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Neutron diffraction by perfect crystals

C. Stassis
Ames Laboratory-USAEC and Department of Physics, Iowa State University, Ames, Iowa 50010

J. A. Oberteuffer*
Francis Bitter National Magnet Laboratory, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
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The dynamical theory of neutron diffraction has been formulated to include the reflected waves from the boundaries of a crystal. This formulation allows a unified treatment of the neutron optical and diffraction phenomena in crystals. It is shown that the neutron propagation in the crystal is determined by two structure factors characterizing the lattice: the total structure factor and the structure factor of the neutron-spin–neutron-orbit interaction. Diffraction by a parallel crystal plate has been studied in considerable detail. It has been found that for a definite neutron-spin orientation, the diffracted and transmitted beams are modulated by six terms periodic in the thickness of the crystal. The period of the dominant term, in this Pendellösung fringe structure, has been calculated in several cases of experimental importance. If the glancing angle of incidence substantially exceeds the critical angle for total reflection, the results are identical with those obtained by a simple extension, to the neutron case, of the x-ray dynamical theory. The diffraction by a magnetized crystal has been examined in some detail and it is shown that measurement of the Pendellösung periods for the two neutron-spin orientations may be used to determine both the nuclear and magnetic neutron scattering amplitude.

I. INTRODUCTION

The appearance of Pendellösung fringe structure within the Bragg reflection of neutrons from perfect crystals has been observed by Shull.[1] These experiments[1-3] demonstrated that the fringe patterns permit a precise determination of the coherent nuclear scattering amplitude. The quantitative analysis of these, as well as earlier experiments[4] has been performed using a simple generalization of the x-ray dynamical theory. In the present work we examine the dynamical theory of neutron diffraction with particular emphasis on the interference phenomena observed in the diffraction of neutrons by perfect crystals.

The theory of x-ray diffraction has been formulated by Darwin,[5] Ewald,[6] and Laue.[7] A more recent review of the x-ray dynamical theory is given by Batterman and Cole.[8] The dynamical theory of electron diffraction has been developed by Bethe.[9] More recently, after the original investigation of Goldberger and Seitz,[10] similar studies have been undertaken in the diffraction of neutrons by perfect crystals.[11]

In the usual formulation of the dynamical theory the reflected waves from the boundaries of the crystal are neglected. This introduces an artificial separation in the treatment of the optical and diffraction phenomena. In addition one faces the apparent paradox[12] of having more equations, from the boundary conditions, than are necessary for the determination of the integration constants. This formulation of the dynamical theory will be referred to as the two-wave approximation.

In the present work we formulate the neutron dynamical theory to include the reflected waves from the boundaries of the crystal. This formulation allows a unified treatment of the neutron optical phenomena and neutron diffraction by crystals. In our treatment we follow the general lines of Zachariasen's treatment[13] of the x-ray dynamical theory. In Sec. II we formulate the fundamental equations of the dynamical theory. In Sec. III we apply the theory to solve some simple problems of neutron optics. In Sec. IV we examine the diffraction of neutrons by a crystal oriented so that the Bragg condition is nearly satisfied by only one reciprocal-lattice vector. In Sec. V we consider the simple problem of diffraction by a parallel crystal plate. In the same section we briefly consider the diffraction of neutrons by a magnetized crystal. In Sec. VI we summarize our results.

II. EQUATIONS OF THE DYNAMICAL THEORY

We consider the elastic scattering of slow neutrons by a perfect crystal in the presence of an external magnetic field. The incident-neutron wave function ψ_i, in the vacuum, is written

$$\psi_i = e^{i\vec{k}_e \cdot \vec{r}}, \tag{1}$$

where $\vec{k}_e$ is the incident-neutron wave vector. The neutron wave of Eq. (1) is assumed to enter the crystal through a plane boundary, whose orientation will be described by a unit normal vector $\vec{n}$ pointing into the crystal. If the origin of the coordinate system is chosen in the boundary plane, the equation of this plane is simply $\vec{n} \cdot \vec{r} = 0$.

The neutron wave function ψ in the crystal satisfies the Schrödinger equation, which may be written

$$\frac{1}{k_e^2}\nabla^2\psi + \left(1 - \frac{2mV(\vec{r})}{\hbar^2 k_e^2}\right)\psi = 0, \tag{2}$$

where m is the neutron mass, k_e is the magnitude of the incident-neutron wave vector, and $V(\vec{r})$ is the neutron-lattice interaction potential. The neutron-lattice interaction potential may be written as a sum of the individual neutron-atom interaction terms

$$V(\vec{r}) = \sum_a V_a(\vec{r} - \vec{r}_a), \tag{3}$$

where $\vec{r}_a$ denotes the position vector of the nucleus of the ath atom. Since the neutron-lattice interaction potential is invariant under translation by any lattice vector, it can be expanded in a Fourier series

$$\frac{2m}{\hbar^2 k_e^2} V(\vec{r}) = \sum_g e^{-i\vec{g}\cdot\vec{r}} V_g, \tag{4}$$

where the sum is over all vectors $\vec{g}$ of the reciprocal lattice. The Fourier coefficients V_g in Eq. (4) depend on the neutron momentum as a result of the neutron-spin–neutron-orbit term in the interaction potential. They may formally be written

$$V_g = \frac{2mN_c}{\hbar^2 k_e^2}\int_{\text{unit cell}} d\vec{r}\, e^{i\vec{g}\cdot\vec{r}} V(\vec{r}), \tag{5}$$

where N_c denotes the number of unit cells per unit volume of the crystal.

A. Fourier coefficients of the interaction Hamiltonian

The neutron-atom interaction may be written as the sum of the nuclear and electromagnetic interaction terms

$$V_a = V_{a\mathrm{N}} + V_{a\,\mathrm{EM}}. \tag{6}$$

For slow neutrons the nuclear interaction term may be written in the form of the Fermi pseudopotential[14]

$$V_{a\mathrm{N}} = (2\pi\hbar^2/m)(b - ib' + B\vec{I}\cdot\vec{\sigma})\delta(\vec{r} - \vec{r}_a), \tag{7}$$

where

$$B = (b_+ - b_-)/(2I+1) \tag{8}$$

and

$$b' = \sigma_t/2\lambda. \tag{9}$$

In these equations, b is the coherent nuclear scattering length, b' is the imaginary part of the nuclear scattering amplitude, $\vec{I}$ is the spin of the atomic nucleus, $\vec{\sigma}$ is the Pauli matrix, b_+ and b_- are the nuclear scattering lengths for the $I+\frac{1}{2}$ and $I-\frac{1}{2}$ neutron-nucleus states, respectively, σ_t is the total neutron-nucleus cross section and λ is the neutron wavelength. The electromagnetic interaction term may be written

$$V_{a\,\mathrm{EM}} = -\mu\vec{\sigma}\cdot\vec{H} - \frac{\mu\vec{\sigma}\cdot(\vec{E}\times\vec{P})}{mc} - \frac{\mu\hbar}{2mc}(\nabla\cdot\vec{E}), \tag{10}$$

where $\mu = \gamma_n e\hbar/2mc$ is the neutron magnetic moment ($\gamma_n = -1.91$), $\vec{P}$ is the neutron momentum, and $\vec{E}$ and $\vec{H}$ are the electric and magnetic field of the atom, respectively. In Eq. (10) the first term is the well known magnetic dipole interaction,[15] the second term is the neutron spin-neutron orbit interaction,[16] and the third is the Foldy interaction term.[17]

