

Theory of the Refraction and the Diffraction of Neutrons by Crystals

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The equations for the elastic scattering of neutrons by a single crystal, governing simple refraction, reflection, and Laue-Bragg scattering, are derived under the assumption that the scattering and absorption cross sections are independent of spin. A brief summary of the results is given in the final section of the paper.

1. INTRODUCTION

THE experiments on the scattering of neutrons by single crystals carried out at the Argonne Laboratories by Fermi and Zinn and at the Clinton Laboratories by Borst and Wollan have given conclusive evidence that an appreciable part of the scattered intensity is coherent. In fact, a substantial part of the scattering takes place in accordance with the Laue-Bragg equations. The purpose of the present paper is to investigate the theoretical background for the scattering somewhat more fully than has been done previously¹ and to summarize the results in a form that may be of use in the course of the development of the experimental work.

The scattering of slow neutrons by crystals has been of considerable interest since the earliest days of neutron physics. Following Fermi's development² of a simplified or semi-empirical method of treating the interaction between neutron and nucleus, Wick³ showed that one should expect highly crystalline media to scatter slow neutrons in a way that is very different from that expected for gases or completely

amorphous materials because of the interference effects which occur. Wick's work has formed the basis for much of the theoretical work in this field. Following a very similar line of reasoning, Teller⁴ pointed out that one should expect ortho- and parahydrogen to possess markedly different scattering cross sections because of interference, provided the large cross section for the scattering of slow neutrons by protons could be ascribed to a virtual singlet level of the type used in the Breit-Wigner formalism of resonance scattering. The subsequent experimental verification⁵ of the quantitative predictions of Teller and Schwinger⁴ on the basis of Teller's original suggestion demonstrated that one can expect to obtain a reasonable description of the scattering of slow neutrons by polyatomic systems with the use of wave mechanics and the Breit-Wigner formalism.

In the period following Wick's work, numerous investigators extended his treatment of the scattering of neutrons by crystals. Most prominent among these are the work of Pomerantschuk,⁶ Van Vleck,⁷ Halpern, Hamermesh and Johnson,⁸ Seeger and Teller,⁹ and Weinstock.¹⁰ Pomerantschuk examined more carefully than Wick the influence of low temperatures upon the scattering cross section. Van Vleck investigated the scatter-

¹ This document is based on work performed under Contract No. W-35-058-eng-71 for the Manhattan Project. Part of the information covered in this document appeared in Report CP-2419, and a more complete survey will appear in volume IIIB, Division IV of the Manhattan Project Technical Series, as part of the contribution of the Clinton Laboratories. Some of the results derived in this report, particularly those for the index of refraction, were derived earlier by Fermi for simple cases. Fermi's measurements of the total reflection of thermal neutrons by graphite and subsequent measurements of Bragg scattering by Zinn and Borst furnished the incentive for much of the work described here. Professor W. E. Lamb has informed us that he investigated theoretical aspects of the problem of neutron refraction as early as 1940.

² E. Fermi, *Ricerca Scientifica*, **7**, Part 2, 13 (1936).

³ G. C. Wick, *Phys. Zeits.* **38**, 403 (1937).

⁴ J. Schwinger and E. Teller, *Phys. Rev.* **51**, 775 (1937); J. Schwinger and E. Teller, *Phys. Rev.* **52**, 286 (1937).

⁵ J. Halpern, I. Estermann, and O. Stern, *Phys. Rev.* **52**, 142 (1937); L. W. Alvarez and K. S. Pitzer, *Phys. Rev.* **55**, 596 (1939).

⁶ I. Pomerantschuk, *Phys. Zeits. Sowjetunion* **13**, 65 (1938).

⁷ J. H. Van Vleck, *Phys. Rev.* **55**, 924 (1939).

⁸ O. Halpern, M. Hamermesh, and M. H. Johnson, *Phys. Rev.* **59**, 981 (1941).

⁹ R. J. Seeger and E. Teller, *Phys. Rev.* **62**, 37 (1942).

¹⁰ R. Weinstock, *Phys. Rev.* **65**, 1 (1944).

ing of neutrons by paramagnetic media. Halpern, Hamermesh, and Johnson considered the elastic or Laue-Bragg scattering of neutrons by a simple lattice. Seeger and Teller treated in a qualitative fashion the consequences of the selection rules which govern inelastic collisions of neutrons with a lattice in the approximation in which one thermal quantum is emitted or absorbed in the process. Finally, Weinstock presented a more complete treatment of the theory of inelastic collisions and applied his results to a computation of the influence of temperature on the scattering cross section of a polycrystalline medium as a function of temperature. His work was carried out in the approximation in which each crystal scatters a negligible portion of the intensity of a monochromatic beam of neutrons which impinges upon it. Use of the foregoing theoretical work will be made in the following presentation.

It should be emphasized that a number of experiments which were carried out prior to those at Argonne and Clinton gave strong indications that polycrystalline media scatter differently from non-crystalline ones. In this connection should be mentioned the work of Beyer and Whitaker¹¹ on the scattering of neutrons by salts, that of Anderson¹² and co-workers on the penetration of very slow neutrons through thick layers of graphite, and the experiments of Rainwater and Havens¹³ on the variation with neutron velocity of the scattering cross section of solids.

The present paper will treat the theory of refraction and diffraction from several points of view and will derive equations both for the complex index of refraction and for the reflectivity when the Laue-Bragg conditions are satisfied. For simplicity it will be assumed that the scattering cross sections are independent of spin orientation. This condition is satisfied when the scattering nuclei have zero spin, as is true for the isotopes of even atomic mass above N¹⁴. There is considerable evidence that the equations based on this assumption are reasonably accurate for many nuclei having a finite spin. For ex-

ample, the alkali halides exhibit good Bragg reflection.

2. EQUATIONS FOR A SCATTERING MEDIUM

According to conventional collision theory,¹⁴ the wave function describing an incident plane wave of particles and the waves scattered by a spherically symmetric center of force is

$$\psi = e^{i\mathbf{k}\cdot\mathbf{r}} + e^{i\mathbf{k}r}f(\theta)/r, \quad (1)$$

at large distances from the center, where \mathbf{k} is the wave number vector of the incident beam of particles; \mathbf{r} is the positional vector; and

$$f(\theta) = \frac{1}{2ik} \sum_n (2n+1)(e^{2i\eta(n)} - 1)P_n(\cos\theta). \quad (2)$$

The center of force is assumed to be at the origin of coordinates. In Eq. (2), P_n is a Legendre polynomial of order n ; $\eta(n)$ is the shift in phase of the radial wave function associated with P_n relative to the phase in the absence of the force field. This phase shift is real if the center does not absorb; however, it is complex in the more general case in which the center may absorb the particles as well as scatter them.¹⁵ In order to treat the case in which $\eta(n)$ is complex we shall write it in the form

$$\eta(n) = \eta_r(n) + i\eta_i(n) \quad (3)$$

in which both $\eta_r(n)$ and $\eta_i(n)$ are real.

An analysis of the amplitude of the scattered wave in (1) shows that the scattering cross section σ_s of the center is given by

$$\sigma_s = \frac{2\pi}{k^2} \sum_n (2n+1)e^{-2\eta_i(n)} \times [\cosh 2\eta_i(n) - \cos 2\eta_r(n)]. \quad (4)$$

Similarly an examination of the net flux of current through a sphere surrounding the center shows that the absorption cross section is

$$\sigma_a = \frac{2\pi}{k^2} \sum_n (2n+1)e^{-2\eta_i(n)} \sinh 2\eta_i(n). \quad (5)$$

¹¹ H. G. Beyer and W. D. Whitaker, Phys. Rev. **57**, 976 (1940). See also the more recent work by F. C. Nix and G. F. Clement, Phys. Rev. **68**, 159 (1945).

¹² Anderson, Fermi, and Wood, CP-718, CP-781 (Manhattan District Reports).

¹³ Rainwater and Havens, CP-1962 (Manhattan District Reports).

¹⁴ See for example N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, 1933).

¹⁵ We are indebted to Professor Schwinger for an informative discussion of complex phase shifts.

The total cross section, $\sigma_t = \sigma_s + \sigma_a$, is given by the relation

$$\sigma_t = \text{Im}(4\pi f(\theta)/k)_{\theta=0} \quad (6)$$

in which Im implies "imaginary part of." In the present case

$$\sigma_t = \frac{2\pi}{k^2} \sum_n (2n+1)(1 - \cos 2\eta_r(n)e^{-2\eta_i(n)}). \quad (7)$$

In ordinary problems of nuclear scattering the phase shifts are small, corresponding to the fact that cross sections are usually small compared to π/k^2 (about 2.6×10^{-17} cm² or 2.6×10^7 barns for thermal neutrons). In this approximation Eqs. (4), (5), and (7) become:

$$\sigma_a = \frac{4\pi}{k^2} \sum_n (2n+1)\eta_i(n)(1 - 2\eta_i(n)); \quad (8)$$

$$\sigma_s = \frac{4\pi}{k^2} \sum_n (2n+1)(\eta_i^2(n) + \eta_r^2(n)); \quad (9)$$

$$\sigma_t = \frac{4\pi}{k^2} \sum_n (2n+1)(\eta_r^2(n) + \eta_i(n) - \eta_i^2(n)). \quad (10)$$

We readily see from these equations that $\eta_i(0)$ is very small compared with $\eta_r(0)$, except when σ_a is much larger than σ_s . The ratio of the two components is

$$\eta_i/\eta_r = k\sigma_a/(4\pi\sigma_s)^{\frac{1}{2}}.$$

The components of phase become comparable only when σ_a is of the order of 10^4 barns for ordinary values of σ_s .

