THEORY OF SCATTERING OF SLOW NEUTRONS IN MAGNETIC CRYSTALS

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CONTENTS

INTRODUCTION

SLOW, or thermal, neutrons interacting with the atoms of a scatterer are subject to two types of scattering: nuclear and magnetic. The first is caused by the interaction of the neutron with the nucleus via purely nuclear forces and has a scattering cross section of the order of one barn. The second type of scattering is due to the presence of the magnetic moment of the neutron which interacts with the magnetic moment of the atom so long as it is different from zero. The cross section for magnetic scattering, like nuclear scattering, is of the order of a barn.

In the scattering of slow neutrons in a crystal the de Broglie wave lengths of which are comparable with interatomic spacings, one gets the typical diffraction scattering picture: for scattering angles corresponding to the Wulff-Bragg conditions, there appear sharp peaks in the intensity of coherently scattered neutrons. If the crystal does not contain magnetic atoms, the entire interference picture is caused by the nuclear scattering of the neutrons from the atoms occupying periodic positions in this space. When the crystal contains magnetic atoms, but these do not form a magnetic order (of the ferro- or antiferromagnetic type), the magnetic scattering of the neutrons will not be coherent because of the chaotic orientation of the magnetic moments of the atoms, and thus the coherent picture will once more be caused by the nuclear scattering.

However, if there is magnetic order in the crystal over a volume of one or several unit cells, the magnetic scattering of the neutrons will also be coherent. In general the conditions for Bragg magnetic reflections will be different from those for nuclear reflections, so that the locations of the coherent peaks in the magnetic scattering may not coincide with those of the nuclear peaks.

In the scattering of unpolarized neutrons there is no interference between nuclear and magnetic scattering, so that we have a simple superposition of the intensities for the two; then, depending on the magnetic structure of the crystal, the magnetic peaks may be superposed on the nuclear peaks (since each magnetic atom also gives a nuclear scattering of the neutron), but they may also appear independently of the nuclear peaks.

As we see from the foregoing, the study of coherent scattering of neutrons in crystals permits one to understand the crystal-chemical and magnetic structure of the crystal. This constitutes the method of neutronography, which at present has already developed into an extensive region of experimental physics and becomes more and more important, especially for the science of magnetic materials. So-called magnetic neutronography is the basis on which the modern theory of ferro- and antiferromagnetism is based.

But the method of neutron diffraction is not limited to the possibility of studying just crystal structures. The coherent Bragg peaks which are associated with

the determination of the structure are those directions along which neutrons are scattered elastically for the most part, i.e., without exchange of energy with the crystal. But neutrons can also be scattered inelastically, giving up a part of their energy to the crystal or getting some from it.

It is well known that inelastic nuclear scattering of neutrons occurs via absorption or emission by the neutron of a definite number of phonons. Magnetic inelastic scattering in the presence of magnetic order occurs via the absorption or emission of magnons— quanta of the spin waves. Phonons and magnons are collective motions of the atoms coupled by the crystalline forces and by the exchange forces between the magnetic moments of the atoms in the crystal. It therefore follows that the study of inelastic scattering of neutrons in crystals permits one to study the dynamics of the crystal: the spectrum of thermal lattice vibrations (phonons) and the spectrum of thermal vibrations of the spin system (magnons).

We can say immediately that the greatest information about the state of the magnetic system of a crystal which has magnetic order comes from a study of the scattering of neutrons near the transition point— magnetic order-disorder, and also from the study of the scattering of polarized neutrons, where one gets interference between the nuclear and magnetic scattering. Even such a brief glance at the possibilities of neutronography shows that experimenters have at their disposal a powerful method for studying the solid state.

The survey as a whole will consistently and systematically present the theory of scattering of slow neutrons in crystals. Since the theory of nuclear scattering in crystals was worked out in detail in the monograph of Akhiezer and Pomeranchuk,[1], our main attention will be devoted to magnetic scattering, especially to questions which have become important in recent years: inelastic scattering, critical scattering, and also the scattering of polarized neutrons. Various applications of elastic magnetic scattering have been treated earlier in the monograph of Bacon[2] and also in the surveys [3,4]. At the same time we have tried to maintain a definite equilibrium between the different parts of the theory in order to cover a wide range of problems. The survey does not pretend to complete explanation of the problem, and only those aspects are considered which have an application to experiment, although very few experimental data are given.* In this connection we have not considered at all problems of multi-phonon and multi-magnon scattering, limiting ourselves merely to a description of their main features.

The presentation is given within a unified mathematical scheme corresponding to a description of the

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*A survey of various applications of the neutronographic method is contained in the paper of Zhdanov and Ozerov.[46]

scattering in the Born approximation. By introducing the so-called time formalism (Van Hove [5,6]), the problem of calculating the scattering cross section per unit solid angle and per unit energy range reduces to computing the Fourier components of the correlations between positions of two atoms in the lattice at different moments in time for the nuclear scattering, and of the correlation functions of the spin projections for the magnetic scattering. The appropriate mathematical apparatus is developed in part I. Later it is applied to various problems of scattering theory.

In part II we consider elastic nuclear and magnetic scattering of neutrons and present the fundamentals of neutronography—nuclear and magnetic. •Part III considers inelastic scattering of neutrons. Here only one-quantum scattering is considered, in which one phonon or one magnon is absorbed or emitted. The theory of this question lies at the basis of the experimental method for reconstructing the spectra of phonon and spin waves from the data on inelastic scattering. In part IV we present the features of magnetic scattering of neutrons near the Curie point. Under conditions of a phase transition of the second kind, where fluctuations in the magnetization increase, one gets "critical" scattering of neutrons which is similar to the scattering of light in a medium in the critical state (opalescence). And finally, part V is devoted to the scattering of polarized neutrons. Here we consider two classes of questions: 1) scattering cross sections of polarized neutrons, 2) change in the polarization vector of the incident neutron beam on scattering in ferro- and antiferromagnets.

I. GENERAL EXPRESSIONS FOR SCATTERING CROSS SECTIONS

1. Time formalism in scattering theory

In problems of scattering of slow neutrons in materials, under conditions remote from resonance capture by the atomic nuclei, one usually starts from the Born approximation which corresponds to the first order of perturbation theory. When the scatterer consists of a large number of particles (for example, a crystal), it is convenient in calculating scattering cross sections to introduce the time formalism. In its most general formulation the problem consists of the following.

The scatterer is in a state of statistical equilibrium at a given temperature and is described by the statistical operator $\rho = e^{-\beta \mathcal{H}}/\text{Tr } e^{-\beta \mathcal{H}}$, where $\mathcal{H}$ is the Hamiltonian and $\beta = 1/kT$. Let the initial state of the scatterer by characterized by the wave function $| n_0)$, which is an eigenfunction of the scatterer Hamiltonian so that

$$\mathcal{H} | n_0) = E_{n_0} | n_0).$$

During interaction with the neutron the scatterer goes over into another stationary state, and the neutron

can change its momentum and spin. The initial state of the neutron is described by the wave function $| p\sigma)$ where p is the wave vector and σ is the spin. We shall determine the total probability for a process in which the neutron, after interacting with the scatterer, goes over into the state $| p'\sigma')$.

The total Hamiltonian of the system, scatterer plus neutron, consists of two parts:

$$H = H_0 + H',$$

where $H_0 = \mathscr{H} + \mathscr{H}_n$ is the Hamiltonian of the scatterer and the neutron, and H' is the operator for interaction between them.

To study the development of the system, scatterer plus neutron, in time, it is convenient to use the evolution operator, [7] expanding it in powers of the interaction:

$$e^{-\frac{i}{\hbar}HT} = e^{-\frac{i}{\hbar}H_0T}\left(1 - \frac{i}{\hbar}\int_0^T e^{\frac{i}{\hbar}H_0t_1}H'e^{-\frac{i}{\hbar}H_0t_1}dt_1 + \ldots\right).$$
(1.1)

We go over to a second-quantization representation for the neutrons, in which we have

$$\mathscr{H}_n = \sum_{p\sigma} E_p a^+_{p\sigma}a_{p\sigma}, \quad H' = \sum_{pp'\sigma\sigma'} V_{p'\sigma',\,p\sigma}a^+_{p'\sigma'}a_{p\sigma},$$
(1.2)

where E_p is the neutron energy, $V_{p'\sigma',p\sigma}$ is the matrix element for the interaction operator taken between the neutron states.

If at the initial time the system was described by the wave function $| p\sigma) | n_0)$, then at time T the wave function of the system will be

$$e^{-\frac{i}{\hbar}HT}| p\sigma) | n_0) = e^{-\frac{i}{\hbar}H_0T}\left[1 - \frac{i}{\hbar}\sum_{pp'\sigma\sigma'}\int_0^T dt_1 e^{\frac{i}{\hbar}(E_{p'}-E_p)t_1}\right.$$

$$\left.\times V_{p'\sigma',\,p\sigma}(t_1)a^+_{p'\sigma'}a_{p\sigma} + \ldots\right] | p\sigma) | n_0),$$
(1.3)

where

$$V_{p'\sigma',\,p\sigma}(t) = e^{\frac{i}{\hbar}\mathscr{H}t}V_{p'\sigma',\,p\sigma}e^{-\frac{i}{\hbar}\mathscr{H}t}$$
(1.4)

is the Heisenberg representative of the interaction operator for the scatterer Hamiltonian.

From expression (1.3) it follows that the total probability of transition of the neutron to the state $| p'\sigma')$ at time T in which the scatterer leaves from the initial state $| n_0)$, is equal to

$$\frac{1}{\hbar^2}\left(n_0 \middle| \int_0^T dt_2 \int_0^T dt_1 e^{\frac{i}{\hbar}(E_{p'}-E_p)(t_1-t_2)} V^+_{p'\sigma',\,p\sigma}(t_2) V_{p'\sigma',\,p\sigma}(t_1) \middle| n_0\right).$$
(1.5)

We average this probability over the initial states of the scatterer, i.e., we multiply (1.5) by ρ_{n_0} and sum over n_0. We note that this is equivalent to taking the trace of the product of ρ with the operator appearing in (1.5) under the matrix element symbol. In addition, we make a change of variables of integration in (1.5), introducing $t = t_1 - t_2$. Noting that under the trace

sign we can make a cyclic permutation of the operators, we obtain for the averaged transition probability the expression

$$\frac{1}{\hbar^2}\int_0^T dt_2 \int_{-t_2}^{T-t_2} dt e^{\frac{i}{\hbar}(E_{p'}-E_p)t}\langle V^+_{p'\sigma',\,p\sigma}V_{p'\sigma',\,p\sigma}(t)\rangle,$$
(1.6)

where $\langle \ldots \rangle$ is a symbol for statistical averaging over the states of the scatterer, i.e.,

$$\langle \ldots \rangle = \mathrm{Sp}\,(e^{-\beta\mathscr{H}}\ldots)/\mathrm{Sp}\,e^{-\beta\mathscr{H}}.$$
(1.7)

In many statistical systems, including crystals, the correlation functions decrease rapidly with time (frequently exponentially). If the correlation function in (1.6) decreases rapidly with some characteristic time τ_c, then for times $T \gg \tau_c$ we can find the asymptotic behavior of (1.6) by replacing the limits in the second integral by $+\infty$ and $-\infty$. Now we see that under these conditions the transition probability is proportional to the time of the transition, and we can introduce the transition probability per unit time

$$W_{p'\sigma',\,p\sigma} = \frac{1}{\hbar^2}\int_{-\infty}^{+\infty} dt e^{\frac{i}{\hbar}(E_{p'}-E_p)t}\langle V^+_{p'\sigma',\,p\sigma}V_{p'\sigma',\,p\sigma}(t)\rangle.$$
(1.8)

If the wave functions of the neutron are normalized to unity (to a δ function), the effective cross section for scattering into unit solid angle per unit energy range $d^2\sigma/d\Omega dE_{p'}$ is related to this probability by the equation [8]

$$\frac{d^2\sigma}{d\Omega\,dE_{p'}} = \frac{m^2}{(2\pi\hbar)^3}\frac{p'}{p}W_{p',\,p}.$$
(1.9)

Here m is the mass of the neutron, $W_{p',p}$ is the probability $W_{p'\sigma',p\sigma}$ averaged over the spin states in the initial beam and summed over the spin states in the final beam. Thus the effective scattering cross section is equal to

$$\frac{d^2\sigma}{d\Omega dE_{p'}} = \frac{m^2}{(2\pi)^3\hbar^5}\frac{p'}{p}\int_{-\infty}^{+\infty} dt e^{\frac{i}{\hbar}(E_{p'}-E_p)t}\overline{\langle V^+_{p',\,p}V_{p',\,p}(t)\rangle},$$
(1.10)

where $V_{p',p}$ is the matrix element of the operator for interaction of the neutron with the scatterer taken only with respect to the momentum states of the neutron. The bar over the operator means

$$\bar{L} = \mathrm{Sp}\,\rho_\sigma L,$$
(1.11)

where ρ_σ is the spin density operator in the initial beam.

Thus in the general case the effective cross section for scattering of neutrons in a material is proportional to the Fourier component of the correlator of the interaction. Time correlations in the theory of scattering of neutrons were first considered by Van Hove [5,6] for the problems of nuclear and magnetic scattering.

It is useful also to put Eq. (1.8) in matrix form (in the representation of the scatterer Hamiltonian $\mathscr{H}$), after integration over the time:

$$W_{p'\sigma', p\sigma} = \frac{2\pi}{\hbar} \sum_{nn_0} \varrho_{n_0} |(n_0|V_{p'p}|n)|^2 \delta(E_p - E_{p'} - E_n + E_{n_0}).$$
(1.12)

From this we see that the method developed here is equivalent to the first approximation in the Born theory of scattering.

2. Interaction of Slow Neutrons with Magnetic Materials

The energy of interaction of a neutron with a magnetic material consists of two parts: the interaction energy with the nuclei and the magnetic interaction energy with the electrons. Generally speaking, there is also an interaction of the neutron with the electrons which is independent of spin, and a magnetic interaction with the magnetic moments of the nuclei. But both these interactions are very small and will be neglected in what follows.

To calculate scattering cross sections using the formalism developed in Sec. 1, we must find expressions for the matrix elements $V_{p',p}$ of the operator for interaction of the neutron with the scatterer.

1. Matrix element of nuclear interaction. The energy of interaction of a neutron with a nucleus is conveniently described by introducing the so-called pseudo-potential. For slow neutrons, where the scattering is mainly by S-wave, the scattering amplitude consequently does not depend on the scattering angle, and the pseudo-potential can be taken in the following form: [1]

$$V(r_n) = \alpha\delta(r_n - R),$$
(2.1)

where r_n and R are the coordinates of the neutron and nucleus and α is determined by the scattering amplitude of the free nucleus.

If the nucleus has a spin, the scattering amplitude differs depending on the orientations of the spins of the nucleus and neutron. This can be taken into account by writing α in the form

$$\alpha = A + B(S_nI),$$
(2.2)

where S_n and I are the spins of the neutron and nucleus, and A and B are constants. From the well-known properties of the operators S_n^x, S_n^y and S_n^z, expression (2.2) is the most general form for α.

In the case of interaction with a system of N nuclei, we have

$$V = \sum_{l=1}^{N} \alpha_l\delta(r_n - R_l).$$
(2.3)

The matrix element $V_{p',p}$ of the operator V between states of the neutron with momenta $\hbar p$ and $\hbar p'$ is given on the basis of (2.3) in the form

$$V_{p',p} = \Sigma_l\alpha_l \exp[i(p - p')\cdot R_l].$$
(2.4)

2. Matrix element of magnetic interaction. By magnetic interaction of the neutron with the scatterer we should understand the interaction of the magnetic field produced by the neutron with the electron currents forming unclosed shells of the scatterer atoms. The energy operator for such an interaction can be written in the form

$$V = \sum_l \frac{1}{c} A_n(r_l)j(r_l),$$
(2.5)*

where $A_n(r) = [\mu_n \times (r - r_n)]/|r - r_n|^3$ is the vector-pontential of the field at point r produced by the neutron located at point r_n, $\mu_n = 2\gamma\mu_nS_n$ is the magnetic moment of the neutron ($\gamma = -1.93$ is the value of the magnetic moment of the neutron in nuclear Bohr magnetons μ_n), $j(r_l)$ is the current produced by the l'th electron. Summing in (2.5) is done over all the unpaired electrons of the scatterer.

