle \psi(\mathbf{r}_\pi, \mathbf{r}_\pi+\mathbf{r})\rangle. \tag{5.33}$$

In fact, according to Eq. (5.3),

$$\psi(\mathbf{r}_\nu-\mathbf{r}, \mathbf{r}_\nu) = \Phi_0(\mathbf{r}_\nu-\mathbf{r}/2, r) + \sum_{L=1}^{\infty} \varphi_L(\mathbf{r}_\nu-\mathbf{r}/2, r)\, Y_L. \tag{5.34}$$

Since there is only s scattering, the functions φ_L for small r vanish as r^L or faster. The occurrence of $r/2$ in the combination $\mathbf{r}_\nu-r/2$ in φ_L brings in a dependence on the direction of $\mathbf{r}$ in addition to that included in Y_L. Expanding the φ_L in Taylor's series, one obtains terms vanishing at least as fast as r^2. Such terms will not matter in the statement of a boundary condition such as (5.32) because they disappear from ψ as r approaches zero. One is concerned, therefore, only with

$$\begin{aligned}\langle \Phi_0(\mathbf{r}_\nu-\mathbf{r}/2, r)\rangle &= (1+a/r)\langle \Phi(|\mathbf{r}_\nu-\mathbf{r}/2|)\rangle \\ &= (1+a/r)\langle \Phi(\mathbf{r}_\nu) + (x^2/8)(\partial^2\Phi/\partial x_\nu^2) + \cdots\rangle \\ &= (1+a/r)[\Phi(\mathbf{r}_\nu) + (r^2/24)\Delta\Phi(\mathbf{r}_\nu) + \cdots].\end{aligned} \tag{5.35}$$

In the condition expressed by Eq. (5.32), it does not matter, therefore, whether one averages over angles with fixed center of mass coordinates or whether one keeps the neutron coordinates fixed,

averages over angles of $\mathbf{r}$, and then makes $\mathbf{r}_\nu$ approach $\mathbf{R}$. The same holds for $\mathbf{r}_\pi$. Combining this result with the consideration of the φ_L which was mentioned right after Eq. (5.34), one may restate Eq. (5.32) in the form

$$\lim_{r=0}[\langle\psi(\mathbf{r}_\pi, \mathbf{r}_\pi+\mathbf{r})\rangle-(1+a/r)\Phi(\mathbf{r}_\pi)]=0. \tag{5.4}$$

If now ψ is defined by

$$\psi(\mathbf{r}_\pi, \mathbf{r}_\nu)=\psi_0(\mathbf{r}_\pi, \mathbf{r}_\nu)+2a\sum_s, \tag{5.5}$$

where $\sum_s$ is as in Eq. (4.9), then simply as a matter of rearranging terms

$$\psi=\psi_0+B+af(\mathbf{r}_\pi)/r, \tag{5.51}$$

with B given by Eq. (5′). Averaging (5.51) over angles in order to substitute into Eq. (5.4) one has to consider first of all the term ψ_0. One has for it

$$\langle\psi_0(\mathbf{r}_\pi, \mathbf{r}_\pi+\mathbf{r})\rangle=\psi_0(\mathbf{r}_\pi, \mathbf{r}_\pi)+(r^2/6)[\Delta_\nu\psi(\mathbf{r}_\pi, \mathbf{r}_\nu)]_{\mathbf{r}_\nu=\mathbf{r}_\pi}+\cdots, \tag{5.52}$$

so that in (5.4) one may replace this term by $\psi_0(\mathbf{r}_\pi, \mathbf{r}_\pi)$. Substituting all terms that matter into (5.4) one has finally

$$(1+a/r)\Phi(\mathbf{r}_\pi)=\psi_0(\mathbf{r}_\pi, \mathbf{r}_\pi)+a\langle B\rangle_{r=0}+af(\mathbf{r}_\pi)/r+O(r), \tag{5.6}$$

where $O(r)$ designates terms of order r. Identifying coefficients of equal powers of r in Eq. (5.6) one has

$$\Phi=f;\ \Phi(\mathbf{r}_\pi)=\psi_0(\mathbf{r}_\pi, \mathbf{r}_\pi)+a\langle B\rangle_{r=0}. \tag{5.7}$$

These two equations are equivalent to Eq. (5).

It has thus been shown that the boundary condition statements of Eqs. (5.32), (5.4) require the validity of the integral equation (5) if it is assumed that ψ can be expressed in the form obtained by substituting for the integral on the right side of Eq. (4.8) its limiting form as in Eq. (4.9). The limiting contraction process has dropped out of the picture. Its only remnant is the suggestion of a possible form for ψ, and this suggestion is not necessary since one can show that $\langle B\rangle_{r=0}$ is a well defined quantity as will be seen in connection with Eq. (6.1).

5. COMPARISON WITH FERMI'S EQUATION

In the present paragraph a comparison with Fermi's equation[1] will be made from the point of view of expressing the quantities occurring in one in terms of those occurring in the other. The numerical comparison is postponed until formulas for the evaluation of quantities occurring in Eq. (5.1) are worked out.

