Dynamical theory of thermal neutron scattering. I. Diffraction from magnetic crystals*

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A general two-beam dynamical theory of the elastic scattering of a thermal neutron from *arbitrary* magnetic structures is presented. Using a density-matrix formalism, general expressions are developed to compute the scattering cross section as well as the final state of polarization of the emerging neutron. Emphasis is placed on those features of scattering which arise due to the spin of the neutron. Detailed calculations have been carried out for spiral structures, ferromagnetic and antiferromagnetic spin arrangements, and the results are compared with those of kinematical theory. As an illustration, the calculation for the flipping ratio R for the MnF_2 (210) peak in the symmetrical Laue configuration indicates that according to dynamical theory R can take arbitrary values when the thickness of the crystal or wavelength of the incident neutron is varied.

INTRODUCTION

The dynamical theory of diffraction for x rays and electrons as probe particles has been known for almost sixty years,[1] and the well-known formulation for scalar particles has appeared in many places. Thermal neutrons as probe particles offer two main advantages in the analysis of the structure of materials. The first advantage is that the spin of the scattered neutron carries information on the magnetic state of the material. A general treatment of the polarization dependence of scattering from magnetic materials using the kinematical theory was given by Blume,[2] and a comprehensive account of thermal-neutron scattering in the Van Hove formulation[3] appears in Marshall and Lovesey,[4] and Izyumov and Ozerov.[5] The second useful feature of thermal neutrons as probe particles lies in the fact that the energy analysis of the scattered beam is possible to a much greater precision than is commonly done with x rays or electrons. This has led to the measurement of inelastic peaks in the scattered beam and, as a consequence, the phonon dispersion curves of many solids have been determined accurately.

A general treatment of the thermal-neutron scattering in dynamical theory taking into account the spin of the neutron and the effect of this theory on the inelastic peaks has not been given so far. In this paper (I), we treat the elastic scattering (diffraction) of a neutron from an arbitrary magnetic structure in dynamical theory; and in a second paper (II), we evaluate dynamical effects in one-phonon inelastic peaks. After we completed our work and were in the process of writing this paper, we became aware of similar work by Stassis and Oberteuffer[6] and by Sivardiere.[7] Their treatment is similar to ours, but the treatment given here deals with all the magnetic structures, including spirals, in a comprehensive way. We have also used the density-matrix formalism to derive the expressions for intensities of the diffracted beams and thus have included the case of partially polarized incident beams in our treatment.

In the following, we derive the dynamical theory of neutron scattering from magnetic materials, taking into account the spin of the neutron. We are interested in quantities like the cross section, the polarization of the diffracted beam, and the flipping ratio. In the past, there have been applications of the dynamical theory of polarized neutrons to specific models or materials. Hamilton[8] computed the extinction effects of dynamical theory treating the up and down components of the spin of the neutron separately. Nityananda and Ramseshan[9] took a one-dimensional model of the continuous magnetization density spiral and arrived at the result that the direction of the spin of the emerging neutron depended upon the length of the spiral (or the thickness of the spiral material). Felcher[10] extended their results to the spiral in three-dimensional space—a more realistic case. However, they did not take their spiral to be made up of localized spins on a discrete lattice, and some of the qualitative effects are lost in this case. Brown[11] has computed the flipping ratio for Cr_2O_3 essentially using Hamilton's approach. Recently, Alperin[12] reported some experiments on rotation of the polarization for Cr_2O_3. In the following, we give a systematic development of the general theory. The basis of our work is a paper by Ekstein,[13] and we aim at extending the results of Blume[2] to dynamical theory.

The arrangement of the material in this paper is as follows. In Sec. I we determine the wave function of the neutron in the crystal corresponding to an incident neutron of definite energy. The wave function is written as a linear combination of degenerate eigenfunctions of the neutron inside the crystal; all these eigenfunctions have energy equal to the incident energy. For perfect crystals, to which we limit our discussion, these eigenfunctions are simply Bloch wave spinors with different indices k. For simplicity we take these Bloch waves in the plane-wave representation. In Sec. II, we determine the constant amplitudes of spinors by matching the total wave functions to the incident wave and to the scattered waves at the boundary of the crystal. Once the wave function inside the crystal is determined, the intensities, the change in the direction of polarization, etc., can be easily found. We use the density-matrix formalism to derive expressions for these quantities.

Section III deals with the application of the formalism to specific physical examples. We also consider interference between nuclear and magnetic scattering. Throughout the paper we emphasize only those aspects of dynamical theory which arise owing to the spinor nature of the neutron. The *Pendellösung* effects which occur in scalar theory are indicated but are not discussed in detail, as these are well known and have been elaborated upon by many workers (for example, Refs. 6 and 14).

I. SPINOR WAVE FUNCTION IN THE CRYSTAL

The Hamiltonian for the neutron in the crystal is given by

$$H=-\frac{\hbar^2}{2m}\nabla_{\vec{x}}^2+V_n(\vec{x})+V_m(\vec{x}), \tag{1}$$

where V_n and V_m are the nuclear and magnetic energies of the neutron, respectively, and, in general, are operators in the neutron spin space. Following Ekstein,[13] we take the wave function of the neutron inside the crystal to be of the following form:

$$\psi(\vec{x})=\sum_{\vec{g}} e^{i(\vec{k}+\vec{g})\cdot\vec{x}}\chi_g=\sum_{\vec{g}} e^{i(\vec{k}+\vec{g})\cdot\vec{x}}\begin{pmatrix}\chi_{g\uparrow}\\ \chi_{g\downarrow}\end{pmatrix}. \tag{2}$$

Here, the χ_g are constant (space-independent) spinors corresponding to the reciprocal-lattice vector $\vec{g}$ of the periodic potential. To take χ_g as space independent does not pose any restriction on the problem, because it can be easily seen that for more than one nonzero term in the sum (2) the spin of the neutron is a function of its position $\vec{x}$. The spinor solution of Herring[15] as employed by Nityananda[9] and Felcher[10] to investigate the diffraction from the spiral structures is a special case of Eq. (2).

In order that $\psi(\vec{x})$ be an eigenfunction of H with energy $E=\hbar^2|\vec{k}_0|^2/2m$, the spinors χ_g must satisfy an homogeneous algebraic equation

$$[(|\vec{k}+\vec{g}|^2-|\vec{k}_0|^2)\underline{1}+V(0)]\chi_g+\sum_{g'\neq g}[V_n(\vec{g}-\vec{g}')+V_m(\vec{g}-\vec{g}')]\chi_{g'}=0. \tag{3}$$

$V_n(\vec{g})$ and $V_m(\vec{g})$ are Fourier transforms of the potential energies $V_n(\vec{x})$ and $V_m(\vec{x})$ in units of $2m/\hbar^2$. Equation (3) is the basic equation of dynamical theory and is exactly the same as that of the band theory of solids except that here V_n and V_m, instead of being scalars, are 2×2 matrices, and the χ's are two-component vectors in the spin space of the neutron.