The Fourier coefficients V_g of the neutron-lattice interaction potential, specified by Eqs. (3), (6), (7), and (10), are easily obtained if one notices that they are simply related, by Eq. (5), to the neutron scattering amplitudes. It is easily seen that as a result of the neutron spin-neutron orbit term these coefficients are operators, linear in the momentum of the neutron

$$V_g\left(\frac{\vec{P}}{\hbar}\right) = V_{1g} + V_{2g}\left(\frac{\vec{P}}{\hbar}\right) = \frac{4\pi N_c}{k_e^2}\left[F_{1g} + F_{2g}\left(\frac{\vec{P}}{\hbar}\right)\right]. \tag{11}$$

In Eq. (11), F_{1g} is the structure factor of the lattice associated with the momentum-independent terms of the interaction Hamiltonian and is given by

$$F_{1g} = \sum_i e^{-W_i}[b_i + \gamma_i + \langle B_i I_{ig}\rangle\vec{h}\cdot\vec{\sigma} + p_i(\vec{g})\vec{q}_g\cdot\vec{\sigma} - ib_i']e^{i\vec{g}\cdot\vec{R}_i}. \tag{12}$$

In Eq. (12), e^{-W} is the Debye-Waller factor, $\vec{R}_i$ are the equilibrium positions of the nuclei in the unit cell, and we defined

$$\langle B I_g\rangle = \frac{(b_+ - b_-)(I+1)\mu_{\mathrm{nuc}}H_{\mathrm{nuc}}}{3(2I+1)KT} \tag{13}$$

and

$$\gamma = (\gamma_n e^2/2mc^2)\, Z[1 - f_c(\vec{g})]. \tag{14}$$

In these equations μ_{nuc} is the magnetic moment of the nucleus, H_{nuc} is the magnetic field seen by the nucleus, T is the absolute temperature, Z is the atomic number of the atom, $f_c(\vec{g})$ is the atomic charge form factor, and $p(\vec{g})$ is the magnetic scattering amplitude. The magnetic scattering vector $\vec{q}_g$ is given by

$$\vec{q}_g = \vec{e}_g(\vec{e}_g\cdot\vec{h}) - \vec{h}, \tag{15}$$

with

$$\vec{e}_g = \vec{g}/|\vec{g}|, \tag{16}$$

and $\vec{h}$ is a unit vector along the magnetization in the crystal. The second term in Eq. (11) is the structure factor operator associated with the spin-orbit interaction term and is given by

$$F_{2g}\left(\frac{\vec{P}}{\hbar}\right) = \sum_i e^{-W_i}\left(-2i\gamma_i\vec{\sigma}\cdot\frac{(\vec{P}/\hbar)\times\vec{g}}{g^2}\right)e^{i\vec{g}\cdot\vec{R}_i}, \tag{17}$$

where $g = |\vec{g}|$. Equations (12) and (17) together with Eq. (11) determine the Fourier coefficients of the interaction potential.

B. Crystal wave functions

If $\vec{k}_0$ is an allowed neutron wavevector in the crystal, the corresponding wave function will be the Bloch function

$$e^{i\vec{k}_0\cdot\vec{r}}\, U_{k_0,s}(\vec{r})\,|s\rangle ,$$

where s labels the neutron spin states and $U_{k_0,s}(\vec{r})$ has the translational symmetry of the crystal lattice. Since $U_{k_0,s}(\vec{r})$ is periodic, it can be expanded in a Fourier series

$$U_{k_0,s}(\vec{r}) = \sum_{g'} u_{k_0,g',s} e^{i\vec{g}'\cdot\vec{r}} ,$$

where the summation is over the vectors $\vec{g}'$ of the reciprocal lattice. Thus the neutron wave function corresponding to an allowed wave vector $\vec{k}_0$ may be written

$$\psi_{k_0} = \sum_{g',s} u_{k_0,g',s} e^{i(\vec{k}_0+\vec{g}')\cdot\vec{r}}\,|s\rangle . \tag{18}$$

It is seen that for every allowed neutron wave vector $\vec{k}_0$ the wave function in the crystal consists of a primary plane wave propagating along $\vec{k}_0$ and any number of secondary plane waves whose wavevectors differ from $\vec{k}_0$ by a reciprocal lattice vector. Substituting the wave function of Eq. (18) into the Schrödinger equation (2), the coefficients $u_{k_0,g',s}$ are found to be determined by the following set of algebraic equations:

$$\left(1 - \frac{(\vec{k}_0+\vec{g}')^2}{k_e^2}\right) u_{k_0,g',s} - \sum_{g} V_g(\vec{k}_0+\vec{g}')\, u_{k_0,g+g',s} = 0. \tag{19}$$

The allowed neutron waves propagating in the crystal are then determined by Eq. (19) and the boundary conditions. The coefficients $u_{k_0,g',s}$ are negligibly small unless the corresponding resonance factors $[1 - (\vec{k}_0+\vec{g}')^2/k_e^2]$ are small. That is, only waves whose wave vectors nearly satisfy the Laue vector equation have an appreciable magnitude.

The allowed neutron wave vectors $\vec{k}_0$ in the crystal are determined from the secular equation associated with Eqs. (19). The solution of the secular equation is considerably simplified by taking into account the additional restrictions imposed on the allowed neutron wave vectors by the boundary conditions at the entrance surface of the crystal. The boundary conditions at the entrance plane $\vec{n}\cdot\vec{r} = 0$ require the continuity of the wave function and its gradient. Since the neutron wave function in the vacuum as well as in the crystal consists of plane waves, the continuity of the wave function can be assured only if the exponentials agree at every point in the plane $\vec{n}\cdot\vec{r} = 0$: the tangential components of the various wavevectors must be the same. Consequently, the allowed wave vectors $\vec{k}_0$ in the crystal may be written

$$\vec{k}_0 = \vec{k}_e + \Delta\vec{n} . \tag{20}$$

It follows that the tangential components of the wave vectors of the secondary waves differ from the tangential component of $\vec{k}_e$ by the tangential component of a reciprocal-lattice vector. It should be pointed out that the continuity of the wave function at the entrance boundary of the crystal and Eq. (20) assure the continuity of the tangential component of the gradient of the wave function. Thus the boundary conditions at the entrance surface of the crystal are reduced to the continuity of the wave function and its normal derivative.

Using Eq. (20), the secular equation that determines the allowed wave vectors $\vec{k}_0$ in the crystal is reduced to an algebraic equation in Δ. In fact it is easily seen that

$$1 - k_0^2/k_e^2 = -2\delta - \frac{\delta^2}{\gamma_e^2} \tag{21}$$

and

$$1 - (\vec{k}_0+\vec{g})^2/k_e^2 = -(2/b_1)\delta - \delta^2/\gamma_e^2 - \alpha , \tag{22}$$

where, using Zachariasen's notation,[13] we defined

$$\delta = \Delta\gamma_e/k_e , \tag{23}$$

$$1/b_1 = [\vec{n}\cdot(\vec{k}_e+\vec{g})]/k_e\gamma_e , \tag{24}$$

$$\alpha = (g^2 + 2\vec{k}_e\cdot\vec{g})/k_e^2 , \tag{25}$$

and

$$\gamma_e = \vec{k}_e\cdot\vec{n}/k_e . \tag{26}$$

The potential coefficients in Eqs. (19) depend on the vector $\vec{k}_0\times\vec{g}/g^2$, which may also be expressed in terms of the dimensionless parameter δ,

$$\vec{k}_0\times\vec{g}/g^2 = [(\vec{k}_e\times\vec{g})/g^2](1 + y\delta) , \tag{27}$$

where

$$y = \frac{k_e}{\gamma_e}\frac{(\vec{n}\times\vec{g})\cdot(\vec{k}_e\times\vec{g})}{|\vec{k}_e\times\vec{g}|^2} . \tag{28}$$

Using Eqs. (21), (22), and (27) the coefficients of Eqs. (19) may be expressed in terms of δ. The allowed values of δ, or what is equivalent, the allowed wave vectors $\vec{k}_0$, are obtained from the secular equation associated with Eqs. (19). Once the allowed wave vectors $\vec{k}_0$ have been determined, the amplitudes of the various plane waves propagating in the crystal (and in the vacuum) are determined from Eqs. (19) and the boundary conditions.