Combining Eqs. (4.8), (4.9) one obtains

$$\psi=\psi_0+2a\sum_s u_s(\mathbf{r}_\pi)\int u_s^*(\mathbf{r}_\pi')f(\mathbf{r}_\pi')\frac{e^{i\kappa_s|\mathbf{r}_\pi'-\mathbf{r}_\nu|}}{|\mathbf{r}_\pi'-\mathbf{r}_\nu|}d\mathbf{r}_\pi'. \tag{6}$$

It follows from this and Eq. (5.1) that

$$(H_0-E)\psi=(ah^2/\pi M)f(\mathbf{r}_\pi)\delta(\mathbf{r}_\pi-\mathbf{r}_\nu). \tag{6.1}$$

This relation has some similarity to Fermi's equation:

$$(H_0-E)\bar{\psi}=(ah^2/\pi M)\bar{\psi}\delta_R(\mathbf{r}_\pi-\mathbf{r}_\nu), \tag{6.2}$$

where $\bar{\psi}$ is the average of ψ over positions of the neutron within a sphere of radius R for fixed proton positions. The radius R is supposed to be large in comparison with nuclear dimensions and small in comparison with the size of the molecule. The delta function on the right side of Eq. (6.2) is first introduced by Fermi in such a way as to have a constant value within the sphere of radius R and so that its integral through the spherical volume is unity. In the applications of the equation Fermi

replaces the function δ_R by Dirac's δ function, and the function $\bar{\psi}$ on the right side of his equation he replaces by the incident wave in the spirit of Born's approximation.

Comparison of the exact equation (6.1) with Fermi's approximation (6.2) shows some points of similarity and also an obvious difference. Eq. (3) shows that $f(\mathbf{r}_\pi)$ is approximately Fermi's $\bar{\psi}$:

$$f(\mathbf{r}_\pi)\cong\bar{\psi}. \tag{6.3}$$

It follows, therefore, that if one is interested only in the scattering, then, to within the limits of validity of (6.3), the Eqs. (6.1) and (6.2) are nearly equivalent because for the calculation of the scattering the distinction between ψ and $\bar{\psi}$ on the left side of the two equations is immaterial. One may look, therefore, at Eq. (6.1) as a substantiation of the approximate validity of Fermi's method of calculation. One sees further that if Fermi's equation is used not exactly but in Born's first approximation and with the replacement of δ_R by Dirac's δ, then the only error involved is that of approximating $f(\mathbf{r}_\pi)$ by the incident wave. Equation (5) shows that $f(\mathbf{r}_\pi)$ is only approximately equal to ψ_0 and that more accurately one should add to ψ_0 the term in a on the left side of (5). This term will be referred to as the "background" for the following reason. It arose as the difference between the term in $2a$ on the right side of Eq. (4.95) and the quantity af/r. The term in $2a$ is, according to Eqs. (4.8), (4.9), equal to $\psi-\psi_0$ and represents, therefore, the effect of the diverging waves emanating from the source density f in the vicinity of $r=0$. A part of this term represents af/r. The excess over this is the "background" term.

Disregarding the "background" term there is no difference between the results obtained here and Fermi's method in Born's first approximation. The validity of Fermi's result is, on the other hand, no better than that of Born's first approximation as may be seen by noting that

$$\bar{\psi}(\mathbf{r}_\pi,\mathbf{r}_\pi)\cong\frac{3}{4\pi R^3}\int_0^R\left(1+\frac{a}{r}\right)f(\mathbf{r}_\pi)d\mathbf{r}_\pi=\left(1+\frac{3a}{2R}\right)f, \tag{6.4}$$

and that calculation with Fermi's Eq. (6.2) in the second Born's approximation would bring in terms having an order of magnitude relative to the zeroth of a divided by the linear molecular dimensions.

6. SIMPLIFIED EXPLANATION OF FERMI'S EQUATION

The end result of Fermi's averaging of the wave equation is the replacement of the nuclear interaction potential $g(r)$ by an interaction energy

$$V_F=-\frac{ah^2}{\pi M}\delta_R(\mathbf{r}_\pi-\mathbf{r}_p)=\frac{3a}{R}\frac{h^2}{MR^2}\quad(r<R). \tag{7}$$

$$V_F=0\quad(r>R)$$

For R slightly greater than ρ this quantity is large in the region $r<R$. The introduction of V_F is then not of much use and would even lead to erroneous results for scattering if one used Fermi's equation (6.2) exactly. In fact, the law in accordance with which V_F and R should be varied together in order to obtain equivalence for scattering is much more closely $V_FR^2=$constant than $V_FR^3=$constant, and it is the latter way of varying V_F with R that follows from Eq. (7). This way is therefore not right, and one should not apply Fermi's equation in this manner. It is thus seen also that Fermi's equation cannot give even approximately correct results for scattering if one replaces the function δ_R by Dirac's δ function and calculates with the resultant equation exactly. The latter replacement corresponds to approaching the limit of $R=0$ in Eq. (7) which corresponds to varying the internal phase as

$$\left(\frac{M}{\hbar^2}|V_F|\right)^{\frac{1}{2}}R=\left[\frac{3|a|}{R}\right]^{\frac{1}{2}}$$

which gives for F of Eq. (2.3) a limiting behavior for $R \ll a$

$$\left(\frac{rdF}{Fdr}\right)_{r=R} \cong \left[\frac{3|a|}{R}\right]^{\frac{1}{2}} \cot\left[\frac{3|a|}{R}\right]^{\frac{1}{2}}$$

which is indeterminate for $R \to 0$ while the limiting value of this quantity should be

$$\left(\frac{rdF}{Fdr}\right)_{r\cong R} = \left[\frac{rd(r+a)}{(r+a)dr}\right]_{r=R} = \frac{R}{R+a} \cong \frac{R}{a}\left(1-\frac{R}{a}\right).$$

These two results are obviously inconsistent, indicating that one should only use Dirac's delta function in Fermi's equation for purposes of calculating the scattering to the first order of Born's method, but that an exact solution of this equation would lead to incorrect results. For this reason the explanation in the present section of the paper is concerned not with the equation which Fermi recommends for solution by the Born procedure but with the form (6.2) in which the δ_R function is employed. A simplified presentation of Fermi's equation is taken up next.