For unique solutions of χ from the homogeneous Eq. (3), $\vec{k}$ must satisfy the well-known vanishing of the determinant condition

$$\mathrm{Det}\,D=0, \tag{4}$$

where the elements of D are

$$D_{ii}=(|\vec{k}+\vec{g}_i|^2-|\vec{k}_0|^2)\underline{1}+V_n(0)+V_m(0),$$
$$D_{ij}=V_n(\vec{g}_i-\vec{g}_j)+V_m(\vec{g}_i-\vec{g}_j)$$

and $\underline{1}$ is a unit 2×2 matrix. Equation (4) cannot be solved for all the components of $\vec{k}$, nor is it necessary. From the boundary condition of the continuity of the wave function one of the conditions which we obtain is that the tangential component of $\vec{k}$ is the same as that of $\vec{k}_0$. In order to solve Eq. (4) for the normal component of $\vec{k}$ we define the following parameters of dynamical theory:

$$\gamma=\vec{k}\cdot\hat{n},\quad \gamma_g=(\vec{k}+\vec{g})\cdot\hat{n},$$
$$\Gamma_0=\vec{k}_0\cdot\hat{n},\quad \Gamma_g^0=(\vec{k}_0+\vec{g})\cdot\hat{n}, \tag{5}$$
$$\Gamma_g=+[|\vec{k}_0|^2-|(\vec{k}_0+\vec{g})_t|^2]^{1/2},$$

where $\hat{n}$ is the inward normal to the incident plane $\hat{n}\cdot\vec{x}=0$; note that in general $\Gamma_g\neq\Gamma_g^0$.

It is possible to solve Eq. (4) and then Eq. (3) for the n-beam case, but in the following we concentrate on the two-beam case because the *Pendellösung* phenomenon can be anticipated in the two-beam case only. Then

$$\psi(x)=e^{i\vec{k}\cdot\vec{x}}\begin{pmatrix}\chi_\uparrow\\ \chi_\downarrow\end{pmatrix}+e^{i(\vec{k}+\vec{g})\cdot\vec{x}}\begin{pmatrix}\chi_{g\uparrow}\\ \chi_{g\downarrow}\end{pmatrix}. \tag{6}$$

Matrix D for the two-beam case is a 4×4 matrix and its elements in terms of smaller 2×2 matrices are

$$D_{11}=(\gamma^2-\Gamma_0^2)\underline{1}+V(0),$$
$$D_{22}=\gamma_g^2-\Gamma_g^2=[(\gamma+g_n)^2-\Gamma_g^2]\underline{1}+V(0), \quad (7)$$
$$D_{12}=V(0-g)\equiv V(-g),\quad D_{21}=V(g-0)\equiv V(+g).$$

Equation (4) is now an *eighth*-order polynomial in γ. That means that for an incident plane-wave spinor represented by wave vector $\vec{k}_0$ there are *eight*, in general different, plane-wave components in the forward direction (γ) and *eight* in the diffracted direction (γ_g). However, in Laue transmission geometry four of the wave vectors in each of the two directions are merely reflections from the boundary $\hat{n}\cdot\vec{x}=T$. A detailed analysis[6,7,14] of the amplitudes of various components shows that the reflected components are of negligible amplitudes compared to the forward-traveling ones. Now, if we take only four γ's and four γ_g's as describing the state of the neutron inside the crystal, then, the system of equations obtained by invoking the continuity of the wave function *and* its normal derivative across *both* the boundaries is an overdetermined system. However, for such a case, Zachariasen-type boundary conditions,[16] *viz.* (a) the total amplitude of the forward traveling waves is equal to the incident amplitude at $\hat{n}\cdot\vec{x}=0$; and (b) no diffracted wave enters the crystal from the incident side, are physically and mathematically consistent.[17] This is the system of the boundary conditions which we shall employ here. To a very good *approximation* the four forward-traveling waves in the crystal can be obtained by writing $\gamma=\Gamma_0+\delta$ and neglecting the second-order terms appropriately in Eq. (4).

For some special forms of the potentials and geometry, the matrix D and hence the polynomial $\mathrm{Det}D=0$ take a simple form and give degenerate solutions. An obvious example would be if all the spin-flipping potentials were zero, corresponding to the neglect of magnetic interactions altogether and writing nuclear potentials in the scalar form. Then one has to solve the following equation for γ:

$$[\gamma^2-\Gamma_0^2+V(0)][(\gamma+g_n)^2-\Gamma_g^2+V(0)] - V_n(+\vec{g})V_n(-\vec{g})=0. \quad (8)$$

This equation and its two forward-traveling γ's give the *Pendellösung* phenomena of the scalar theory.

For the magnetic crystal case when γ has four values corresponding to the traveling plane waves, and for each of the values, the system of Eq. (3) can be solved for the components $\chi_\uparrow$, $\chi_\downarrow$, $\chi_{g\uparrow}$, and $\chi_{g\downarrow}$. The wave function inside the crystal becomes

$$\psi(\vec{x})=\sum_{i=1}^{4} e^{i[\gamma^i(\vec{x}\cdot\hat{n})+\vec{k}_{0t}\cdot\vec{x}_{\parallel}]}\begin{pmatrix}\chi_\uparrow^i\\ u_\downarrow^i\chi_\uparrow^i\end{pmatrix} + \sum_{i=1}^{4} e^{[(\gamma^i+g_n)\vec{x}\cdot\hat{n}+(\vec{k}_0+\vec{g})_t\cdot\vec{x}_{\parallel}]}\begin{pmatrix}u_{g\uparrow}^i\chi_\uparrow^i\\ u_{g\downarrow}^i\chi_\uparrow^i\end{pmatrix}, \quad (9)$$

where,

$$\chi_\uparrow^i=u_\uparrow^i\chi_\uparrow^i,\quad \chi_{g\uparrow}^i=u_{g\uparrow}^i\chi_\uparrow^i,\quad \chi_{g\downarrow}^i=u_{g\downarrow}^i\chi_\uparrow^i.$$

Every term in Eq. (9) is known except the four arbitrary constants $\chi_\uparrow^i$. In some physical cases it may be more convenient to choose some other components as arbitrary constants. In order to calculate various parameters entering Eq. (9) we have to know the explicit form of the potentials V_n and V_m. These have been given by Halpern and Johnson.[18] We use them in the form given in Ref. 2 (B6). Equations of Ref. 2 henceforth will be denoted by (B6), (B7), etc.

For simplification, we shall assume the scalar form of the *nuclear* potential, i.e., we shall neglect that part of the potential which gives rise to polarization in incoherent scattering. This assumption has been made only to delineate the effects of magnetic scattering.

In the following we write the magnetic part of the potential $V_m(g)$ for some cases of interest and discuss features of the scattering from these potentials in Sec. III.