Let us calculate the matrix element between states of the neutron with momenta $\hbar p$ and $\hbar p'$ and states of the scatterer Ψ_a and $\Psi_{a'}$. We have

$$(a'|V_{p',p}|a) = \sum_l \int\int \frac{[\mu_n \times (r_l - r_n)]}{|r_l - r_n|^3}$$

$$\times \frac{1}{c} \Psi_a^* j(r_l) \Psi_a e^{i(p-p')r_n} dr_n(d\tau).$$
(2.6)

Integration over $d\tau$ is done over the coordinates of all electrons included in (2.5). It is well known [8] that the matrix elements of the current are equal to

$$\frac{1}{c}\Psi_{a'}^* j(r_l)\Psi_a = i\mu_0(\Psi_a\nabla_l\Psi_{a'}^* - \Psi_{a'}^*\nabla_l\Psi_a) + 2\mu_0\,\mathrm{rot}_l(\Psi_{a'}^*, s_l\Psi_a),$$
(2.7)†

where s_l is the spin operator of the l'th electron, μ_0 is the Bohr magneton. The first term on the right of (2.7) describes the current produced by the orbital motion of the electron, and the second gives the spin current. For the present we shall consider only the spin part of the current. Substituting the expression for it into (2.6) and introducing the relative coordinates $r_l - r_n = R$, we write the expression for the matrix element (2.6) in the form

$$(a'|V_{p',p}|a)$$

$$= -\sum_l \left[\mu_n \times \int \frac{e^{-iqR}R\,dR}{R^3} \right] \int 2\mu_0 e^{iqr_l}\,\mathrm{rot}_l(\Psi_a^* s_l\Psi_a)\,d\tau,$$
(2.8)

where $q = p - p'$ is the vector of scattering. Noting that

$$\int \frac{R\,dR}{R^3}e^{-iqR} = -\frac{4\pi iq}{q^2},$$

$$\int e^{iqr_l}\,\mathrm{rot}_l(\Psi_a^* s_l\Psi_a)\,dr_l = -i\left[q \times \int e^{iqr_l}\Psi_a^* s_l\Psi_a\,dr_l \right],$$

we now have in place of (2.8)

$$(a'|V_{p',p}|a)$$

$$= -\frac{4\pi\hbar^2}{m}r_0\gamma\left(\left(a'\left|\sum_l e^{iqr_l}s_l\right|a\right), S_n - (eS_n)e \right).$$
(2.9)

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*(ab) or (a, b) = a·b.
†rot = curl.

The expression in parentheses gives the scalar product of the vectors, $r_0 = e^2/m_0c^2$ is the electromagnetic radius of the electron, and $e = q/q$ is the unit scattering vector.

In expression (2.9) the spin variables of the neutron and scatterer are separated. A further simplification can be achieved if we break up the summation over l into a sum over electrons of the individual atoms $\sum_\nu$ and a sum over all atoms of the scatterer $\sum_j$. We shall consider purely magnetic scattering, when the state of the lattice does not change, while $|$ a) characterizes the set of spin variables for the electrons. In this case we can write

$$\left(a' \,\Big|\, \sum_l^N e^{iqr_l}s_l \,\Big|\, a \right) = \sum_j^N e^{iqR_j} \left(a' \,\Big|\, \sum_\nu^{z_j} e^{iqr_\nu}s_\nu \,\Big|\, a \right), \quad (2.10)$$

where z_j is the number of unpaired electrons in atom j.

For slow neutrons we can assume that they do not produce transitions of the atoms into excited states, but produce only a reorientation of the atomic spins. Thus the transition $|$ a) $\rightarrow$ $|$ a') has the form $|$ αm) $\rightarrow |$ αm'), where m and m' are the sets of spin quantum numbers for the scatterer atoms, while α is the set of all the remaining quantum numbers of the atom. From general theorems of quantum mechanics* it follows that the matrix element in (2.10) can be written in our case as

$$\left(a' \,\Big|\, \sum_\nu^{z_j} e^{iqr_\nu}s_\nu \,\Big|\, a \right) = (m' |\, S_j \,| m) \left(\alpha m \,\Big|\, \sum_\nu^{z_j} \frac{e^{iqr_\nu}(s_\nu S_j)}{S_j(S_j+1)} \,\Big|\, \alpha m \right),$$
$$(2.11)$$

where $S_j = \sum_\nu^{z_j} s_\nu$ is the spin operator for atom j, and S_j is the value of the spin. The expression

$$F_j(q) \equiv \left(\alpha m \,\Big|\, \sum_\nu^{z_j} \frac{e^{iqr_\nu}(s_\nu S_j)}{S_j(S_j+1)} \,\Big|\, \alpha m \right)$$

$$= \int \Psi_j^* \sum_\nu^{z_j} \frac{e^{iqr_\nu}(s_\nu S_j)}{S_j(S_j+1)} \, \Psi_j \, d\tau_j, \quad (2.12)$$

where Ψ_j is the wave function of the electrons of the j-th atom, $d\tau_j$ is the element of volume in configuration space of the electrons of the j-th atom, and does not depend on the quantum numbers m, i.e., on the

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*In quantum mechanics it is shown (cf., for example, [9]), that if the vector quantities $\hat{T}_k(k = x, y, z)$ satisfy the commutation relation $[\hat{J}_i, \hat{T}_k] = i\hbar e_{ikl}T_l$, where $\hat{J}_i$ is the projection of the angular momentum, then we have the relation

$$j(j+1)(\alpha jm \,|\, \mathbf{T} \,|\, \alpha'jm') = (\alpha jm \,|\, \mathbf{J} \,|\, \alpha jm')(\alpha jm' \,|\, (\mathbf{JT}) \,|\, \alpha'jm'),$$

where j is the total angular momentum of the system, m is the projection of the total angular momentum. Applying this relation to the operator $\hat{T} = \sum_\nu^{z_j} e^{iqr_\nu}s_\nu$, we get formula (2.11).

orientation of the atomic spin and is a characteristic of the scattering power of the atom. This quantity is called the magnetic form factor of the atom (it should more precisely be called the spin form factor). $F_j(q)$ characterizes the distribution of the spin density in the atom. For $z_j = 1$, $F_j(q)$ is simply the Fourier component of the spin density.

Thus the transformation (2.10) and (2.11) allowed us to express the matrix element (2.6) in terms of matrix elements $(m \,|\, S_j \,| m')$ of the spin operators of the individual scatterer atoms. Combining expressions (2.9)—(2.12), we get the following expression for the magnetic interaction operator:

$$V_{p',p} = -\frac{4\pi\hbar^2}{m} r_0\gamma \sum_j F_j(q) e^{iqR_j}(S_j, \, S_n - (eS_n)e), \quad (2.13)$$

which was first given by Halpern and Johnson.[10]

Similar calculations can also be made for the orbital part of the electron current, but they are more complicated since the orbital angular momentum operator does not commute with $e^{iq \cdot r}$. The corresponding results are given in [11]. Obviously the expression corresponding to (2.13) in the case of scattering by the orbital angular momentum of an atom must contain in place of the operators S_j, the operators L_j of the orbital angular momenta of the atoms. Also, in ferromagnets containing elements of the first transition group, orbital angular momenta are suppressed because of the fact that the crystalline field acting on the atom does not have axial symmetry, so that the average value of the projection of the angular momentum of the atom in the ground state is either equal to zero or much less than the value of the orbital moment of the atom. Therefore, scattering because of interaction of the neutron with orbital motion of electrons in such ferromagnets need not be considered.

3. Differential Cross Sections for Scattering of Unpolarized Neutrons

The expressions for the matrix elements of nuclear (2.4) and magnetic (2.13) interaction of the neutron with a scatterer allow one, by using the fundamental formula (1.10), to get the effective differential cross sections for scattering of unpolarized neutrons. For nuclear scattering

$$\frac{d^2\sigma}{d\Omega \, dE_{p'}} = \frac{m^2}{(2\pi)^3 \hbar^5} \frac{p'}{p} \sum_{ll'} \overline{\langle a_l a_{l'} \rangle}$$
$$\times \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}(E_{p'}-E_p)t} \langle e^{-iqR_l(0)} e^{iqR_{l'}(t)} \rangle \, dt, \quad (3.1)$$

where $R_l(t)$ is the Heisenberg representative of the quantity R_l with the scatterer Hamiltonian $\mathcal{H}$,

$$R_l(t) = e^{\frac{i}{\hbar}\mathcal{H}t} R_l e^{-\frac{i}{\hbar}\mathcal{H}t}. \quad (3.2)$$

For magnetic scattering we find the expression

$$\frac{d^2\sigma}{d\Omega\,dE_{p'}} (r_0\gamma)^2 \frac{p'}{p} \sum_{jj'} F_j(\mathbf{q}) F_{j'}(\mathbf{q}) \sum_{\alpha\beta} (\delta_{\alpha\beta} - e_\alpha e_\beta)$$

$$\times \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}(E_{p'}-E_p)t}$$

$$\times \langle S_j^\alpha(0) e^{-i\mathbf{q}\mathbf{R}_j(0)} e^{i\mathbf{q}\mathbf{R}_{j'}(t)} S_{j'}^\beta(t)\rangle\, dt \quad (\alpha, \beta = x,\, y,\, z), \quad (3.3)$$

where $S_j^\alpha(t)$ is the Heisenberg representative of the spin operator S_j^α

$$S_j^\alpha(t) = e^{\frac{i}{\hbar}\mathscr{H}t} S_j^\alpha e^{-\frac{i}{\hbar}\mathscr{H}t}. \quad (3.4)$$

In getting (3.3) we have, in accordance with the requirements of formula (1.10), averaged over the spin orientations in the neutron beam:

$$\overline{[S_n^\alpha - (\mathbf{eS}_n)\,e_\alpha]\,[S_n^\beta - (\mathbf{eS}_n)\,e_\beta]} = \frac{1}{4}(\delta_{\alpha\beta} - e_\alpha e_\beta). \quad (3.5)$$

It is easy to see that in the scattering of unpolarized neutrons there is no interference of nuclear and magnetic scattering, so that for a magnetic material

$$\frac{d^2\sigma}{d\Omega\,dE_{p'}} = \frac{d^2\sigma_n}{d\Omega\,dE_{p'}} + \frac{d^2\sigma_m}{d\Omega\,dE_{p'}}.$$

When the correlations in the positions of the atom and its spin projections can be neglected, i.e., when spin-lattice interaction is unimportant, the correlation function in (3.3) can be written approximately in the form

$$\langle S_j^\alpha(0) e^{-i\mathbf{q}\mathbf{R}_j(0)} e^{i\mathbf{q}\mathbf{R}_{j'}(t)} S_{j'}^\beta(t)\rangle \approx \langle e^{-i\mathbf{q}\mathbf{R}_j(0)} e^{i\mathbf{q}\mathbf{R}_{j'}(t)}\rangle \langle S_j^\alpha(0) S_{j'}^\beta(t)\rangle, \quad (3.6)$$

where the averaging on the right side is done independently: in the first factor over the states of the lattice, and in the second factor over the states of the spin system. The Heisenberg representatives of the quantities $\mathbf{R}_j(t)$ and $S_j^\alpha(t)$ are taken with the corresponding Hamiltonians.

If we neglect lattice vibrations, i.e., we set

$$\langle e^{-i\mathbf{q}\mathbf{R}_j(0)} e^{i\mathbf{q}\mathbf{R}_{j'}(t)}\rangle \approx e^{-i\mathbf{q}(\mathbf{R}_j - \mathbf{R}_{j'})}, \quad (3.7)$$

the expression for the cross section for magnetic scattering takes the form

$$\frac{d^2\sigma}{d\Omega\,dE_{p'}}$$

$$= (r_0\gamma)^2 \frac{p'}{p} \sum_{jj'} F_j(\mathbf{q}) F_{j'}(\mathbf{q}) e^{-i\mathbf{q}(\mathbf{R}_j - \mathbf{R}_{j'})} \sum_{\alpha\beta} (\delta_{\alpha\beta} - e_\alpha e_\beta)$$

$$\times \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}(E_{p'}-E_p)t} \langle S_j^\alpha(0) S_{j'}^\beta(t)\rangle\, dt. \quad (3.8)$$

In the following, however, we shall use the approximation (3.6) taking account of the lattice vibrations by introducing the so-called temperature factor.

Expressions (3.1) and (3.8) will be basic in our presentation of the scattering theory. We see that the cross sections for nuclear and magnetic scattering are simply the Fourier components of the correlation functions:[5,6]

$$\langle e^{-i\mathbf{q}\mathbf{R}_l(0)} e^{i\mathbf{q}\mathbf{R}_{l'}(t)}\rangle, \quad \langle S_j^\alpha(0) S_{j'}^\beta(t)\rangle. \quad (3.9)$$

II. ELASTIC SCATTERING

4. Nuclear Scattering in Single and Polycrystals

The differential cross section for elastic scattering of neutrons by nuclei can be gotten from (3.1) if we take out of the corresponding correlation function the term independent of the time. We can break up the correlation function most naturally as follows:

$$\langle e^{-i\mathbf{q}\mathbf{R}_l(0)} e^{i\mathbf{q}\mathbf{R}_{l'}(t)}\rangle = \langle e^{-i\mathbf{q}\mathbf{R}_l(0)} e^{i\mathbf{q}\mathbf{R}_{l'}(\infty)}\rangle$$

$$+ \{\langle e^{-i\mathbf{q}\mathbf{R}_l(0)} e^{i\mathbf{q}\mathbf{R}_{l'}(t)}\rangle - \langle e^{-i\mathbf{q}\mathbf{R}_l(0)} e^{i\mathbf{q}\mathbf{R}_{l'}(\infty)}\rangle\}. \quad (4.1)$$

Since the positions of the atoms are not correlated over infinitely long times, the first term on the right of (4.1), which is responsible for the elastic scattering, is equal to

$$\langle e^{-i\mathbf{q}\mathbf{R}_l(0)} e^{i\mathbf{q}\mathbf{R}_{l'}(\infty)}\rangle = \langle e^{-i\mathbf{q}\mathbf{R}_l}\rangle \langle e^{i\mathbf{q}\mathbf{R}_{l'}}\rangle. \quad (4.2)$$

Substituting the expansion (4.1) in (3.1) and integrating over the energy of the scattered neutron, we get for the effective cross section for elastic scattering into unit solid angle the expression

$$\frac{d\sigma_0}{d\Omega} = \frac{m^2}{4\pi^2\hbar^4} \sum_{ll'} \overline{\langle a_l a_{l'}\rangle} \langle e^{-i\mathbf{q}\mathbf{R}_l}\rangle \langle e^{i\mathbf{q}\mathbf{R}_{l'}}\rangle. \quad (4.3)$$

For simplicity, we consider in the following a crystal consisting of atoms of one kind, assuming, however, that there may be different isotopes. Expression (4.3) must be averaged over the distributions of isotopes. We note first of all that if we expand the radius vector $\mathbf{R}_l$ into its equilibrium part $\mathbf{R}_l^0$ and the displacement $\mathbf{U}_l$:

$$\mathbf{R}_l = \mathbf{R}_l^0 + \mathbf{U}_l, \quad (4.4)$$

then in the expression $\langle e^{-i\mathbf{q}\cdot\mathbf{R}_l}\rangle \equiv e^{-i\mathbf{q}\cdot\mathbf{R}_l^0} \langle e^{-i\mathbf{q}\cdot\mathbf{U}_l}\rangle$ the average value of the displacement function $\mathbf{U}_l$ should be independent of l. Averaging in the sum over l and l' of (4.3) over the isotope distribution, as well as over the orientations of spins in the neutron beam, in the case where the nuclei of the scatterer have spins, we write the expression (4.3) in the form

$$\frac{d\sigma_0}{d\Omega} = \left\{\sigma^{(0)} \left| \sum_l e^{i\mathbf{q}\mathbf{R}_l^0}\right|^2 + N\sigma'\right\} e^{-2W}\mathbf{q}, \quad (4.5)$$

where we have introduced the notation

$$\sigma^{(0)} = \frac{m^2}{4\pi^2\hbar^4} \overline{A}^2, \quad \sigma' = \frac{m^2}{4\pi^2\hbar^4}\left[\overline{A^2} - \overline{A}^2 + \frac{1}{4}\overline{B^2 I(I+1)}\right], \quad (4.6)$$

$$e^{-2W}\mathbf{q} = |\langle e^{i\mathbf{q}\mathbf{U}_l}\rangle|^2. \quad (4.7)$$

In the expression (4.6) the bar above means an average over the isotope distribution; for example, $\overline{A} = \sum_s A_s C_s$, where C_s is the concentration of the isotope for which $A_l = A_s$, N is the number of nuclei in the crystal, I is the spin of the nucleus. The

quantity W_q introduced in (4.5) is the Debye-Waller temperature factor.[12] It can be calculated using the relation (4.7).