The radius R can be made several times a, and the potential energy V_F can thereby be made small compared with the nuclear interaction potential $g(r)$ and yet large in comparison with the molecular potential energy acting on the proton. By making R sufficiently large one can make the modification of the wave function due to the action of V_F quite gentle and keep the term of $a\psi/R$ small compared with ψ. Born's first approximation can be thus made to be a good approximation for Eq. (6.2). The margin of available orders of magnitude is not exceedingly great for this choice of R but is nevertheless sufficient to make this point of view have good sense. Thus, e.g., one can make

$$R = 20(\hbar/(Mm)^{\frac{1}{2}}c) = 1.8\times 10^{-11} \text{ cm},$$

which is reasonably large compared with the maximum value of a that comes under consideration, *viz.* $a = 2\times 10^{-12}$ cm. The averaging sphere is still small in comparison with the molecular vibration amplitude which is of the order 10^{-9} cm. This choice gives

$$V_F = -\frac{3a}{R}\frac{mc^2}{20^2} = -\frac{1}{3}\frac{510000}{400} \text{ ev} = -433 \text{ ev}.$$

The kinetic and potential energies of molecular motion are seen to be small compared with V_F and can be neglected in the region $r<R$. Under these conditions the dependence of ψ on r inside $r<R$ is expressible as the product of a nearly constant factor and the function χ. The dependence of the latter on r is for an attractive V_F, i.e., $a>0$

$$F = r\chi = \text{const.}\times\sin[(M|V_F|/\hbar^2)^{\frac{1}{2}}r]$$

so that

$$(rdF_-/F_-dr)_{r=R} \cong 1-\frac{1}{3}\left[\frac{3a}{R}\frac{\hbar^2}{MR^2}\right]\frac{M}{\hbar^2}R^2 = 1-\frac{a}{R}, \tag{7.1}$$

which is precisely the value needed to join on smoothly to the function $F=r+a$ for $r>R$. In fact for the latter

$$(rdF_+/F_+dr)_{r=R} = R/(R+a) = 1-a/R+\cdots. \tag{7.2}$$

If V_F is repulsive rather than attractive, the sign of the terms in $1/R$ in *both* of the above expressions is changed, and the internal function can be still joined smoothly to the external one. It is seen, thus, that the potential energy V_F is such that for $R \gg a$ the solution of Eq. (6.2) gives the correct value of $rd\chi/\chi dr$. Within the limitations already discussed this equation must give, therefore, the solution of the problem.

It has been noted above that the margin available for the choice of R is not very great. The question naturally arises as to the order of precision of calculations that assume the validity of Eq. (6.2) which has been seen to imply the possibility of choosing R so that it is both large in comparison with the range of nuclear forces and small as compared with molecular dimensions.

7. TRANSFORMATIONS OF THE BACKGROUND

In order to estimate the accuracy of the calculation, one has to know the coefficient of a in Eq. (5). For this purpose it will be transformed into a different form. By means of Eq. (1.1) one obtains

$$\int u_s^*(\mathbf{r}')f(\mathbf{r}')\frac{e^{i\kappa_s|\mathbf{r}'-\mathbf{r}_\nu|}}{|\mathbf{r}'-\mathbf{r}_\nu|}d\mathbf{r}'=\frac{1}{E_s}\int f(\mathbf{r}')\,U(\mathbf{r}')u_s^*(\mathbf{r}')\frac{e^{i\kappa_s|\mathbf{r}'-\mathbf{r}_\nu|}}{|\mathbf{r}'-\mathbf{r}_\nu|}d\mathbf{r}'-\frac{\hbar^2}{2ME_s}\int f(\mathbf{r}')\frac{e^{i\kappa_s|\mathbf{r}'-\mathbf{r}_\nu|}}{|\mathbf{r}'-\mathbf{r}_\nu|}\Delta u_s^*(\mathbf{r}')d\mathbf{r}', \tag{8}$$

and one further has for any regular $\varphi(\mathbf{r})$

$$\int\frac{e^{i\kappa r}}{r}(\Delta+\kappa^2)\varphi(\mathbf{r})d\mathbf{r}=-4\pi\varphi(0). \tag{8.1}$$

Letting

$$\varphi(\mathbf{r})=f(\mathbf{r})u_s^*(\mathbf{r})$$

and combining Eqs. (8), (8.1) one obtains

$$\sum_s u_s(\mathbf{r}_\pi)\int u_s^*(\mathbf{r}_\pi')f(\mathbf{r}_\pi')\frac{2e^{i\kappa_s|\mathbf{r}_\pi'-\mathbf{r}_\nu|}}{|\mathbf{r}_\pi'-\mathbf{r}_\nu|}d\mathbf{r}_\pi'=(2\pi\hbar^2/M)f(\mathbf{r}_\nu)\sum_s u_s^*(\mathbf{r}_\nu)u_s(\mathbf{r}_\pi)/E_s+\text{other terms}. \tag{8.2}$$