In the following sections of this paper we will examine two simple problems of considerable experimental interest. In the first we will assume that the direction of incidence is such that the Bragg

condition is not satisfied by any reciprocal lattice vector of the crystal. In this case, only primary waves are of appreciable magnitude and the crystal behaves like an isotropic medium. In the second we will assume that the direction of incidence is such that the Bragg condition is nearly satisfied by only one reciprocal lattice vector $\vec{G}$. In this case for every allowed wave vector $\vec{k}_0$, only waves propagating along $\vec{k}_0$ and $\vec{k}_0+\vec{G}$ are of appreciable magnitude.

III. NEUTRON OPTICS

If the direction of incidence is such that no reciprocal lattice vector satisfies the Bragg condition, only the amplitude $u_{k_0,0,s}$ is of appreciable magnitude and Eqs. (19) reduce to

$$(1-k_0^2/k_e^2-V_{0s})u_{k_0,0,s}=0\ . \tag{29}$$

Note that $V_{0s}=V_{10s}$, since the spin-orbit amplitude vanishes in the forward direction. Using Eq. (21), the secular equation for a definite neutron spin state may be written

$$\delta^2+2\gamma_e^2\delta+\gamma_e^2V_{10}=0\ , \tag{30}$$

where the subscript s is omitted for simplicity. The roots of this equation are

$$\delta_\pm=-\gamma_e^2(1\pm\beta)\ , \tag{31}$$

where

$$\beta=(1-V_{10}/\gamma_e^2)^{1/2}\ . \tag{32}$$

Thus there are two allowed primary wave vectors

$$\vec{k}_{0\pm}=\vec{k}_e-k_e\gamma_e(1\pm\beta)\vec{n}\ , \tag{33}$$

and the general solution for the neutron wave function in the crystal is

$$\psi=C_1e^{i\vec{k}_{0+}\cdot\vec{r}}+C_2e^{i\vec{k}_{0-}\cdot\vec{r}}\ , \tag{34}$$

where C_1, C_2 are constants to be determined from the boundary conditions.

A. Semi-infinite crystal

We examine first the case of a semi-infinite crystal limited by the plane $\vec{n}\cdot\vec{r}=0$. The neutron wave function in the vacuum is written

$$e^{i\vec{k}_e\cdot\vec{r}}+\sqrt{r}\,e^{i\vec{k}'_e\cdot\vec{r}}\ , \tag{35}$$

where r is the reflectivity of the crystal and $\vec{k}'_e$ the wave vector of the reflected wave. Since the tangential components of the incident and reflected wave vectors are equal and $|\vec{k}'_e|=|\vec{k}_e|$, it follows that $\vec{k}'_e\cdot\vec{n}=-\vec{k}_e\cdot\vec{n}$. From the two possible neutron waves of Eq. (34) only the second satisfies the boundary condition at infinity ($\vec{k}_0\cdot\vec{n}>0$).

The amplitudes of the reflected and refracted waves are determined from the boundary conditions at the plane $\vec{n}\cdot\vec{r}=0$,

$$1+\sqrt{r}=C_2,\quad 1-\sqrt{r}=\beta C_2\ . \tag{36}$$

Thus, the reflectivity and the amplitude of the refracted wave are given by

$$r=|(1-\beta)/(1+\beta)|^2 \tag{37}$$

and

$$|C_2|^2=|2/(1+\beta)|^2\ . \tag{38}$$

It is seen that total reflection of the neutrons occurs for $\beta=0$, or for a direction of incidence such that

$$\gamma_e^2=V_{10}\ . \tag{39}$$

For $\gamma_e>V_{10}$ the refracted wave is exponentially attenuated and the penetration depth E is given by

$$E=1/k_e\gamma_e|\beta|\ . \tag{40}$$

These results may be written in a familiar form by introducing the index of refraction n and the glancing angle of incidence $\theta=\frac{1}{2}\pi-\arccos\gamma_e$. Since by definition $n\equiv k_0/k_e$, the secular equation gives

$$n^2=1-V_{10}=1-\frac{\lambda^2}{\pi}\times\sum_i N_i[b_i\mp p_i(0)\pm\langle B_i I_{iz}\rangle-ib'_i]\ , \tag{41}$$

where N_i is the number of atoms of the ith type per unit volume. Using Eqs. (37) and (40) the reflectivity and penetration depth may be expressed in terms of n and θ,

$$r=\left(\frac{(n^2-\cos^2\theta)^{1/2}-\sin\theta}{(n^2-\cos^2\theta)^{1/2}+\sin\theta}\right)^2\ , \tag{37'}$$

$$E=\lambda/2\pi(n^2-\cos^2\theta)^{1/2}\ . \tag{40'}$$

The critical glancing angle θ_c for total reflection of the neutrons is obtained from Eq. (39),

$$\cos\theta_c=n\ . \tag{39'}$$

It is seen that the amplitude of the reflected wave is unity for $\theta\le\theta_c$ and drops sharply for $\theta\ge\theta_c$. For an incident wavelength of 1 Å and a typical scattering amplitude of 10^{-12} cm the Fourier coefficient V_{10} is of the order of 10^{-6}. Thus the corresponding critical glancing angle is of the order of a few minutes of arc.

B. Parallel crystal plate

We examine next the case of a parallel crystal plate limited by the planes $\vec{n}\cdot\vec{r}=0$ and $\vec{n}\cdot\vec{r}=t$. In the vacuum the neutron wave function is written

$$e^{i\vec{k}_e\cdot\vec{r}}+Re^{i\vec{k}'_e\cdot\vec{r}}\quad\text{for } \vec{n}\cdot\vec{r}<0$$

and

$$C_3e^{i\vec{k}_e\cdot\vec{r}}\quad\text{for } \vec{n}\cdot\vec{r}>t. \tag{42}$$

The neutron wave function in the crystal is given by Eq. (34). The boundary conditions at $\vec{n}\cdot\vec{r}=0$

and $\vec{n}\cdot\vec{r}=t$ are

$$C_1+C_2=1+R,\quad -\beta C_1+\beta C_2=1-R,$$
$$C_3e^{ik_e\gamma_e t}=C_1e^{-ik_e\gamma_e\beta t}+C_2e^{ik_e\gamma_e\beta t}, \tag{43}$$
$$C_3e^{ik_e\gamma_e t}=-\beta C_1e^{-ik_e\gamma_e\beta t}+\beta C_2e^{ik_e\gamma_e\beta t},$$

where β is defined by Eq. (32). The reflected and transmitted intensities are obtained from Eqs. (43) by straightforward manipulations

$$I_r=|R|^2=\frac{4r\sin^2(k_e\gamma_e\beta t)}{(1-r)^2+4r\sin^2(k_e\gamma_e\beta t)}, \tag{44}$$

$$I_t=|C_3|^2=\frac{(1-r)^2}{(1-r)^2+4r\sin^2(k_e\gamma_e\beta t)}, \tag{45}$$

where r is defined by Eq. (37).