The sum appearing in (4.5) can also be calculated easily. If in the crystal there is one atom per unit cell, we have the relation [1,13]

$$\Big| \sum_l e^{i q R_l^0} \Big|^2 = \frac{(2\pi)^3 N}{V_0} \sum_\tau \delta\,(q - \tau), \qquad (4.8)$$

where τ is a vector of the reciprocal lattice multiplied by 2π, V_0 is the volume of a unit cell. If in a unit cell there are several atoms, the phase sum over all the atoms should be split into a sum over atoms within a single unit cell and a sum over all of the unit cells. This gives [1]

$$\Big| \sum_l e^{i q R_l^0} \Big|^2 = \frac{(2\pi)^3 N}{V_0}\,S\,(q) \sum_\tau \delta\,(q - \tau), \qquad (4.9)$$

where

$$S\,(q) = \Big| \sum_v e^{i q R_v^0} \Big|^2 \qquad (4.10)$$

is the structure factor; the summation over v goes over all the atoms of a single unit cell.

Substituting expression (4.8) in (4.5), we get the formula for the differential cross section for elastic nuclear scattering

$$\frac{d\sigma_0}{d\Omega} = \sigma^{(0)} \frac{(2\pi)^3 N}{V_0} \sum_\tau \delta\,(q - \tau)\,e^{-2W_q} + N\sigma' e^{-2W_q}. \qquad (4.11)$$

The first term gives sharp maxima in the intensity of scattered neutrons given by the Wulff-Bragg formula

$$p' - p = \tau. \qquad (4.12)$$

This term describes the coherent neutron scattering. The second term describes the incoherent scattering. If we neglect the factor e^{-2W_q}, it is independent of scattering angle and is similar to the background observed in the scattering of x-rays.

From the relations (4.6) we see that the coherent scattering is determined by the average value (over the distribution of isotopes) of the quantity $\overline{A}$. The incoherent scattering is determined by the quadratic fluctuation of the quantity A and the quantity $B^2 I (I + 1)$, depending on the nuclear spin. Thus the coherent scattering is determined by collisions of the neutron with nuclei without a change in spin direction, while for incoherent scattering the spin of the neutron may change.

Now let us look at relation (4.12). For elastic scattering $p' = p$, which is possible when $p > \tau/2$, so that elastic coherent scattering at angles different from zero is possible only if $p > \tau_{min}/2$, where τ_{min} is the smallest vector of reciprocal lattice. It is useful to express this fact as follows: coherent elastic scattering is impossible if the wave length of the neutron is greater than the Bragg wave length $\lambda_B = 4\pi/\tau_{min}$. One can show that inelastic scattering is also impossible under these conditions. It thus

follows that if a beam of thermal neutrons is incident on a crystal consisting of monoisotopic atoms whose nuclei have no spin, then in the direction of the initial beam, after emergence from the crystal, one will find only those neutrons whose wave vectors are smaller than $\tau_{min}/2$. Thus, one can filter out very slow "cold" neutrons. An example of such a filter is polycrystalline graphite, beryllium, beryllium oxide, etc.

We can now calculate the temperature factor W_q using the definition (4.7). We know that the displacements of the atoms from their equilibrium position can be expanded in Fourier series*,

$$U_l = \sum_{k j} e_j\,(k) \Big[\frac{\hbar}{2M N \omega_j (k)} \Big]^{1/2} (b_{kj} e^{i k R_l^0} + b_{kj}^+ e^{-i k R_l^0}) \qquad (4.13)$$

with quantized Bose-amplitudes which satisfy the commutation relations

$$[b_{kj},\, b_{k'j'}] = 0, \quad [b_{kj},\, b_{k'j'}^+]_- = \delta_{jj'} \delta_{kk'}. \qquad (4.14)$$

Here k and $e_j\,(k)$ are the wave vector and the polarization vector of the phonon, $\omega_j\,(k)$ is its frequency, $j = 1, 2, 3$ is an index for the phonon polarization, and M is the mass of the atom.

The energy spectrum of the lattice vibrations is then a sum over a definite number of phonons:

$$\mathscr{H} = \sum_{k j} \hbar \omega_j\,(k)\, b_{kj}^+ b_{kj}. \qquad (4.15)$$

Using expression (4.13), we can easily write

$$\langle e^{i q U_l} \rangle = \langle \prod_{k j} e^{i[\eta_{kj}^l b_{kj} + \eta_{kj}^{*l} b_{kj}^+]} \rangle, \qquad (4.16)$$

where for brevity we have used the notation

$$\eta_{kj}^l = \Big[\frac{\hbar}{2M N \omega_j (k)} \Big]^{1/2} (q e_j\,(k))\,e^{i k R_l^0}. \qquad (4.17)$$

From formula (4.16), taking account of the additivity of the energy operator (4.15), we get

$$\langle e^{i q U_l} \rangle = \prod_{k j} \langle e^{i[\eta_{kj}^l b_{kj} + \eta_{kj}^{*l} b_{kj}^+]} \rangle_{kj}, \qquad (4.18)$$

where

$$\langle \ldots \rangle_{kj} = \frac{Sp\,[e^{-\beta \hbar \omega_j (k) b_{kj}^+ b_{kj}} \ldots]}{Sp\,e^{-\beta \hbar \omega_j (k) b_{kj}^+ b_{kj}}}. \qquad (4.19)$$

Expanding the exponent in (4.18) in series and calculating the traces of the individual terms, we write the whole expression in the form

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*If the unit cell consists not of one, but several atoms (in general, different atoms), we should write in place of the expansion (4.13),

$$U_{lv} = \sum_{kj} \Big[\frac{\hbar}{2M_v \omega_j (k) N} \Big]^{1/2} [e_j^v\,(k)\,e^{i k R_l^0} b_{kj} + e_j^{*v}\,(k)\,e^{-i k R_l^0} b_{kj}^+],$$

where the complex polarization vectors $e_j^v(k)$ satisfy the orthonormalization relations

$$\sum_v e_j^v\,(k)\,e_j^{*v}\,(k) = \delta_{jj'}, \quad \sum_j e_j^{v\alpha}\,(k)\,e_j^{*v'\beta}\,(k) = \delta_{vv'} \delta_{\alpha\beta}.$$

Here $e_j^{v\alpha}(k)$ is the projection of the vector $e_j^v(k)$ on the axis $\alpha = x, y, z$.

$$\langle e^{iqU_l}\rangle = \prod_{kj}\left\{1 - \tfrac{1}{2}\,|\,\eta_{kj}^l\,|^2\,[2n_j(k)+1] + O\,(N^{-2})\right\}, \quad (4.20)$$

where

$$n_j(\mathbf{k}) \equiv \langle b_{kj}^+ b_{kj}\rangle_{kj} = (e^{\beta\hbar\omega_j(k)}-1)^{-1} \quad (4.21)$$

is the Bose distribution function for the average number of phonons in state k_j at temperature $T = 1/\beta k$. The remaining term contains terms in the expansion $\sim N^{-2}$ and higher order.

If we write

$$a_{kj} = \tfrac{1}{2}\,|\,\eta_{kj}^l\,|^2 [2n_j(k)+1],$$

expression (4.20) can easily be brought to the form[14]

$$\langle e^{iqU_l}\rangle = \prod_{kj}[1 - a_{kj} + O\,(N^{-2})]$$

$$= 1 - \sum_{kj} a_{kj} + \frac{1}{2!}\sum_{kj\neq k'j'} a_{kj}a_{k'j'} - \frac{1}{3!}\sum_{kj\neq k'j'\neq k''j''} a_{kj}a_{k'j'}a_{k''j''}$$

$$+ \sum_{kj} O\,(N^{-2}) + \sum_{kj\neq k'j'} a_{kj}\,O\,(N^{-2}) + \dots \quad (4.22)$$

Since the sum over k contains N terms, all of those terms which contain a sum of products of a_{kj} are of order 1, while terms containing $O(N^{-2})$ in addition to the a_{kj} are at least of order N^{-1}, and can be neglected. From arguments of this sort it is clear that the sum containing m factors a_{kj} can be replaced by $(\sum_{kj} a_{kj})^m$, where we make an error of order N^{-1}, so that instead of (4.22) we get

$$\langle e^{iqU_l}\rangle = 1 - \sum_{kj} a_{kj} + \frac{1}{2}\left(\sum_{kj} a_{kj}\right)^2$$

$$- \frac{1}{3!}\dots + O\,(N^{-1}) \approx e^{-\sum_{kj} a_{kj}}$$

to an accuracy of order N^{-1}.

Substituting this result in (4.7), we get*

$$W_q = \frac{\hbar}{2MN}\sum_{kj}\frac{[qe_j(k)]^2}{\omega_j(k)}\left[n_j(k)+\tfrac{1}{2}\right]. \quad (4.23)$$

This expression can be calculated by going from summation to integration

$$\sum_{k}\dots = \frac{V}{(2\pi)^3}\int d\mathbf{k}\dots \quad (4.24)$$

In a cubic crystal the energy of the phonons is the same for all three branches. If, in addition, we consider that for such a crystal $\sum_j (\mathbf{q}\cdot\mathbf{e}_j(\mathbf{k}))^2 = q^2$, then in the Debye approximation, where it is assumed that $\omega_j(\mathbf{k}) = ck$ (where c is the sound velocity), expression (4.23) reduces to the following:

$$W_q = \frac{3}{2}\frac{\hbar^2 q^2}{M\Theta}\left(\frac{1}{4}+\left(\frac{T}{\Theta}\right)^2\int_0^{\Theta/T}\frac{x\,dx}{e^x-1}\right). \quad (4.25)$$

Here Θ is the Debye temperature.* Thus, for a cubic crystal the dependence of the temperature factor on the direction of scattering is given by the factor $q^2 = 16\pi^2\sin^2\frac{\theta}{2}/\lambda^2$ where θ is the angle between the scattered and incident beams, λ is the wave length of the neutrons in the incident beam. In the presence of anisotropy of the sound velocity in non-cubic crystals, the angular dependence of W_q will be more complicated.

Formulas (4.11) apply to scattering by single crystals. In order to get the cross section for scattering by polycrystals we must average these cross sections over the orientations of the microcrystals, assuming that all orientations are equally probable.

Let us consider elastic coherent scattering.

To average over the orientations of the microcrystals it is sufficient, in the expressions

$$\frac{d\sigma_0^{coh}}{d\Omega} = \sigma^{(0)}\frac{(2\pi)^3}{V_0}\sum_{\tau}\delta(\mathbf{q}-\tau)\,e^{-2W_q} \quad (4.26)$$

to average[1] the δ-function over all orientations τ; in doing this we assume that the dependence of the temperature factor on q is given by the quantity q^2. Since

$$\int d\Omega_\tau\delta(\mathbf{q}-\tau) = \frac{1}{\tau^2}\delta(q-\tau) = \frac{1}{\tau^2}\delta\left(2p\sin\frac{\theta}{2}-\tau\right), \quad (4.27)$$

we have, after averaging (4.26),

$$\left(\frac{d\sigma_0^{coh}}{d\Omega}\right)_{polycr} = \sigma^{(0)}\frac{(2\pi)^3 N}{V_0}\sum_{\tau}\frac{a_\tau}{\tau^2}e^{-2W_\tau}\delta(2p\sin\theta-\tau), \quad (4.28)$$

where a_τ is the number of different vectors of the reciprocal lattice having length τ.

From (4.28) it follows that in place of individual diffraction maxima given by the equation: $\mathbf{p'} = \mathbf{p} + \tau$, which were present for a single crystal, in scattering by a polycrystal there are diffraction cones, with their axis along $\mathbf{p}$ and with the angles between their generator and the axis given by the conditions

$$2p\sin\frac{\theta}{2} = \tau, \quad (4.29)$$

along whose generators the neutrons are scattered.

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*If the unit cell contains several atoms, then for atom ν the temperature factor W_q^ν is again given by expression (4.23) with the appropriate value of the mass of the atom M_ν and the polarization vector $e_j^\nu(\mathbf{k})$.

*Recently attempts have been made to calculate the temperature factor using a more rigorous theory of lattice vibrations than the Debye theory. These papers were stimulated by the discovery of the Mössbauer effect, for which it turned out that the probability of emission of a γ quantum by a nucleus in a crystal without recoil is determined by the expression e^{-W_q}. As was shown by Kagan,[15] the Debye temperature is a satisfactory characteristic of the temperature factor only for a monatomic lattice. Already for the case of a diatomic lattice it is not even an approximate description of the temperature dependence of the temperature factor. In the case of polyatomic lattices the optical vibration branches play an important part.

Integrating (4.28) with respect to $d\Omega$, we get the total cross section for coherent scattering of a polycrystal:

$$(\sigma_0^{coh})_{polycr} = \sigma^{(0)} \frac{4\pi^3 N}{V_0 p^2} \sum_{\tau \leqslant 2p} \frac{a_\tau}{\tau} e^{-2W_\tau}. \qquad (4.30)$$

From formula (4.30) we see that with increasing p the cross section jumps when p reaches a value equal to half of any reciprocal lattice vector τ. It then decreases in inverse proportion to p^2, i.e., the neutron energy, until p reaches half the modulus of the next larger reciprocal lattice vector. With increasing p more and more planes characterized by vectors τ begin to participate in the reflection, so that the cross section becomes a smoothly varying function of the neutron energy.

From (4.30) it also follows that the total coherent scattering of a polycrystal is equal to zero if $p < \tau_{min}/2$. This is entirely reasonable, since under this condition coherent scattering is not possible for the individual single crystals.

5. Magnetic Scattering in Single and Polycrystals

The differential cross section for magnetic scattering by atomic spins is given by formula (3.8). First let us consider the scattering in paramagnets for which the interaction of the atomic spins can be neglected. In this case $S_j^\alpha(t) \equiv S_j^\alpha$, so that we see from (3.8) that the scattering will be elastic. Since there is no correlation between the orientations of the atomic spins of a paramagnet, and all orientations are equally probable, we have the relation

$$\langle S_j^\alpha S_{j'}^\beta \rangle = \delta_{\alpha\beta} \delta_{jj'} \langle (S_j^\alpha)^2 \rangle = \frac{1}{3} S(S+1) \delta_{\alpha\beta} \delta_{jj'}. \qquad (5.1)$$

Substituting this expression in (3.8) and integrating over the energy of the scattered neutrons, we get [10]

$$\frac{d\sigma}{d\Omega} = N \frac{2}{3} S(S+1)(r_0\gamma)^2 F^2(\mathbf{q}). \qquad (5.2)$$

Thus the angular dependence of the intensity of neutrons scattered from a paramagnet is given completely by the angular dependence of the magnetic form factor.

In the case of a ferromagnet there is a strong exchange interaction between the atomic spins which leads to a spontaneous ordering of the spins. Every reorientation of the spin of an individual atom is associated with an expenditure of energy against the exchange forces, so that magnetic scattering of neutrons in a ferromagnet can be either elastic or inelastic.

In order to take out of the cross section (3.8) the elastic part, we note, as in the case of nuclear scattering, that the time correlator $\langle S_j^\alpha(0) S_{j'}^\beta(t) \rangle$ is to be replaced by the expression $\langle S_j^\alpha(0) S_{j'}^\beta(\infty) \rangle$ which is independent of time. Since there is no correlation between the orientations of the spins over an infinitely long time interval, we can write

$$\langle S_j^\alpha(0) S_{j'}^\beta(\infty) \rangle \cong \langle S_j^\alpha \rangle \langle S_{j'}^\beta \rangle. \qquad (5.3)$$

Suppose that the average value of the spin at lattice site j along the direction of the spontaneous moment is $S_j(T)$; this is a function of temperature proportional to the magnetization of the ferromagnet.