A. Simple spiral of *continuous* magnetization density

This has been discussed by Felcher[10] and Nityananda[9] and we give results for comparison with the spiral on a lattice.

$$V_m(\vec{x})=4\pi\mu_N M\frac{2m}{\hbar^2}\begin{pmatrix}0 & e^{-i\vec{q}\cdot\vec{x}}\\ e^{i\vec{q}\cdot\vec{x}} & 0\end{pmatrix},$$

$$V_m(\mp\vec{G})=4\pi\mu_N M\frac{2m}{\hbar^2}\begin{pmatrix}0 & \delta_{G,q}\\ \delta_{G,-q} & 0\end{pmatrix}.$$

With this form of the interaction, where magnetization is a *continuous* function, it is possible to discuss only $(000)^{\pm}$ satellites. For a particular peak, say the + satellite

$$V_m(-\vec{q})=C\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix},\quad V_m(+\vec{q})=C\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix};$$

$$V_m(0)=0 \text{ for } \vec{q}\neq0 \text{ and } C\equiv4\pi\mu_N M(2m/\hbar^2).$$

B. Ferromagnetic spiral due to spins on a lattice

When the magnetic properties of the crystal can be described by ions having localized spins on a lattice the potential is given by (B9)–(B11)

$$V_m(\mp\vec{G}) = \frac{2m}{\hbar^2}\frac{2\pi\hbar^2}{m}\frac{2\gamma e^2}{m_e c^2}\frac{1}{V} \times\left(\sum_{\vec{l},j} e^{\pm i\vec{G}\cdot(\vec{l}+\vec{d}_j)} f_{lj}(\mp\vec{G})(\hat{G}\times\vec{S}_{lj}\times\hat{G})\right)\cdot\vec{s}. \tag{10}$$

We have used the notation of Ref. 2 except for a change of sign in the definition of the Fourier transform to make it agree with the conventional definition. $\vec{G}$ is the general scattering vector at which the peak is observed, and f_{lj} is the form factor of the ion with the spin $\vec{S}_{lj} = \hat{\eta}_{lj}S$ at the site $(\vec{l}, j)$.

$$V_m(\mp\vec{G}) = C\sum_{\vec{l},j} e^{\mp iG\cdot(\vec{l}+\vec{d}_j)} f_{lj}(\mp\vec{G})[(\hat{\eta}_{lj}\cdot\hat{G}^{\perp})(\vec{s}\cdot\hat{G}^{\perp})]; \tag{11}$$

$$C \equiv \frac{2m}{\hbar^2}\frac{2\pi\hbar^2}{m}\frac{2\gamma e^2}{m_e e^2}\frac{S}{V}, \quad \hat{G}^{\perp}\cdot\hat{G} = 0, \tag{12}$$

$$V_m(0) = C\left(\sum_{\vec{l},j} f_{lj}(0)(\hat{\eta}_{lj}\cdot\hat{G}^{\perp})(s\cdot\hat{G}^{\perp})\right).$$

This expression shows that the component of the spin along the direction of the scattering vector does not contribute to magnetic scattering. This is also obvious from Eq. (10). So far no fixed set of coordinate axes has been chosen, nor has the spin structure on the lattice been fixed. In this sense expressions (11) and (12) are valid for an arbitrary spin structure and any experimental geometry.

For a spiral structure on a Bravais lattice

$$\vec{\eta}_l = \tfrac{1}{2}(\hat{u}_- e^{i\vec{q}\cdot\vec{l}} + \hat{u}_+ e^{-i\vec{q}\cdot\vec{l}})\sin\beta + \hat{q}\cos\beta,$$

where $\vec{q}$ is the wave vector of the spiral, β is the angle that the spin direction makes with $\vec{q}$, $\hat{u}_- = \hat{u}_1 - i\hat{u}_2$, $\hat{u}_+ = \hat{u}_1 + i\hat{u}_2$, and u_1 and u_2 are orthogonal unit vectors perpendicular to $\hat{q}$.

For a + satellite around $\vec{g}$, $\vec{G} = \vec{g} + \vec{q}$,

$$V_m^{+}(\mp\vec{G}) = C_{\mp}^{+}[\tfrac{1}{2}(\hat{u}_{\pm}\cdot\hat{G}^{\perp})\sin\beta](\vec{s}\cdot\hat{G}^{\perp}), \tag{13}$$

and for a – satellite

$$V_m^{-}(\mp\vec{G}) = C_{\mp}^{-}[\tfrac{1}{2}(\hat{u}_{\mp}\cdot\hat{G}^{\perp})\sin\beta](\vec{s}\cdot\hat{G}^{\perp}), \tag{14}$$
$$C_{\mp}^{+} = Cf(\mp(\vec{g}+\vec{q})), \quad C_{\mp}^{-} = Cf(\mp(\vec{g}-\vec{q})).$$

This is the most general form of the potential. However, in order to do computations for dynamical theory we have to choose some geometrical configuration. For illustration, we choose the geometry employed by Koehler *et al.*[19]

$$\hat{q} = \hat{z}; \quad \hat{G} = \hat{z}\cos\phi + \hat{x}\sin\phi,$$
$$V_m^{+}(-\vec{G}) = C_{-}[\tfrac{1}{2}s_{+} - \tfrac{1}{2}(s_z\cos\phi + s_x\sin\phi)\sin\phi]$$
$$= \tfrac{1}{2}C_{-}\begin{pmatrix} -\cos\phi\sin\phi & 2-\sin^2\phi \\ -\sin^2\phi & \cos\phi\sin\phi \end{pmatrix}. \tag{15}$$

This potential correctly gives the form factor of Koehler *et al.*[19] for unpolarized neutrons, i.e., $\frac{1}{4}(1+\cos^2\phi)f^2$. When ϕ is zero, i.e., when the scattering vector $\vec{G}$ and spiral wave vector $\vec{q}$ are parallel, we get the same form as in Sec. I A.

C. Ferromagnets and antiferromagnets

For ferromagnets as well as for antiferromagnets we can write V_m from Eq. (11) as

$$V_m(\mp\vec{G}) = CF_m(\mp\vec{G})\begin{pmatrix} 0 & \eta_x - i\eta_y \\ \eta_x + i\eta_y & 0 \end{pmatrix}. \tag{16}$$

F_m is the form factor of the magnetic unit cell and includes the geometrical structure factor, which determines the selection rules for antiferromagnetic peaks. Here we have chosen $\hat{G} = \hat{z}$, a convention different from that for spiral case. Also,

$$V_m(0) = CF_M(0)\begin{pmatrix} 0 & \eta_x - i\eta_y \\ \eta_x + i\eta_y & 0 \end{pmatrix},$$

and $\hat{\eta}$ is the direction of magnetization.

II. INTENSITY AND FINAL POLARIZATION

In this section we derive expressions for the intensity and the state of polarization of the diffracted beam for the two-beam case of dynamical theory. The approach followed is a straightforward extension of the scalar neutron theory. First we calculate the intensity for a fixed polarization state of the incident beam and then derive the expressions for a partially polarized incident beam. We consider the Laue transmission geometry explicitly, but calculations for the forward beam as well as for the other experimental geometry (Bragg reflection) are straightforward and are given in Sec. III for specific spin structures.

In the Laue transmission geometry we take the spinor wave function of the neutron in the exit vacuum region to be

$$\psi_e(\vec{x}) = e^{i[\Gamma_0(\vec{x}\cdot\hat{n}) + \vec{k}_{0t}\cdot\vec{x}_{\parallel}]}\begin{pmatrix}\chi_{e\uparrow}\\ \chi_{e\downarrow}\end{pmatrix} + e^{i[\Gamma_g(\vec{x}\cdot\hat{n}) + (\vec{k}_0+\vec{g})_t\cdot\vec{x}_{\parallel}]}\begin{pmatrix}\chi_{e\uparrow}\\ \chi_{eg\downarrow}\end{pmatrix},$$

where

$$e^{i(\Gamma_0 \vec{x}\cdot\hat{n} + \vec{k}_{0t}\cdot\vec{x}_{(\parallel)})} = e^{i\vec{k}_0\cdot\vec{x}},$$

and, since $\Gamma_g^2 + |(\vec{k}_0+\vec{g})_t|^2 = |\vec{k}_0|^2$, $\psi_e(\vec{x})$ satisfies the free space Schrodinger equation for a neutron of energy $\hbar^2|\vec{k}_0|^2/2m$.