Equations (44) and (45) are equivalent to the well-known Airy's formulas in optics.[18] If we define the order of interference m by

$$m=k_e\gamma_e\beta t/\pi, \tag{46}$$

it may be seen that the transmitted intensity exhibits maxima and minima for integral and half integral values of m respectively. The reflected intensity, on the other hand, exhibits maxima and minima for half-integral and integral values of m, respectively. Thus, both the reflected and transmitted intensity exhibit an interference fringe structure. The reflected (and transmitted) intensity is modulated by a term periodic in the thickness of the plate with a period T given by

$$T=\frac{\lambda}{2\gamma_e(1-V_{10}/\gamma_e^2)^{1/2}}. \tag{46'}$$

Finally, let us examine the propagation of the neutron waves in the plate when the glancing angle of incidence θ substantially exceeds the critical angle θ_c for total reflection of the neutron. In this case

$$\delta_+\simeq -2\gamma_e^2+\tfrac{1}{2}V_{10},$$
$$\delta_-\simeq -\tfrac{1}{2}V_{10},$$

and the corresponding allowed crystal wave vectors are

$$\vec{k}_{0+}\simeq(\vec{k}_{et}-\vec{k}_{en})+(V_{10}/2\gamma_e^2)\vec{k}_{en}$$

and

$$\vec{k}_{0-}\simeq(\vec{k}_{et}+\vec{k}_{en})-(V_{10}/2\gamma_e^2)\vec{k}_{en}.$$

In the last two equations the subscripts t and n denote the tangential and normal component of a vector respectively. Thus, one of the waves in the plate propagates close to the incident direction $\vec{k}_e$ and the other close to the reflected direction $(\vec{k}_{et}-\vec{k}_{en})$. Since $V_{10}\sim 10^{-6}$, the allowed values of δ are of the order of $-2\gamma_e^2$ and V_{10}, respectively. Therefore, if $\theta\gg\theta_c$, the reflected waves by the boundaries of the plate could be neglected by restricing δ in the secular equation to values of the order of the potential coefficients. The refelcted intensity as well as the modulation of the transmitted intensity may be neglected, since for $\theta\gg\theta_c$, r is of the order of $V_{10}^2\sim 10^{-12}$.

IV. NEUTRON DIFFRACTION

A. General solution

In examining the diffraction of neutrons by a perfect crystal, we will assume that the incident wave enters the crystal through the plane boundary $\vec{n}\cdot\vec{r}=0$. In addition, we will assume that the direction of incidence is such that the Bragg condition is nearly satisfied for only one reciprocal lattice vector $\vec{G}$. In this case only the amplitudes $u_{k_0,0,s}$ and $u_{k_0,G,s}$ are of appreciable magnitude and Eqs. (19) are reduced to four simultaneous equations

$$\left(1-\frac{k_0^2}{k_e^2}-V_{10s}\right)u_{k_0,0,s}-[V_{1Gs}+V_{2Gs}(\vec{k}_0)]u_{k_0,G,s}=0,$$
$$\left(1-\frac{(\vec{k}_0+\vec{G})^2}{k_e^2}-V_{10s}\right)u_{k_0,G,s}-[V_{1\bar{G}s}+V_{2\bar{G}s}(\vec{k}_0)]u_{k_0,0,s}=0, \tag{47}$$

where $\bar{G}$ stands for the vector $-\vec{G}$. Note that V_{20s} does not appear in Eqs. (47) as a result of the vanishing of the spin-orbit scattering amplitude in the forward direction.

The secular equation associated with Eqs, (47) determines the allowed primary wave vectors $\vec{k}_0$ in the crystal. Using Eqs. (21), (22), and (27) the secular equation reads

$$\delta_s^4+a\delta_s^3+b_1'\delta_s^2+c\delta_s+d=0, \tag{48}$$

where

$$a=2\gamma_e^2(1+1/b),$$
$$b_1'=\gamma_e^4\left(\frac{4}{b_1}+\frac{\alpha}{\gamma_e^2}+\frac{2}{\gamma_e^2}V_{10s}-y^2V_{2Gs}(\vec{k}_e)V_{2\bar{G}s}(\vec{k}_e)\right), \tag{49}$$
$$c=2\gamma_e^4\{\alpha+V_{10s}+(1/b_1)V_{10s}-y[V_{Gs}(\vec{k}_e)V_{2\bar{G}s}(\vec{k}_e)+V_{\bar{G}s}(\vec{k}_e)V_{2Gs}(\vec{k})]\},$$

and

$$d=\gamma_e^4[\alpha V_{10s}+V_{10s}^2-V_{Gs}(\vec{k}_e)V_{\bar{G}s}(\vec{k}_e)].$$

To each solution δ_{js} of Eq. (48) corresponds an allowed wave vector $\vec{k}_{0js}$ and two plane waves, the primary propagating along $\vec{k}_{0js}$ and the secondary propagating along $\vec{k}_{0js}+\vec{G}$. The ratio of the amplitudes of these waves is obtained from Eq. (47),

$$x_{js}=\frac{u_{k_0,G,s}}{u_{k_0,0,s}}$$

$$= - \frac{2\delta_{js} + \delta_{js}^2/\gamma_e^2 + V_{10s}(\vec{k}_e)}{V_{1Gs}(\vec{k}_e) + (1 + y\delta_{js}) V_{2Gs}(\vec{k}_e)} \quad . \tag{50}$$

Thus, for a definite neutron spin orientation, the general solution in the crystal is the superposition of *eight* plane waves, four travelling along the primary wave vectors $\vec{k}_{0js}$ and four along $\vec{k}_{0js} + \vec{G}$. Defining the phase parameter $\varphi_{js}(\vec{n} \cdot \vec{r})$ by

$$\varphi_{js}(\vec{n} \cdot \vec{r}) = (k_e \delta_{js}/\gamma_e) \vec{n} \cdot \vec{r} , \tag{51}$$

the general solution in the crystal may be written

$$\psi = e^{i\vec{k}_e \cdot \vec{r}} \sum_{j=1}^{4} C_{js} e^{i\varphi_{js}(\vec{n} \cdot \vec{r})} + e^{i(\vec{k}_e + \vec{G}) \cdot \vec{r}} \times \sum_{j=1}^{4} x_{js} C_{js} e^{i\varphi_{js}(\vec{n} \cdot \vec{r})} . \tag{52}$$

In Eq. (52), C_{js} ($j = 1, 2, 3, 4$) are constants to be determined from the boundary conditions.

B. Discussion

The existence of eigh waves propagating in the crystal may be easily understood. The energy states of the neutron in the crystal are arranged into allowed and forbidden energy bands, and the values of the wave vector for which the bands of forbidden energy occur are simply those satisfying the Bragg reflection conditions. If the direction of incidence is such that the Bragg condition is nearly satisfied, the diffracted and transmitted beams will each consist of two plane waves whose wave vectors are slightly different from the wave vectors $\vec{k}_e + \vec{G}$ and $\vec{k}_e$, respectively. Thus, an incident neutron wave, whose wave vector nearly satisfies the Bragg condition, generates four plane waves in the crystal: two waves propagating close to the direction of incidence and two along the direction of the diffracted beam. With each of these waves is associated a reflected wave from the lower limiting boundary of the crystal. If the glancing angle of incidence substantially exceeds the critical angle for total reflection of the neutrons the amplitudes of the various reflected waves are negligibly small. The characteristic fringe structure of the diffracted and transmitted beam is due to the interference of the waves propagating close to the direction of the diffracted and transmitted beam, respectively.