From the theory of ferromagnetism it is known that for temperatures below the Curie point, but not close to it, the average value of spin components perpendicular to the direction of the spontaneous moment is equal to zero. Taking this fact into account, after substituting (5.3) in (3.8) and integrating over the energy of the scattered neutrons we get an expression for the differential cross section for elastic scattering in ferromagnets

$$\frac{d\sigma_0}{\partial\Omega} = (r_0\gamma)^2 \sum_{jj'} F_j(\mathbf{q}) F_{j'}(\mathbf{q}) e^{-i\mathbf{q}\cdot(\mathbf{R}_j - \mathbf{R}_{j'})} S_j(T) S_{j'}(T) [1 - (\mathbf{em})^2], \qquad (5.4)$$

where $\mathbf{m}$ is a unit vector in the direction of the spontaneous magnetic moment of the crystal. In (5.4) the summation over j extends over all the magnetic atoms of the crystal. If the ferromagnetic material consists of identical magnetic atoms, then $F_j(\mathbf{q}) = F(\mathbf{q})$ and $S_j(T) = S(T)$ is independent of the location of the lattice site and can be taken out of the summation sign. The sum over phase factors can be transformed to the form (4.8), after which the expression for the elastic scattering cross section is written as

$$\frac{d\sigma_0}{d\Omega} = (r_0\gamma)^2 S^2(T) F^2(\mathbf{q}) [1 - (\mathbf{em})^2]^2 \frac{(2\pi)^3 N}{V_0} \sum_\tau \delta(\mathbf{q} - \tau) e^{-2W_q}. \qquad (5.5)$$

For ferromagnetic materials consisting of magnetic and non-magnetic atoms, the magnetic unit cell coincides with the chemical cell, but the arrangement of the magnetic moments within the unit cell leads to the appearance in the scattering cross section of a structure factor for magnetic scattering analogous to the nuclear factor (4.10).

Thus, in the scattering of neutrons by a ferromagnet we get coherent maxima of the intensity at angles corresponding to the Wulff-Bragg conditions (4.12). These maxima are superposed on the maxima in the intensity of nuclear scattering. Since the cross section for magnetic scattering is proportional to the square of the magnetization, the coherent magnetic scattering should disappear above the Curie point, and thus the coherent maxima in the paramagnetic region correspond to nuclear scattering.

The angular dependence of coherent elastic magnetic scattering is much more complicated than that of the corresponding nuclear scattering, since it is determined by the additional angular dependence of the magnetic form factor as well as by the factor $1 - (\mathbf{e}\cdot\mathbf{m})^2$, depending on the orientation of the scattering vector relative to the vector $\mathbf{m}$ of the spontaneous magnetic moment.

In the case of a complex magnetic material (ferrite or antiferromagnet), one must take into account the

fact that the unit magnetic cell does not coincide with the chemical cell, but is larger than it. Such a magnetic material frequently can be considered as consisting of several ($\nu = 1, 2, \ldots, n$) identical sublattices superimposed upon one another, in which the directions of the spontaneous moments are characterized by unit vectors m_ν. For the averaging of the spin $S_\nu(T)$ in each of these sublattices, the same arguments hold as were given for a simple ferromagnet consisting of one sublattice (cf. the relation (5.3) and the following text). Breaking up the sum $\sum_j$ in (3.8) into a sum $\sum_s$ over magnetic cells and a sum $\sum_\nu$ over magnetic atoms within a single magnetic cell, or, what is the same thing, over the sublattices (since we associate a sublattice with each of the magnetic atoms in the unit magnetic cell), we obtain for the scattering cross section the expression

$$\frac{d\sigma_0}{d\Omega} = (r_0\gamma)^2 \frac{(2\pi)^3 N'_m}{V_{0m}} \sum_{\nu\nu'} F_\nu(q) F_{\nu'}$$

$$\times (q) S_\nu(T) S_{\nu'}(T) e^{iq(r_\nu - r_{\nu'})} e^{-W_{\nu q} - W_{\nu' q}} \cdot [m_\nu m_{\nu'}$$

$$- (em_\nu)(em_{\nu'})] \cdot \sum_{\tau_m} \delta(q - \tau_m). \tag{5.6}$$

Here N'_m is the number of magnetic unit cells in the crystal, V_{0m} is the volume of the unit magnetic cell, τ_m is a vector of the reciprocal lattice (multiplied by 2π), $W_{\nu q}$ is the temperature factor* corresponding to an atom of the ν-th sublattice.

In getting the expression (5.6) we have used the relation

$$\left| \sum_s e^{iqR_s} \right|^2 = \frac{(2\pi)^3 N'_m}{V_{0m}} \sum_{\tau_m} \delta(q - \tau_m), \tag{5.7}$$

which is analogous to (4.8).

Thus, in magnetic elastic scattering of neutrons in magnetic materials, coherent maxima of the intensity appear in places corresponding to Bragg reflections from the planes of the magnetic lattice. If the unit magnetic cell is larger than the chemical cell, we should get purely magnetic scattering maxima, not necessarily coincident with the nuclear maxima. Above the Curie point or the Néel point these are not present. Experimental study of these maxima, using relations of the type (5.6), permit one to determine the magnetic structure of the material. A relation of type (5.6) is the basis of magnetic neutronography.

From (5.6) we easily obtain the special formula for the cross section for scattering by an antiferro-

magnet consisting of two equivalent collinear sublattices:

$$\frac{d\sigma_0}{d\Omega} = (r_0\gamma)^2 F^2(q) S^2(T) e^{-2Wq} (1 - e_z^2)$$

$$\times [1 - \cos(qr_{12})] \frac{(2\pi)^3 N'_m}{V_{0m}} \sum_{\tau_m} \delta(q - \tau_m). \tag{5.8}$$

Here e_z is the projection of the scattering vector on the direction of one of the sublattices, r_{12} is a vector from one magnetic atom to the neighboring atom of the second sublattice. Formula (5.8) is equivalent to formula (5.5) for the scattering by a ferromagnet. The essential difference consists in the fact that the sets of vectors $\{\tau\}$ and $\{\tau_m\}$ are different. The magnetic unit cell in the present case is twice as large as the chemical cell. The temperature dependence of the intensity of antiferromagnetic peaks is determined by the square of the magnetization of either sublattice.

Recently new magnetic structures have been discovered ($MnAu_2$, Ho, Dy, Er et al.) in which there is a completely special magnetic order. These structures are characterized by the fact that along some crystal direction, which is a symmetry axis of high order, the orientations of the spins as one goes from one atom to the next change periodically, and the period of this variation does not coincide with the period of the crystal lattice and may change with temperature. Among a large class of such structures, which have been called helicoidal or screw structures, the simplest is the so-called ferromagnetic spiral (FS). The components of the spins along the base planes in such spirals go through a periodic rotation with a certain angle φ, while the components along the axis of the helicoid are constant. Such a crystal as a whole is a ferromagnet. A special case of the FS structure is the simple spiral (SS) which does not have a ferromagnetic component.

If the spin of the atom located at the origin is called S_0, the spin of the atom at lattice site j can be given by the following transformation:

$$S_j = S_0^z m + \frac{1}{2} S_0^- e^{-ik_0 R_j} m^+ + \frac{1}{2} S_0^+ e^{ik_0 R_j} m^-,$$

where m is the unit vector along the axis of the helicoid, $m^\pm = m^x \pm im^y$, where m^x and m^y are unit vectors in the base plane, k_0 is a vector directed along the axis of the helicoid ($k_0 \parallel m$) of such a length that $k_0 c = \varphi$ is the angle between two neighboring spins of the helicoid (c is the distance between two magnetic atoms along the helicoid axis).

From expression (3.8) it follows that the cross section for elastic magnetic scattering in the case of identical magnetic atoms in a crystal is equal to

$$\frac{d\sigma_0}{d\Omega} = (r_0\gamma)^2 F^2(q) \sum_{jj'} e^{-iq(R_j - R_{j'})} \sum_{\alpha\beta} (\delta_{\alpha\beta} - e_\alpha e_\beta) \langle S_j^\alpha S_{j'}^\beta \rangle.$$

Using the preceding relations we can rewrite the sum over α and β in the form

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*In getting (5.5) from (5.4) we have also taken account of the effect on the magnetic scattering of neutrons of thermal vibrations of the lattice, in the scheme of the relations (3.3), (3.6), and (4.7). It reduces to the appearance of a factor e^{-Wq} in the cross section for pure magnetic scattering. In the following all expressions obtained from the general formula (3.8) for the magnetic scattering cross sections are to be corrected by the temperature factor e^{-2Wq}.

$$\sum_{\alpha\beta} (\delta_{\alpha\beta} - e_\alpha e_\beta) \langle S_j^\alpha S_{j'}^\beta \rangle = \langle (S_0^z)^2 \rangle [1 - (em)^2]$$

$$+ \frac{1}{4} \langle (S_0^- S_0^+) \rangle [1 + (em)^2] e^{-ik_0 (R_j - R_{j'})}$$

$$+ \frac{1}{4} \langle (S_0^+ S_0^-) \rangle [1 + (em)^2] e^{ik_0 (R_j - R_{j'})} + \dots$$

The terms which have not been written down contain phase factors of the form $e^{\pm ik_0(R_j + R_{j'})}$.

After substituting this expression in the formula for $d\sigma_0/d\Omega$, the terms with factors $e^{\pm ik_0 (R_j + R_{j'})}$ drop out of the summations over j and j'; then using relation (4.8) we finally get

$$\frac{d\sigma_0}{d\Omega} = (r_0\gamma)^2 F^2(q) S^2(T) \frac{(2\pi)^3 N}{V_0} \sum_\tau \Big\{ \cos^2\alpha \, [1 - (em)^2] \, \delta(q - \tau)$$

$$+ \frac{1}{4} \sin^2\alpha \, [1 + (em)^2] \, \delta(q - \tau + k_0)$$

$$+ \frac{1}{4} \sin^2\alpha \, [1 + (em)^2] \delta(q - \tau - k_0) \Big\} e^{-2W_q}, \qquad (5.8')$$

where $S(T)$ is the average, at a given temperature, of the projection of the spin on to the equilibrium position, and α is the angle between the axis of the helicoid and the direction of the equilibrium orientation of the spins.

From formula (5.8) we see that for each τ there are three magnetic peaks. One peak, for the condition $q = \tau$, is caused by the "ferromagnetic" component of the spin; it is absent for the case of a simple spiral. The two others at $q \pm k_0 = \tau$ are associated with the projections of the spin on the base plane. Usually $k_0 \ll \tau$, so that the latter two magnetic peaks should be located close to the nuclear peak $q = \tau$. The presence of such a "trident" consisting of a nuclear peak at the center and two magnetic peaks at the sides led to the discovery of the helicoidal structure.*

Formula (5.5) applies to scattering by a ferromagnetic single crystal. To get the scattering cross section for a polycrystal, we must average over the direction of τ. We then get[17]

$$\left(\frac{d\sigma_0}{d\Omega}\right)_{\text{polycr}}$$

$$= (r_0\gamma)^2 S^2(T) (1 - e_z^2) \frac{2\pi^2 N}{V_0} \sum_{\tau \leqslant 2p} \frac{a_\tau F^2(\tau)}{\tau^2} e^{-2W_\tau} \delta(q - \tau). \quad (5.9)$$

As in the case of nuclear scattering by a polycrystal, the magnetically scattered neutrons move along the generators of cones with their axes along the vector p and an opening angle 2θ. The angular dependence of the intensity is, however, more complicated than for nuclear scattering.

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*Such a "trident" was first discovered on a neutronogram of MnO_2 by Erick32son.[49] The interpretation of such neutronograms in terms of a helicoidal structure was given by Yoshimori.[50] In a paper of Koehler[51] a general method was given for the interpretation of neutronograms of helicoidal structures. The theory of helicoidal ordering was developed by Kaplan.[52] The temperature variation in the spiral step was calculated theoretically in [53].

It is also of interest to compute the total scattering in a polycrystal, for which purpose we must integrate expression (5.9) over all angles of scattering of neutrons, i.e., over $d\Omega = \sin\theta \, d\theta \, d\varphi$; θ is the polar angle of the vector p' in the coordinate system where the z axis is taken along the direction of p. It is not difficult to show that e_z^2 is expressed in the following fashion in terms of the angles θ and φ:

$$e_z^2 = \left(\cos\frac{\theta}{2} \sin\varphi \sin\xi - \sin\frac{\theta}{2} \cos\xi \right)^2, \qquad (5.10)$$

where ξ is the angle between p and the magnetization m, and φ is the azimuthal angle of the vector p' taken in the plane perpendicular to the vector p from an axis directed along the vector $p \times m$.

Substituting (5.10) in (5.9) and integrating over $d\Omega$, we find the total cross section for the polycrystal

$$(\sigma_0)_{\text{polycr}} = (r_0\gamma)^2 S^2(T) \frac{(2\pi)^3}{4V_0 p^2} \sum_{\tau \leqslant 2p} \frac{c_\tau F^2(\tau)}{\tau} e^{-2W}\tau$$

$$\times \left[1 + \cos^2\xi + \frac{\tau^2}{4p^2}(1 - 3\cos^2\xi) \right]. \qquad (5.11)$$

The essential difference between this expression and (4.30) is that the total cross section depends on the orientation of the initial neutron beam with respect to the magnetic moment of the sample. Just as for nuclear scattering, it increases abruptly as the energy of the neutrons is increased.

III. INELASTIC ONE-QUANTUM SCATTERING

6. Scattering with Emission and Absorption of a Phonon

In this section we shall consider in detail the nuclear scattering by a single crystal. We shall start from the general formula (3.1) for the differential scattering cross section. As in Sec. 4, we expand the nuclear coordinates R_l into an equilibrium part R_l^0 and the displacement U_l. Expanding the displacement U_l in Fourier series (4.13), we write the expression (3.1) in the form

$$\frac{d^2\sigma}{d\Omega \, dE_{p'}} = \frac{m^2}{(2\pi)^2 \hbar^4} \frac{p'}{p} \sum_{ll'} \langle a_l a_{l'} \rangle I_{ll'}(q) e^{-iq(R_l^0 - R_{l'}^0)}, \qquad (6.1)$$

where

$$I_{ll'}(q) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dt \, e^{\frac{i}{\hbar}(E_{p'} - E_p)t}$$

$$\times \prod_{kj} \langle e^{-i[\eta_{kj}^l b_{kj} + \overset{*l}{\eta}_{kj} b_{kj}^+]} \cdot e^{i[\eta_{kj}^{l'} b_{kj}(t) + \overset{*l'}{\eta}_{kj} b_{kj}^+(t)]} \rangle_{kj}. \qquad (6.2)$$

Here

$$b_{kj}(t) = b_{kj} e^{-i\omega_j(k)t}, \quad b_{kj}^+(t) = b_{kj}^+ e^{i\omega_j(k)t} \qquad (6.3)$$

are the operators b_{kj} and b_{kj}^+ in the Heisenberg representation.

We expand the exponent under the average sign in expression (6.2) in series of powers of the argument.