If we expand the wave function (1) in the vicinity of $r=0$, we find that in the approximation in which $f(\theta) = \eta/k$ the leading terms are

$$\psi = \eta/kr + 1 + \dots \quad (11)$$

Thus near the origin ψ in general has the form

$$\psi = a_{-1}/r + a_0 + \dots, \quad (12)$$

where

$$ka_{-1}/a_0 = \eta. \quad (13)$$

In view of Eqs. (8)–(10), this means that

$$\frac{ka_{-1}}{a_0} = \pm \left[\frac{k^2\sigma_s}{4\pi} - \left(\frac{k^2\sigma_a}{4\pi} \right)^{\frac{1}{2}} \right]^{\frac{1}{2}} + i \frac{k^2\sigma_a}{4\pi}. \quad (14)$$

3. WAVE FUNCTIONS IN A CRYSTAL¹⁶

We are now in a position to examine neutron wave functions in a crystal. We shall attempt to find a function of the form

$$\psi(r) = \chi(r)e^{i\mathbf{k}' \cdot \mathbf{r}}, \quad (15)$$

in which χ has the periodicity of the lattice, \mathbf{r} is the positional vector, and \mathbf{k}' , is the wave number vector. For simplicity we may assume that the crystal is a simple cubic lattice although the results which we shall obtain are easy to generalize to a more complicated case. We shall also assume that the energy E of the wave function is related to the wave number k outside the crystal through the relation

$$E = \hbar^2 k^2 / 2m. \quad (16)$$

Since the wave function possesses a $1/r$ singularity of the type (12) at the position of each nucleus in the lattice, and since the potential of the neutron can be taken to be zero in the region of space between nuclei, it follows that the equation satisfied by the wave functions within the lattice is

$$\Delta\psi + k^2\psi = -4\pi a_{-1} \sum_n e^{i\mathbf{k}' \cdot \mathbf{r}} \delta(\mathbf{r} - \mathbf{r}_n). \quad (17)$$

The right-hand side of this equation is a sum of delta-functions over the positions \mathbf{r}_n of the various nuclei, appropriately modified by a phase factor in accordance with the form of (15), because the Laplacian applied to $1/r$ gives $-4\pi\delta(r)$. The corresponding form of the equation for the function $\chi(r)$ is

$$\nabla^2\chi + 2i\mathbf{k}' \cdot \text{grad}\chi - (k'^2 - k^2)\chi = -4\pi a_{-1} \sum_n \delta(\mathbf{r} - \mathbf{r}_n). \quad (18)$$

Since χ is a periodic function, it can be expanded in a Fourier series

$$\chi = \sum_{\mathbf{K}} c_{\mathbf{K}} e^{i\mathbf{K} \cdot \mathbf{r}}. \quad (19)$$

The summation is to be carried out over all vectors \mathbf{K} of the reciprocal lattice, that is, over all vectors the components of which are integer multiples of $2\pi/a$, where a is the lattice constant.

¹⁶ The mathematical approach presented in this section was proposed to us by Professor Wigner. The results obtained with this method were first obtained by the somewhat less rigorous method described in Section 5.

If we introduce (19) into (18) and expand the sum of the delta-functions into a Fourier series, we obtain

$$c_{\mathbf{K}}(-\mathbf{K}^2 - 2\mathbf{k}' \cdot \mathbf{K} - \mathbf{k}'^2 + \mathbf{k}^2) = -4\pi a_{-1}/v, \quad (20)$$

where $v = a^3$ is the volume of the unit cell of the lattice. Thus when we solve for $c_{\mathbf{K}}$ and substitute into (19) and (15)

$$\psi = \frac{4\pi a_{-1}}{v} \sum_{\mathbf{K}} \frac{\exp[i(\mathbf{k}' + \mathbf{K}) \cdot \mathbf{r}]}{(\mathbf{k}' + \mathbf{K})^2 - \mathbf{k}^2}. \quad (21)$$

The series converges very slowly; in fact its convergence behavior is the same as for the series expansion of the function of $1/r$. It is convenient for subsequent use to place (21) in the form

$$\psi = \frac{4\pi a_{-1}}{v} \int \sum_{\mathbf{K}} \delta(\mathbf{u} - \mathbf{K}) \frac{\exp[i(\mathbf{k}' + \mathbf{u}) \cdot \mathbf{r}]}{(\mathbf{k}' + \mathbf{u})^2 - \mathbf{k}^2} d\tau(\mathbf{u}). \quad (22)$$

It now remains to relate a_{-1} to the physically interesting quantities σ_s and σ_a (see Eq. (14)). In order to use Eq. (14) we must first determine a_0 from (22). To do this, we subtract from (22) the quantity

$$\begin{aligned} \frac{a_{-1}}{r} &= 4\pi a_{-1} \int \frac{\exp(i\mathbf{u} \cdot \mathbf{r})}{(2\pi)^3 \mathbf{u}^2} d\tau(\mathbf{u}) \\ &= 4\pi a_{-1} \int \frac{\exp[i(\mathbf{k}' + \mathbf{u}) \cdot \mathbf{r}]}{(2\pi)^3 (\mathbf{k}' + \mathbf{u})^2} d\tau(\mathbf{u}) \end{aligned} \quad (23)$$

and obtain

$$\begin{aligned} \psi - \frac{a_{-1}}{r} &= \frac{4\pi a_{-1}}{v} \int d\tau(\mathbf{u}) \exp[i(\mathbf{k}' + \mathbf{u}) \cdot \mathbf{r}] \\ &\times \left[\sum_{\mathbf{K}} \frac{\delta(\mathbf{u} - \mathbf{K})}{(\mathbf{k}' + \mathbf{u})^2 - \mathbf{k}^2} - \frac{v}{(2\pi)^3 (\mathbf{k}' + \mathbf{u})^2} \right]. \end{aligned} \quad (24)$$

This expression converges for $r=0$, and its limiting value is

$$a_0 = \frac{4\pi a_{-1}}{v} \int d\tau(\mathbf{u}) \left[\sum_{\mathbf{K}} \frac{\delta(\mathbf{u} - \mathbf{K})}{(\mathbf{k}' + \mathbf{u})^2 - \mathbf{k}^2} - \frac{v}{(2\pi)^3 (\mathbf{k}' + \mathbf{u})^2} \right]. \quad (25)$$

If (14) is used to replace the ratio a_{-1}/a_0 , this equation may be employed to determine the

relation between \mathbf{k}' , \mathbf{k} , and the observed cross sections of the nucleus involved.

In the remainder of this section we shall restrict our attention to the case in which k'^2 and k^2 are very nearly equal, as will be true whenever the phase shifts are small, and in which $(\mathbf{k}' + \mathbf{K})^2$ and \mathbf{k}^2 are nearly equal only when $\mathbf{K} = 0$. This is the case in which the Laue-Bragg conditions for diffraction are not satisfied so that the crystal behaves like a simple optical medium. We shall consider Bragg reflection in detail in the next section. Under these conditions the first term in the sum in (25) is much larger than the other terms appearing behind the integral sign. As a result the equation can be written

$$\frac{a_0}{a_{-1}} = \frac{4\pi}{v} \frac{1}{k'^2 - k^2} \quad (26)$$

or

$$k'^2 - k^2 = \frac{4\pi n_0}{k} \left(\pm \left[\frac{k^2 \sigma_s}{4\pi} - \left(\frac{k^2 \sigma_a}{4\pi} \right)^2 \right]^{\frac{1}{2}} + i \frac{k^2 \sigma_a}{4\pi} \right) \quad (27)$$

in which n_0 is the number of atoms per unit volume.

It is interesting to note that k' will be complex in the general case in which σ_a does not vanish. Thus in this case the functions (15) have the form of attenuated waves.

If σ_a is zero, Eq. (27) becomes

$$k'^2 - k^2 = \pm n_0 (4\pi \sigma_s)^{\frac{1}{2}}. \quad (28)$$

The index of refraction n of the crystalline medium, defined by the relation

$$k' = nk \quad (29)$$

is given by the equation

$$n^2 - 1 = \pm \frac{n_0 (4\pi \sigma_s)^{\frac{1}{2}}}{k^2} = \pm \frac{\hbar^2 n_0 (4\pi \sigma_s)^{\frac{1}{2}}}{8\pi^2 m E}. \quad (30)$$

It is to be noted that there is an arbitrariness in sign before the square root in Eqs. (14), (28), and (30). This sign cannot be determined merely from knowledge of the scattering cross sections, but requires additional information. According to the Breit-Wigner formalism of resonance levels, the sign which appears before the root depends upon the distribution of resonance levels of the compound nucleus relative to the zero energy represented by the energy of the incident

neutron plus that of the nucleus. Resonance levels which have higher energy contribute to the positive sign, those with lower energies to the negative sign, just as in the corresponding optical case.

In cases in which the nuclear scattering cross section is of the order of 10^{-24} cm², as is commonly the case, $n^2 - 1$ is of the order of 10^{-6} for thermal neutrons ($k \sim 5 \times 10^8$ cm⁻¹). Thus the index of refraction differs from unity by a very small amount, in close analogy with the situation for x-rays.