Since we have taken only four γ's (associated with the forward-traveling waves) to specify the wave function inside the crystal, in the following, we apply approximate (Zachariasen-type) boundary conditions and obtain

$$\begin{aligned} &\sum_{i=1}^{4} \chi_\uparrow^i = \chi_{in\uparrow}; \quad \sum_{i=1}^{4} u_\downarrow^i \chi_\uparrow^i = \chi_{in\downarrow}, \\ &\sum_{i=1}^{4} u_{g\uparrow}^i \chi_\uparrow^i = 0; \quad \sum_{i=1}^{4} u_{g\downarrow}^i \chi_\uparrow^i = 0. \end{aligned} \tag{17}$$

The above four inhomogeneous equations unambiguously determine the four constants $\chi_\uparrow^i$ to give uniquely the wave function inside the crystal. Finally, from boundary conditions at the exit surface $\hat{n}\cdot\vec{x} = T$ we obtain the amplitude of the diffracted wave function in the exit region:

$$A = e^{ig_n T}\begin{pmatrix} \sum_{i=1}^{4} e^{i\gamma^i T} u_{g\uparrow}^i \chi_\uparrow^i \\ \sum_{i=1}^{4} e^{i\gamma^i T} u_{g\downarrow}^i \chi_\uparrow^i \end{pmatrix}. \tag{18}$$

The intensity of the diffracted beam, and consequently the cross section (except for kinematical factors) is $A^\dagger A$, and the orientation of the spin of the neutron in the diffracted beam is given by $A^\dagger(\frac{1}{2}\vec{\sigma})A$.

The above procedure, exact for an incident beam of unit polarization, can be easily cast into the density-matrix formalism by defining an average of the incident spinor over the various spin directions.[20] If $|\chi\rangle$ is a spinor representing an incident neutron, then the density matrix ρ of the incident neutron beam is defined by

$$\rho \equiv (|\chi\rangle\langle\chi|)_{\text{av}},$$

where the $(\ )_{\text{av}}$ represents an average over the neutrons in the incident beam. The density matrix can be written generally as $\rho = \frac{1}{2}\underline{1} + \vec{p}\cdot\vec{s}$, where $\frac{1}{2}\vec{p} = \langle\vec{s}\rangle$ is the polarization of the incident beam; similarly if $|\chi'\rangle$ is the spin wave function of neutron in the scattered beam then $|\chi'\rangle = M|\chi\rangle$, where M is a 2×2 matrix, and

$$\rho' = (|\chi'\rangle\langle\chi'|)_{\text{av}} = M\rho M^\dagger$$

is proportional to the density matrix of the diffracted beam.

In terms of the density matrix the cross section is given by

$$\frac{d\sigma}{d\Omega} = \text{Tr}\rho' = \text{Tr}M\rho M^\dagger \tag{19}$$

and the polarization vector of the diffracted beam by

$$\frac{\vec{p}}{2} = \frac{\text{Tr}\vec{s}\rho'}{\text{Tr}\rho'} = \frac{\text{Tr}\vec{s}M\rho M^\dagger}{\text{Tr}M\rho M^\dagger}. \tag{20}$$

The cross-section for an unpolarized beam would be simply $\text{Tr}M^\dagger M$. All the above quantities can be easily computed once the matrix M, which gives the amplitude of the diffracted spinor in terms of the incident spinor of unit polarization, is known. Various trace relations (B7) in the product matrices of Pauli spin matrices facilitate this computation.

From the form of the amplitude of the diffracted beam—Eq. (18)—one can note that since γ, in general, has four values, the usual feature of dynamical theory associated with two distinct values of γ (*Pendellösung* phenomena) will not be observed unless some special geometry or form of the potential yields only two distinct values of γ. Second, the role played by the matrix M can be compared with the role played by the interaction potential V.[21] Since in kinematical theory the intensity formula is given by $\text{Tr}\rho V^\dagger V$, we observe that if the structure of the matrix M turns out to be the same as that of V (for some special physical example and experimental geometry) the polarization features of the scattering will not show any dynamical effects. More precisely, if M differs from V only by a thickness-dependent scale factor, the final state of polarization $\vec{p}'$ and the flipping ratio will be given by the expressions of kinematical theory.[22] In effect, M plays the role of a scattering matrix as compared to V of the first Born approximation (kinematical theory).

Finally, the flipping ratio is defined as the ratio of the intensities for two different directions of the initial polarization. In many experiments one measures first the intensity for the polarization vector parallel to some preferred axis and then antiparallel to the same axis. This defines two density matrices ρ_+ and ρ_-. The ratio of the two intensities, or flipping ratio, is

$$R = \text{Tr}\rho_+ M^\dagger M / \text{Tr}\rho_- M^\dagger M. \tag{21}$$

III. PHYSICAL EXAMPLES

In the following we apply the techniques of dynamical theory developed above to three important spin structures: spirals, ferromagnets, and antiferromagnets. The main emphasis is on the dynamical effects in the polarization of the scattered beam. We first consider two special cases of

high-symmetry spirals and treat ferromagnets and antiferromagnets in general in Sec. III A.

A. Spiral structures on a lattice

The potentials in the matrix D for a + satellite are given by Eq. (15),

$$D_{12}=V_{-g}=p\begin{pmatrix}-\cos\phi\sin\phi & 2-\sin^2\phi\\ -\sin^2\phi & \cos\phi\sin\phi\end{pmatrix},$$

$$D_{21}=V_{+g}=p^*\begin{pmatrix}-\cos\phi\sin\phi & -\sin^2\phi\\ 2-\sin^2\phi & \cos\phi\sin\phi\end{pmatrix},$$

with

$$p=\tfrac{1}{2}C_-\sin\beta=\tfrac{1}{2}Cf(-(\vec{g}+\vec{q}))\sin\beta$$
$$=2\pi(2\gamma e^2/m_ec^2)(v_0)^{-1}Sf_-\sin\beta$$

where v_0 is the volume per lattice site.

1. Case A

We take $\phi=0$, i.e., $\hat{q}\cdot\hat{G}=1$. This occurs when the axis of the spiral (z axis) is parallel to the scattering vector. This will be the case for the $(00l)$ satellites of holmium.[19] Equations (3) are

$$(\gamma^2-\Gamma_0^2)\chi_\uparrow+2p\chi_{g\downarrow}=0,\quad (\gamma^2-\Gamma_0^2)\chi_\downarrow+0=0,$$
$$0+[(\gamma+g_n)^2-\Gamma_g^2]\chi_{g\uparrow}=0,$$
$$2p^*\chi_\uparrow+[(\chi+g_n)^2-\Gamma_g^2]\chi_{g\downarrow}=0.$$

The four solutions for γ and the corresponding arbitrary coefficients are

$$\gamma^{1,2}=\Gamma_0+\delta^{1,2};$$
$$\delta^{1,2}=-\frac{1}{4\Gamma_g^0}(\Gamma_g^{0^2}-\Gamma_g^2)\pm\left(\frac{1}{4\Gamma_g^0}(\Gamma_g^{0^2}-\Gamma_g^2)^2+\frac{|p|^2}{\Gamma_0\Gamma_g^0}\right)^{1/2},$$
$$\gamma^3=\Gamma^0,\quad \gamma^4=\Gamma_g-g_n;$$
$$\chi_\uparrow^{1,2},\quad \chi_\downarrow^3,\quad \text{and}\quad \chi_{g\uparrow}^4.$$