To terms of order $|\eta^l_{kj}|^2$ we obtain after averaging

$$I_{ll'}(\mathbf{q}) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dt\, e^{\frac{i}{\hbar}(E_{\mathbf{p'}} - E_{\mathbf{p}})t} \prod_{kj} \{1 - |\eta^l_{kj}|^2 \cdot [2n_j(\mathbf{k}) + 1]$$

$$+ \eta^l_{kj}\eta^{l'*}_{kj}[1 + n_j(\mathbf{k})]\, e^{i\omega_j(\mathbf{k})t} + \eta^{l*}_{kj}\eta^{l'}_{kj}n_j(\mathbf{k})\, e^{-i\omega_j(\mathbf{k})t} + \ldots\},$$

(6.4)

where $n_j(\mathbf{k})$ is the distribution function for the phonons, determined by expression (4.21). In addition, to terms of order N^{-1} the product in (6.4) can be written in the form

$$\prod_{kj} \ldots \approx \prod_{kj} \{1 - |\eta^l_{kj}|^2(2n_j(\mathbf{k}) + 1)\}\{1 + \eta^l_{kj}\eta^{l'*}_{kj}[1 + n_j(\mathbf{k})]\, e^{i\omega_j(\mathbf{k})t}$$

$$+ \eta^{l*}_{kj}\eta^{l'}_{kj}n_j(\mathbf{k})\, e^{-i\omega_j(\mathbf{k})t} + \ldots\}$$

$$\approx e^{-\sum_{kj}|\eta^l_{kj}|^2(2n_j(\mathbf{k})+1)} \{1 + \sum_{kj}[\eta^l_{kj}\eta^{l'*}_{kj}(1 + n_j(\mathbf{k}))\, e^{i\omega_j(\mathbf{k})t}$$

$$+ \eta^{l*}_{kj}\eta^{l'}_{kj}n_j(\mathbf{k})\, e^{-i\omega_j(\mathbf{k})t}]\}.$$

(6.5)

Integrating over the time in (6.4) we now get

$$I_{ll'}(\mathbf{q}) = e^{-2W_{\mathbf{q}}} \{\delta(E_{\mathbf{p'}} - E_{\mathbf{p}})$$

$$+ \sum_{kj}[\eta^l_{kj}\eta^{l'*}_{kj}(1 + n_j(\mathbf{k}))\,\delta(E_{\mathbf{p'}} - E_{\mathbf{p}} + \hbar\omega_j(\mathbf{k}))$$

$$+ \eta^{l*}_{kj}\eta^{l'}_{kj}n_j(\mathbf{k})\,\delta(E_{\mathbf{p'}} - E_{\mathbf{p}} - \hbar\omega_j(\mathbf{k}))]\}.$$

Now we substitute this expression into (6.1). Averaging the sum $\sum_{ll'}$ over the distribution of isotopes, and using the transformation (4.8), we find the following expression for the differential scattering cross section:

$$\frac{d^2\sigma}{d\Omega\, dE_{\mathbf{p'}}} = N\left\{\sigma^{(0)}\frac{(2\pi)^3}{V_0}\sum_{\tau}\delta(\mathbf{q} - \boldsymbol{\tau}) + \sigma'\right\} e^{-2W_{\mathbf{q}}}\delta(E_{\mathbf{p'}} - E_{\mathbf{p}})$$

$$+ N\frac{p'}{p}\sum_{kj}\left\{\sigma^{(0)}\frac{(2\pi)^3}{V_0}\sum_{\tau}\delta(\mathbf{q} - \mathbf{k} - \boldsymbol{\tau}) + \sigma'\right\}$$

$$\times e^{-2W_{\mathbf{q}}}\frac{\hbar(\mathbf{qe}_j(\mathbf{k}))^2}{2MN\omega_j(\mathbf{k})}(1 + n_j(\mathbf{k}))\,\delta(E_{\mathbf{p'}}$$

$$- E_{\mathbf{p}} + \hbar\omega_j(\mathbf{k})) + N\frac{p'}{p}\sum_{kj}$$

$$\times \left\{\sigma^{(0)}\frac{(2\pi)^3}{V_0}\sum_{\tau}\delta(\mathbf{q} + \mathbf{k} - \boldsymbol{\tau}) + \sigma'\right\} e^{-2W_{\mathbf{q}}}\frac{\hbar(\mathbf{qe}_j(\mathbf{k}))^2}{2MN\omega_j(\mathbf{k})}$$

$$\times n_j(\mathbf{k})\,\delta(E_{\mathbf{p'}} - E_{\mathbf{p}} - \hbar\omega_j(\mathbf{k})),$$

(6.6)

where $\sigma^{(0)}$ and σ' are the constants (4.6) which determine the coherent and incoherent scattering. The individual terms in (6.6) have the following meaning.

The first term represents the differential cross section for elastic nuclear scattering. If we integrate over the energies of the scattered neutrons, we get the expression for the scattering cross section per unit solid angle identical with (4.11). The second term, and also the third, describe the inelastic scattering. The first of these gives the cross section for

scattering with emission of a phonon, and the second with absorption of a phonon. As we see from (6.6), these processes lead both to coherent, as well as to incoherent scattering. The δ-functions appearing in (6.6) take account of the conservation laws for energy and quasimomentum in collision of a neutron with a phonon.

The inelastic scattering terms given in (6.6) correspond to one-quantum scattering, i.e., to scattering in which the number of phonons of the scatterer changes by unity. If the expansion of the exponent in (6.2) is carried to higher degree, we can obtain an expression for the cross sections for scattering with multiphonon transitions in which several phonons are absorbed or emitted. The role of such processes was studied in reference[18]. We shall not consider them in detail here. It is important only to emphasize that at temperatures below the Debye temperature the main contribution to the inelastic scattering comes from one-phonon processes.

Let us consider in more detail the incoherent one-phonon scattering. The corresponding scattering cross section, according to (6.6), can be written in the form

$$\frac{d^2\sigma^{\pm 1}_{\text{incoh}}}{d\Omega\, dE_{\mathbf{p'}}} = \sigma' e^{-2W_{\mathbf{q}}}\sum_{kj}\frac{\hbar(\mathbf{qe}_j(\mathbf{k}))^2}{2M\omega_j(\mathbf{k})}$$

$$\times \left[n_j(\mathbf{k}) + \frac{1}{2} \pm \frac{1}{2}\right]\frac{p'}{p}\,\delta(E_{\mathbf{p'}} - E_{\mathbf{p}} \pm \hbar\omega_j(\mathbf{k})).$$

(6.7)

The upper sign corresponds to scattering with emission, and the lower with absorption of a phonon. The sum over $\mathbf{k}$ generally cannot be calculated since we do not know the form of the function $\omega_j(\mathbf{k})$. We shall therefore see what physical consequences can follow from an analysis of expression (6.7).

First of all, we find that neutrons scattered in any direction have a continuous energy spectrum covering the interval

$$E_p \leqslant E_{p'} \leqslant E_p + \hbar\omega_{\max}$$

(6.8)

in the case of scattering with absorption, and the interval

$$E_p \geqslant E_{p'} \geqslant \begin{cases} E_p - \hbar\omega_{\max}, & E_p > \hbar\omega_{\max}, \\ 0, & E_p < \hbar\omega_{\max} \end{cases}$$

(6.9)

in the case of scattering with emission of a phonon. In these inequalities $\omega_{\max}$ is the maximum value of the phonon frequency.

In the following, for simplicity we shall restrict ourselves to crystals with cubic symmetry; then

$$\frac{d^2\sigma^{\pm 1}_{\text{incoh}}}{d\Omega\, dE_{\mathbf{p'}}} = \sigma'\frac{NV_0}{(2\pi)^3}\frac{\hbar}{6M}\sum_j \int d\mathbf{k}\frac{e^{-\alpha q^2}}{\omega_j(\mathbf{k})}q^2\frac{p'}{p}$$

$$\times \left[n_j(\mathbf{k}) + \frac{1}{2} \pm \frac{1}{2}\right]\delta(E_{\mathbf{p'}} - E_{\mathbf{p}} \pm \hbar\omega_j(\mathbf{k})),$$

(6.10)

where α is determined by (4.23), and is independent of scattering angle.

We now introduce the frequency distribution function $g(\omega)$ which determines how many normal vibrations there are per unit frequency interval, divided by the total number of vibrations:

$$\left.\begin{array}{l} g(\omega)\,d\omega = \frac{1}{3}\frac{V_0}{(2\pi)^3}\sum_j \int_{\omega\leqslant\omega_j(k)\leqslant\omega+d\omega} dk, \\ g(\omega) = 0, \qquad \text{if} \qquad \omega > \omega_{max}, \end{array}\right\} \quad (6.11)$$

after which expression (6.10) can be written as [19]

$$\frac{d^2\sigma^{\pm 1}_{incoh}}{d\Omega\,dE_{p'}} = N\sigma'\,\frac{\hbar}{2M}\,\frac{p'}{p}\,e^{-\alpha q^2}\,\frac{q^2}{|E_p - E_{p'}|}$$

$$\times g\left(\frac{|E_p - E_{p'}|}{\hbar}\right)\left(\frac{1}{e^{\beta|E_p - E_{p'}|}-1} + \frac{1}{2} \pm \frac{1}{2}\right), \quad (6.12)$$

where the limits of variation of $E_{p'}$ are given by expressions (6.8) and (6.9). Thus for a cubic crystal the cross section for incoherent one-phonon scattering is proportional to the frequency distribution function $g(\omega)$. In the case of crystals of arbitrary symmetry this is no longer true because of the presence of polarization terms in the expression for the cross section. This leads to difficulties in the determination of $g(\omega)$ in crystals which do not have cubic symmetry. However, the polarization terms in the cross section can be eliminated under certain definite conditions. First of all, we note that at temperatures below the Debye temperature the temperature factor is close to 1. Oskot-skiĭ[20] has shown that in this case the polarization terms in (6.7) are eliminated if we consider scattering in a composite sample.

We form the sample of twelve plates in the following fashion. We arbitrarily orient a Cartesian coordinate system X, Y, Z in the first plate. In the second plate the crystal axes should be turned relative to the central line of the axial cross through 120°, in the third through 240°. In the fourth, seventh, and tenth plates the crystal axes are turned through 180° about the axes X, Y, Z respectively. Relative to these orientations, the remaining three pairs of plates are oriented just as in the first triple. The cross section for scattering from all of the plates is the sum of the cross sections for scattering from the individual plates (where t labels the plates). In the twelve sums $\sum_k$ in expressions (6.7) we shall consider simultaneously those k_t which are identically oriented with respect to the crystal axes of their plates. Then $\omega^t_j(k) = \omega_j(k)$, where the quantity without the superscript t refers to the first plate. Now only $|q\,e^t_j(k_t)|^2$ depends on the label t. It is easy to show that

$$\sum_t |e_j(k_t)\,q|^2 = 4q^2.$$

Thus, neglecting the temperature factor the cross section for scattering from the composite plate is given by formula (6.12), which is appropriate for a cubic lattice, multiplied by 4, i.e., the cross section

turns out to be proportional to the frequency function $g(\omega)$. If the crystal contains a three- or four-fold axis, then four or three plates are sufficient. For a cubic crystal, naturally, we need only a single "plate."

A simpler method for eliminating the polarization terms has been proposed by Kagan.[21] Namely, for a fixed scattering direction we want to determine $d^2\sigma^{\pm 1}_{inc}/d\Omega dE_{p'}$ for three orientations of the single crystal which differ from one another by cyclic permutation of the coordinates. It is not hard to see that the sum of these three cross sections (for $e^{-2W_q} \approx 1$) is

$$\frac{1}{3}\sum_l^3 \frac{d^2\sigma^{\pm 1}_{incoh}}{d\Omega\,dE_{p'}}\Bigg|_{lt} = N\sigma'\,\frac{\hbar}{2M}\,\frac{p'}{p}\,\frac{q^2}{|E_p - E_{p'}|}$$

$$\times g\left(\frac{|E_p - E_{p'}|}{\hbar}\right)\left(\frac{1}{e^{\beta|E_p - E_{p'}|}-1} + \frac{1}{2} \pm \frac{1}{2}\right)$$

and allows us to determine the frequency function $g(\omega)$. In the case of uniaxial crystals two orientations of the crystal are sufficient. In a cubic crystal a single position of the sample is enough, and we arrive at the formula of Placzek and Van Hove [19] (6.12).

If the crystal consists of atoms of different types, the quantity

$$\sum_l \frac{d^2\sigma^{\pm 1}_{incoh}}{d\Omega\,dE_{p'}}\left(\frac{d\sigma^0_{incoh}}{d\Omega}\right)^{-1}\Bigg|_l$$

also is proportional to the function $g(\omega)$.[21] Thus a measurement of the cross section for three orientations of a single crystal allows us in any case to reestablish the frequency function $g(\omega)$.

As was shown in reference [22], the function $g(\omega)$ in the crystal has a finite number of singularities ω_s which are roots of the equation

$$\nabla\omega_j(k) = 0. \quad (6.13)$$

In the neighborhood of the singular points, the function $g(\omega)$ has one of the forms

$$g(\omega) = \begin{cases} A|\omega - \omega_s|^{1/2} + o(\omega - \omega_s), & \omega < \omega_s, \\ O(\omega - \omega_s), & \omega > \omega_s \end{cases} \quad (6.14)$$

or the same thing with the relations $\omega < \omega_s$ and $\omega > \omega_s$ interchanged. The symbol $O(\omega - \omega_s)$ denotes the remainder term in the series, of order $|\omega - \omega_s|$ for $\omega \to \omega_s$.

Because of (6.12) the cross section for one-phonon incoherent scattering for scattering energies $E_{p'}$ satisfying the relation $|E_p - E_{p'}| \approx \hbar\omega_s$ also has a singularity of the type (6.14), where this singularity in the spectrum of scattered neutrons is independent of the scattering direction. Moreover, one can show that the energy distribution of multi-phonon incoherent scattering has a continuous derivative with respect to the energy of the scattered neutrons.[18] On the other

hand, the singularities in the energy distribution of coherently scattered neutrons depend on the scattering angle and on the orientation of the crystal relative to the direction of the incident neutrons, so that they can be separated experimentally from the singularities considered above. Thus, incoherent one-phonon scattering is the simplest phenomenon from which one can determine the singularities in the frequency function of the crystal (and the function itself, of course).

The preceding discussion refers to a single crystal. For inelastic scattering by a powder, the expression (6.7) should be averaged over the orientations of the microcrystals. Since the singularities in the energy distribution do not depend on direction, they remain even after the averaging is done.

Now we go on to one-phonon coherent scattering. From (6.6) we get

$$\frac{d^2\sigma_{coh}^{\pm 1}}{d\Omega \, dE_{p'}} = N\sigma^{(0)} \frac{\hbar}{2M} \sum_j \sum_\tau \int dk e^{-2W_q} \frac{p'}{p} \frac{(qe_j(k))^2}{\omega_j(k)}$$

$$\times \left[n_j(k) + \frac{1}{2} \pm \frac{1}{2} \right] \delta(q \mp k - \tau) \delta(E_{p'} - E_p \pm \hbar\omega_j(k)).$$

$$(6.15)$$

Using the δ-function in the momenta, we eliminate the integral over k, replacing k in each term by $q + \tau$. All the terms in (6.15) depend on k through a function with periods equal to the basis vectors of the reciprocal lattice multiplied by 2π, so that

$$\omega_j(q+\tau) = \omega_j(q), \quad e_j(q+\tau) = e_j(q). \qquad (6.16)$$

Taking this into account we find from (6.15), for a reflection in the neighborhood of the vector τ, the expression

$$\frac{d^2\sigma_{\tau, coh}^{\pm 1}}{d\Omega \, dE_{p'}} = N\sigma^{(0)} \frac{\hbar}{2M} \sum_j e^{-2W_q} \frac{p'}{p} \frac{(qe_j(q))^2}{\omega_j(q)}$$

$$\times \left[n_j(q) + \frac{1}{2} \pm \frac{1}{2} \right] \delta(E_{p'} - E_p \pm \hbar\omega_j(q)). \qquad (6.17)$$

Scattering with emission and absorption of a phonon will occur when the energy conservation conditions are satisfied

$$E_{p'} - E_p \pm \hbar\omega_j(q) = 0,$$

or

$$\pm (p^2 - p'^2) - \frac{2M}{\hbar} \omega_j(p - p') = 0. \qquad (6.18)$$

Here the plus sign corresponds to scattering with emission, the minus sign with absorption of a phonon. Let us consider these two cases separately.

We start with scattering accompanied by absorption, and show that equation (6.18) has a solution for p' for any angle of scattering and any p. It is obvious that for a given p the range of admissible values of p' is determined by the inequalities (6.8). We construct the function[19]

$$\varphi_j^-(p, \, p') = p'^2 - p^2 - \frac{2M}{\hbar} \omega_j(p - p').$$

For $p^{12} = p^2 + 2M/\hbar \, \omega_{max}$, $\varphi_j^-(p, \, p') \geq 0$, and when $p' = p$, $\varphi_j^-(p, p') \leq 0$, but it follows from this that, in the case of absorption of a phonon, equation (6.17) for any p has at least one solution for any scattering angle, and all the solutions lie between two concentric spheres C and C_{max} with radii p and $p_{max} = \sqrt{p^2 + (2M/\hbar)\omega_{max}}$, having their centers at the origin. These solutions form surfaces S_j^- in p-space, lying completely between the two spheres. Any radius vector taken at any point of the surface S_j^- is permissible, by virtue of the energy and momentum conservation laws, as a wave vector of the scattered neutron. It is obvious that in each scattering direction there is a finite number of possible values of p' (in general, no fewer than three, which corresponds to the three possible polarizations of the phonons), and consequently the spectrum of neutrons scattered in any direction as a result of one-phonon coherent scattering is discrete.