The wave functions of the form (15) may also be derived with the use of the cellular approximation, which has proved very useful in the treatment of electron waves in solids, in the case in which the phase shift is real (i.e., $\sigma_a = 0$). A straightforward application of this procedure shows that as long as the phase shift is small, the form of χ within any given cell of the lattice is accurately¹⁷ represented by the function

$$\chi_0 = 1 + \eta_0/k_0 r \quad (31)$$

in which k_0 is the value of k for which k' is zero, that is, according to (28),

$$k_0^2 = \pm n_0(4\pi\sigma_s)^{\frac{1}{2}},$$

and η_0 is the phase shift for $k = k_0$, that is,

$$\eta_0 = \pm (k_0^2 \sigma_s / 4\pi)^{\frac{1}{2}}.$$

This form of χ is valid for values of k' outside the first zone, provided k' is not too close to the surfaces of the Brillouin zones. The same type of calculation shows that the effective neutron mass inside the crystal is the actual mass. This conclusion is, of course, apparent from Eq. (27) in the approximation in which σ_a vanishes since the coefficients of k^2 and k'^2 are equal.

Equation (31) may also be represented in the form

$$\chi_0 = 1 - r_0/r, \quad (32)$$

in which r_0 is the "extrapolation distance" of the wave function near the origin, which is related

¹⁷ In the approximation in which the cells of the crystal lattice are replaced by spheres, as is possible in reasonably close-packed lattices, the wave function χ_0 will have the form

$$\chi_0 = (1/k_0 r) \sin k_0(r - r_0).$$

to the other quantities by the equations

$$k_0 r_0 = -\eta_0; \quad k_0^2 = 4\pi n_0 r_0; \quad r_0 = \pm (\sigma_s / 4\pi)^{\frac{1}{2}}. \quad (33)$$

Since $(\sigma_s / 4\pi)^{\frac{1}{2}}$ is of the order of 10^{-13} for most nuclei, it follows from the last of the relations (33) that the second term on the right-hand side of (32) is negligible when r corresponds to distances midway between atoms. In other words the function χ_0 is almost constant everywhere except in the immediate vicinity of the nucleus when the scattering cross section is of the order of 10^{-24} cm².

When r_0 is used in place of $(\sigma_s)^{\frac{1}{2}}$, the equation for the refractive index n is

$$n^2 - 1 = -k_0^2/k^2 = -4\pi n_0 r_0/k^2. \quad (34)$$

In the event that there is more than one atom per unit cell, the more general form of Eq. (17) is

$$\nabla^2 \psi + k^2 \psi = -4\pi \sum_{n,j} \exp(i\mathbf{k}' \cdot \mathbf{r}) a_{-1}(j) \times \delta(\mathbf{r} - \mathbf{r}_j - \mathbf{r}_n). \quad (35)$$

Here the vector \mathbf{r}_n is summed over the cells of the lattice whereas \mathbf{r}_j represents the positional coordinate of the j th atom in the unit cell and is summed over the atoms in this cell. $a_{-1}(j)$ is the coefficient of $1/|\mathbf{r} - \mathbf{r}_j|$ in the expansion of the wave function about the point \mathbf{r}_j . We shall let $a_0(j)$ designate the corresponding value of the constant term in the expansion about \mathbf{r}_j . The relation between $a_0(j)$ and $a_{-1}(j)$ analogous to (14) is

$$\frac{k a_{-1}(j)}{a_0(j)} = \pm \left[\frac{k^2 \sigma_s^j}{4\pi} - \left(\frac{k^2 \sigma_a^j}{4\pi} \right)^2 \right]^{\frac{1}{2}} + i \frac{k^2 \sigma_a^j}{4\pi} \equiv k \xi(j), \quad (36)$$

in which σ_s^j and σ_a^j are the scattering and absorption cross sections for the j th nucleus.

The equation for $c_{\mathbf{K}}$ in the expansion of (19), analogous to (20) is readily found to be

$$c_{\mathbf{K}} [\mathbf{k}^2 - (\mathbf{k}' + \mathbf{K})^2] = -4\pi n_0 \sum_j a_{-1}(j) \exp(-i\mathbf{K} \cdot \mathbf{r}_j), \quad (37)$$

in which n_0 is the number of unit cells per unit volume of the crystal. Similarly the family of equations, analogous to (25), relating the $a_0(j)$

and $a_{-1}(j)$ are

$$a_0(i) = 4\pi n_0 \int d\tau(\mathbf{u}) \left[\frac{\sum_{K,j} \delta(\mathbf{u}-\mathbf{K}) a_{-1}(j) \exp[i\mathbf{K} \cdot (\mathbf{r}_i - \mathbf{r}_j)]}{(\mathbf{k}' + \mathbf{u})^2 - k^2} - \frac{a_{-1}(i)}{n_0(2\pi)^3(\mathbf{k}' + \mathbf{u})^2} \right]. \quad (38)$$

The vector \mathbf{u} has the same meaning as in (25).

As previously, only the first term in the sum (38) is large when k'^2 and k^2 are very nearly equal (and $(\mathbf{k}' + \mathbf{K})^2$ is not nearly equal to k^2 for any K different from zero). Thus in this case Eq. (38) may be written

$$a_0(i) = 4\pi n_0 \sum_j a_{-1}(j) / (k'^2 - k^2). \quad (39)$$

Since the right-hand side of this is independent of i , it follows that

$$a_0(i) = a_{-1}(i) / \xi(i) = C, \quad (40)$$

in which C is a constant independent of i . Using this relation, we find that (39) may be placed in the form

$$k'^2 - k^2 = 4\pi n_0 \sum_i \xi(i) \quad (41)$$

which replaces Eq. (27). The new form of ψ is

$$\begin{aligned} \psi &= 4\pi n_0 C \exp(i\mathbf{k}' \cdot \mathbf{r}) \sum_{\mathbf{K}} \frac{\sum_j \xi(j) \exp[i\mathbf{K} \cdot (\mathbf{r} - \mathbf{r}_j)]}{(\mathbf{k}' + \mathbf{K})^2 - k^2} \\ &= 4\pi n_0 C \exp(i\mathbf{k}' \cdot \mathbf{r}) \chi_{\mathbf{k}'}(\mathbf{r}). \end{aligned} \quad (41a)$$

Equation (41) may also be derived with the use of the cellular approximation in the case in which the σ_a^i are zero. In this case one surrounds each nucleus with a polyhedral cell and determines the wave functions within the cell by means of the usual boundary conditions. As previously, it is found that the wave function has the form (32) in each sub-cell of the unit cell of the lattice; that is, the function χ is constant everywhere except in the immediate vicinity of the nuclei.

The fact that χ is constant at regions not too close to the immediate vicinity of the nuclei has very important consequences when the solid is treated like an optical medium. In the conventional treatment of the refracting properties of a continuous optical medium, the relations between incident, transmitted, and reflected rays are determined by fitting boundary conditions at the surface of the solid, which in the simplest cases is taken to be a plane. Since χ is constant at

distances of the order of 10^{-8} cm from the nuclei in the present problem, it follows that the neutron wave functions may be taken to have the form $\exp(i\mathbf{k}' \cdot \mathbf{r})$ at a mathematical surface of the solid which lies at the periphery of the outermost layer of atoms of the crystal. If this surface is reasonably flat in the sense that large areas of the crystal surface are composed of the same continuous crystallographic plane, the conventional results relating index of refraction, reflection, and transmission of a continuous optical medium, derived for the planar case, can be employed. For example, in the case in which the index of refraction is real, the reflectivity is given by the relation

$$R = \left[\frac{(n^2 - \sin^2\theta)^{\frac{1}{2}} - \cos\theta}{(n^2 - \sin^2\theta)^{\frac{1}{2}} + \cos\theta} \right]^2,$$

in which θ is the angle of incidence of the incident beam, that is, the angle made with a normal to the surface. If n is greater than unity this remains less than 1; however, if n is less than unity, the reflectivity is unity for values of θ greater than those for which

$$\sin\theta > n.$$

Since n is very near to unity in the cases in which we are principally interested here, we may write $\theta = (\pi/2) - \varphi$, $n = 1 - \mu$ and use the relation $\cos\theta = \sin\varphi \cong \varphi$. The reflectivity then becomes

$$R = \left\{ \frac{1 - [1 - (2\mu/\varphi^2)]^{\frac{1}{2}}}{1 + [1 - (2\mu/\varphi^2)]^{\frac{1}{2}}} \right\}^2 \quad (42)$$

Perfect reflectivity occurs for values of φ less than $(2\mu)^{\frac{1}{2}}$. For typical nuclear cross sections, one finds that the angle at which the reflectivity becomes total is of the order of 10 minutes of arc. This type of reflectivity was first sought for and found by Fermi and Zinn.

As in the conventional optical case, the component of \mathbf{k}' in the direction normal to the crystal surface and inside the solid becomes imaginary when $\sin\theta > n$, if n is less than unity. That is, in the region of total reflection the

transmitted wave is dampened exponentially. The depth of penetration d for which the amplitude falls to $1/e$ times its value at the surface is

$$d = \frac{i}{k(n^2 - \sin^2\theta)^{\frac{1}{2}}} \approx \frac{1}{k(2\mu)^{\frac{1}{2}}} = \frac{\lambda}{2\pi(2\mu)^{\frac{1}{2}}}$$

in which λ is the wave-length. We find that d is of the order of $10^2\lambda$ for typical values of μ , that is, of the order of 100A. This distance is sufficiently small that experimental determinations of the existence of total reflection will be seriously influenced by the presence on the surface of a contaminating layer of the order of 100 atom distances in thickness. For example, the oxide layer on most metals will have an important influence on the reflectivity.