From the form of the potential for the spiral (Sec. I A) and the above equations it follows that the spiral in this configuration acts like a filter. And the magnetic interaction favors the up component of the spin in the forward direction, while only the down component is found in the diffracted beam. From the boundary conditions the amplitude of the scattered beam is given by

$$A_g=e^{iG_nT}\begin{pmatrix}0\\ -\frac{u_{g\downarrow}^1u_{g\downarrow}^2}{u_{g\downarrow}^2-u_{g\downarrow}^1}\chi_{in\uparrow}e^{i\gamma_1T}+\frac{u_{g\downarrow}^1u_{g\downarrow}^2}{u_{g\downarrow}^2-u_{g\downarrow}^1}e^{i\gamma_2T}\chi_{in\uparrow}\end{pmatrix},$$

and the matrix M is

$$M=\frac{u_{g\downarrow}^1u_{g\downarrow}^2}{u_{g\downarrow}^2-u_{g\downarrow}^1}e^{i\gamma_1T}(e^{i\Delta T}-1)\begin{pmatrix}0&0\\1&0\end{pmatrix}=f(T)s_-;$$

$$f(T)\equiv\frac{u_{g\downarrow}^1u_{g\downarrow}^2}{u_{g\downarrow}^2-u_{g\downarrow}^1}e^{i\gamma_1T}(e^{i\Delta T}-1).$$

The cross section and final polarization are then

$$\frac{d\sigma}{d\Omega}=\mathrm{Tr}(\tfrac{1}{2}\underline{1}+\vec{p}\cdot\vec{s})[f^*(T)s_+][f(T)s_-]$$
$$=|f(T)|^2\tfrac{1}{2}(1+p_z),$$
$$\frac{\vec{p}'}{2}\frac{d\sigma}{d\Omega}=|f(T)|^2\tfrac{1}{2}[\hat{z}-\tfrac{1}{2}(\vec{p}\cdot\hat{z})\hat{z}],$$

or

$$\vec{p}'=2\frac{(1-\frac{1}{2}p_z)}{(1+p_z)}\hat{z}.$$

Therefore, we conclude that the polarization of the diffracted beam is independent of the thickness. In the above we have made use of the following relations:

For $M=\alpha+\vec{\beta}\cdot\vec{s}$ and $\rho=\tfrac{1}{2}1+\vec{p}\cdot\vec{s}$

$$\mathrm{Tr}(\rho M^\dagger M)=|\alpha|^2+\tfrac{1}{4}|\beta|^2+\tfrac{1}{2}\alpha^*\vec{p}\cdot\vec{\beta}+\tfrac{1}{4}i\vec{p}\cdot(\vec{\beta}^*\times\vec{\beta}),$$
$$\mathrm{Tr}(\vec{s}M\rho M^\dagger)=\tfrac{1}{2}\alpha^*\beta+\tfrac{1}{2}\alpha\beta^*$$
$$+\tfrac{1}{4}i[-\vec{\beta}^*\times\vec{\beta}+(\vec{\beta}\times\vec{p})\alpha^*+(\vec{\beta}^*\times\vec{p})\alpha]$$
$$+\tfrac{1}{8}[(\vec{p}\cdot\vec{\beta}^*)\vec{\beta}-\vec{p}(\vec{\beta}^*\cdot\vec{\beta})+(\vec{p}\cdot\vec{\beta})\vec{\beta}^*].$$

Exactly the same calculations can be carried out for the negative satellite, *viz.*, $\vec{G}=\vec{g}-\vec{q}$, and the following results are obtained:

$$M=f(T)s_+,\quad \frac{d\sigma}{d\Omega}=|f(T)|^2\tfrac{1}{2}(1-p_z),$$

$$\vec{p}'=2\frac{1+\frac{1}{2}p_z}{1-p_z}\hat{z}.$$

Two points concerning these results should be noted. First, we obtain the same ratio of intensity between the two satellites as obtained by kinematical theory (Ref. 2). Second, no dynamical effects have appeared in the polarization dependence of the intensity. This follows from our earlier assertion (Sec. II) that no dynamical effects in polarization will be observed if the matrices M and V are proportional.

The matrix M_0 in the forward direction does, however, show interesting properties. The amplitude of the forward spinor A_0, for the + satellite, is given by

$$A_0=\begin{pmatrix}\left(e^{i\gamma_1T}\frac{u_{g\downarrow}^2}{u_{g\downarrow}^2-u_{g\downarrow}^1}-e^{i\gamma_2T}\frac{u_{g\downarrow}^1}{u_{g\downarrow}^2-u_{g\downarrow}^1}\right)\chi_{in\uparrow}\\ e^{i\Gamma_0T}\chi_{in\downarrow}\end{pmatrix},$$

and

$$M_0=\begin{pmatrix} e^{i\gamma_1 T}\left(\frac{u^2_{g\downarrow}}{u^2_{g\downarrow}-u^1_{g\downarrow}}-\frac{u^1_{g\downarrow}}{u^2_{g\downarrow}-u^1_{g\downarrow}}e^{i\Delta T}\right) & 0 \\ 0 & e^{i\Gamma_0 T}\end{pmatrix}$$

$$=\tfrac{1}{2}f_+(T)\underline{1}+f_-(T)s_z\,,$$

where

$$f_\pm(T)=e^{i\gamma_1 T}[(u^2_{g\downarrow}-u^1_{g\downarrow})^{-1}(u^2_{g\downarrow}-u^1_{g\downarrow}e^{i\Delta T}) \pm e^{i(\Gamma_0-\gamma_1)T}]\,,$$

with $\Delta=\gamma_2-\gamma_1$. Then

$$\frac{d\sigma}{d\Omega}=\frac{|f_+(T)|^2}{4}+\frac{|f_-(T)|^2}{4}+\frac{f_+^*f_-p_z}{4}+\frac{f_+f_-^*p_z}{4}\,,$$

$$\tfrac{1}{2}\vec{\mathfrak{p}}'=\frac{\frac{1}{4}(f_+^*f_-+f_+f_-^*)\hat{z}+\frac{1}{8}(p_z|f_-|^2\hat{z}-\vec{\mathfrak{p}}|f_-|^2+\hat{z}|f_-|^2p_z)}{d\sigma/d\Omega}\,,$$

and

$$\vec{\mathfrak{p}}'=2\frac{(f_+^*f_-+f_+f_-^*)\hat{z}+p_z|f_-|^2\hat{z}-2|f_-|^2\vec{\mathfrak{p}}}{|f_+|^2+|f_-|^2+p_z(f_+^*f_-+f_\pm f_-^*)}\,.$$

Here the polarization direction does depend upon thickness, and we expect oscillations of polarization direction given by an extinction thickness proportional to $1/\Delta$. For $\vec{\mathfrak{p}}=\hat{z}$,

$$\vec{\mathfrak{p}}'=2\frac{(f_+^*f_-+f_+f_-^*)-|f_-|^2}{|f_+|^2+|f_-|^2+(f_+^*f_-+f_+f_-^*)}\hat{z}\,,$$

and for the opposite direction of polarization

$$\vec{\mathfrak{p}}'=2\frac{(f_+^*f_-+f_-^*f_+)+|f_-|^2}{|f_+|^2+|f_-|^2-(f_+^*f_-+f_+f_-^*)}\hat{z}\,.$$