By means of a similar transformation one finds

$$\sum_s u_s(\mathbf{r}_\pi)\int u_s^*(\mathbf{r}_\pi')\frac{f(\mathbf{r}_\pi')}{|\mathbf{r}_\pi'-\mathbf{r}_\nu|}d\mathbf{r}_\pi'=(2\pi\hbar^2/M)f(\mathbf{r}_\nu)\sum_s u_s^*(\mathbf{r}_\nu)u_s(\mathbf{r}_\pi)/E_s+\text{other terms}. \tag{8.3}$$

In Eqs. (8.2), (8.3) the first term is the same. This term approaches $f(\mathbf{r}_\pi)/r$ for small r. If, therefore, one subtracts (8.3) from (8.2), the result is free of the term in $1/r$. It is thus found that

$$B(\mathbf{r}_\pi,\mathbf{r}_\pi)=E\sum_s\frac{u_s(\mathbf{r}_\pi)}{E_s}\int f(\mathbf{r})\frac{e^{i\kappa_s|\mathbf{r}-\mathbf{r}_\pi|}}{|\mathbf{r}-\mathbf{r}_\pi|}u_s^*(\mathbf{r})d\mathbf{r}+\sum_s\frac{u_s(\mathbf{r}_\pi)}{E_s}\int\frac{e^{i\kappa_s|\mathbf{r}-\mathbf{r}_\pi|}-1}{|\mathbf{r}-\mathbf{r}_\pi|}$$
$$\times\left\{f(\mathbf{r})u_s^*(\mathbf{r})\,U(\mathbf{r})+\frac{\hbar^2}{2M}[2\nabla f(\mathbf{r})\cdot\nabla u_s(\mathbf{r})+u_s^*\Delta f(\mathbf{r})]\right\}d\mathbf{r}. \tag{8.4}$$

The behavior of the first term in this formula will now be discussed. One finds by straightforward calculation that

$$[\Delta_\pi-(2M/\hbar^2)\,U(\mathbf{r}_\pi)]X=-4\pi\delta(\mathbf{r}_\nu-\mathbf{r}_\pi)$$

where

$$X=(2\pi\hbar^2/M)\sum_s u_s^*(\mathbf{r}_\nu)u_s(\mathbf{r}_\pi)/E_s.$$

It follows, therefore, that for small $r=|\mathbf{r}_\pi-\mathbf{r}_\nu|$ X behaves as $1/r$. For large r and fixed $\mathbf{r}_\nu$ the quantity X vanishes much more rapidly than $1/r$ on account of the rapid decrease of the $u_s(\mathbf{r}_\pi)$. In (8.4) the first term contains on performing the summation contributions of the order

$$(M/2\pi\hbar^2)Ef/|\mathbf{r}-\mathbf{r}_\pi|^2$$

for small value of $|\mathbf{r}-\mathbf{r}_\pi|$ modified by the presence of the exponentials. This term has, therefore,

the approximate magnitude

$$Ef(\mathbf{r}_\pi)\frac{2M\bar{R}}{\hbar^2}=\frac{E}{(\hbar^2/2M\bar{R}^2)}\frac{f(\mathbf{r}_\pi)}{\bar{R}}, \tag{8.5}$$

where $\bar{R}$ is a mean length at which the changes in f and in the exponentials containing κ_s decrease the integrand appreciably in comparison with the approximation just mentioned. This length is roughly of the order of $1/\bar{\kappa}$, where $\bar{\kappa}$ is a mean value of κ, and the length is, therefore, of molecular dimensions. The energy of the neutron enters, therefore, in comparison with the centrifugal barrier for molecular dimensions, and besides one, has the factor $f/\bar{R}$. Therefore, one expects the order of magnitude of the effect of the background on the cross section to be 10^{-12} cm/10^{-9} cm $=0.001$, which amounts to a tenth of a percent.

Another convenient form is found by introducing the quantity

$$F(\mathbf{r}_\pi, \mathbf{r}')=\sum_{s=0}^{\infty} u_s(\mathbf{r}_\pi)u_s^*(\mathbf{r}')e^{-2M(E_s-E_0)\tau/\hbar^2}, \tag{8.6}$$

where E_0 is the lowest E_s. One verifies readily that

$$\{\Delta_\pi+(2M/\hbar^2)[E_0-U(\mathbf{r}_\pi)]\}F=\partial F/\partial\tau, \tag{8.7}$$

and one obtains

$$\sum_{s=0}^{\infty} f_s=\sum_{s=0}^{\sigma} f_s+\int_{\tau=0}^{\infty}\frac{\exp\left\{-\dfrac{|\mathbf{r}_\nu-\mathbf{r}'|^2}{4\tau}+\dfrac{2M}{\hbar^2}(E-E_0)\tau\right\}}{2(\pi)^{\frac{3}{2}}\tau^{\frac{3}{2}}}$$
$$\cdot\left[F(\mathbf{r}_\pi, \mathbf{r}')-\sum_{s=0}^{\sigma} u_s(\mathbf{r}_\pi)u_s^*(\mathbf{r}')e^{-2M(E_s-E_0)\tau/\hbar^2}\right]d\tau, \tag{8.8}$$