The recent experiments of Fermi,¹⁸ Zinn, Marshall, Borst,¹⁹ and Wollan, and the somewhat earlier work of Goldberger carried out in cooperation with Zinn, seem to show that most nuclei scatter with negative phase shift, corresponding to index of refraction less than unity. (Manganese appears to be the only exception discovered to date.) This result seems to imply that for most nuclei the influence of stable neutron levels having negative energy on the dispersion properties of nuclei for thermal neutrons is greater than that of the virtual levels which lie above the thermal region. If further work justifies this conclusion we need not be too surprised: Practically all transparent media have an index of refraction greater than unity in the visible portion of the optical spectrum; it would hardly seem more startling to find a similar uniform principle operating for thermal neutrons in cases in which the scattering nucleus does not possess a virtual level lying close to the thermal region.

4. LAUE-BRAGG REFLECTION

We are now in a position to discuss the analog of ordinary x-ray diffraction. From the mathematical viewpoint, this type of diffraction occurs when \mathbf{k}'^2 and $(\mathbf{k}' + \mathbf{K})^2$ become equal for a value of K different from zero. We shall designate

¹⁸ E. Fermi, W. H. Zinn, and L. Marshall, Abstracts E2, E4, and E5, Chicago Meeting, American Physical Society, June, 1946.

¹⁹ As yet unpublished work.

this value of \mathbf{K} by \mathbf{K}' for the purposes of the following discussion. When this condition is satisfied, two terms in the sum under the integral sign in Eq. (38) are large instead of only one, namely that for which \mathbf{K} is equal to 0 and to \mathbf{K}' . Thus the equation relating \mathbf{k} and \mathbf{k}' which replaces (39) is

$$a_0(i) = 4\pi n_0 \left(\frac{\sum_j a_{-1}(j)}{\mathbf{k}'^2 - \mathbf{k}^2} + \exp(i\mathbf{K}' \cdot \mathbf{r}_i) \frac{\sum_j a_{-1}(j) \exp(-i\mathbf{K}' \cdot \mathbf{r}_j)}{(\mathbf{k}' + \mathbf{K}')^2 - \mathbf{k}^2} \right). \quad (43)$$

If we write

$$C_1 = 4\pi n_0 \sum_j a_{-1}(j) / (\mathbf{k}'^2 - \mathbf{k}^2); \quad (44)$$

$$C_2 = 4\pi n_0 \frac{\sum_j a_{-1}(j) \exp(-i\mathbf{K}' \cdot \mathbf{r}_j)}{(\mathbf{k}' + \mathbf{K}')^2 - \mathbf{k}^2}, \quad (45)$$

Eq. (43) may be placed in the form

$$a_0(i) = a_{-1}(i) / \xi(i) = C_1 + \exp(i\mathbf{K}' \cdot \mathbf{r}_i) C_2. \quad (46)$$

When the value of $a_{-1}(j)$ derived from (46) is substituted into (44) and (45), the following two simultaneous equations result:

$$\begin{aligned} [\mathbf{k}'^2 - \mathbf{k}^2] C_1 &= 4\pi n_0 [C_1 \sum_j \xi(j) \\ &+ C_2 \sum_j \xi(j) \exp(i\mathbf{K}' \cdot \mathbf{r}_j)], \\ [(\mathbf{k}' + \mathbf{K}')^2 - \mathbf{k}^2] C_2 &= 4\pi n_0 [C_1 \sum_j \xi(j) \\ &\times \exp(-i\mathbf{K}' \cdot \mathbf{r}_j) + C_2 \sum_j \xi(j)]. \end{aligned} \quad (47)$$

The determinantal compatibility equation associated with (47) gives the relation between \mathbf{k}^2 and \mathbf{k}'^2 . We may expect the roots of this equation to exhibit all of the characteristic features of the theory of Brillouin zones in the case in which the $\xi(i)$ are real. That is \mathbf{k}^2 will be single valued and real for all real values of \mathbf{k}' except at the zone surfaces for which \mathbf{k}'^2 and $(\mathbf{k}' + \mathbf{K}')^2$ are equal. Here \mathbf{k}^2 will be real and double-valued. Conversely, in the neighborhood of the zone surface there will be two real values of \mathbf{k}'^2 associated with each value of \mathbf{k}^2 . These values of \mathbf{k}'^2 will be complex when the $\xi(i)$ are complex. In other words, there are two sets of functions ψ associated with each value of \mathbf{k}^2 when the Laue-Bragg condition is satisfied. From (19), (37), and (46) we

find that these functions have the form

$$4\pi n_0 \exp(i\mathbf{k}' \cdot \mathbf{r}) \left[\sum_{\mathbf{K}} \frac{C_1 \sum_j \xi(j) \exp[i\mathbf{K} \cdot (\mathbf{r} - \mathbf{r}_j)]}{(\mathbf{k}' + \mathbf{K})^2 - \mathbf{k}^2} + \sum_{\mathbf{K}} C_2 \exp(i\mathbf{k}' \cdot \mathbf{r}) \frac{\sum_j \xi(j) \exp[i(\mathbf{K} - \mathbf{K}') \cdot (\mathbf{r} - \mathbf{r}_j)]}{(\mathbf{k}' + \mathbf{K})^2 - \mathbf{k}^2} \right], \quad (48)$$

in which C_1 and C_2 are the solutions of Eqs. (47). We see that these functions may be regarded as the superposition of two waves traveling in the direction \mathbf{k}' and $\mathbf{k}' + \mathbf{K}'$, respectively. The relative amplitude with which each solution appears in the final form of the wave function within the crystal is to be determined by the boundary conditions. These in turn depend upon the physical arrangement in a given experiment. For example, if a neutron beam is diffracted in such a way that it enters and emerges through the same surface (the case of Bragg reflection), the solution within the crystal must join the incident and emergent solutions at the surface of incidence. In addition, it must satisfy the condition that there be no incident wave on the rear face of the specimen.

Fortunately, we may note that Eqs. (47) are identical with those which occur in the dynamical theory of x-ray diffraction²⁰ if C_1 and C_2 are interpreted as being equivalent to the amplitudes D_0^n and $D_{\mathbf{K}'}^0$, respectively, of the displacement vectors which are polarized in a direction normal to the plane containing k and k' , and if the quantities

$$n_0 \sum_j \xi(j) \quad \text{and} \quad n_0 \sum_j \xi(j) \exp(i\mathbf{K}' \cdot \mathbf{r}_j)$$

occurring as coefficients of C_1 and C_2 in the right-hand side of (47) are regarded as being the equivalent of \mathbf{k}^2 times the Fourier components of the complex polarizability of the medium. Moreover, it is conventional to have D_0 and $D_{\mathbf{K}'}$ satisfy exactly the same boundary conditions as the corresponding amplitude constants in our problem do. Thus we may use all of the results of the dynamical theory of x-ray diffraction for the case of the normally polarized wave, after

²⁰ W. H. Zachariasen, *X-Ray Diffraction in Crystals* (Wiley and Sons, New York). See Sec. 9, Chapter 3 in particular. We are deeply indebted to Professor Zachariasen for numerous valuable discussions of the material in this paper and for the use of an advanced copy of the manuscript of his book.

suitably readjusting the constants which appear in the equations.

It is readily seen that Eq. (48) may be placed in the form

$$\psi = 4\pi n_0 [C_1 \exp(i\mathbf{k}' \cdot \mathbf{r}) \chi_{\mathbf{k}'}(\mathbf{r}) + C_2 \exp[i(\mathbf{k}' + \mathbf{K}') \cdot \mathbf{r}] \chi_{\mathbf{k}' + \mathbf{K}'}(\mathbf{r})], \quad (48a)$$

in which $\chi_{\mathbf{k}'}$ and $\chi_{\mathbf{k}' + \mathbf{K}'}$ are identical functions of the variables \mathbf{k}' and $\mathbf{k}' + \mathbf{K}'$, respectively. $\chi_{\mathbf{k}'}$ in (48a) is, in turn, defined by the same series as the corresponding function $\chi_{\mathbf{k}'}$, appearing in (41a), which we have seen to be nearly constant everywhere except in the immediate vicinity of the nuclei. It follows that as long as \mathbf{r} is not in the immediate vicinity of the nuclei (48a) may be written in the approximate form

$$\psi = A_1 \exp(i\mathbf{k}' \cdot \mathbf{r}) + A_2 \exp[i(\mathbf{k}' + \mathbf{K}') \cdot \mathbf{r}], \quad (48b)$$

where $A_1/A_2 = C_1/C_2$.

Now in satisfying conditions of continuity for incoming and transmitted waves in the dynamical theory of x-ray diffraction, it is commonly assumed that the wave inside the crystal has the form (48b). This assumption is highly accurate in the present case near the mathematical boundary of the crystal where boundary conditions are satisfied, as long as this boundary is not too close to the nuclei. In fact the assumption is much more justifiable in the present case than in the case of x-ray diffraction, for in the latter problem the series analogous to (48) has very different convergence properties. In the dynamical theory of x-ray diffraction, it is also common to assume that the surface boundary is a perfect plane. As in the treatment of refraction in the preceding section, this assumption will evidently be accurate only if large areas of the crystal surface are composed of the same plane of atoms in the usual crystallographic sense.