It is seen [Eqs. (48) and (49)] that the allowed neutron wave vectors in the crystal are determined by the geometry of the problem and two structure factors: the total structure factor and the structure factor for the spin-orbit interaction. The latter structure factor appears separately in the secular equation as a result of the momentum dependence of the spin-orbit interaction. These specific spin-orbit effects depend strongly on the geometry of the problem through the parameter y, defined by Eq. (28). In particular, they are absent in the symmetric Bragg case ($y = 0$). For crystals possessing a center of inversion symmetry $V_{Gs} V_{2\bar{G}s} + V_{\bar{G}s} V_{2Gs} = 0$ and the specific spin-orbit effects are quadratic in the spin-orbit amplitude. If the glancing angle of incidence is not of the order of a few minutes of arc, the specific spin orbit effects may be neglected since for $\lambda \sim 1$ Å, $V_{1Gs} \simeq V_{Gs} \simeq V_{10s} \sim 10^{-6}$, whereas V_{2Gs} is of the order of 10^{-9}–10^{-11}.

We have seen that if the glancing angle of incidence substantially exceeds the critical angle for total reflection of the neutrons, the specific spin-orbit effects may be neglected and the amplitudes of the reflected waves in the crystal are small in comparison with those of the transmitted and diffracted waves. The reflected waves, in this case, may be eliminated from the problem by restricting δ to values of the order of the potential coefficients ($\delta \sim 10^{-6}$). Under this assumption Eq. (48) reduces to

$$(4/b)\, \delta_s^2 + 2[\alpha + (1 + 1/b_1)\, V_{10s}]\, \delta_s + (\alpha V_{10s} + V_{10s}^2 - V_{Gs} V_{\bar{G}s}) = 0, \tag{48'}$$

and Eqs. (50) and (52) read

$$x_{js} = - (2\delta_{js} + V_{10s})/V_{Gs} , \tag{50'}$$

$$\psi = e^{i\vec{k}_e \cdot \vec{r}} \sum_{j=1}^{2} C_{js} e^{i\varphi_{js}(\vec{n} \cdot \vec{r})} + e^{i(\vec{k}_e + \vec{G}) \cdot \vec{r}} \times \sum_{j=1}^{2} x_{js} C_{js} e^{i\varphi_{js}(\vec{n} \cdot \vec{r})} . \tag{52'}$$

Equations (48′), (50′) are identical in structure with those of the dynamical x-ray theory. In this approximation the neutron wave function in the crystal consists of four plane waves, two traveling close to the forward direction and two close to the direction of incidence. We will refer to this approximation as the two-wave approximation to the dynamical theory.

V. PARALLEL CRYSTAL PLATE

In this section we explicitly solve the diffraction problem for a crystal plate bounded by the planes $\vec{n} \cdot \vec{r} = 0$ and $\vec{n} \cdot \vec{r} = t_0$, where t_0 is the thickness of the plate. The incident neutron wave enters the crystal through the boundary $\vec{n} \cdot \vec{r} = 0$ and the diffracted wave may leave the crystal either from the boundary $\vec{n} \cdot \vec{r} = t_0$ (Laue case) or from the face $\vec{n} \cdot \vec{r} = 0$ (Bragg case).

A. Boundary conditions

The neutron wave function in the crystal is given by Eq. (52), where C_{js} ($j = 1, 2, 3, 4$) are constants

determined from the boundary conditions. In writing the boundary conditions we take the z axis along the inward normal $\vec{n}$ to the plane $\vec{n}\cdot\vec{r}=0$.

The neutron wave functions in the vacuum may be written

$$\psi_i = e^{i\vec{k}_e\cdot\vec{r}} + B_1 e^{i(\vec{k}_{et}-\vec{k}_{en})\cdot\vec{r}} + B_2 e^{i(\vec{k}_{et}+\vec{G}_t+\Gamma\vec{n})\cdot\vec{r}} \quad \text{for } z<0$$

and (53)

$$\psi_e = \psi_1 e^{i\vec{k}_e\cdot\vec{r}} + \psi_2 e^{i(\vec{k}_{et}+\vec{G}_t+\Gamma'\vec{n})\cdot\vec{r}} \quad \text{for } z>t_0,$$

where t and n denote the normal and tangential components of the wave vectors, respectively. In writing Eqs. (53), the continuity of the tangential components of the wave vectors has been taken into account. The normal components Γ and Γ' must be such that

$$|\vec{k}_{et}+\vec{G}_t+\Gamma\vec{n}| = |\vec{k}_{et}+\vec{G}_t+\Gamma'\vec{n}| = k_e ,$$

with

$$\Gamma<0 \text{ and } \Gamma' = -\Gamma > 0. \tag{54}$$

The constants C_{js} $(j=1,2,3,4)$, B_1, B_2, ψ_1, ψ_2 are determined by expressing the continuity of the wavefunction and its normal derivative at the plane boundaries $\vec{n}\cdot\vec{r}=0$ and $\vec{n}\cdot\vec{r}=t_0$,

$$1+B_1 = \sum_{j=1}^{4} C_j , \qquad B_2 = \sum_{j=1}^{4} x_j C_j ,$$

$$1-B_1 = \sum_{j=1}^{4} C_j + \frac{1}{k_{en}} \sum_{j=1}^{4} \Delta_j C_j ,$$

$$B_2 = \frac{k_{en}+G_n}{\Gamma} \sum_{j=1}^{4} x_j C_j + \frac{1}{\Gamma} \sum_{j=1}^{4} \Delta_j x_j C_j ,$$

$$\sum_{j=1}^{4} \Delta_j C_j e^{i\varphi_j(t_0)} = 0 , \tag{55}$$

$$(k_{en}+G_n+\Gamma) \sum_{j=1}^{4} x_j C_j e^{i\varphi_j(t_0)} + \sum_{j=1}^{4} x_j C_j \Delta_j e^{i\varphi_j(t_0)} = 0,$$

$$\psi_1 = \sum_{j=1}^{4} C_j e^{i\varphi_j(t_0)} ,$$

$$\psi_2 = e^{i(k_{en}+G_n+\Gamma)t_0} \sum_{j=1}^{4} x_j C_j e^{i\varphi_j(t_0)} .$$

It is easily seen that the constants C_j $(j=1,2,3,4)$ are determined from the following set of algebraic equations :

$$\sum_{j=1}^{4} \left(2+\frac{\Delta_j}{k_{en}}\right) C_j = 2,$$

$$\sum_{j=1}^{4} \left(\frac{k_{en}+G_n+\Delta_j}{\Gamma} - 1\right) x_j C_j = 0 ,$$

$$\sum_{j=1}^{4} \Delta_j C_j e^{i\varphi_j(t_0)} = 0 ,$$

$$\sum_{j=1}^{4} (k_{en}+G_n+\Gamma+\Delta_j) x_j C_j e^{i\varphi_j(t_0)} = 0, \tag{56}$$

Equations (56) determine the integration constants C_j for both the Laue and Bragg case.