Now let us go on to scattering with emission of a phonon. If $p^2 \geq p_1^2 \equiv 2M/\hbar \, \omega_{max}$, the range of possible values of p', because of (6.9), runs from p to $p_{min} = \sqrt{p^2 - p_1^2}$, and just as in the case of scattering with absorption of a phonon, we get surfaces S_j^+, located between concentric spheres C_{min} and C, with radii p_{min} and p. To each scattering angle there again correspond definite discrete values of p'. If, however, $p < p_1$, then $p_{min} = 0$ and the function

$$\varphi_j^+(p, \, p') = p^2 - p'^2 - \frac{2M}{\hbar} \omega_j(p - p')$$

for $p' = 0$ is equal to $p^2 - (2M/\hbar)\omega_j(p)$. No conclusion can be drawn concerning the sign of this expression without taking a specific form for the function $\omega_j(p)$, and we can only assert that for $p < p_1$ neutrons in general will not be scattered over all directions when a phonon is emitted.

Furthermore if p is sufficiently small, scattering with emission of a phonon is not possible. In fact, from the momentum conservation law it follows that for $\tau \neq 0$, $\tau - k = p' - p$. This equality is possible only if $|\tau - k| \leq p' + p$. But for scattering with emission of a phonon $p' + p \leq 2p$, and consequently scattering is possible if $p > \frac{1}{2} |\tau - k|$. Therefore there exists a $p_2 = \frac{1}{2} \tau_{min}$, such that for $p < p_2$ scattering with emission is impossible. If, however, $\tau = 0$ and k is small, scattering with emission is possible[1] only for $V > c$.

Thus, for any direction of scattering, in addition to the continuous spectrum of neutrons which are scattered incoherently and as a result of multi-phonon coherent scattering, one should observe, for definite values of p' peaks due to one-phonon coherent scattering. By studying the location of the one-phonon peaks in the neutron spectrum scattered at different angles and using (6.18), one can easily get $\omega_j(k)$. In

fact, the quantity p is given to us, p' is found directly by measuring the location of the peak. From (6.18) one then determines the quantity $\omega_j(p - p')$. The direction of the vector p' is determined by the assigned scattering angle.

Thus, the peaks of coherent one-phonon scattering allow us to reconstruct the energy spectrum of the crystal vibrations, while the incoherent one-phonon scattering permits us to find the frequency distribution function. The question therefore arises: How do we separate these two types of scattering? If we measure the intensity of neutrons in the scattering direction p', it will consist of both types of scattering together.

However, by changing the technique of measurement one can eliminate the coherent one-phonon scattering in certain cases (Kagan[23]). In fact, let us consider formulas (6.10) and (6.17), which determine the cross sections for incoherent and coherent scattering. From these formulae we see that the cross sections are functions of the two quantities $\Delta E \equiv E_{p'} - E_p$ and q—the energy and momentum transferred by the neutron to the crystal.

In the general case both these quantities can be considered to be independent. Once this is the case, we can fix q and study the cross section as a function of ΔE alone. Let us set $q = \tau$; then, as we see from (6.17), the coherent cross section will be different from zero if $\Delta E = \pm \hbar\omega_j(0)$, since $\omega_j(q)$ is a periodic function of q with period τ. For the acoustic branches $\omega_j(0) = 0$, so that, in the case of an arbitrary monatomic lattice, by measuring the cross section as a function of ΔE for $\Delta E \neq 0$ we will measure the cross section for purely incoherent scattering, i.e., the quantity (6.10). Thus for monatomic lattices we can make a completely rigorous separation.

If there is more than one atom in the unit cell of the crystal, then in addition to the acoustic branches there are also optical branches, for which $\omega_j(0) \neq 0$. If the minimum value of the frequency in the optical branches is above ω_{max}^{ac} for the acoustic branches, then for $\Delta E \leq \omega_{max}^{ac}$ the scattering will again be purely incoherent. For an interval ΔE corresponding to the optical branches there is a superposition of both types of scattering. In the general case we can not assert that $\omega_{max}^{ac} < \omega_{min}^{opt}$, so that the superposition can still occur within the frequency interval $\Delta E/\hbar$ corresponding to the acoustic branches. However, coherent scattering corresponding to the frequencies of the optical branches $\omega_j(0)$ will lead to narrow sharp lines, so that apparently one can get both a clear separation of the coherent scattering at the frequencies $\omega_j(0)$, as well as obtain the cross section for incoherent scattering for the whole range of frequencies in the phonon spectrum.

The coherent one-phonon scattering in principle permits one to determine not only the spectrum of the lattice vibrations, but also the values of the complex vectors of polarization of the vibrations. To do this requires a study of the scattering on samples with different isotopic composition. Such measurements would solve the complete inverse problem—the reconstruction of the frequency function of the distribution, the spectrum of vibrations, and the polarization vectors of the vibrations. Conditions for solvability of the complete reciprocal problem have been investigated recently by Kagan.[23] Practically such a problem apparently can be solved only for lattices which are monatomic and diatomic and in which each lattice site is a center of inversion.

7. Scattering with Emission and Absorption of a Spin Wave

We now proceed to study magnetic scattering in ferromagnets. We shall start from the simplest Heisenberg model of a ferromagnet: The crystal consists of N magnetic atoms each of which has spin **S**. We include only the isotropic exchange interaction of the spins, taking the Hamiltonian of the system in the form

$$\mathscr{H} = - \sum_{j \neq j'} J(\mathbf{R}_j - \mathbf{R}_{j'})(\mathbf{S}_j \mathbf{S}_{j'}). \tag{7.1}$$

The differential scattering cross section in the magnetic material is determined by the expression (3.8) multiplied by $e^{-2W}q$. In the general case, the spin correlator $\langle S_j^\alpha(0) S_j^\beta(t) \rangle$ cannot be computed since we do not know the eigenvalues of the energy operator (7.1). However, in two limiting cases one can develop an approximate theory of ferromagnetism, namely, for temperatures much less than the Curie temperature and in the immediate vicinity of the Curie point. In this section we shall consider the case of low temperatures. The other limiting case will be treated specially in part IV.

In the case of low temperatures, when the magnetization of the crystal (we are thinking of a single domain) does not differ very much from the saturation magnetization at 0°K, the average value of the projection of the spin along the direction of the spontaneous magnetic moment differs little from S, while the average value of the transverse components of the spin is small. In this case we can use the well-known relations [24] which express the spin operators $\mathbf{S}_j$ of the individual sites approximately in terms of the Bose operators b_j and b_j^+:

$$S_j^+ = (2S)^{1/2}b_j, \quad S_j^- = (2S)^{1/2}b_j^+, \quad S_j^z = S - b_j^+ b_j, \tag{7.2}$$

where $S_j^\pm = S_j^x \pm i S_j^y$.

If we change from the Bose amplitudes b_j and b_j^+ to their Fourier components $b_\mathbf{k}$ and $b_\mathbf{k}^+$,

$$b_j = \frac{1}{\sqrt{N}} \sum_\mathbf{k} e^{i\mathbf{k}\mathbf{R}_j} b_\mathbf{k}, \quad b_j^+ = \frac{1}{\sqrt{N}} \sum_\mathbf{k} e^{-i\mathbf{k}\mathbf{R}_j} b_\mathbf{k}^+, \tag{7.3}$$

the Hamiltonian (7.1) will be diagonal:

$$\mathcal{H} = \sum_k \varepsilon_k b_k^+ b_k + \text{const.} \tag{7.4}$$

Since the eigenvalues of the operator $b_k^+ b_k$ are integers $0, 1, 2, 3, \ldots$, this result can be treated as follows: At low temperatures the state of the ferromagnet is equivalent to the state of an ideal Bose gas of spin waves with energy

$$\varepsilon_k = 2S \sum_R \mathbf{J}(\mathbf{R})(1 - e^{i\mathbf{k}\mathbf{R}}). \tag{7.5}$$

Since the exchange integral falls off rapidly with distance, the main contribution to the sum over $\mathbf{R}$ in (7.5) comes from the nearest neighbors. For small k the exponent in (7.5) can be expanded in series where, for example, for a cubic lattice we get the following expression for the energy of a spin wave:

$$\varepsilon_k = \frac{1}{3} SzJ_0(ak)^2, \tag{7.6}$$

where J_0 is the exchange integral between nearest neighbors, z is the number of nearest neighbors. In the expression for the magnetic scattering cross section

$$\frac{d^2\sigma}{d\Omega dE_{p'}} = (r_0\gamma)^2 F^2(q) \frac{p'}{p} e^{-2W_q} \sum_{jj'} e^{-i\mathbf{q}\,(\mathbf{R}_j - \mathbf{R}_{j'})} \sum_{\alpha\beta} (\delta_{\alpha\beta} - e_\alpha e_\beta)$$

$$\times \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}(E_{p'} - E_p)\,t} \langle S_j^\alpha(0) S_{j'}^\beta(t)\rangle \, dt \tag{7.7}$$

we can neglect "non-diagonal" correlators $\langle S_j^\pm S_{j'}^z(t)\rangle$, $\langle S_j^\pm S_{j'}^\pm(t)\rangle$ and $\langle S_j^z S_{j'}^\pm(t)\rangle$. One can also show that at low temperatures they are unimportant compared to the others, not only for the phenomenon of neutron scattering, but also for other phenomena in ferromagnets. In this approximation expression (7.7) is written as

$$\frac{d^2\sigma}{d\Omega dE_{p'}} = (r_0\gamma)^2 F^2(q) \frac{p'}{p}$$

$$\times \sum_{jj'} e^{-i\mathbf{q}(\mathbf{R}_j - \mathbf{R}_{j'})} e^{-2W_q} \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}(E_{p'} - E_p)\,t} \, dt \left\{ \frac{1}{4} \langle S_j^- S_{j'}^+(t) \right.$$

$$\left. + S_j^- S_{j'}^+(t)\rangle [1 + (em)^2] + \langle S_j^z S_{j'}^z(t)\rangle [1 - (em)^2] \right\}. \tag{7.8}$$

Using (7.2), (7.3) and (4.8) we get

$$\frac{d^2\sigma}{d\Omega dE_{p'}} = (r_0\gamma)^2 F^2(q) e^{-2W_q} \left(S^2 - \frac{2S}{N} \sum_k n_k \right) [1 - (em)^2] \frac{(2\pi)^3 N}{V_0}$$

$$\times \sum_\tau \delta(\mathbf{q} - \tau) \delta(E_{p'} - E_p) + (r_0\gamma)^2 F^2(q) e^{-2W_q} \frac{S}{2} \frac{p'}{p}$$

$$\times [1 + (em)^2] \frac{(2\pi)^3}{V_0} \sum_\tau \sum_k \{\delta(\mathbf{q} - \mathbf{k} - \tau) Q_k'(E_{p'} - E_p)$$

$$+ \delta(\mathbf{q} + \mathbf{k} - \tau) Q_k''(E_{p'} - E_p)\}, \tag{7.9}$$

where

$$Q_k'(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar} Et} \langle b_k b_k^+(t)\rangle \, dt, \quad Q_k''(E)$$

$$= \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar} Et} \langle b_k^+ b_k(t)\rangle \, dt, \quad n_k = \frac{\text{Sp}(e^{-\beta\mathcal{H}} b_k^+ b_k)}{\text{Sp}\, e^{-\beta\mathcal{H}}} \tag{7.10}$$

is the average number of spin waves with momentum k at a given temperature.

If we restrict ourselves to a description of a ferromagnet using an ideal system of spin waves, i.e., if we use (7.4) as the Hamiltonian of the scatterer, the expression (7.10) is easily calculated:

$$Q_k'(E) = (1 + n_k)\,\delta(E + \varepsilon_k), \quad Q_k''(E) = n_k \delta(E - \varepsilon_k), \tag{7.11}$$

where

$$n_k = (e^{\beta\varepsilon_k} - 1)^{-1} \tag{7.12}$$

is the Bose distribution function for the spin waves. We also note that one of the factors in the first term of expression (7.9) can be written approximately as

$$S^2 - \frac{2S}{N} \sum_k n_k \approx \left(S - \frac{1}{N} \sum_k n_k \right)^2 = S^2(T).$$

Taking these remarks into account, the differential cross section for magnetic scattering is equal to

$$\frac{d^2\sigma}{d\Omega dE_{p'}} = (r_0\gamma)^2 F^2(q) S^2(T) e^{-2W_q} [1 - (em)^2] \frac{(2\pi)^3 N}{V_0} \sum_\tau \delta(\mathbf{q} - \tau)\,\delta$$

$$\times (E_{p'} - E_p) + (r_0\gamma)^2 F^2(q) \frac{S}{2} e^{-2W_q} \frac{p'}{p} [1 + (em)^2] \frac{(2\pi)^3}{V_0}$$

$$\times \sum_\tau \sum_k \{\delta(\mathbf{q} - \mathbf{k} - \tau)\,\delta(E_{p'} - E_p + \varepsilon_k)(1 + n_k)$$

$$+ n_k \delta(\mathbf{q} + \mathbf{k} - \tau)\,\delta(E_{p'} - E_p - \varepsilon_k)\}. \tag{7.13}$$

The first term of this expression describes the elastic scattering. After integration over $dE_{p'}$ it goes over into expression (5.5) which we found earlier. The second term gives the cross section for scattering of a neutron with emission or absorption of a spin wave. The structure of this expression is very close to that of the coherent part of the one-phonon scattering given by formula (6.6). The essential feature of the magnetic one-magnon scattering is the additional angular dependence of the coherent maxima through the quantities $F^2(q)$ and $1 + (\mathbf{e} \cdot \mathbf{m})^2$. We also note that if we consider terms of higher order in expression (7.7) for the expansion of the spin operator in terms of Bose amplitudes, which one can do using the formalism of Holstein and Primakoff,[24] we can easily supplement expression (7.13) by terms corresponding to multi-magnon scattering with absorption and emission of several spin waves. Estimates made by Maleev[25] show that for low temperatures the contribution to the inelastic magnetic scattering from these processes can be neglected.

Thus the cross section for one-magnon scattering in a single crystal is equal to

$$\frac{d^2\sigma^{\pm 1}}{d\Omega dE_{p'}} = N(r_0\gamma)^2 F^2(q) \frac{S}{2} e^{-2W_q} [1 + (em)^2] \sum_\tau \int dk \frac{p'}{p}$$

$$\times \left[n_k + \frac{1}{2} \pm \frac{1}{2} \right] \delta(\mathbf{q} \mp \mathbf{k} - \tau)\,\delta(E_{p'} - E_p \pm \varepsilon_k). \tag{7.14}$$

The upper sign refers to scattering with emission, the lower to scattering with absorption of a spin wave.