The analogy between x-ray diffraction and neutron diffraction, in the ideal case we are

considering, extends even more deeply than might be supposed at first sight, as we shall see more clearly in the next section.

We shall examine the equations for neutron diffraction further after discussing another method by which the problem may be treated.

5. APPLICATION OF THE METHOD OF THE PSEUDO-POTENTIAL

The results derived in the preceding sections can be obtained in a very straightforward manner with the use of the pseudo-potential, first employed by Fermi.² In this method the actual interaction potential between neutron and nucleus is replaced with a simple function that will lead to the same phase shifts as the actual potential for a range of energy of interest. This range will be taken to be that near thermal energies in the present problem.

To begin with, we shall consider the case in which the pseudo-potential is taken to have the form of a simple square well of depth $u\hbar^2/2m$ and breadth a . In the general case in which the nucleus absorbs neutrons, u will be complex. The relation between u and the phase shift η outside the potential well is found by requiring that the wave function and its derivative be continuous at the boundary of the square well. The corresponding condition is¹⁴

$$\frac{\sin(ua)^{\frac{1}{2}}}{u \cos(ua)^{\frac{1}{2}}} = \frac{\sin(ka + \eta)}{k \cos(ka + \eta)}. \quad (49)$$

If $(ua)^{\frac{1}{2}}$, ka , and η are all small compared with unity, both sides of this equation may be expanded. The resulting equation is

$$\eta = ka^3 u / 3 \quad (50)$$

or

$$u = 3\eta / ka^3. \quad (51)$$

We note from (51) that the product ua^3 , which is proportional to the volume integral of the pseudo-potential is a constant in the present approximation if the cross sections are constant. Hence as long as the pseudo-potential is multiplied by functions which vary very slowly over the potential well, as when the neutron wavelength is long compared with a , the square well may be replaced by a delta-function. In this

approximation the pseudo-potential V_j associated with the j th nucleus can be written in the form

$$V_j = \frac{\hbar^2}{2\pi m} \left(\pm \left[\frac{\sigma_s^j}{4\pi} - k^2 \left(\frac{\sigma_a^j}{4\pi} \right)^2 \right]^{\frac{1}{2}} + \frac{ik\sigma_a^j}{4\pi} \right) \delta(\mathbf{r} - \mathbf{r}_j). \quad (52)$$

It should be noted again that the conditions under which (52) is valid are that η , a , and the wave-length, λ , satisfy the inequality relation

$$\eta/k \ll a \ll \lambda. \quad (53)$$

These conditions stand in contrast with those for the methods employed in the previous sections. In these cases it was only necessary that λ be large compared with η/k .

It is easy to show that the relation (52) is valid even if the original well is not taken to be square, provided the phase shift is sufficiently small. To prove this we note that the left hand side of Eq. (49) is the value of R/R' at the outer edge of the potential barrier, regardless of the form it is assumed to have, where R is r times the radial part of the s wave function, and R' is its derivative. Now R/R' satisfies the equation

$$\frac{d}{dr} \left(\frac{R}{R'} \right) = 1 - \frac{RR''}{R'^2} = 1 + u(r) \frac{R^2}{R'^2}, \quad (54)$$

in which $u(r)$ is $-2m/h^2$ times the pseudo-potential. Since $R/R' = r$ for small phase shifts, it follows that at the outer boundary of the potential ($r = a$)

$$\left(\frac{R}{R'} \right)_{r=a} = a + \int_{r=a} u(r) r^2 dr = a + \frac{1}{4\pi} \int u(r) d\tau.$$

Equating this to the right-hand side of (49) we obtain

$$\frac{\eta}{k} = \frac{1}{4\pi} \int u(r) d\tau. \quad (55)$$

Thus the pseudo-potential can be taken to have the form (52) wherever the conditions (53) are satisfied.

To summarize, we may take the Schrodinger equation inside the crystal to have the form

$$\Delta\psi + k^2\psi = -\alpha\psi, \quad (56)$$

where

$$\alpha = 4\pi \sum_{\nu} \left(\pm \left[\frac{\sigma_{\nu}}{4\pi} - k^2 \left(\frac{\sigma_{\nu}}{4\pi} \right)^2 \right]^{\frac{1}{2}} + ik \frac{\sigma_{\nu}}{4\pi} \right) \times \delta(\mathbf{r} - \mathbf{r}_{\nu}), \quad (57)$$

in which r_{ν} is summed over all atoms in the lattice. It is clear that Eq. (35) is much more general since the only condition on its applicability is that λ be large compared with η/k for all nuclei. Actually, as we shall see below, the results obtained with the use of Eq. (56) and the type of perturbation theory that was employed in connection with Eq. (17) for the index of refraction and the Laue-Bragg diffraction are the same as those found in the previous sections. This indicates that the results obtained with the use of the pseudo-potential are more general than the equations from which they are derived.

We shall now resolve α appearing in (57) into a Fourier series of the form

$$\alpha = \sum_{\mathbf{K}} a_{\mathbf{K}} \exp(i\mathbf{K} \cdot \mathbf{r}), \quad (58)$$

in which the $a_{\mathbf{K}}$ are constants and the vectors \mathbf{K} extend over the reciprocal lattice of the crystal. It is readily found from (57) that

$$a_{\mathbf{K}} = 4\pi n_0 \sum_j \xi(j) \exp(-i\mathbf{K} \cdot \mathbf{r}_j), \quad (59)$$

where n_0 is the density of unit cells, \mathbf{r}_j is summed over the atoms in the unity cell, and $\xi(j)$ is defined by Eq. (36).

As previously, we may now solve Eq. (56) with a function of the form

$$\psi = \exp(i\mathbf{k}' \cdot \mathbf{r}) \left(\sum_{\mathbf{K}} c_{\mathbf{K}} \exp(i\mathbf{K} \cdot \mathbf{r}) \right), \quad (60)$$

in which the $c_{\mathbf{K}}$ are constants, and \mathbf{k}' is an unknown vector. When (59) and (60) are substituted in Eq. (56) and the coefficients of each term $e^{i\mathbf{K} \cdot \mathbf{r}}$ are equated, we obtain the following family of equations.

$$\sum_{\mathbf{K}'} a_{\mathbf{K}-\mathbf{K}'} c_{\mathbf{K}'} = [(\mathbf{k}' + \mathbf{K})^2 - k^2] c_{\mathbf{K}}. \quad (61)$$

Again there are two interesting cases to treat.

(a) No Bragg Reflection

In this case c_0 is larger than all other values of $c_{\mathbf{K}}$ and Eqs. (61) may be written

$$\begin{aligned} a_0 c_0 &= [\mathbf{k}'^2 - k^2] c_0; \\ a_{\mathbf{K}} c_0 &= [(\mathbf{k}' + \mathbf{K})^2 - k^2] c_{\mathbf{K}}. \end{aligned} \quad (62)$$

The first equation leads to (41) when the relation (59) is employed, whereas the second reduces to Eq. (37) when Eq. (40) is used to express $a_{-1}(j)$ in (37) in terms of $\xi(j)$.

(b) Near Bragg Reflection

When $(\mathbf{k}' + \mathbf{K}')^2$ is near to \mathbf{k}'^2 for a particular value \mathbf{K}' of \mathbf{K} , the constants c_0 and $c_{\mathbf{K}'}$ become comparable. There are then two equations analogous to the first of (62), namely

$$\begin{aligned} a_0 c_0 + a_{-\mathbf{K}'} c_{\mathbf{K}'} &= [\mathbf{k}'^2 - k^2] c_0; \\ a_{\mathbf{K}'} c_0 + a_0 c_{\mathbf{K}'} &= [(\mathbf{k}' + \mathbf{K}')^2 - k^2] c_{\mathbf{K}'}. \end{aligned} \quad (63)$$

These equations are identical in form with (47) so that the allowed values of \mathbf{k}' are identical in the two cases. Moreover, it is readily found that when the value (46) for $a_{-1}(j)$ is substituted into Eq. (37) for $c_{\mathbf{K}}$, the result is identical with the equation for $c_{\mathbf{K}}$ obtained from (61), namely

$$[(\mathbf{k}' + \mathbf{K})^2 - k^2] c_{\mathbf{K}} = a_{\mathbf{K}} c_0 + a_{\mathbf{K}-\mathbf{K}'} c_{\mathbf{K}'}. \quad (64)$$

Hence the method based on the pseudo-potential yields the results we obtained previously.

A close comparison between Eqs. (63) and the corresponding equations for x-ray diffraction²⁰ shows that the function $\alpha/4\pi k^2$ can be regarded as the equivalent of the complex electrical polarizability of the medium in which the x-rays are diffracted. In a region of wave-length not too close to an absorption band, the polarizability $\mu(\mathbf{r})$ for a monatomic substance is given by the equation

$$\mu(\mathbf{r}) = (e^2 Z / mc^2 k^2) \rho_e(\mathbf{r}), \quad (65)$$

in which $\rho_e(\mathbf{r})$ is the electron charge distribution, which is normalized to unity for a single atom; Z is the atomic number; m is the electronic mass; and c is the velocity of light. This is to be contrasted with $\alpha/4\pi k^2$ which in a non-absorbing monatomic substance is

$$\frac{\alpha}{4\pi k^2} = \pm \frac{1}{k^2} \left(\frac{\sigma_s}{4\pi} \right)^{\frac{1}{2}} \rho(\mathbf{r}), \quad (66)$$

where $\rho(\mathbf{r})$ is the density of scattering centers. Since Ze^2/mc^2 is of the same order of magnitude as $(\sigma_s/4\pi)^{\frac{1}{2}}$ in regions not too close to resonance peaks, it follows that we may expect nearly quantitative agreement for the two cases.