where

$$f_s=u_s(\mathbf{r}_\pi)u_s^*(\mathbf{r}')e^{i\kappa_s|\mathbf{r}'-\mathbf{r}_\nu|}/|\mathbf{r}'-\mathbf{r}_\nu|, \tag{8.9}$$

which is useful for the evaluation of B (Cf. Appendix II). This transformation is especially convenient for $E=E_0$. It can be employed also for other values of E. In applying Eq. (8.8), one represents the collection of terms due to the -1 in the numerator of Eq. (5′) as

$$-\frac{1}{r}=-\frac{1}{2\pi^{\frac{1}{2}}}\int_0^{\infty}\frac{\exp(-r^2/4\tau)}{\tau^{\frac{3}{2}}}d\tau. \tag{8.9′}$$

It is found then that in the limit of $r=0$, the two definite integrals over τ entering the representation of B combine to give a convergent integral. In evaluating B for $E>E_0$ the number σ in (8.8) must be chosen so as to make $E_\sigma<E<E_{\sigma+1}$. The terms $\sum_{s=0}^{\sigma}f_s$ represent the effect of the diverging waves.

8. FREE PROTONS

The equations will be illustrated first in the case of free protons. There might be reasonable doubt regarding their applicability because the free protons recoil and the proton waves have sources of diverging waves on a par with the neutron waves. These sources are not obviously present in Eq. (6), however.

The protons will be quantized in a fundamental volume with a periodic boundary condition. The wave function ψ_0 will be taken to be

$$\psi_0=e^{i\mathbf{k}_0\mathbf{r}_\nu},\quad \mathbf{k}_0=i\mathbf{p}_0/\hbar \tag{9}$$

corresponding to the collision of neutron and proton waves of unit amplitude. The momentum

of the incident neutrons is $\mathbf{p}_0$. The proper functions for the protons are

$$u_s(\mathbf{r}_\pi) = V^{-\frac{1}{2}} e^{i\mathbf{k}_s \mathbf{r}_\pi}, \quad \mathbf{k}_s = \mathbf{p}_s/\hbar, \tag{9.1}$$

where V is the fundamental volume. In the usual manner the summation over s can be replaced by

$$V \int d\mathbf{k}_s/2\pi^2. \tag{9.2}$$

One has thus for the sum that is multiplied by $2a$ on the right of Eq. (6)

$$\sum_s = \frac{1}{8\pi^3} \int\int |\mathbf{r}' - \mathbf{r}_\nu|^{-1} \exp\{i[\mathbf{k}(\mathbf{r}_\pi - \mathbf{r}') + \mathbf{k}_0 \mathbf{r}' + (k_0^2 - k^2)^{\frac{1}{2}} |\mathbf{r}' - \mathbf{r}_\nu|]\} d\mathbf{r}' d\mathbf{k}, \tag{9.21}$$

where in accordance with the convention that has been followed for κ one must set

$$(k_0^2 - k^2)^{\frac{1}{2}} = |(k_0^2 - k^2)^{\frac{1}{2}}| \quad (k_0 > k) \tag{9.22}$$

$$(k_0^2 - k^2)^{\frac{1}{2}} = i|(k^2 - k_0^2)^{\frac{1}{2}}| \quad (k > k_0). \tag{9.23}$$

The quantity needed for the integral equation is

$$\langle \sum_s \rangle = \frac{1}{8\pi^3} \int\int \frac{\sin kr}{kr|\mathbf{r}' - \mathbf{r}_\nu|} \cdot \exp\{i[\mathbf{k}(\mathbf{r}_\nu - \mathbf{r}') + \mathbf{k}_0 \mathbf{r}' + (k_0^2 - k^2)^{\frac{1}{2}} |\mathbf{r}' - \mathbf{r}_\nu|]\} d\mathbf{r}' d\mathbf{k}. \tag{9.24}$$

On introducing $\mathbf{r}'' = \mathbf{r}' - \mathbf{r}_\nu$ and integrating over directions of $\mathbf{r}''$ one finds

$$\langle \sum_s \rangle = \frac{e^{i\mathbf{k}_0 \mathbf{r}_\nu}}{2\pi^2} \int \left\{ \int_0^\infty \frac{\sin(kr) \sin(|\mathbf{k}_0 - \mathbf{k}| r'')}{kr|\mathbf{k}_0 - \mathbf{k}|} \exp[i(k_0^2 - k^2)^{\frac{1}{2}} r''] dr'' \right\} d\mathbf{k}, \tag{9.25}$$

and integration over directions of $\mathbf{k}$ gives

$$\langle \sum_s \rangle = \frac{2e^{i\mathbf{k}_0 \mathbf{r}_\nu}}{\pi k_0 r} \int_0^\infty \int_0^\infty (1/r'') \sin(kr) \sin(k_0 r'') \sin(kr'') \exp\{i(k_0^2 - k^2)^{\frac{1}{2}} r''\} dr'' dk. \tag{9.26}$$

It will be noted that the integrals over r'' converge and that the integrations can be performed first over r'' by straightforward calculation.