The δ-function in the momenta removes the integral over k. Since in the spin-wave approximation $ak \ll 1$, the quasi-momentum of the spin wave is much less than the magnitude of the principal vectors of the reciprocal lattice, we can replace q by τ in (7.14). The result is

$$\frac{d^2\sigma_{\tau}^{\pm 1}}{d\Omega dE_{p'}} = N\,(r_0\gamma)^2 F^2(\tau)\frac{S}{2}\,e^{-2W\tau}\frac{p'}{p}\left[1 + \frac{(\tau m)^2}{\tau^2}\right]\left[n_q + \frac{1}{2} \pm \frac{1}{2}\right]$$

$$\times\ \delta\,(E_{p'} - E_p \pm \varepsilon_{q+\tau}). \qquad (7.15)$$

It follows that in the energy distribution of neutrons scattered with emission or absorption of a spin wave one should see peaks whose location is determined by the energy conservation law

$$E_{p'} - E_p \pm \varepsilon_{q+\tau} = 0, \qquad (7.16)$$

or, considering that ε_k is a periodic function, by the equation

$$\frac{\hbar^2 p'^2}{2m} - \frac{\hbar^2 p^2}{2m} \pm \varepsilon_{p-p'} = 0. \qquad (7.16')$$

The width of these peaks turns out to be equal to zero which is shown by the presence of the δ-functions in (7.15). This is connected with the assumption that the state of a ferromagnet is described by a system of non-interacting spin waves which are in a stationary state. Actually, because of the interaction of these waves with one another and with the lattice, their states are not stationary, but they can be considered as quasi-stationary for temperatures which are much below the Curie point. They are characterized by a finite lifetime τ_k, or equivalently by a level width Γ_k. The effect of the finite lifetime of the spin waves can be taken into account phenomenologically if, in the expression determining the time dependence of the spin wave operators, we replace ε_k by $\varepsilon_k - i\Gamma_k$. Thus we have

$$b_k(t) = b_k e^{-i\frac{\varepsilon_k}{\hbar}t} e^{-\frac{\Gamma_k}{\hbar}|t|}, \quad b_k^+(t) = b_k^+ e^{i\frac{\varepsilon_k}{\hbar}t} e^{-\frac{\Gamma_k}{\hbar}|t|}.$$

Substituting these expressions in (7.10), we find

$$Q_k'(E) = (1 + n_k)\,I_k(-E), \quad Q_k''(E) = n_k I_k(E),$$

where

$$I_k(E) = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}(E-\varepsilon_k)t - \frac{\Gamma_k}{\hbar}|t|}\,dt = \frac{1}{\pi}\frac{\Gamma_k}{(E-\varepsilon_k)^2 + \Gamma_k^2}.$$

From expression (7.9) it follows that the cross section for one-magnon scattering is described by formulas (7.13)–(7.15), in which we simply should replace $\delta(E_{p'} - E_p \pm \varepsilon_k)$ by $I_k(\pm|E_{p'} - E_p|)$. The peaks in the energy distribution of the neutrons are thus described by a Lorentz-shaped line with half-width Γ_k equal to the energy of damping of the corresponding spin wave. Γ_k is a complicated function of quasimomentum and temperature, determined by the mechanism of interaction of the spin waves. At low temperatures $\Gamma_k \ll \varepsilon_k$, so that the peaks described by the function $I_k(E)$ are sharp and have maxima at

points given by equation (7.16). In the limit as $\Gamma_k \to 0$, $I_k(E)$ goes over into a $\delta(E - \varepsilon_k)$-function. The Lorentz shape of the peak comes from the assumption of exponential damping of the stationary states. In the general case, the shape of the peaks is determined by expression (7.10), which can be computed, for example, using temperature Green's functions.[26] By this method Krivoglaz and Kashcheev [27] have computed the broadening of the one-magnon line because of interaction of spin waves with phonons and with one another. Izyumov [28] treated the broadening of the line in a ferromagnetic metal because of interaction of the spin waves with the conduction electrons. The experimental investigation of the broadening (after removing the apparatus broadening) of one-magnon peaks would allow one to get valuable information about the interaction of atomic spins within a ferromagnet (or an antiferromagnet).*

Now let us consider in more detail scattering with absorption of a spin wave, assuming that the dispersion law for the spin waves in quadratic.

In this case the energy conservation law can be rewritten as

$$p'^2 = p^2 + \alpha(q+\tau)^2, \quad \alpha = \frac{SZJ}{\hbar^2/2ma^2}, \qquad (7.17)$$

from which we get two possible values for the wave vector of the scattered neutrons:

$$p'_\pm = \frac{\alpha P}{\alpha - 1}\{\cos\theta \pm \sqrt{\cos^2\theta - \cos^2\theta_0}\}. \qquad (7.18)$$

Here θ is the scattering angle measured from the direction of the vector $P = p + \tau$:

$$\cos^2\theta_0 = \frac{\alpha - 1}{\alpha}\left(1 + \frac{p^2}{\alpha P^2}\right). \qquad (7.19)$$

Integrating (7.15) over the energies of the scattered neutrons, we find, taking account of the possible values of $p'_\pm$, the differential cross section per unit solid angle (Maleev [17]):

$$\frac{d\sigma^{-1}}{d\Omega} = N\frac{S}{2}(r_0\gamma)^2\sum_\tau F^2(\tau)e^{-2W\tau}\left(1 + \frac{(\tau m)^2}{\tau^2}\right)\frac{P\alpha}{p(\alpha-1)^2}$$

$$\times(\cos^2\theta - \cos^2\theta_0)^{-1/2}[n(k_+)(\cos\theta + \sqrt{\cos^2\theta - \cos^2\theta_0})^2$$

$$+ n(k_-)(\cos\theta - \sqrt{\cos^2\theta - \cos^2\theta_0})^2], \qquad (7.20)$$

where

$$k_\pm^2(\cos\theta) = \frac{P^2\alpha}{(\alpha-1)^2}[(\cos\theta \pm \sqrt{\cos^2\theta - \cos^2\theta_0})^2 - \left(\frac{\alpha-1}{\alpha}\right)^2\frac{p^2}{P^2}] \qquad (7.21)$$

is the square of the quasimomentum of the spin wave which participates in the scattering.

Thus the scattering depends essentially on the

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*All these remarks concerning broadening of one-magnon peaks also apply to one-phonon coherent peaks. The magnitude of the broadening of these peaks has been considered by Krivoglaz [29] for various types of interaction of the phonons with one another and with lattice defects (cf. also [30]).

magnitude of the parameter α. For ferromagnets with a Curie temperature of the order of several hundreds of degrees, the parameter $\alpha \sim 100$, so that it follows from (7.19) that $\cos^2 \theta_0 > 1 - 1/\alpha$, so that $\theta_0 < \alpha^{-1/2}$. Since according to (7.18) the limits of variation of $\cos \theta$ are

$$1 \geqslant \cos \theta \geqslant \cos \theta_0 > 0, \qquad (7.22)$$

the angle $\theta < \alpha^{-1/2}$. This means that scattering with absorption of a magnon is possible only within a narrow cone with the axis $\mathbf{P} = \mathbf{p} + \boldsymbol{\tau}$, where to each direction of scattering lying on the cone there correspond two values (7.18) of the momenta of the scattered neutrons.

Furthermore we note that since $\cos^2 \theta_0 < 1$,

$$\frac{p^2}{P^2} < \frac{\alpha}{\alpha - 1} \quad \text{or} \quad \cos \Psi > -\frac{1}{2}\left(\frac{\tau}{p} + \frac{1}{\alpha}\frac{p}{\tau}\right), \qquad (7.23)$$

where Ψ is the angle between $\mathbf{p}$ and $\boldsymbol{\tau}$.

Now let us consider scattering with emission of a magnon. Just as in the case of scattering accompanied by absorption, we get

$$\frac{d\sigma^{+1}}{d\Omega} = N \frac{S}{2} (r_0 \gamma)^2 \sum_{\tau} F^2(\tau) e^{-2W} \tau \left[1 + \frac{(\tau m)}{\tau^2}\right] \frac{Pa}{p(\alpha + 1)^2}$$

$$\times \left[\cos\theta - \frac{\alpha + 1}{\alpha}\left(1 - \frac{1}{\alpha}\frac{p^2}{P^2}\right)\right]^{1/2} \times \{[1 + n(k'_+)]$$

$$\times \left[\cos\theta + \sqrt{\cos^2\theta - \frac{\alpha+1}{\alpha}\left(1 - \frac{1}{\alpha}\frac{p^2}{P^2}\right)}\right]^2 + [1 + n(k'_-)]$$

$$\times \left[\cos\theta - \sqrt{\cos^2\theta - \frac{\alpha+1}{\alpha}\left(1 - \frac{1}{\alpha}\frac{p^2}{P^2}\right)}\right]^2\}. \qquad (7.24)$$

Here the wave vectors of the magnon and the scattered neutron have the values

$$k_{\pm}'^2 (\cos\theta) = \frac{\alpha P^2}{(\alpha+1)^2} \left\{\left(\frac{\alpha+1}{\alpha}\right)^2 \frac{p^2}{P^2}\right.$$

$$\left. - \left[\sqrt{\cos^2\theta - \frac{\alpha+1}{\alpha}\left(1 - \frac{1}{\alpha}\frac{p^2}{P^2}\right)} \pm \cos\theta\right]^2\right\}, \qquad (7.25)$$

$$p'_{\pm} = \frac{\alpha P}{\alpha+1} \left[\cos\theta \pm \sqrt{\cos^2\theta - \frac{\alpha+1}{\alpha}\left(1 - \frac{1}{\alpha}\frac{p^2}{P^2}\right)}\right]. \qquad (7.26)$$

Scattering is possible only if

$$\frac{p^2}{P^2} > \frac{\alpha}{\alpha+1} \quad \text{or} \quad \cos\psi < -\frac{1}{2}\left(\frac{\tau}{p} - \frac{1}{\alpha}\frac{p}{\tau}\right). \qquad (7.27)$$

Since $\cos \Psi \geq -1$, it follows from (7.27) that scatter-with emission of a magnon is possible only when

$$p > \alpha\tau\left(\sqrt{1 + \frac{1}{\alpha}} - 1\right) \approx \frac{\tau}{2}\left(1 - \frac{1}{4\alpha}\right). \qquad (7.28)$$

We must consider the two cases:

$$(1) \quad \frac{\alpha+1}{\alpha}\left(1 - \frac{p^2}{\alpha P^2}\right) \equiv \cos^2\theta_1 > 0; \quad (2) \quad 1 - \frac{p^2}{\alpha P^2} < 0. \quad (7.29)$$

We first consider case one. Just as for scattering with absorption, $\cos \theta$ varies within the limits

$$1 \geqslant \cos\theta \geqslant \cos\theta_1 > 0 \qquad (7.30)$$

and to each scattering angle θ there correspond two

values of the momentum of the scattered neutron (7.26). The structure of this expression is completely analogous to (7.18).

Now we consider case two. It can occur only if

$$\tau\sqrt{\alpha}(\sqrt{\alpha} + 1)^{-1} < p < \tau\sqrt{\alpha}(\sqrt{\alpha} - 1)^{-1},$$

i.e., when p differs only very little from τ. From (7.26) it follows that in this case $p'_- < 0$ and, consequently, to each scattering angle there corresponds only one value p'_+ for the momentum of the scattered neutron, and the scattering angle can change from zero to π.

In conclusion we note that, as follows from (7.24) and (7.27), scattering with emission can occur simultaneously with scattering with absorption of a magnon only if

$$-\left(\frac{\tau}{p} + \frac{1}{\alpha}\frac{p}{\tau}\right) \leqslant 2\cos\Psi \leqslant -\left(\frac{\tau}{p} - \frac{1}{\alpha}\frac{p}{\tau}\right), \qquad (7.31)$$

i.e., within that range of values of Ψ where both cross sections reach their maximum values.

We shall now give a geometric interpretation of the one-quantum coherent scattering. As already pointed out above, it is determined by the energy and momentum conservation laws:

$$\left.\begin{array}{c} \frac{\hbar^2 p^2}{2m} - \frac{\hbar^2 p'^2}{2m} = \pm \, \varepsilon_q, \\ \mathbf{p} - \mathbf{p}' + \boldsymbol{\tau} = \pm \mathbf{q}, \end{array}\right\} \qquad (7.32)$$

where $\mathbf{q}$ is the wave vector of the spin wave (or phonon) participating in the scattering and ε_q is its energy. The upper sign applies to emission and the lower to absorption of a spin wave. Both these equations together determine a surface in the reciprocal lattice space, on which the ends of the wave vectors $\mathbf{p}'$ of the scattered neutrons lie (for fixed orientation of the incident beam relative to the reciprocal lattice vector of the reflection plane). Thus the scattering surface determines the possible values of the energies of neutrons scattered in a given direction.

In the special case of a quadratic dispersion law for the spin waves, we have from (7.32) (cf. (7.17)), for absorption, a scattering surface given by the equation

$$p'^2 = p^2 + \alpha (\mathbf{p}' - \mathbf{P})^2, \qquad (7.33)$$

where

$$\mathbf{P} = \mathbf{p} + \boldsymbol{\tau}. \qquad (7.34)$$

Let us find the geometrical picture of this equation (Fig. 1). We choose a rectangular coordinate system (xyz) so that the x and y axes lie in the plane of the vectors $\mathbf{p}$, $\boldsymbol{\tau}$ (the vector $\mathbf{p}'$ also lies in this plane). Then the left side of equation (7.33), $p'^2 = p_x'^2 + p_y'^2$, is a paraboloid of revolution with axis along z (in Fig. 1 we show the parabola a which is the section of the paraboloid by a plane passing through the z axis). The right side of the equation is a paraboloid with vertex B taken above the plane (x, y) at a value p^2
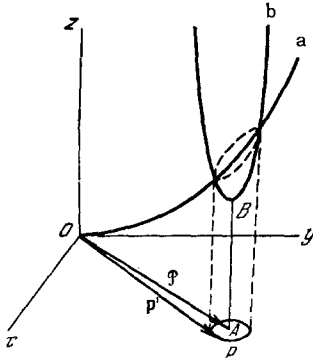
FIG. 1. Geometrical interpretation of scattering with absorption of a spin wave, $AB = p^2$.

and projected on the point A, which is the end of the vector P taken from the coordinate origin (shown in Fig. 1 as a paraboloid b lying in the same vertical plane as paraboloid a).

The intersection of these two paraboloids gives a curve which is shown dotted in Fig. 1. The projection of this curve onto the (x, y) plane gives a closed curve on which all the possible values of the ends of vectors p' lie, i.e., the scattering surface, or more precisely, the scattering curve which is obtained by the intersection of the spatial scattering surfaces and the plane in which the scattering occurs. It is not hard to see that this "surface" of scattering is a circle with its center at a point lying in the neighborhood of the end of the vector P. For $\alpha \gg 1$ the center of the circle practically coincides with the end of the vector P. From Fig. 1 we see that scattering is possible within a narrow sector near the direction P. The opening angle θ_0 in which scattering is possible is determined by the expression (7.19) which was found earlier.

In the case of scattering with emission of a spin wave there should be a minus sign in the last term of equation (7.33). Geometrically this corresponds to the fact that paraboloid b is turned so that it opens downward. From this we see that scattering with emission is not always possible, but only for those values of p for which the segment $AB = p^2$ intersects the parabola a, i.e., when the neutron energy is greater than the energy of the emitted spin wave.

We also note that in the case of a linear dispersion law for the spin waves (or in the case of acoustic phonons) in place of the paraboloid b we should have a cone with its vertex at point B, so that qualitatively the picture remains a similar one, but the scattering surface will be not a circle, but an ellipse.

One interesting result follows from Fig. 1: If we shift the point A further from the coordinate origin, the scattering surface will spread out. To develop experimental methods for studying inelastic scattering we must find the relation between the value of the vector P and the radius of the scattering surface. Let us consider Fig. 2 which essentially shows a more detailed scattering picture in the (x, y) plane of Fig.
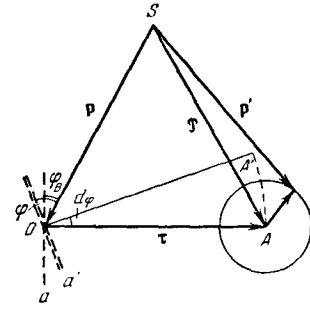

FIG. 2. Momentum conservation law in absorption of a spin wave. Reflection from a crystal plane shown by the dotted line a, when the neutron beam is incident on it at a Bragg angle φ_B. The double line a' shows the reflecting plane when the crystal is turned through an angle $d\varphi$ from the Bragg position a.

1. Here scattering with absorption of a spin wave is shown in the reciprocal lattice space. The dashed line a shows the crystalline reflection plane which goes perpendicular to the plane of the figure. Its location is determined by the reciprocal lattice vector τ. The relative arrangement of the vectors p, p', τ and q satisfies the momentum conservation law for the scattering. A circle drawn from point A is the scattering surface. The ends of the vectors p' should necessarily lie on this circle, since only in this case will the energy conservation law be satisfied, as well as the momentum conservation law.

Let the orientation of the crystal plane a relative to the incident neutron beam correspond to the Bragg position, given by the conditions

$$\mathbf{p'} = \mathbf{p} + \tau, \quad p' = p, \qquad (7.35)$$

or the equivalent

$$\sin \varphi_B \tau = 2\pi p. \qquad (7.36)$$

Leaving the energy of the neutrons in the incident beam unchanged, i.e., fixing p, we turn the crystal from the Bragg position through an angle $d\varphi = \varphi - \varphi_B$. In this case the value of the vector P will change along with $d\varphi$. To find this dependence we square (7.34). We have

$$p^2 + \tau^2 + 2(\mathbf{p}\tau) = P^2. \qquad (7.37)$$

Obviously

$$(\mathbf{p}\tau) = p\tau \cos\left(\frac{\pi}{2} + \varphi\right) = -p\tau \sin(\varphi_B + d\varphi).$$

For small deviations $\sin(\varphi_B + d\varphi)$ can be expanded in a series in $d\varphi$; substituting the expansion in (7.37) and using (7.36), we find approximately

$$p - P \approx \tau(\varphi - \varphi_B)\cos\varphi_B. \qquad (7.38)$$

As we have seen from Fig. 1, with increasing P the scattering surfaces (at least in the case of a quadratic dispersion law) spread out. By means of (7.38) we can now relate this change in the scattering surface to the angular deviation of the crystal from the Bragg position. This lies at the basis of the exper-

imental determination of the dispersion law for mag-nons (and phonons). It was shown earlier that in the energy distribution of neutrons scattered in a given direction coherently with absorption or emission of one quasiparticle (spin wave or phonon) there should be peaks whose positions are determined by the energy conservation law. There are several experimental techniques* which allow one to determine the momentum of the quasiparticle participating in the scattering. Of these the most important are the following.