This close analogy is not as valid in the vicinity of absorbing regions as it is the case of pure scattering. Absorption cross sections of the order of 10^{-20} cm² or larger are very common in the case of x-rays, particularly when the material contains heavy elements. Similar large absorption cross sections occur for thermal neutrons only in crystals containing cadmium, gadolinium, or one of the other elements possessing a resonance peak in the thermal region.

6. APPLICATION OF EQUATIONS FOR LAUE-BRAGG SCATTERING

We shall now apply the results of diffraction theory to a few typical problems of interest in connection with neutron diffraction, restricting our attention to cases in which absorption is negligible, unless the contrary is stated.

(1) Depth of Penetration

In the conventional treatments of the diffraction of x-rays, it is customary to distinguish two cases, namely that of a "thin" crystal and that of a "thick" crystal. Only a small portion of the incident wave is diffracted before passing through the crystal in the first case, whereas the wave is diffracted a number of times in the second case. The conditions on the thickness t_0 determining whether or not the crystal is to be regarded as thin or thick are, respectively, that the quantity A defined by the equation

$$A = a_K |t_0| / 2k (|\gamma_0| |\gamma_K|)^{\frac{1}{2}} \quad (67)$$

be much smaller or much larger than unity (cf. Zachariasen, Eq. (3.140)). Here \mathbf{K} is the reciprocal vector for the diffracting plane; γ_0 is the cosine of the angle between the direction of the incident wave and the normal to the surface through which the wave enters the crystal; γ_K is the cosine of the angle the diffracted ray makes with the same normal; and the other quantities are as defined previously. The two cosines are equal in magnitude in the case in which the incident wave undergoes Bragg-reflection from crystallographic planes that are parallel to the surface plane of the specimen.

Thus the reciprocal of the coefficient of t_0 in Eq. (67) provides a measure of the depth to which a wave penetrates before being attenuated to the maximum degree. This distance, which we

shall designate as d_K is

$$d_K = (2k/|a_K|) (|\gamma_0| |\gamma_K|)^{\frac{1}{2}}. \quad (68)$$

In the case of a monatomic substance this is

$$d_K = (k/2\pi n_0) (4\pi/\sigma_s)^{\frac{1}{2}} (|\gamma_0| |\gamma_K|)^{\frac{1}{2}}.$$

This is closely comparable with the corresponding distance for x-rays for²⁰ all ordinary values of σ_s , as we might expect from what has been said previously. For example, if we take

$$k = 3.5 \cdot 10^8 \text{ cm}^{-1}, \quad n_0 = 3 \times 10^{22} \text{ cm}^{-3},$$

$$\text{and } \sigma_s/4\pi = 10^{-24} \text{ cm}^2,$$

and

$$(|\gamma_0| |\gamma_K|)^{\frac{1}{2}} = 0.2,$$

we find

$$d = 3.7 \times 10^{-4} \text{ cm}.$$

As a more specific example let us consider the case of thermal neutrons diffracted by the (100) faces of magnesium oxide, which possesses the sodium-chloride lattice. We shall take the neutron energy to be $3k_0T/2$ (k_0 is Boltzmann's constant, and T will be chosen as 300°K) for which the neutron wave number k is 4.57×10^8 cm⁻¹. The most reliable values for the cross sections appear to be $\sigma_s(Mg) = 4.0 \times 10^{-24}$ cm² and $\sigma_s(0) = 4.0 \times 10^{-24}$ cm². If we assume that both nuclei scatter with the same phase $a_{100} = 7.6 \times 10^{11}$ cm⁻². Since $(|\gamma_0| |\gamma_K|)^{\frac{1}{2}} = 0.653$, we obtain

$$d_{100} = 7.84 \times 10^{-4} \text{ cm}.$$

It is to be noted that in this case a_{100} would vanish to a first approximation if the phases of the scattering nuclei were opposite since the cross sections are almost identical. In fact the cancellation would occur for all orders of reflection from the (100) planes since

$$a_{N00} = 8\pi n_0 \left[\pm \left(\frac{\sigma_s(Mg)}{4\pi} \right)^{\frac{1}{2}} \pm \left(\frac{\sigma_s(0)}{4\pi} \right)^{\frac{1}{2}} \right] \times (1 + \cos N\pi). \quad (69)$$

If the (100) reflections vanish, it is still possible to obtain reflections from the (111) planes since

$$a_{NNN} = 4\pi n_0 \left[\pm \left(\frac{\sigma_s(Mg)}{4\pi} \right)^{\frac{1}{2}} \pm \left(\frac{\sigma_s(0)}{4\pi} \right)^{\frac{1}{2}} \right] \times (\cos 3N\pi + 3 \cos N\pi). \quad (70)$$

This close correspondence between the penetration distance for the two types of radiation shows us that the upper limit on the size of mosaic blocks for which primary extinction is negligible for a strong x-ray reflection is about the same for neutrons.

(2) The Intensity of Reflection from a Crystal

Let us now consider the intensity of a reflected neutron beam under the somewhat idealized conditions we are discussing in the present treatment. To begin with, let us assume that a polychromatic beam impinges upon a perfect crystal and makes an angle with the plane of the crystal. We shall assume that this plane coincides with the planes responsible for diffraction so that the situation is that typical of Bragg reflection. In addition we shall assume that the number of neutrons per second in the beam having wavelength lying in the range from λ to $\lambda + d\lambda$ is given by $\nu_\lambda d\lambda$. The incident beam will possess a small angular divergence so that the wave-length which is diffracted with maximum effectiveness will differ for each ray of which the beam is composed. We shall assume that the angular divergence is sufficiently small that the distribution function ν_λ does not vary appreciably over the range of wave-lengths which are diffracted most efficiently.

According to Zachariasen (cf. Eqs. (3.152) and (3.156)) the integrated intensity N_R which is reflected from the crystallographic plane associated with \mathbf{K} for a *thick* crystal is

$$N_R = (\pi |a_{\mathbf{K}}| \lambda_B / 2k^2 \sin^2 \theta_B) \nu_\lambda(\lambda_B), \quad (71)$$

in which λ_B satisfies the equation

$$\lambda_B / 2\pi = 1/k_B = 2 \sin \theta_B / |\mathbf{K}|. \quad (72)$$

N_R represents the net neutron flux per unit time across the entire area of the reflected beam. If the distribution spectrum of the incident beam is expressed in terms of wave number instead of wave-length, Eq. (71) is replaced by

$$N_R = \pi |a_{\mathbf{K}}| \nu_k(k) / 2k \sin^2 \theta_B, \quad (73)$$

where

$$\nu_k(k) dk = \nu_\lambda(\lambda) d\lambda. \quad (74)$$

If the incident neutron beam has a net intensity N_I neutrons per second and is derived from

a thermal source by collimation, the distribution function ν_k is given by

$$\nu_k = \frac{2N_I}{k} \left(\frac{\hbar^2 k^2}{2mk_0 T} \right)^2 \exp(-\hbar^2 k^2 / 2mk_0 T), \quad (75)$$

in which k_0 is Boltzmann's constant, T is the neutron temperature; and the other quantities are as designated in previous sections. Using Eq. (73) we find

$$\begin{aligned} \frac{N_R}{N_I} &= \frac{\pi |a_{\mathbf{K}}|}{k^2 \sin^2 \theta_B} \left(\frac{\hbar^2 k^2}{2mk_0 T} \right)^2 \exp(-\hbar^2 k^2 / 2mk_0 T) \\ &= \frac{\pi |a_{\mathbf{K}}|}{k^2 \sin^2 \theta_B} \left(\frac{\epsilon}{k_0 T} \right)^2 e^{-\epsilon/k_0 T} \end{aligned} \quad (76)$$

in which ϵ is the neutron energy. If we set $\epsilon = \frac{3}{2} k_0 T$, we find that (76), which measures the effective reflectivity of the crystal, is of the order of 10^{-5} for a typical monatomic scatterer. Actually the reflectivity will be this small only for a very perfect crystal. We may expect values between 10 and 100 times larger for a moderately imperfect crystal containing mosaic blocks which are tilted relative to one another.

It is interesting to compute N_R/N_I for MgO. We shall consider second-order diffraction from the 100 planes and first-order diffraction from 111 planes. Here $k = 4.57 \times 10^8 \text{ cm}^{-1}$, $|a_{100}| = |a_{111}| = 7.61 \times 10^{11} \text{ cm}^{-2}$, $\theta_{B100} = 40^\circ 45'$; $\theta_{B111} = 16^\circ 26'$; and we find $(N_R/N_I)_{100} = 1.35 \times 10^{-5}$, $(N_R/N_I)_{111} = 7.10 \times 10^{-5}$.