$$I.P. \int_0^\infty (1/r'') \sin k_0 r'' \sin kr'' \exp[i(k_0^2 - k^2)^{\frac{1}{2}}] dr''$$

$$= (i/4) \int_0^\infty (1/r) \{\sin A_1 r + \sin A_2 r - \sin A_3 r - \sin A_4 r\} dr \tag{9.27}$$

with

$$\begin{aligned} A_1 &= \surd + k_0 - k; \quad A_2 = \surd - k_0 + k; \\ A_3 &= \surd + k_0 + k; \quad A_4 = \surd - k_0 - k; \end{aligned} \tag{9.28}$$

and

$$\surd = (k_0^2 - k^2)^{\frac{1}{2}}.$$

Contributions to the imaginary part are present only if $k_0 > k$. For this reason A_1, A_2, A_3 are positive, while A_4 is negative in Eq. (9.27). The right side of (9.27) becomes $\pi i/4$ and

$$I.P.\langle \sum_s \rangle = ie^{i\mathbf{k}_0 \mathbf{r}_\nu} \frac{1 - \cos k_0 r}{2k_0 r^2} \cong ie^{i\mathbf{k}_0 \mathbf{r}_\nu} k_0/4. \tag{9.3}$$

Similarly one obtains

$$R.P.\langle\Sigma_s\rangle=\frac{e^{ik_0r_\nu}}{2\pi k_0 r}\int_0^\infty \sin kr\,\log\left[\frac{k+k_0}{|k-k_0|}\right]dk=\frac{e^{ik_0r_\nu}}{2k_0r^2}\sin(k_0r)\cong\frac{e^{ik_0r_\nu}}{2r}\left(1-\frac{k_0^2r^2}{6}\right), \tag{9.4}$$

and in the limit of $r=0$, and $\mathbf{r}_\nu=\mathbf{r}_\pi$ one has from Eqs. (9.3), (9.4)

$$a\langle B\rangle_{r=0}=iak_0e^{ik_0r_\pi}/2. \tag{9.5}$$

Here use was made of the fact that one may keep either $\mathbf{r}_\pi$ or $\mathbf{r}_\nu$ fixed in the averaging over directions of $\mathbf{r}$ as has been explained in connection with Eq. (5.34). One may replace, therefore, the $\mathbf{r}_\nu$ in Eqs. (9.3), (9.4) by $\mathbf{r}_\pi$.

In the above calculation one has introduced into the calculation of B the approximate value of $f\cong\psi_0$ which follows from (5) if one neglects $a\langle B\rangle$, i.e., if one solves (5) by iteration. On account of Eq. (9.5) the corrected value of f is

$$f(\mathbf{r}_\pi)\cong(1+ik_0a/2)e^{ik_0r_\pi}. \tag{9.6}$$

The asymptotic behavior of the angular average over directions of $\mathbf{r}$ is

$$\langle\psi\rangle_{r=0}\cong(1+ik_0a/2)(1+a/r)e^{ik_0r_\pi}, \tag{9.7}$$

which can be compared with the exact value following from

$$\psi=\psi_0(\mathbf{r}_\pi,\,\mathbf{r}_\nu)+e^{ik_0R}\frac{\sin(k_0a/2)}{k_0r/2}e^{ik_0(r+a)/2} \tag{9.8}$$

according to which

$$\langle\psi\rangle_{r=0}\sim1+\frac{\sin(k_0a/2)}{k_0/2}e^{ik_0a/2}(1/r+ik_0/2)=e^{ik_0a/2}\left[\frac{a}{r}\frac{\sin k_0a/2}{k_0a/2}+\cos k_0a/2\right]\cong(1+ik_0a/2)(1+a/r). \tag{9.8'}$$

It is seen from Eq. (9.8′) that the wave function is not quite of the form $1+a/r$. The deviations from this form are seen, however, to be of the order $k_0^2a^2$, which is a very insignificant factor for thermal neutrons.

It is satisfying that to the order k_0a there is agreement between (9.8′) and (9.7). While even the terms in $ik_0a/2$ affect the cross section only by the insignificant factor $1+k_0^2a^2/4$, it is satisfactory to have the *phase* of the scattered wave correct to the order $k_0a/2$.

The agreement between (9.7) and (9.8) is seen to be no worse than the assumption that the factor $1+a/r$ represents correctly the variation with r of the s part of ψ at small r. The exact dependence is of the type

$$\frac{1}{kr}(\sin ka\,\cos kr+\cos ka\,\sin kr)\sim\cos ka\left[1+\frac{\tan ka}{ka}\cdot\frac{a}{r}\right].$$

The deviations from the assumed form are themselves representable by correction factors $1+k^2a/3$, and there is no apparent reason for expecting the agreement to be closer than that found.

If one makes a calculation for the cross section along standard lines with ψ_0 in place of f in Eq. (6), then one finds without difficulty that the differential cross section per unit solid angle in any given direction when corrected for the factor $1+k_0^2a^2/4$ is

$$\sigma_\omega=(4a^2+k_0^2)p_\nu/p_0.$$

The last correction goes outside of the limits of accuracy of the method and does not represent an

improvement over the simpler result

$$\sigma_\omega \cong 4a^2 p_v/p_0,$$

since this correction is given by the factor

$$\sin^2 k_0 a/2.$$

If all the corrections obtainable from the equations were as small as that just discussed, there would be no purpose in presenting the equations. It is found, however, that the actual correction factor involves the ratio of a to molecular dimensions to the first rather than to the second power and is not negligible, therefore.