1. Laue case

In this case the diffracted beam leaves the crystal from the face $\vec{n}\cdot\vec{r}=t_0$. Using Eqs. (55) the transmitted I_t, diffracted I_d, and reflected intensities I_{r1} and I_{r2} may be expressed in terms of the integration constants C_j,

$$I_t = |\Psi_1|^2 = \left|\sum_{j=1}^{4} C_j e^{i\varphi_j(t_0)}\right|^2 , \tag{57}$$

$$I_d = |\Psi_2|^2 = \left|\sum_{j=1}^{4} x_j C_j e^{i\varphi_j(t_0)}\right|^2 , \tag{58}$$

$$I_{r1} = |B_1|^2 = \frac{1}{4k_{en}^2}\left|\sum_{j=1}^{4} \Delta_j C_j\right|^2 , \tag{59}$$

$$I_{r2} = |B_2|^2 = \left|\sum_{j=1}^{4} x_j C_j\right|^2 . \tag{60}$$

2. Bragg case

In this case the diffracted beam leaves the crystal from the face $\vec{n}\cdot\vec{r}=0$. The transmitted, diffracted, and reflected intensities are

$$I_t = |\Psi_1|^2 = \left|\sum_{j=1}^{4} C_j e^{i\varphi_j(t_0)}\right|^2 , \tag{57'}$$

$$I_d = |B_2|^2 = \left|\sum_{j=1}^{4} x_j C_j\right|^2 , \tag{58'}$$

$$I_{r1} = |B_1|^2 = \frac{1}{4k_{en}^2}\left|\sum_{j=1}^{4} \Delta_j C_j\right|^2 , \tag{59'}$$

$$I_{r2} = |\Psi_2|^2 = \left|\sum_{j=1}^{4} x_j C_j e^{i\varphi_j(t_0)}\right|^2 . \tag{60'}$$

3. Two-wave approximation

In the two-wave approximation, the general solution [Eq. (52′)] involves only two constants and the boundary conditions provide more equations than are necessary for their determination. This apparent paradox is resolved if one recognizes that in this approximation δ is assumed to be of the order of the potential coefficients ($\sim 10^{-6}$). This is equivalent to assuming that Δ is small compared to the normal component of the incident wave vector. Thus the boundary conditions expressing the continuity of the normal component of the wave func-

tion are approximately satisfied. The integration constants are obtained by expressing the continuity of the wave function at the plane boundaries of the plate

$$\sum_{j=1}^{2} C_{js} = 1, \quad \sum_{j=1}^{2} x_{js} C_{js} = 0$$

(Laue case) (61)

and

$$\sum_{j=1}^{2} C_{js} = 1, \quad \sum_{j=1}^{2} x_{js} C_{js} e^{i\varphi_{js}(t_0)} = 0$$

(Bragg case). (61′)

B. Explicit solutions

Next, some diffraction problems of practical importance will be explicitly solved. In each case an expression for the period of the Pendellösung fringes will be derived. First, the general solution in the two-wave approximation will be given for the Laue case. Then, in two simple cases, the Pendellösung period will be obtained without neglecting the reflected waves, and it will be compared with the result of the two-wave approximation. Finally, we will briefly discuss the diffraction of neutrons by a magnetized crystal.

1. General solution in the two-wave approximation: Laue case

In this approximation the diffracted intensity [Eq. (58)] is given by

$$I_{ds} = \left| \sum_{j=1}^{2} x_{js} C_{js} e^{i\varphi_{js}(t_0)} \right|^2, \tag{62}$$

where [Eq. (50′)]

$$x_{js} = -(2\delta_{js} + V_{10s})/V_{Gs}, \quad j = 1, 2, \tag{63}$$

and δ_{js} $(j = 1, 2)$ are the roots of Eq. (48′). The constants of integration obtained from the boundary conditions [Eq. (61)] are

$$C_{1s} = x_{2s}/(x_{2s} - x_{1s}) \quad C_{2s} = -x_{1s}/(x_{2s} - x_{1s}) . \tag{64}$$

Substituting the integration constants into Eq. (62) one obtains

$$I_{ds} = 4 \left| \frac{x_{1s} x_{2s}}{x_{2s} - x_{1s}} \right|^2 e^{-(\varphi''_{1s} + \varphi''_{1s})} \times \left[\sinh^2 \left(\frac{\varphi''_{1s} - \varphi''_{2s}}{2} \right) + \sin^2 \left(\frac{\varphi'_{1s} - \varphi'_{2s}}{2} \right) \right],$$

where φ'_{js}, φ''_{js} are the real and imaginary part of $\varphi_{js}(t_0)$, respectively,

$$\varphi_{js}(t_0) = (k_e \delta_{js}/\gamma_e) t_0 = \varphi'_{js} + i\,\varphi''_{js}. \tag{65}$$

Using Eqs. (62) and (48′) we obtain

$$\varphi'_{1s} - \varphi'_{2s} = (b_1 k_e/4\gamma_e) t_0 \,\mathrm{Re}(D_s^{1/2}), \tag{66}$$

$$\varphi''_{1s} - \varphi''_{2s} = (b_1 k_e/4\gamma_e) t_0 \,\mathrm{Im}(D_s^{1/2}), \tag{67}$$

$$\varphi''_{1s} + \varphi''_{2s} = -[(1 + b_1)/2\gamma_e] t_0 k_e \,\mathrm{Im}(V_{10s}), \tag{68}$$

where D_s is the discriminant of Eq. (48′),

$$D_s = 4[\alpha + (1 - 1/b_1) V_{10s}]^2 + (16/b_1) V_{Gs} V_{\bar{G}s}. \tag{69}$$

It is easily seen that $[(1 + b_1)/2\gamma_e]\, t_0$ is the average neutron path in the crystal and $-k_e \mathrm{Im}(V_{10s})$ is the linear attenuation coefficient μ of the crystal

$$\bar{t} = [(1 + b_1)/2\gamma_e] t_0, \qquad \mu = -k_e \mathrm{Im}(V_{10s}). \tag{70}$$

Using Eqs. (68) and (70) the diffracted intensity may be written

$$I_{ds} = 4 \left| \frac{x_{1s} x_{2s}}{x_{2s} - x_{1s}} \right|^2 e^{-\mu \bar{t}} \left[\sinh^2 \left(\frac{\varphi''_{1s} - \varphi''_{2s}}{2} \right) + \sin^2 \left(\frac{\varphi'_{1s} - \varphi'_{2s}}{2} \right) \right]. \tag{71}$$

The second term in Eq. (71) exhibits the Pendellösung fringe structure that arises from the interference of the neutron waves propagating close to the direction of diffraction. It is seen [Eq. (66)] that this oscillatory term is periodic in the thickness of the crystal, with a period given by

$$T_s = \frac{8\pi\gamma_e}{k_e b_1 \mathrm{Re}(D_s^{1/2})} = \frac{4\gamma_e \lambda}{b_1 \mathrm{Re}(D_s^{1/2})}. \tag{72}$$

It is seen that the Pendellösung period depends on the geometry and the potential coefficients. Therefore, measurement of this period may be used to obtain information about the neutron lattice interaction. If one choses the direction of incidence so that the Bragg condition is exactly satisfied ($\alpha = 0$), the expression for the period in the symmetric Laue case ($b_1 = 1$) is reduced to a very simple form:

$$T_s = \gamma_e \lambda / \mathrm{Re}(V_{Gs} V_{\bar{G}s})^{1/2}. \tag{73}$$

If the imaginary part of the nuclear scattering amplitude and the spin-orbit scattering amplitude may be neglected, then $V_{\bar{G}s} = V^*_{Gs}$ and the period is given by

$$T_s = \gamma_e \lambda / |V_{Gs}|. \tag{73′}$$

For a monatomic nonmagnetic crystal in the absence of an external magnetic field

$$|V_{Gs}| = |V_G| = (4\pi N_c/k_e^2) e^{-W_G} |S_G(b + \gamma)|, \tag{74}$$

where e^{-W_G} is the Debye-Waller factor and S_G is the geometrical structure factor of the crystal. Since the Foldy scattering term is small in comparison to the nuclear scattering amplitude, the Pendellösung period, in this case, is inversely proportional to the nuclear scattering amplitude. Thus the experi-

mental determination of the Pendellösung period may be used to determine the nuclear scattering amplitude. It is seen from Eq. (74) that the data must be corrected for the Debye-Waller factor and the small Foldy scattering term. The precision of the measurement is essentially limited by the precision of the measurement of the Debye-Waller factor.