The difference in the results for the forward direction and the diffracted direction is due to the fact that in the forward direction there is interference between the incident beam and the forward scattered beam, while such interference does not occur in the diffracted direction. All the above results are also found for Bragg geometry, which differs from Laue geometry only in the boundary conditions.[16] The diffracted amplitude A_g and matrix M for Bragg geometry are

$$A_g=\begin{pmatrix} 0 \\ -\frac{u^1_{g\downarrow}u^1_{g\downarrow}e^{i\gamma_2 T}}{u^2_{g\downarrow}e^{i\gamma_2 T}-u^1_{g\downarrow}e^{i\gamma_1 T}}+\frac{u^1_{g\downarrow}u^2_{g\downarrow}e^{i\gamma_1 T}}{u^2_{g\downarrow}e^{i\gamma_2 T}-u^1_{g\downarrow}e^{i\gamma_1 T}}\end{pmatrix}\chi_{\text{in}\uparrow}\,,$$

$$M_g=f(T)\begin{pmatrix}0&0\\1&0\end{pmatrix}=f(T)s_-\,,$$

$$f(T)\equiv-\frac{u^1_{g\downarrow}u^2_{g\downarrow}}{u^2_{g\downarrow}e^{i\Delta T}-u^1_{g\downarrow}}(e^{i\Delta T}-1)\,.$$

Except for trivial changes, this gives the same results as obtained for Laue geometry because M is the same in both cases, except for the redefinition of $f(T)$.

2. Case B

This will be the approximate situation for the $(l00)^\pm$ satellites when l is large (Ref. 19). In Laue geometry, the amplitude of the diffracted wave is given by

$$e^{i\gamma_1 T}(1-e^{i\Delta T})\frac{u^1_{g\uparrow}u^2_{g\uparrow}}{u^2_{g\uparrow}-u^1_{g\uparrow}}\begin{pmatrix}\chi_{\text{in}\uparrow}\\-\chi_{\text{in}\downarrow}\end{pmatrix},$$

leading to

$$M_g=f(T)\begin{pmatrix}0&1\\-1&0\end{pmatrix}=2f(T)s_x\,,$$

$$\frac{d\sigma}{d\Omega}=|f(T)|^2\,,\quad \vec{\mathfrak{p}}'=2(\vec{\mathfrak{p}}\cdot\hat{x}-\tfrac{1}{2}\vec{\mathfrak{p}})\,.$$

This result is remarkable for the fact that the cross section is independent of polarization, but the final state of polarization is different from the initial state. We also note that since the axis of the spiral is perpendicular to the scattering vector, from the point of view of the magnetic interaction there is no preferred component of the spinor. As a consequence, both the components, up and down, are affected equally. Similar results can be easily obtained for the – satellite and for the Bragg geometry.

3. Case C: spiral, general case: $\phi\neq0$ and $\phi\neq\frac{1}{2}\pi$

As an illustration we give the formalism for general potential when $V(0)=0$. Equations (3) are

$$(\gamma^2-\Gamma_0^2)\chi+V(-\vec{\mathfrak{g}})\chi_g=0\,, \tag{22}$$

$$V(+\vec{\mathfrak{g}})\chi+[(\gamma+g_n)^2-\Gamma_g^2]\chi_g=0\,. \tag{23}$$

For $\gamma=\Gamma_0+\delta$, δ being a small deviation, Eqs. (22) and (23) can be transformed to the following set of eigenvalue equations

$$\frac{V_-}{\Gamma_0}\chi_g=-2\delta\chi\,;\quad V_-\equiv V(-\vec{\mathfrak{g}})\,; \tag{24}$$

$$\frac{V_+}{\Gamma_g^0}\chi+\frac{(\Gamma_g^0)^2-\Gamma_g^2}{\Gamma_g^0}\chi_g=-2\delta\chi_g\,;\quad V_+\equiv V(+\vec{\mathfrak{g}})\,. \tag{25}$$

The problem of determining γ (or δ) is reduced to solving the above eigenvalue problem. The eigenvalues δ (or the values of γ) are given by

$$2\delta\Gamma_0(2\delta\Gamma_g^0+\Gamma_g^{02}-\Gamma_g^2)-\lambda_{1,2}=0\,, \tag{26}$$

where $\lambda_{1,2}$ are eigenvalues of the matrix

$$V_+V_-=|p|^2[(1+\cos^2\phi)\underline{1}-2\cos^2\phi\sigma_z-\sin2\phi\sigma_x]\,, \tag{27}$$

$$\lambda_{1,2}=|p|^2(1\pm\cos\phi)^2\,. \tag{28}$$

Finally, from Eq. (26) we obtain the following four

values of γ:

$$\gamma=\Gamma_0+\frac{1}{4}\left(\Gamma_g^0-\frac{\Gamma_g^2}{\Gamma_g^0}\right)\pm\frac{1}{4\Gamma_g^0}\left([(\Gamma_g^0)^2-\Gamma_g^2]^2-\frac{4\Gamma_g^0}{\Gamma_0}|p|^2(1\pm\cos\phi)^2\right)^{1/2}. \tag{29}$$

If $\phi\neq 0$ and $\phi\neq\frac{1}{2}\pi$, all the values of γ are distinct. The neutron wave function inside the crystal is

$$\begin{aligned}\psi(z)=&(e^{i\gamma^1 z}\chi_\uparrow^1+e^{i\gamma^2 z}\chi_\uparrow^2)\begin{pmatrix}1\\-\frac{V_{11}-\lambda_1}{V_{12}}\end{pmatrix}+(e^{i\gamma^3 z}\chi_\uparrow^3+e^{i\gamma^4 z}\chi_\uparrow^4)\begin{pmatrix}1\\-\frac{V_{11}-\lambda_2}{V_{12}}\end{pmatrix}\\&-V_+\begin{pmatrix}1\\-\frac{V_{11}-\lambda_1}{V_{12}}\end{pmatrix}(u_g^1e^{i\gamma_g^1 z}\chi_\uparrow^1+u_g^2e^{i\gamma_g^2 z}\chi_\uparrow^2)-V_+\begin{pmatrix}1\\-\frac{V_{11}-\lambda_2}{V_{12}}\end{pmatrix}(u_g^3e^{i\gamma_g^3 z}\chi_\uparrow^3+u_g^4e^{i\gamma_g^4 z}\chi_\uparrow^4),\end{aligned} \tag{30}$$

$$u_g=-[(\gamma+g_n)^2-\Gamma_g^2]^{-1}\simeq[2\delta\Gamma_g^0+(\Gamma_g^{02}-\Gamma_g^2)]^{-1}.$$