A general idea of what one may expect can be obtained by considering the background for free protons as made of two parts, one of which comes from the region $k_s > k_0$, and the other from $k_s < k_0$. The evaluation can be carried out by means of Eq. (9.4) by replacing the integral by

$$\int_{k_0}^{\infty} \sin kr \log\frac{k+k_0}{k-k_0} dk = \frac{\cos k_0 r}{r}[C - Ci(2k_0 r) + \log 2k_0 r)] + \frac{\pi}{r}\sin(k_0 r) - \frac{\sin k_0 r}{r} Si(2k_0 r) \tag{9.9}$$

with

$$C = 0.5772\cdots = \text{Euler-Mascheroni constant}$$

$$Si(x) = \int_0^x \frac{\sin u}{u} du; \quad Ci(x) = -\int_x^\infty \frac{\cos u}{u} du.$$

By means of the above Eq. (9.9), one finds on substitution into Eq. (9.4) and on passing to the limit of $r \to 0$

$$R.P.\langle \sum_{k>k_0} \rangle \to e^{ik_0 r\pi}\left(\frac{1}{2r} - \frac{k_0}{2\pi}\right), \tag{10}$$

and one has similarly

$$R.P.\langle \sum_{k<k_0} \rangle \to e^{ik_0 r\pi}\left(\frac{ik_0}{4} + \frac{k_0}{2\pi}\right). \tag{10.1}$$

It is seen that the singularity in $1/r$ is contributed by the region of high k as could be expected since the representation of the δ function in Eq. (6.1) is impossible without the extension of the sum over the eigenfunctions to those of infinitesimal wave-length. It is seen also that there are two real contributions to $a\langle B\rangle$, one of amount

$$-ak_0/\pi = \text{part of } \langle B\rangle_{r=0} \text{ for } k > k_0, \tag{10.2}$$

and another of equal and opposite amount which comes from $k < k_0$. The effect of each of these parts on f is of the order of a fractional change of amount $2a/\lambda_0$, where λ_0 is the wave-length of the incident neutron which is of the order 10^{-3} for 1 ev neutrons, and 10^{-2} for 100 ev neutrons. When the protons are chemically bound, the balance of the contributions from $k > k_0$ and $k < k_0$ is upset, and there is a residual effect which can be expected to give changes in the scattering cross section of the order of tenths of a percent, since the molecular energies are of the order of 0.5 ev or 0.2 ev.

The evaluation of the background for neutrons having very small energies incident on harmonically bound protons is made in the next paper in this issue.[5] The results agree with the estimates made here in Section 7 above.

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[5] G. Breit and P. R. Zilsel, Phys. Rev. **71**, 232 (1947).

ACKNOWLEDGMENTS

The work has received support from the Wisconsin Alumni Research Foundation and from the Office of Naval Research of the Navy Department.

APPENDIX I

Derivation of Eq. (4.9)

Substitution of K into the left side of Eq. (4.9) by means of Eqs. (4.2), (4.5) gives

$$\int \mathbf{K}(\ ,\ ')g(r')\psi(\ ')d\mathbf{r}_\pi' d\mathbf{r}_\nu' = \frac{2\pi M}{h^2}\sum_s \int u_s(\mathbf{r}_\pi)u_s^*(\mathbf{r}_\pi')f(\mathbf{r}_\pi')\left\{\int \frac{e^{i\kappa_s|\mathbf{r}_\nu-\mathbf{r}_\nu'|}}{|\mathbf{r}_\nu-\mathbf{r}_\nu'|}g(\mathbf{r}')\chi(r')d\mathbf{r}'\right\}d\mathbf{r}_\pi' \quad \text{(I, 1)}$$

where the replacement

$$\psi(\mathbf{r}_\pi, \mathbf{r}_\nu) = f(\mathbf{r}_\pi)\chi(r) \quad \text{(I, 2)}$$

has also been made. The latter involves the harmless approximations which have been justified in connection with Eqs. (1.2), (2.1), and (3). This discussion showed that to a very good approximation

$$\left[-\frac{\hbar^2}{M}\Delta + g(r)\right]\chi(r) = 0. \quad \text{(I, 3)}$$

As the range of nuclear forces ρ contracts in the process discussed for Eq. (3), one can make it small enough, for any pre-assigned $\mathbf{r}_\pi'$, $\mathbf{r}_\nu$, so as to have

$$|\mathbf{r}_\pi' - \mathbf{r}_\nu| \gg \rho. \quad \text{(I, 4)}$$

When this condition is satisfied, one can set

$$\int \frac{e^{i\kappa_s|\mathbf{r}_\nu-\mathbf{r}_\nu'|}}{|\mathbf{r}_\nu-\mathbf{r}_\nu'|}g(r')\chi(\mathbf{r}')d\mathbf{r}' \cong \frac{e^{i\kappa_s|\mathbf{r}_\nu-\mathbf{r}_\pi'|}}{|\mathbf{r}_\nu-\mathbf{r}_\pi'|}\cdot I \quad \text{(I, 4.1)}$$

where

$$I = \int g(r')\chi(\mathbf{r}')d\mathbf{r}', \quad \text{(I, 4.2)}$$

and the employment of Eq. (I, 3) in the above formula gives

$$I = -\frac{h^2 a}{\pi M}. \quad \text{(I, 4.3)}$$

In the calculation just described a appears as the value of $-r^2 d\chi/dr$ at the outer boundary of the region where $g(r) \neq 0$. Substitution of (I, 4.3) into (I, 4.2), of the latter into (I, 4.1), and of the result into (I, 1) yields Eq. (4.9) of the text.