In some cases the spin-orbit scattering amplitude is negligible in comparison with the imaginary part of the nuclear scattering amplitude. If, in addition, the crystal posesses a center of inversion symmetry then

$$V_{Gs} = V_{\bar{G}s}, \tag{75}$$

and the period is given by

$$T_s = \gamma_e \lambda / \mathrm{Re}(V_{Gs}). \tag{73''}$$

For a monatomic nonmagnetic crystal in the absence of a magnetic field

$$\mathrm{Re}(V_{Gs}) = (4\pi N_c/k_e^2) e^{-W_G} \mathrm{Re}[S_G(b + \gamma - ib')]. \tag{76}$$

In the general case, the period is calculated from Eq. (73). It should be pointed out that Eq. (75) is not valid for a crystal with inversion symmetry, due to the fact that the spin-orbit amplitude changes sign under the transformation $G \to \bar{G}$. As an example let us take an fcc, monatomic, nonmagnetic crystal in the absence of an external magnetic field. Then for an allowed reflection defined by the reciprocal-lattice vector $\vec{G}$

$$V_{Gs} = V_G = \frac{16\pi N_c}{k_e^2} e^{-W_G}(b + \gamma - ib' + ib_{s,G})$$

and

$$V_{\bar{G}s} = V_{\bar{G}} = \frac{16\pi N_c}{k_e^2} e^{-W_G}(b + \gamma - ib' - ib_{s,G}), \tag{77}$$

where $b_{s,G}$ denotes the spin-orbit amplitude. The period will be given by Eq. (73) with

$$\mathrm{Re}(V_{Gs} V_{\bar{G}s})^{1/2} = (16\pi N_c/k_e^2) e^{-W_G} \times [(b + \gamma)^2 + b_{s,G}^2 - b'^2]^{1/2} \tag{78}$$

Since the spin-orbit amplitudes are in most cases smaller, by a factor of 10^3–10^5, than the nuclear scattering amplitudes the spin-orbit correction to the experimental data is small.

To summarize, if the conditions of the two-wave approximation are fulfilled, the measurement of the Pendellösung period may be used to determine the nuclear scattering amplitude. The corrections due to the imaginary part of the nuclear scattering amplitude, the spin-orbit and Foldy scattering amplitude are small and can easily be taken into account. The precision of the measurement is essentially limited by the precision of the measurement of the Debye-Waller factor.

2. *General case*

The results obtained above are valid provided the glancing angle of incidence substantially exceeds the critical angle for total reflection of the neutrons. If this condition is not satisfied, the diffracted intensity will be given by Eq. (58) or (58′) with the constants of integration determined from the boundary conditions Eq. (56). The solution is straightforward but involves tedious algebraic manipulations. We will consider two simple diffraction problems by a nonmagnetic crystal in the absence of an external magnetic field. In both problems we will assume that the geometry of the problem is that of the symmetric Laue case ($b_1 = 1$), with the Bragg condition exactly satisfied ($\alpha = 0$).

a. Let us first examine the diffraction of neutrons by a crystal possessing a center of inversion symmetry. In addition we will assume, for simplicity, that the imaginary part of the nuclear amplitude and the spin-orbit scattering are negligible. Under these assumptions

$$V_{Gs} = V_{\bar{G}s} = V_{1Gs} = V_{10s} = V, \tag{79}$$

and the secular equation reduces to

$$\delta^4 + 4\gamma_e^2 \delta^3 + \gamma_e^4[4 + (2/\gamma_e^2)V]\,\delta^2 + 4\gamma_e^4 V \delta = 0. \tag{80}$$

The roots of this equation are

$$\begin{aligned} &\delta_1 = 0, \quad \delta_2 = -\gamma_e^2(1 - \beta_1) \cong -V, \\ &\delta_3 = -\gamma_e^2(1 + \beta_1) \cong -2\gamma_e^2 + V, \\ &\delta_4 = -2\gamma_e^2, \end{aligned} \tag{81}$$

where

$$\beta_1 = (1 - 2V/\gamma_e^2)^{1/2}, \tag{82}$$

and the approximate expressions for δ_2, δ_3 are valid if $V \ll \gamma_e^2$. Thus, the allowed neutron wave vectors in the crystal are given by

$$\begin{aligned} &\vec{k}_{01} = \vec{k}_0, \\ &\vec{k}_{02} = \vec{k}_e - k_e\gamma_e(1 - \beta_1)\vec{n} \cong \vec{k}_e - (k_e/\gamma_e) V \vec{n}, \\ &\vec{k}_{03} = \vec{k}_e - k_e\gamma_e(1 + \beta_1)\vec{n} \cong (\vec{k}_{et} - \vec{k}_{en}) + (k_e/\gamma_e) V \vec{n}, \\ &\vec{k}_{04} = \vec{k}_{et} - \vec{k}_{en}. \end{aligned} \tag{83}$$

Note that in the present problem $G_n = 0$ and $\Gamma = -k_{en}$ [Eq. (54)]. Using these relations the boundary conditions [Eqs. (56)] are

$$\begin{aligned} &\sum_j \left(1 + \frac{\delta_j}{2\gamma_e^2}\right) C_j = 1, \quad \sum_j \left(1 + \frac{\delta_j}{2\gamma_e^2}\right) x_j C_j = 0, \\ &\sum_j \delta_j C_j e^{i\varphi_j} = 0, \quad \sum_j \delta_j x_j C_j e^{i\varphi_j} = 0. \end{aligned} \tag{84}$$

Using Eqs. (81) it is easily seen [Eq. (50)] that

$$x_1 = x_4 = -1$$

and

$$x_2 = x_3 = 1. \tag{85}$$

Making use of Eqs. (85) and (81) into Eqs. (84) one obtains

$$C_1 = \tfrac{1}{2}, \quad C_2 = \frac{r_1 + 1}{2(1 - r_1^2 e^{i(\varphi_2 - \varphi_3)})},$$
$$C_3 = \frac{-r_1(r_1+1)e^{i(\varphi_2-\varphi_3)}}{2(1 - r_1^2 e^{i(\varphi_2-\varphi_3)})}, \tag{86}$$
$$C_4 = 0,$$

where we define

$$r_1 = (1 - \beta_1)/(1 + \beta_1), \tag{87}$$

and φ_2, φ_3 expressed in terms of the parameter β_1 and the thickness t_0 of the crystal are given by

$$\varphi_2 = -k_e \gamma_e (1 - \beta_1) t_0,$$
$$\varphi_3 = -k_e \gamma_e (1 + \beta_1) t_0. \tag{88}$$

Using Eqs. (58), (85), and (86) the intensity of the diffracted beam may be written

$$I_d = [(1 + r_1)\sin^2 \tfrac{1}{2}\varphi_2 + r_1(r_1 + 1)\sin^2 \tfrac{1}{2}\varphi_3 - r_1 \sin^2 \tfrac{1}{2}(\varphi_2 - \varphi_3)] \times [(1 - r_1^2)^2 + 4 r_1^2 \sin^2 \tfrac{1}{2}(\varphi_2 - \varphi_3)]^{-1}. \tag{89}$$