(3) Influence of Mosaic Structure

In a single crystal x-ray spectrometer, the mosaic structure seriously interferes with the resolving power in cases in which the highest detail is required, for example when it is desired to resolve the natural breadth of emission lines. The corresponding problem is probably not as grave for a neutron spectrometer, at least from present standards. For example, if we require an energy resolution ΔE in the energy range near E the allowed angular spread of the beam must be less than

$$\Delta\theta = (\Delta E/E)(1/2 \cot\theta), \quad (77)$$

in which θ is the angle at which observations are made. When θ is about 5×10^{-2} , which is a

typical small value that would be of interest in the diffraction of thermal neutrons from a crystal such as calcite, we find that an energy resolution of 5×10^{-3} , which would be of high quality compared to present standards of resolution, can be achieved with an angular divergence of about 10^{-4} radian or about 0.4 second of arc. Thus both the degree of divergence of the neutron beam and the degree of variation of the orientation of mosaic blocks could be considerably larger for the case of neutrons than for x-rays for "good" results.

The quantitative importance of mosaic structure in determining the reflectivity of a crystal can be estimated approximately in the following fashion. If the crystal were perfect and were thick compared to d_K given by Eq. (69), its reflectivity would be unity for monochromatic waves incident at the Bragg angle for a range of angular deviation ω given by (cf. Zachariasen (3.151) and (3.155))

$$\omega = 1.15 |a_K| / k^2 \sin 2\theta_B. \quad (78)$$

This width is of the order of a second of arc for a typical case. In the case of magnesium oxide we find that when $k = 4.57 \times 10^8 \text{ cm}^{-1}$, $\omega = 0.875''$ for second-order reflection from the (100) planes, and $\omega = 1.59''$ for first-order reflection from (111) planes. The net reflectivity for a polychromatic beam is given by Eqs. (71) and (73).

The angular distribution of mosaic blocks relative to perfect orientation will, in the simplest case, be given by a distribution function of the form

$$f = \exp[-\Delta_a^2 / \eta^2] / (2\pi)^{1/2} \eta, \quad (79)$$

in which Δ_a is the angular deviation from the mean, and η measures the breadth of the distribution. η is very small, of the order of a few seconds of arc or less, in a few natural crystals. However, in most crystals η is much wider, of the order of a minute of arc or more.

In the case of a thick crystal (i.e., a calcite crystal 1 cm thick) we may expect to obtain unit reflectivity over a range of angle equal to η instead of over the range ω given by Eq. (78) if we assume that absorption is not large for the thickness of the specimen. Thus in the cases of interest to us, the reflectivity is equal to (76) times η/ω . The reflectivity then may be of the

order of 10^{-4} or larger instead of the value given by Eq. (76).

In the corresponding problem for x-rays, the absorption of the incident beam is usually so great that the simple reasoning of the previous paragraph cannot be employed. It is readily shown that when the absorption is great the quantity multiplying (76) is (cf. Zachariasen (4.40))

$$\pi(\sigma_s/4\pi)^{1/2} / k\sigma_a, \quad (80)$$

provided (Zachariasen (4.34))

$$\frac{2\pi^2 n_0}{(2\pi)^{1/2} k^3 \sin 2\theta_B} \frac{1}{\sigma_a} \ll \eta, \quad (81)$$

in which η is expressed in radians. The condition (81) is generally not met for neutrons in the cases of interest. For example, η is of the order of 3×10^{-4} , whereas the expression on the left-hand side is of the order of 10^{-2} . The approximation (81) becomes valid if σ_a is about 10^3 times σ_s . However (80) is then near unity.

7. ADDITIONAL INFLUENCE OF DISORDERING UPON THE INTENSITY OF BRAGG REFLECTION

We have seen in the previous section that the angular disorientation of the mosaic blocks of which real single crystals are composed increases the reflectivity of a specimen for polychromatic radiation by increasing the range of angles of incidence for which a monochromatic component can be reflected. Most other types of crystalline disorder decrease the reflectivity. Two disorders of this type which should be mentioned are the disordering arising from the thermal (and zero point) oscillations of the atoms and the disordering which can occur when the atoms are polyisotopic.

The influence of atomic oscillation has been discussed in detail by Weinstock¹⁰ for a monoatomic lattice in the case in which primary extinction is negligible, that is, in the case in which each mosaic is so small that only a small fraction of the monochromatic radiation which satisfies the Bragg condition is scattered. In this case the reflectivity is reduced from the value for a crystal in which the atoms are at rest by a factor

$$e^{-2W} \quad (82)$$

where

$$W = \frac{3\hbar^2 K^2}{2Mk_0\theta} \left[\frac{1}{4} + \left(\frac{T}{\theta} \right)^2 Q \left(\frac{\theta}{T} \right) \right] \quad (83)$$

with

$$Q(z) = \int_0^z \frac{\beta d\beta}{e^\beta - 1}.$$

Here \mathbf{K} is the vector in the reciprocal lattice associated with the reflecting plane; θ is the Debye characteristic temperature; k_0 is Boltzmann's constant; and M is the mass of the atoms of which the lattice is composed. It is readily seen that W is of the order of m/M for thermal neutrons when T is near θ and θ is near room temperature, as is the case for the crystals with comparatively large elastic constants that would normally be used in a neutron spectrometer. m is the neutron mass. Thus the factor (82) is usually very close to unity and will not influence the conclusions drawn previously in an appreciable way.

We shall discuss the influence of isotopes for a monatomic lattice since the results can readily be generalized. Let us consider a small crystal upon which is incident a wave possessing the wave number vector \mathbf{k} . The quantity which determines the intensity of reflection in the direction for which the wave number vector is \mathbf{k}' is

$$\sum_j f_j \exp[i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{r}_j], \quad (84)$$

in which \mathbf{r}_j is the position of the j th atom in the lattice, and f_j is proportional to $\pm(\sigma_s^j)^{\frac{1}{2}}$. If the element is monoisotopic, the factor f_j is independent of j and may be removed from the summation. The square of the absolute value of the resulting summation may then be approximated by a sum of delta-functions with constant multipliers which are centered about the points for which $\mathbf{k}-\mathbf{k}'=\mathbf{K}$, where as before the \mathbf{K} are the reciprocal vectors. On the other hand if two or more isotopes are present, and if the values of f_i for these isotopes are different, the value of (84) in a given direction for which $\mathbf{k}-\mathbf{k}'=\mathbf{K}$ is

$$\sum_j f_j = N\bar{f}, \quad (85)$$

where N is the number of atoms, and \bar{f} is the average value of f_j . This average is taken in such a way that each isotope is weighted with its abundance and due recognition is taken of the sign before $(\sigma_s^j)^{\frac{1}{2}}$. Thus even when the values of

σ_s^j are nearly identical for the isotopes the reflectivity may be decreased, provided the major isotopes are present in comparable abundance and have opposite phases. Conversely the isotopic mixture will be unimportant if all isotopes have nearly equal cross sections and the same phases.

It is readily shown that the distribution of the scattered radiation is described by a set of delta-functions peaked at positions for which $\mathbf{k}-\mathbf{k}'=\mathbf{K}$ upon which is superimposed a diffuse isotopic component of scattered radiation. The diffuse component is isotopic only when the isotopes are distributed at random among the various lattice sites. To demonstrate this, we set

$$f_j = f + \delta f_j, \quad (86)$$

where $\sum_j \delta f_j = 0$. We may then write (84) in the form

$$\bar{f} \sum_j \exp[i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{r}_j] + \sum_j \delta f_j \exp[i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{r}_j]. \quad (87)$$

The first sum is sharply peaked at $\mathbf{k}-\mathbf{k}'=\mathbf{K}$, as when the δf_j are zero. Hence any diffuse scattering must be described by the second term. The square of the absolute value of this term is

$$\sum_{j,p} \delta f_j \delta f_p^* \exp[i(\mathbf{k}-\mathbf{k}') \cdot (\mathbf{r}_j - \mathbf{r}_p)]$$

which may also be written in the form

$$\sum_{j,s} \delta f_j \delta f_{j+s}^* \exp[i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{r}_s], \quad (88)$$

where $\mathbf{r}_s = \mathbf{r}_j - \mathbf{r}_{j+s}$. The summation for fixed s may be separated from that over j , that is the summation may be written as

$$\sum_s \exp[i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{r}_s] \sum_j \delta f_j \delta f_{j+s}^*. \quad (89)$$

When the isotopes are randomly distributed, the sum over j vanishes if s is not zero since for each particular value of δf_j that occurs f_{j+s} will range over all values at random and the resultant is zero. When s vanishes the second sum is a finite constant which is, of course, independent of s and may be removed entirely to the left of the summation over s . In this case $\mathbf{r}_s = 0$ so that the expression for the scattered radiation is independent of $(\mathbf{k}-\mathbf{k}')$. Thus in addition to the Laue-Bragg scattering there is an isotropically distributed diffuse component.

If the isotopes were correlated, $\sum_i \delta f_i \delta f_{i+s}^*$ would be a function of s which is different from zero when $s \neq 0$ and diffuse, but anisotropic scattering would occur. This scattering would resemble closely the type of diffuse x-ray scattering observed for liquids. There is, of course, no reason for expecting a correlation between the positions of isotopes in the heavier solids.