Applying the boundary conditions,

$$\begin{aligned}A_g=&V_+\begin{pmatrix}1\\\frac{V_{11}-\lambda_1}{V_{12}}\end{pmatrix}(e^{i\gamma^1 T}-e^{i\gamma^2 T})\frac{u_g^2u_g^1}{u_g^2-u_g^1}\frac{1}{\lambda_1-\lambda_2}[(V_{11}-\lambda_2)\chi_{in\uparrow}-V_{12}\chi_{in\downarrow}]+V_+\begin{pmatrix}1\\\frac{V_{11}-\lambda_2}{V_{12}}\end{pmatrix}(e^{i\gamma^4 T}-e^{i\gamma^3 T})\\&\times\frac{u_g^4u_g^3}{u_g^4-u_g^3}\frac{1}{\lambda_1-\lambda_2}[(V_{11}-\lambda_1)\chi_{in\uparrow}-V_{12}\chi_{in\downarrow}],\\=&f_{12}(T)V_+\begin{pmatrix}V_{11}-\lambda_2&-V_{12}\\-\frac{(V_{11}-\lambda_1)(V_{11}-\lambda_2)}{V_{12}}&V_{11}-\lambda_1\end{pmatrix}\begin{pmatrix}\chi_{in\uparrow}\\\chi_{in\downarrow}\end{pmatrix}+f_{34}(T)V_+\begin{pmatrix}V_{11}-\lambda_1&-V_{12}\\-\frac{(V_{11}-\lambda_1)(V_{11}-\lambda_2)}{V_{12}}&V_{11}-\lambda_2\end{pmatrix}\begin{pmatrix}\chi_{in\uparrow}\\\chi_{in\downarrow}\end{pmatrix}.\end{aligned} \tag{31}$$

Within the small δ approximation,

$$\begin{aligned}f_{12}(T)=&\frac{e^{i\gamma^1 T}(1-e^{i\Delta T})}{2\Delta}\frac{1}{(\lambda_1-\lambda_2)},\\f_{34}(T)=&\frac{e^{i\gamma^4 T}(1-e^{-i\Delta' T})}{2\Delta'}\frac{1}{\lambda_1-\lambda_2},\end{aligned} \tag{32}$$

$$\Delta\equiv\gamma^2-\gamma^1,\quad \Delta'\equiv\gamma^4-\gamma^3.$$

The matrix M for the diffracted beam is, finally, given by

$$M=V_+[A_1f_{12}(T)+A_2f_{34}(T)]. \tag{33}$$

It is easy to observe then that the diffracted intensity

$$\begin{aligned}\mathrm{Tr}\rho M^\dagger M=&\mathrm{Tr}\rho[A_1^\dagger f_{12}(T)+A_2^\dagger f_{34}^*(T)]\\&\times V_+^\dagger V_+[A_1f_{12}(T)+A_2f_{34}(T)]\end{aligned}$$

is different from the kinematical expression $\mathrm{Tr}\rho V^\dagger V$. If we define

$$A_1f_{12}(T)+A_2f_{34}(T)\equiv F(T)$$

then we observe that all the formulas of kinematical theory are valid if we compute them with a new density matrix

$$\bar{\rho}=F(T)\rho F^\dagger(T). \tag{34}$$

The cross section and other quantities are given by this new density matrix $\bar{\rho}$. Also, if $F(T)=f(T)\overline{A}$, where $f(T)$ is a scalar function, then there is no thickness-dependent rotation of the polarization direction of the incident beam as it passes through the crystal, but the final direction of polarization is different from that given by the kinematical expression $\mathrm{Tr}\rho V^\dagger\vec{S}V$ by a constant angle.

B. Ferromagnets and antiferromagnets

First, we find γ (or δ) using techniques similar to those used for spirals. The matrix D can be easily written using the potentials given in Eq. (16). Finding the values of δ is equivalent to finding the eigenvalues of the following partitioned matrix:

$$D'=\begin{pmatrix}C_{00}(A+\vec{B}\cdot\vec{\sigma})&C_-(A+\vec{B}\cdot\vec{\sigma})\\C_+(A+\vec{B}\cdot\vec{\sigma})&C_{0g}(A+\vec{B}\cdot\vec{\sigma})+C_{gg}\underline{1}\end{pmatrix}, \tag{35}$$

where,

$$C_{00}=\frac{CF_M(0)}{2\Gamma_0},\quad C_{0g}=\frac{CF_M(0)}{2\Gamma_g^0},\quad C_{gg}=-\frac{\Gamma_g^{02}-\Gamma_g^2}{2\Gamma_g^0},$$

$$C_+=\frac{CF_M(+\vec{g})}{2\Gamma_g^0},\quad C_-=\frac{CF_M(-\vec{g})}{2\Gamma_0}.$$

$A\equiv 0$, $\vec{B}=(\eta_x,\eta_y,0)$. (See Sec. III A for the con-

vention.) We have written the matrix in this form so that it may be applicable to a general case, including the nuclear interaction.

We compute the matrix M by a procedure quite similar to the one detailed in the preceding sections. The matrix M is given by

$$M = h^{-1}\begin{pmatrix} f_{12}(T) & 0 \\ 0 & f_{34}(T) \end{pmatrix} h ,$$

where h is a unitary matrix which diagonalizes the Hermetian matrix

$$\begin{pmatrix} 0 & \eta_x - i\eta_y \\ \eta_x + i\eta_y & 0 \end{pmatrix} .$$

The matrix h is the spin-$\frac{1}{2}$ representation of the rotation operator which brings the projection of spin $\hat{\eta}$ onto the x-y plane (or more precisely the vector $[\hat{\eta} - (\hat{\eta}\cdot\hat{G})\hat{G}]$) into the z axis (or in the direction of $\hat{G}$). If this projection makes an angle β with the x axis, then

$$h = \begin{pmatrix} \frac{e^{+i\beta/2}}{\sqrt{2}} & \frac{e^{-i\beta/2}}{\sqrt{2}} \\ -\frac{e^{+i\beta/2}}{\sqrt{2}} & \frac{e^{-i\beta/2}}{\sqrt{2}} \end{pmatrix}, \tag{36}$$

$$\begin{aligned} M &= \begin{pmatrix} f_{12}+f_{34} & (f_{12}-f_{34})e^{-i\beta} \\ (f_{12}-f_{34})e^{i\beta} & f_{12}+f_{34} \end{pmatrix} \\ &= \tfrac{1}{2}(f_{12}+f_{34})\underline{1} + (f_{12}-f_{34})(\cos\beta s_x + \sin\beta s_y) . \end{aligned} \tag{37}$$

The cross section is given by

$$2\frac{d\sigma}{d\Omega} = (|f_{12}|^2 + |f_{34}|^2) + (|f_{12}|^2 - |f_{34}|^2) \times \frac{\vec{p}\cdot[\hat{\eta} - (\hat{\eta}\cdot\hat{G})\hat{G}]}{\sin\phi} . \tag{38}$$

Obviously, for $\vec{p}$ in the direction of the scattering vector the last term is zero, and there is no polarization dependence of the scattering.