It is seen that the diffracted intensity is modulated by three terms periodic in the thickness of the crystal. Since $r_1 < 1$ the dominant term in Eq. (89) is the one involving $\sin^2(\varphi_2/2)$ which is periodic in the thickness of the crystal with a period

$$T = \frac{\lambda}{\gamma_e(1 - \beta_1)} = \frac{\lambda}{\gamma_e[1 - (1 - 2V/\gamma_e^2)^{1/2}]}. \tag{91}$$

If $V/\gamma_e^2 \ll 1$ the period given by Eq. (91) reduces to

$$T = \lambda \gamma_e / V, \tag{92}$$

which is identical with the result that one would obtain using the two-wave approximation. Note that the deviation of the period given by Eq. (91) from the two-wave approximation result [Eq. (92)] decreases with decreasing scattering angle.

b. In the general case the calculation of the diffracted intensity involves the solution of a fourth-order secular equation. The calculation is straightforward but involves tedious algebraic manipulations. The diffracted intensity [Eq. (58)] is modulated by six terms periodic in the thickness of the crystal. If the glancing angle of incidence exceeds the angle for total reflection of the neutrons, an approximate expression for the period of the dominant term in the diffracted intensity may be derived.

Since the specific spin-orbit effects (discussed in Sec. IV) are negligible in most cases, the secular equation may be written

$$\delta^4 + 4\gamma_e^2 \delta^3 + \gamma_e^4[4 + (2/\gamma_e^2) V_{10}] \delta^2 + 4\gamma_e^4 V_{10} \delta + \gamma_e^4 (V_{10}^2 - V_G V_{\bar{G}}) = 0. \tag{93}$$

The solution of Eq. (93) is considerably simplified if one notices that for glancing angles of incidence exceeding the critical angle for total reflection of the neutrons, two of the roots (δ_1, δ_2) are of the order of the potential coefficients. The other two roots may be written

$$\delta_3 = -2\gamma_e^2 + \delta_3', \quad \delta_4 = -2\gamma_e^2 + \delta_4', \tag{94}$$

where δ_3', δ_4' are also of the order of the potential coefficients. In addition it is easily seen that

$$\delta_3' + \delta_4' = -(\delta_1 + \delta_2). \tag{95}$$

The primary neutron waves corresponding to δ_1, δ_2 propagate close to the direction of incidence and those corresponding to δ_3, δ_4 propagate close to the direction of the reflected beam. Using Eqs. (93)–(95) one finds that

$$\delta_{1,2} \cong \tfrac{1}{2}[-V_{10}(1 + \nu) \pm (V_G V_{\bar{G}})^{1/2}(1 + \nu')], \tag{96}$$

where

$$\nu = (V_{10}^2 + V_G V_{\bar{G}})/4\gamma_e^2 V_{10} \tag{97}$$

and

$$\nu' = \nu(V_{10}^2 + V_G V_{\bar{G}})/2 V_G V_{\bar{G}}. \tag{98}$$

Thus the period of the dominant term in the diffracted intensity is given by

$$T = \frac{\lambda \gamma_e}{\mathrm{Re}(\delta_1 - \delta_2)} \cong \frac{\lambda \gamma_e}{\mathrm{Re}[(V_G V_{\bar{G}})^{1/2}(1 + \nu')]}. \tag{99}$$

If the imaginary part of the nuclear scattering amplitude and the spin-orbit scattering may be neglected, Eq. (99) reduces to Eq. (91). For $\nu' = 0$ the period is identical with the result of the two-wave approximation [Eq. (73)].

3. *Magnetic scattering*

Let us finally discuss the neutron diffraction problem by a magnetized perfect crystal plate. For simplicity we will assume that the geometry of the problem is that of the symmetric Laue case ($b_1 = 1$) and that the Bragg condition is exactly satisfied ($\alpha = 0$). The magnetization will be assumed to be perpendicular to the scattering plane, the usual experimental arrangement. For simplicity, the problem will be discussed in the two-wave approximation.

If the neutron beam is unpolarized the Pendellösung fringe structure will consist of the incoherent superposition of two terms periodic in the thickness of the crystal. The periods of these terms are given by Eq. (73),

$$T_{\pm} = \gamma_e \lambda / \mathrm{Re}(V_{G,\pm} V_{\bar{G},\pm})^{1/2}, \quad (100)$$

where ± label the two neutron spin states (parallel and antiparallel to the magnetization of the crystal). If the beam is completely polarized (parallel or antiparallel to the magnetization of the crystal) the Pendellösung fringe structure will consist of a single term periodic in the thickness of the crystal. The period of the fringe structure will be T_+ or T_- depending on whether the polarization is parallel or antiparallel to the magnetization of the crystal. Since highly polarized beams are presently available, the periods corresponding to the two neutron spin states may be separately determined. It is easily seen that a measurement of these two periods will determine both the nuclear and the magnetic scattering amplitude. In fact for a monatomic fcc crystal

$$V_{G,\pm} = \frac{16\pi N_c}{k_e^2} e^{-W_G}(b \pm p_G + \gamma - ib' + ib_{s,G}),$$
$$V_{\bar{G},\pm} = \frac{16\pi N_c}{k_e^2} e^{-W_G}(b \pm p_G + \gamma - ib' - ib_{s,G}). \quad (101)$$

where p_G is the magnetic scattering amplitude for the reflection specified by the reciprocal-lattice vector $\vec{G}$. The periods are obtained from Eq. (100), where

$$\mathrm{Re}(V_{G,\pm} V_{\bar{G},\pm})^{1/2} = (16\pi N_c/k_e^2)\, e^{-W_G} \times [(b + \gamma \pm p_G)^2 + b_{s,G}^2 - b'^2]. \quad (102)$$

It is seen that measurement of these periods determines both $b + p_G$ and $b - p_G$. If the nuclei possess a nonzero magnetic moment, a nuclear polarization term must be included. If the measurements are not performed at very low temperatures, this term is, in most cases of practical interest, negligibly small.

VI. SUMMARY

The dynamical theory of neutron diffraction has been formulated to include the reflected waves from the boundaries of the crystal. This formulation allows a unified treatment of the neutron optical and diffraction phenomena in crystals. Neutron propagation in the crystal can be described in terms of two structure factors characterizing the crystal: the total structure factor and the structure factor of the neutron spin-neutron orbit interaction. This latter structure factor appears separately in the problem as a result of the neutron momentum dependence of the spin-orbit interaction.

The diffraction of neutrons by a parallel crystal plate has been studied assuming that the direction of incidence is such that the Bragg condition is nearly satisfied by only one reciprocal lattice vector. For a definite spin orientation the diffracted and transmitted intensity are modulated by six terms periodic in the thickness of the crystal. This Pendellösung fringe structure of the diffracted and transmitted beam arises from the interference of neutron waves propagating close to the diffracted and transmitted direction, respectively. The period of the dominant term in the diffracted intensity has been calculated in several cases of practical importance. If the glancing angle of incidence substantially exceeds the critical angle for total reflection of the neutrons the results of the theory are reduced to those of the two-wave approximation. In the diffraction by a magnetized crystal there are two periods associated with the two spin states of the neutron. Measurement of these periods could be used to determine both the nuclear and magnetic scattering amplitude.

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*Present address: Sala Magnetics Inc., Cambridge, Mass. 02141.

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