SUMMARY

1. The equations for the elastic scattering of neutrons by a single crystal are examined in detail in the approximation in which inelastic scattering is neglected. This procedure is equivalent to treating the case of a perfectly ordered crystal of rigidly fixed atoms by methods analogous to those employed in the dynamical theory of x-ray scattering. Three methods of deriving the results are employed: The first, which is the most rigorous method takes account of the singularity produced on the wave function in the region near but just outside the nucleus in the general case in which the nucleus both scatters and absorbs. This method is accurate as long as the square of the wave-length is large compared with the cross sections. The second method is based on the use of the cellular approximation that has found wide use in the treatment of electron wave functions in solids. It is applied only when the absorption cross section vanishes, but is then as accurate as the first method. The third method is based on the use of a pseudo-potential, which replaces the actual potential between neutron and nucleus in the Schroedinger equation. This method, which was first used by Fermi, can be justified only when the wave-length is large compared with the diameter of the pseudo-potential well, which must in turn be large compared with the "displacement distance."

2. It is shown that the index of refraction n and the extinction coefficient $n\kappa$ are given by the following equations when the wave-length and direction of incidence of the neutrons are not such that the Bragg conditions are satisfied:

$$n = 1 + n_0 \sum_j \pm \frac{2\pi}{k^2} \left(\frac{\sigma_s^j}{4\pi} - k^2 \left(\frac{\sigma_a^j}{4\pi} \right)^2 \right)^{\frac{1}{2}},$$

$$n\kappa = n_0 \sum_j \frac{\sigma_a^j}{2k}.$$

These are generalizations of a similar set of equations derived by Fermi. Here n_0 is the number of unit cells per unit volume of the crystal; k is the wave number, which is equal to $2\pi/\lambda$, where λ is the wave-length; σ_s^j is the scattering cross section of the j th atom in the unit cell; and σ_a^j is the corresponding absorption cross section. The signs which appear before the radicals in the first equation are related to the sign of the shift in phase of the wave scattered by the corresponding atom. These equations may be used for highly disordered materials in the case in which the wave-length is so large that the material is homogeneous over a distance comparable to the wave-length. In this case n_0 is to be taken as the number of chemical molecules per unit volume, and the summations extend over the constituents of the chemical molecule. It is interesting to note that the second equation can be written in the form

$$n\kappa = \lambda/2L_a,$$

in which L_a is the mean free path for absorption in the material.

3. A crystal will reflect neutrons which strike it at grazing incidence provided the index of refraction is less than unity. This is to be expected from the general laws of optics and has been pointed out previously by Fermi in connection with his derivation of the equations discussed in paragraph 2. The reflectivity for a monochromatic beam of neutron is given by the equation

$$R = \left[\frac{1 - (1 - 2\mu/\varphi^2)^{\frac{1}{2}}}{1 + (1 + 2\mu/\varphi^2)^{\frac{1}{2}}} \right]^2$$

in which φ is the angle that the beam makes with the reflecting surface and $\mu = 1 - n$. Absorption influences the reflectivity only when there is a resonance level in the thermal region.

The depth of penetration of the ray reflected at grazing incidence is given by the equation

$$d = \lambda/2\pi(2\mu)^{\frac{1}{2}}.$$

This distance is of the order of magnitude 100λ for a typical case.

The experiments carried out by Fermi, Zinn, Marshall, Borst, and Wollan seem to show that the index of refraction is usually less than unity.

It is pointed out that this observation may be no more surprising than the fact that most transparent optical media have an index greater than unity in the visible portion of the spectrum.

4. It is found that there is a very close correlation between the diffraction of neutrons and of x-rays which are polarized in the direction normal to the plane of incidence. This correlation is almost quantitative in the non-absorbing cases because the cross section for Thomson scattering, which is related to the classical electron radius, is almost equal to the typical cross section for nuclear scattering. The absorption cross section for neutrons is comparable to the corresponding typical cross section for x-rays only in the special case in which one of the nuclei present possesses a resonance level in the thermal region of the energy spectrum, that is, when elements like cadmium or gadolinium are present. Only in cases of this type does the absorption of neutrons affect the properties of a material for diffracting neutrons.

5. The depth of penetration of a diffracted wave which satisfies the Laue-Bragg condition is determined for a perfect crystal. The result is

$$d = 2k/|a_{\mathbf{K}}| \sin\theta_B$$

in which θ_B is the Bragg angle and

$$a_{\mathbf{K}} = n_0 \sum_j 4\pi \left[\pm \left(\frac{\sigma_s^j}{4\pi} - k^2 \left(\frac{\sigma_a^j}{4\pi} \right)^2 \right)^{\frac{1}{2}} + i \frac{k\sigma_a^j}{4\pi} \right] \times \exp(-i\mathbf{K} \cdot \mathbf{r}_j).$$

Here all quantities are as in paragraph 2 above, and \mathbf{K} is the reciprocal vector of the lattice that is to be associated with the crystallographic plane from which the incident beam is reflected in the Bragg sense.

$a_{\mathbf{K}}$ plays much the same role in neutron diffraction as the x-ray structure factor does in x-ray diffraction.

In the case of a non-absorbing monatomic substance this equation simplifies to

$$d = \frac{\sin\theta_B (4\pi)^{\frac{1}{2}}}{\lambda n_0 (\sigma_s)^{\frac{1}{2}}}.$$

This distance is of the order of 10^{-4} in typical cases, just as in the case of strongly reflected x-ray beams.

6. The reflectivity R of a perfect single crystal for a stream of thermal neutrons is given by the equation

$$R = \frac{\pi |a_{\mathbf{K}}|^2}{k^2 \sin^2\theta_B} \left(\frac{\epsilon}{k_0 T} \right)^2 e^{-\epsilon/k_0 T}.$$

Here k_0 is Boltzmann's constant, and ϵ is the energy of the neutrons which undergo Bragg reflection for the geometrical arrangement employed. This reflectivity is of the order of 0.001 percent when the angle of incidence is adjusted so that the neutrons at the peak of the thermal distribution function in the incident beam are diffracted.

7. It is pointed out that the reflectivity will be much larger than the equations given in paragraph 6 indicate if the crystal possesses well-developed disorientation of the type in which the mosaic blocks are tilted relative to one another. If the mean spread in angular disorientation is η , the expression for the reflectivity given in the preceding paragraph should be multiplied by a factor η/ω where ω is the rocking angle for which high reflectivity is obtained when a highly collimated monochromatic beam is incident on a perfect crystal near the Bragg angle. ω is of the order of several seconds of arc. This multiplicative factor is to be used only when $\eta/\omega \gg 1$. Thus we see that by selecting a crystal with the proper mosaic structure, it is possible to enhance the reflectivity by a factor of one or two decades.

8. If it is desired to maintain a resolving power that is considered "good" from present standards, that is, an energy resolution of the order of 5×10^{-3} ev for 1 ev neutrons, the mean angular disorientation caused by the mosaic structure must be no more than a few minutes of arc. The angular aperture of the entrance and exit slits of the system should also be no larger than this if the same resolving power is specified.

9. The decrease in intensity of Bragg reflection arising from the thermal oscillations is discussed on the basis of Weinstock's calculations. It is shown that this decrease is not important for crystals which possess high elastic constants, as those used in a neutron spectrometer probably would.

10. It is shown that the reflectivity may be decreased if the atoms in the crystal are polyisotopic and if the isotopes for a given element are present in comparable abundance, possess nearly equal scattering cross sections and opposite phases. More explicitly the effective scattering strength of a given element is proportional to

$$\sum_i \pm g_i (\sigma_s^i)^{\frac{1}{2}},$$

in which g_i is the fractional abundance of the i th isotope, and σ_s^i is its scattering cross section. The contribution from isotopes with opposite phases tend to cancel one another. The presence

of isotopes may also add a diffuse background to the inelastically scattered radiation.

11. It should be emphasized that the present paper does not contain a discussion of the coherent inelastic scattering of neutrons from crystals. This type of scattering actually can be very important in practical cases and can alter some of the qualitative viewpoints which were obtained.

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A Proposed Focusing Cosmic-Ray Telescope

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A magnetic lens which will focus charged particles entering its aperture parallel to the axis can be constructed in the form of a toroidal winding. For an air or iron core toroid, the cross section of the winding is parabolic. If partial iron filling is used, trapezoidal or rectangular cross sections may be employed to produce sharp focusing. The focal length is proportional to the particle momentum, and hence a telescope of this type is also a spectrograph. By using coincidence counters and anticoincidence guard counters for observations, a collimating tube effect can be obtained, permitting full use of the properties of the telescope lens without a background due to particles which do not pass through the lens. There are some advantages to an installation in a deep shaft in the earth having two lenses. With such a device charged and uncharged components can be studied separately.

INTRODUCTION

AS a consequence of Maxwell's equation

$$\text{curl } H = 4\pi i,$$

it is clear that the magnetic field strength inside a long straight solenoid is uniform over the cross section of the solenoid, regardless of the shape of the cross section. If the solenoid is formed into a toroid, H varies inside the cross section as $1/r$, regardless of the shape of the cross section of the toroidal winding.

If a toroidal coil is to serve as a lens to focus a parallel beam of particles of like energies and e/m through the point F (Fig. 1), it is necessary that the radial momenta imparted to the par-

ticles increase directly as r . This can be accomplished in either of two ways.

(1) Air core toroid. Since in an air core toroid the field varies as $1/r$, the width of the cross section must increase as r^2 , in order that the time in which a particle is accelerated radially may compensate the decrease in field strength and yield a radial impulse which is proportional to r . This leads to a toroidal lens having the parabolic shape shown in Fig. 1.

(2) Toroidal lens containing iron. If iron is distributed inside the toroid, and the iron is regarded as being transparent to the particles, several choices of lens design are possible. In this case we must deal with the continuous magnetic