The flipping ratio for $\vec{p}$ in the scattering plane, but perpendicular to $\vec{G}$ is given by

$$R = \frac{(|f_{12}|^2 + |f_{34}|^2) + (|f_{12}|^2 - |f_{34}|^2)(\cos\beta/\sin\phi)}{(|f_{12}|^2 + |f_{34}|^2) - (|f_{12}|^2 - |f_{34}|^2)(\cos\beta/\sin\phi)} . \tag{39}$$

In the above,

$$f_{12} \equiv f_{12}(T) = e^{i\gamma^1 T}\frac{(1 - e^{i\Delta T})}{\Delta} C_+\lambda_1 ,$$

$$f_{34} \equiv f_{34}(T) = e^{i\gamma^3 T}\frac{(1 - e^{i\Delta' T})}{\Delta'} C_+\lambda_2 ,$$

$$\lambda_{1,2} = \pm\sin\phi .$$

C. Calculations for MnF_2

For an antiferromagnet we obtain some interesting results so far as rotation of the polarization direction is concerned. We illustrate this by taking the case of MnF_2. The various elements of the matrix D are given by

$$D_{11} = [\gamma^2 - \Gamma_0^2 + V_n(0)]\underline{1} , \quad D_{22} = [(\gamma + g_n)^2 - \Gamma_g^2 + V_n(0)]\underline{1} ,$$

$$D_{12} = \begin{pmatrix} V_n(-\vec{g}) & cF_M(-\vec{g})(\eta_x - i\eta_y) \\ cF_M(-\vec{g})(\eta_x + i\eta_y) & V_n(-\vec{g}) \end{pmatrix} , \tag{40}$$

$$D_{21} = \begin{pmatrix} V_n(+\vec{g}) & cF_M(+\vec{g})(\eta_x - i\eta_y) \\ cF_M(+\vec{g})(\eta_x + i\eta_y) & V_n(+\vec{g}) \end{pmatrix} .$$

We have studied this case in detail and therefore have included nuclear potentials in the matrix D. If we analyze a purely magnetic peak, i.e., $V_n(+g) = 0$, then the two equations [similar to Eq. (26)] determining δ are degenerate, leading to the conclusion that $|f_{12}|^2 = |f_{34}|^2$. This will happen only if the form factor of the ion is real and spherical. In the following, we assume that covalency effects and the nonsphericity of the form factor can be neglected. Therefore, we observe that for *purely magnetic* peaks the flipping ratio will be one and the cross section will not depend upon the polarization—a fact borne out by kinematical theory also.

The strongest mixed peak in MnF_2 is (210). For this peak the following numerical values of the structure factors can be easily evaluated.[23]

$$F_N(\vec{g}) = -4b_F \sin(2\pi uh)\sin(2\pi uk) ,$$

$$u = 0.31 \simeq \tfrac{1}{3} .$$

$(hkl) \equiv (210)$; b_F, the scattering length for flourine ions, is 0.55×10^{-12} cm.

$$F_N(\mp\vec{g}) = 1.39 \times 10^{-12} \text{ cm} ;$$

$$F_N(0) = 2b_{Mn} + 4b_F = 1.52 \times 10^{-12} \text{ cm} ;$$

$$b_{Mn} = -0.36 \times 10^{-12} \text{ cm} ;$$

$$F_M(-\vec{g}) = \frac{2\gamma e^2}{m_e c^2} S(1 - e^{i\pi(2+1+0)})f .$$

Taking $f = 0.7$ and $S = \frac{5}{2}$ (Ref. 24)

$$F_M(\mp\vec{g}) = 3.8 \times 10^{-12} \text{ cm}$$

$V = F \times 4\pi/(v_0)$; v_0, the volume of the unit cell, is 114 Å^3. For illustration, we choose a simple geometry. We take a crystal oriented in the (001) direction (the direction of $\hat{\eta}$) and analyze the (210) peak in symmetrical Laue geometry, i.e., the scattering vector $\vec{G}$ is parallel to the incident face of the crystal. For this case eigenvalues λ_1 and λ_2 are $(F_N + F_M)4\pi/v_0$ and $(F_N - F_M)4\pi/v_0$, respec-

tively. At the peak

$$\Delta = \frac{|F_N + F_M|}{\Gamma_0}\frac{4\pi}{v_0}, \quad \Delta' = \frac{|F_N - F_M|}{\Gamma_0}\frac{4\pi}{v_0}, \tag{41}$$

and

$$f_{12}(T) = \frac{1}{4}\sin\left(\frac{|F_N + F_M|}{2\Gamma_0}\frac{4\pi}{v_0}T\right),$$

$$f_{34}(T) = \frac{1}{4}\sin\left(\frac{|F_N - F_M|}{2\Gamma_0}\frac{4\pi}{v_0}T\right).$$

Next we compute the flipping ratio for $\vec{p}\cdot\hat{\eta} = \pm 1$. In this case $\vec{p}$ will be automatically perpendicular to $\hat{G}$ if we choose it to be parallel to $\hat{\eta}$.

$$R = \frac{|f_{12}(T)|^2}{|f_{34}(T)|^2}$$

$$= \sin^2\left(\frac{F_N + F_M}{2\Gamma_0}\frac{4\pi}{v_0}T\right)\Big/\sin^2\left(\frac{F_N - F_M}{2\Gamma_0}\frac{4\pi}{v_0}T\right)$$

$$= \left(\frac{\sin(p+1)x}{\sin(p-1)x}\right)^2,$$

where

$$p \equiv F_N/F_M, \quad x \equiv (F_M/2\Gamma_0)(4\pi/v_0)T.$$

For the (210) reflection of MnF_2

$$F_N/F_M = 0.366 \simeq 0.37.$$

The flipping ratio versus x is shown in Fig. 1, where

$$x = 0.033(\lambda T/\cos\theta_B),$$

λ is in Å, T is in μm.

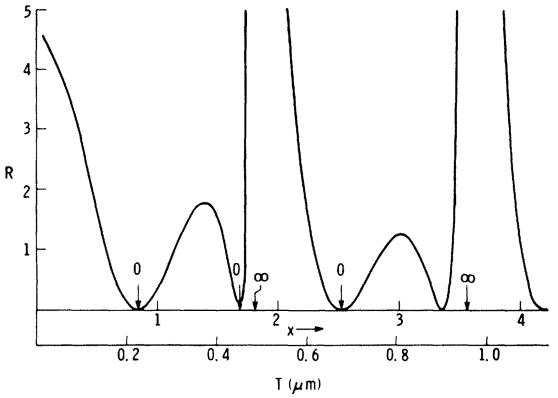

FIG. 1. Flipping ratio R for MnF_2 (210) peak in symmetrical Laue configuration. x is a dimensionless parameter (see text). Thickness T is for incident neutrons of wavelength 2.5 Å.

IV. CONCLUSION

We have extended the dynamical theory of diffraction to include the effects of magnetic ordering on the polarization dependence of the scattered intensity and on the polarization of the scattered beam. The theory is given for arbitrary magnitude and direction of incident polarization, and for arbitrary spin arrangement.

The theory appears very similar to kinematical theory except that the interaction potential V between neutron and crystal is replaced by a matrix which can be written as a product of V and some thickness-dependent matrix $F(T)$. Calculations of M have been carried out in detail, for the case of spiral spin structures, ferromagnets, and antiferromagnets. Intensity as well as final polarization states have been computed for some important experimental geometries. When M contains the thickness dependence as a scalar multiple then there is *no rotation* of the spin direction of the neutron as it comes out of the crystal after passing through the magnetic structure. In this aspect the results presented here are different from those of Nityananda, for simple spiral structures. In simple spirals, there is no rotation in the *forward diffracted* beam, but the forward transmitted beam does undergo a rotation of the spin direction which depends upon the thickness. In the case of an antiferromagnet on a body-centered lattice (e.g., MnF_2) there is a rotation of the spin direction only for mixed peaks, i.e., those peaks where both magnetic and nuclear interactions contribute.

Throughout this paper we have concentrated on the phenomenon of rotation of the spin of the neutron and, therefore, have not discussed such topics as depolarization of the diffracted beam, for example. However, the formulation presented is general and these effects can be readily computed.

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