In the above discussion no account was taken of the region in which (I, 4) is not fulfilled. As ρ approaches zero, the volume of the part of the space $\mathbf{r}_\pi'$ in which (I, 4) does not hold also approaches zero, and the contribution to the sum on the right side of Eq. (4.9) due to an individual term is of the order

$$2\pi\rho^2 u_s^*(\mathbf{r}_\nu)f(\mathbf{r}_\nu). \quad \text{(I, 4.4)}$$

This is true only for terms with sufficiently low s. For high s, the strongly negative numbers $i\kappa_s$ make the contributions smaller. The series consists of terms like (I, 4.4) up to the point where $|\kappa_s|$ is of the order $1/\rho$. The sum on the right side of Eq. (4.9) contains thus

$$\sum_{s=0}^{|\kappa_s|\sim 1/\rho} u_s(\mathbf{r}_\pi)u_s^*(\mathbf{r}_\nu) = D(|\mathbf{r}_\pi - \mathbf{r}_\nu|) \quad \text{(I, 4.5)}$$

which is an approximation to the δ function and differs from the δ function by being distributed through a volume of approximate linear dimensions ρ. The whole sum on the right of Eq. (4.9) is thus of the order $f(\mathbf{r}_\pi)/\rho$, if $r=|\mathbf{r}_\pi-\mathbf{r}_\nu|$ is of the order ρ on account of (I, 4.4), (I, 4.5), which has to be true in order to cancel the term in $1/r$ on the left side of Eq. (4.95). In the description of the behaviour of the sum which has just been considered, the quantity ρ has no direct significance as the range of nuclear force, but can be made equal to it if desired. It is thus seen that the contribution to the sum owing to the region $|\mathbf{r}_\pi'-\mathbf{r}_\nu|$ is quite large for $|\mathbf{r}_\pi-\mathbf{r}_\nu|<\rho$ and cannot be said to be negligible everywhere. It is also seen, however, that on account of (I, 4.5), this contribution is very much smaller if $|\mathbf{r}_\pi-\mathbf{r}_\nu|>\rho$, because the D function in (I, 4.5) is concentrated mainly in a region having linear dimensions ρ.

In spite of the fact that the contributions to the sum in (4.9), caused by the region inside a sphere of radius ρ, are responsible for the term $f(\mathbf{r}_\pi)/\rho$, when $|\mathbf{r}_\pi-\mathbf{r}_\nu|=\rho$, the contraction procedure makes it possible to make ρ small enough so that for a given $|\mathbf{r}_\pi-\mathbf{r}_\nu|$ one can satisfy (I, 4).

APPENDIX II

Derivation of Eq. (8.8)

For real values of $i\kappa_s$, one can represent the quantity f_s which is defined by Eq. (8.9) as

$$f_s=[u_s(\mathbf{r}_\pi)u_s^*(\mathbf{r}')/2\pi^{\frac{1}{2}}]\int_{\tau=0}^{\infty}\tau^{-\frac{3}{2}}\exp\{-|\mathbf{r}_\nu-\mathbf{r}'|^2/4\tau-|\kappa_s|^2\tau\}d\tau. \tag{II, 1}$$

This formula can be verified as follows. The factor in (8.9) which multiplies the product of u_s and u_s^* will be temporarily denoted by g_s. One can define g_s by

$$(\Delta_\nu+\kappa_s^2)g_s=0, \tag{II, 1.1}$$

and the requirements: (a) $g_s\to 0$ for $\mathbf{r}_\nu\to\infty$; (b) g_s approaches $|\mathbf{r}_\nu-\mathbf{r}'|^{-1}$ as a limit for $|\mathbf{r}_\nu-\mathbf{r}'|\to 0$. It is seen that

$$h_s=(1/2\pi^{\frac{1}{2}})\int_0^{\infty}\tau^{-\frac{3}{2}}\exp[-|\mathbf{r}_\nu-\mathbf{r}'|^2/4\tau-|\kappa_s|^2\tau]d\tau \tag{II, 1.2}$$

has the property (II, 1.1) of g_s

$$(\Delta_\nu+\kappa_s^2)h_s=(1/2\pi^{\frac{1}{2}})\int_0^{\infty}\frac{d}{d\tau}\{\tau^{-\frac{3}{2}}\exp[-|\mathbf{r}_\nu-\mathbf{r}'|^2/4\tau-|\kappa_s|^2\tau\}d\tau \tag{II, 1.3}$$

and is, therefore, zero unless $|\mathbf{r}_\nu-\mathbf{r}'|=0$. In the latter case the right side of (II, 1.3) is infinite. It is also clear from the form of (II, 1.2) that h_s has the same asymptotic forms at small and at large distances as g_s. It follows that

$$g_s=h_s \tag{II, 1.4}$$

as can be verified by integration of (II, 1.2). Substituting (II, 1.2) for g_s in Eq. (8.9) of the text one obtains Eq. (II, 1) for f_s. This transformation applies only for $\kappa_s^2<0$ because if κ_s is real, then f_s is an outgoing wave. Equation (8.8) now follows by straightforward substitution of (II, 1) for $s=\sigma+1, \sigma+2, \cdots$.