1. Conventional method. The experiment is done as follows: The crystal to be studied is placed in the Bragg position corresponding to reflection from the plane τ. An apparatus recording the scattered neutrons is placed at such a position as to capture neutrons scattered in the direction of the Bragg peak. In such an arrangement one records mainly neutrons which are elastically scattered. The fraction of neutrons scattered inelastically will be negligible. Furthermore, without changing the angle of scattering ψ (the angle between the vectors p and p'), one turns the crystal through some angle from the Bragg position and analyzes the neutrons scattered in the original direction according to their energies. In the energy distribution of the scattered neutrons one observes peaks corresponding to absorption or emission of a quasi-particle. Such measurements are done for different angular deflections of the crystal from the Bragg position; throughout the experiment ψ = const.

In Fig. 3 we show in the reciprocal lattice space the inelastic scattering for three positions of a single crystal. Let us consider position 1. The distance from the point S_1 to point A (site of the reciprocal lattice τ) corresponds to the scattering surface 1 which we have shown by a circle. The points of intersection p' with the scattering surface correspond to the two peaks in the energy distribution of the scattered neutrons. Vectors drawn from point A to these points of intersection give the wave vectors of the quasiparticles participating in the scattering. We see that the angle ψ should be chosen so that the direc-

FIG. 3. Conventional method.
p = const, ψ = const; φ changes.

tion of p' intersects the scattering surface; otherwise there will be no inelastic one-quantum scattering. To the point S_2 which is further from point A (larger value of vector P) there corresponds another scattering surface (2) etc.

If we join the points of intersection of the vectors p' with the scattering surfaces for different orientations of the single crystal, we obtain curves which are also called "scattering surfaces." On these surfaces lie the ends of the vectors p' corresponding to inelastic scattering. The actual scattering surfaces are usually not known to us, and in the experiment we usually obtain the curves which are shown dotted. From these curves one can obtain a series of points for the dependence of ϵ_q, the energy of the quasiparticle, on the wave vector.

However, in this method we can not beforehand control the direction of the wave vector of the quasiparticle q, since we do not know the scattering surface beforehand and can not orient the crystal so that there will be neutrons in the scattering direction which have absorbed or emitted a quasiparticle with a given direction of its wave vector. Therefore in the conventional method we can obtain individual points on the dispersion curve corresponding to different directions of the wave vector. If we want to determine the spectrum of the quasiparticle for a particular direction of the wave vector in reciprocal lattice space, we must make the experimental technique more complicated. This is achieved in the following methods:

2. Method of constant Q. The experiment is carried out so that the vector $Q \equiv p - p'$ = const. There are two variants of this technique.

a) The analyzer crystal is placed at a position where it records a single energy of the scattered neutrons, i.e., a single value of p'. If we hold Q = const, then necessarily q = const; thus we have a given value of the wave vector of the quasiparticle for which we want to measure the corresponding energy.

The energy of the neutrons in the incident beam is changed so that the wave vector p varies. The end of the vector p must lie on an arc of a circle with radius equal to the length of the vector q drawn from the end of the vector p' (Fig. 4, a). Consequently the end of the vector p slides along a circle and, together with its length, the angles φ and ψ change. For each value of p one measures the neutron intensity scattered for fixed energy p'. Step by step we change the length of vector p so that the point S moving along the circle will go further away or approach the point A of the reciprocal lattice. For some value of p the scattering surface passes through point q, and the intensity of the neutrons increases markedly. The position of peaks in the intensity of scattered neutrons as a function of the energy of the initial neutrons determines the energy of

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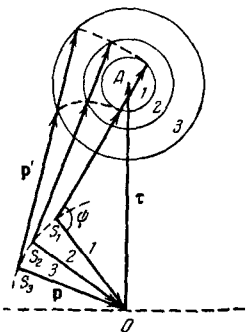*The details of the experimental methods, their possibilities, and a comparison between them are discussed in the survey paper of Brockhouse,[54] who is the author of many of the techniques of neutron spectrometry which are applied at the present time.
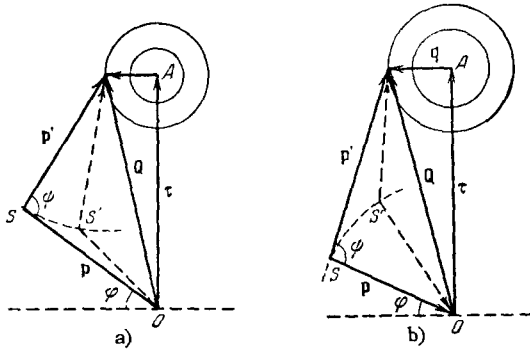
FIG. 5. Method of constant ΔE. ΔE = E − E' = const; φ and ψ change, but in such a way that the vector Q slides along the chosen direction.

FIG. 4. Method of constant Q. a) p, φ, ψ vary; p' = const; b) p', φ, ψ vary; p = const.

the quasiparticles participating in the scattering with a given wave vector q. Thus in this method, keeping q fixed, we vary the initial energy of the neutrons until the energy conservation law is not satisfied for the collision of the quasiparticle with the neutron. Along with the change in the value of p, we must also change φ and ψ according to the scheme corresponding to the scattering picture in the reciprocal lattice space.

Making the measurement of the energy distribution for a given q, we then go to another value of q and repeat the procedure. Consequently this method is a most regular and ordered one. It does not require any previous knowledge of the scattering surface. Technically, however, the method is complicated, since it requires a movement of the crystal monochromator giving the energy of the incident beam to agree with the motion of the crystal sample and the crystal analyzer. Consequently, one should have a so-called triaxial spectrometer. Another variant of the constant Q method can be done with the usual biaxial three-crystal spectrometer.

b) The energy of the incident neutron beam is kept constant throughout. The end of the vector p lies on a circle drawn from the origin—the point O (Fig. 4, b). The crystal analyzer is set to record neutrons with energies corresponding to a given angle φ. The intensity is measured as a function of the energy of the scattered neutrons. The peaks on this curve also determine the energy of the quasiparticles with a given wave vector q participating in the scattering. In the constant Q method (for both variants) we get sections of all the dispersion curves of the quasiparticle for a given direction of the wave vector by the vertical lines q = const. In some cases it is convenient to carry out the experiment so that one gets sections of the dispersion curves by horizontal lines ϵ_q = const.

3. The method of constant ΔE. The energy of the incident neutrons E and the scattered neutrons E' are not changed, so that ΔE = E − E' = const. The angles φ and ψ are changed, but in such a way that the end of the vector Q slides along a chosen direction for the wave vector of the quasiparticles (Fig. 5).
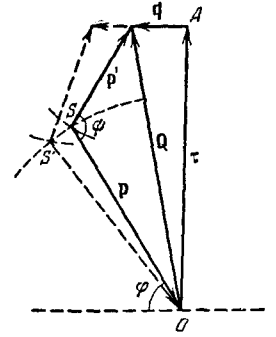
For each value of the angles φ and ψ one measures the intensity of the scattered neutrons as a function of the length of the wave vector q. In the intensity curves one gets peaks when the end of the vector q falls on the scattering surface. The values of q obtained correspond to energies ΔE of the quasiparticles. One then varies ΔE and repeats the whole series of measurements.

In the constant ΔE method one gets sections of the dispersion curves by horizontal lines. This method is convenient in that it permits one to choose the desired value of ΔE, but it obviously is inapplicable for determining the dispersion law for branches of the quasiparticles which vary slowly with q.

The methods considered for determining the dispersion curves of quasiparticles are based on the study of the energy distribution of neutrons scattered in some direction. There also exist methods based on studying the angular width of the inelastic peaks, among which the most widely used is the method of Lowde.

4. The Lowde method.[31] In the case of a quadratic dispersion law, as we have seen, there is a maximum angle θ_0 (angle AOP in Fig. 1), within which there exists one-quantum inelastic scattering. The value of this angle is determined by (7.19). Usually α ≫ 1, so that from (7.19) we get an approximate expression for θ_0:

$$\theta_0 \approx \frac{1}{\sqrt{\alpha P}} \sqrt{2|P-p|}. \qquad (7.39)$$

Substituting (7.38), we get

$$\theta_0 \approx \frac{\sqrt{2\tau \cos \varphi_B}}{\sqrt{\alpha P}} \sqrt{|\varphi - \varphi_B|}. \qquad (7.40)$$

One can show that in the case of a linear dispersion law (ϵ_q = cq, where c is the velocity of the quasiparticle) we have, in place of (7.40), the relation

$$\theta_0 \approx \left(\frac{c^2}{v^2} - 1\right)^{-1/2} \sin 2\varphi_B |\varphi - \varphi_B|, \qquad (7.41)$$

which is applicable only for v > c, where v is the velocity of the incident neutrons. Thus the angular width of the inelastic one-quantum peak varies ~ $\sqrt{|\varphi - \varphi_B|}$ in the case of a quadratic dispersion law for the quasi-particles and varies ~ $|\varphi - \varphi_B|$ for the case of a linear law.

These two dependences open possibilities for the

following experimental technique.[31] The crystal is placed in the Bragg position, and one measures the angular width of the diffuse inelastic peak. Then one turns the crystal through an angle $\varphi - \varphi_B$ from the Bragg peak ("missetting") and again measures the angular width of the diffuse peak. Carrying out a series of measurements, one constructs the dependence of θ_0 on $|\varphi - \varphi_B|$. From the form of this dependence one determines the nature of the dispersion law, i.e., whether it is quadratic or linear. Although this method is very simple (it requires a two-crystal spectrometer), it is clear that using it one can obtain only limited information about the dispersion curves.

In conclusion we consider one important question: the experimental determination of the parameter α in the quadratic dispersion law for spin waves in a ferromagnet. It is simplest to relate α to the experimentally observed quantities if one uses formula (7.18). Let us write the difference between the two possible values of the vectors of the scattered neutrons in the direction of the center of the inelastic peak, i.e., for $\theta = 0$. From (7.18) and (7.39) we have

$$\delta q \equiv [p'_+ - p'_-]_{\theta=0} = \frac{2\alpha P}{\alpha - 1}\sin\theta_0 \approx \frac{2\sqrt{2P}\,|P - p|}{\sqrt{\alpha}}.$$

The quantities p and P are fixed in the experiment so that the last relation can be written as

$$\alpha \sim (\delta q)^{-2}. \qquad (7.42)$$

If α changes under the influence of any physical factor, as for example the temperature, this change can be determined from the change in δq—the distance in k-space between the two peaks of the inelastic scattering. Such measurements were made a long time ago by Brockhouse [59] for magnetite. The appearance of the experiment for two temperatures is shown in Fig. 6. The temperature dependence of the parameter α, determined from (7.42), agreed well with the curve of the temperature dependence of the spontaneous magnetization of the ferromagnet $M(T)$. This result ($\alpha \sim M(T)$) is of fundamental importance since it confirms qualitatively the new theory of the ferro-
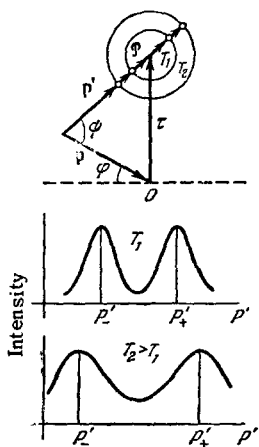
magnetic state of Bogolyubov and Tyablikov,[26,61] according to which spin waves exist at any temperature at which the ferromagnet is still ordered, but their energy depends on temperature, decreasing as the magnetization decreases. The development of these investigations should play an important part in the theory of atomic magnetic ordering. Such temperature measurements of spectra of spin waves should be carried out for different types of magnetic structures. The corresponding theory of spin waves in arbitrary structures is given in [61].

Up to the present time, spectra of spin waves have been investigated experimentally only for a few magnetic materials: magnetite,[55,59] iron,[56] $CO_{0.92}Fe_{0.08}$,[57] franklinite (zinc-manganese ferrite),[58] and hematite.[37] Of these only hematite is an antiferromagnet, while the others are ferromagnetic. In accordance with the conclusions of the theory, in papers[55-58] they obtained a quadratic law for the dispersion of the spin waves in a ferromagnet, while a linear law was found for the antiferromagnet.[37] In [59] for magnetite one first observed an optical branch of the spin waves in a ferromagnet, while the dispersion law for the "acoustic" branch was investigated for the principal directions over the whole Brillouin zone. In papers[58,59] the lifetime of spin waves in ferromagnets is estimated.

IV. MAGNETIC CRITICAL SCATTERING

8. Scattering in the Neighborhood of the Curie or Néel Points

Experiments show a sharp increase in magnetic scattering of neutrons in ferro-[32] and antiferromagnets[33] in the neighborhood of the Bragg magnetic reflections as one approaches the phase transition point, and above it, in the paramagnetic region. This phenomenon, which has been called magnetic critical scattering, in its nature is completely analogous to the scattering of light in a liquid near its critical state (opalescence) or the scattering of x-rays in alloys in the neighborhood of the ordering point.

Magnetic critical scattering of neutrons is related to the increase in large spontaneous fluctuations of the magnetization in the vicinity of the Curie point. Since the fluctuations propagate over distances larger than the interatomic spacing and exist for a long time compared with the time of microscopic relaxation, they produce a magnetic scattering whose distribution in angle and energy is markedly different from the distributions which appear at low temperatures.

The theory of critical scattering of neutrons in a ferromagnet was first developed by Van Hove [6] on the basis of a study of spin correlations near the Curie point. A phenomenological treatment of the phenomenon using the thermodynamic theory of fluctuations was given by Krivoglaz,[34] who expressed

FIG. 6. Scheme of the experiment for determining the dependence of the energy of a spin wave in a ferromagnet on temperature.

the cross section in terms of the magnetic suscepti-
bility in the vicinity of the Curie point. A more com-
plete theory (which we shall proceed now to describe)
using a quasiclassical description of the spin system
near the ordering point was proposed recently by
de Gennes and Villain.[35]

Having in mind application of the theory to crystals
with an arbitrary lattice, whose unit cell may consist
of several magnetic atoms, we shall write the cross
section for magnetic scattering (3.8) in the following
form:

$$\frac{d^2\sigma}{d\Omega\, dE_{\mathbf{p}'}} = (r_0\,\gamma)^2 \frac{p'}{p} \sum_{ij} F_i(\mathbf{q})\, F_j(\mathbf{q}) \sum_{R_i R_j} e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)} \sum_{\alpha\beta} (\delta_{\alpha\beta} - e_\alpha e_\beta)$$

$$\times \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}(E_{\mathbf{p}'}-E_{\mathbf{p}})t}\, \langle S_{R_i}^\alpha(0)\, S_{R_j}^\beta(t)\rangle \; dt, \qquad (8.1)$$

where the summation over the magnetic atoms of the
crystal is split into a sum $\sum_i$ over the limits of one

unit cell and a sum $\sum_{R_i}$ over the atoms of a given type

located in all cells of the crystal.

Since in the ordered phase the average components
of the spin of each atom are not all equal to zero, it
is convenient to write the spin correlator in the form

$$\langle S_{R_i}^\alpha(0)\, S_{R_j}^\beta(t)\rangle = \langle S_{R_i}^\alpha\rangle \langle S_{R_j}^\beta\rangle + \gamma_{\alpha\beta}'(\mathbf{R}_j - \mathbf{R}_i, t). \qquad (8.2)$$

The first term, corresponding to long-range order,
gives elastic Bragg scattering. The second term gives
an additional diffuse scattering which in general is in-
elastic. It is also this part of the correlator which
causes the critical scattering in the neighborhood of
the ordering temperature. The part of the scattering
cross section corresponding to it is equal to

$$\left(\frac{d^2\sigma}{d\Omega dE_{\mathbf{p}'}}\right)_{\text{crit}} = (\tau_0\gamma)^2 \frac{p'}{p}$$

$$\times \sum_{ij} F_i(\mathbf{q})\, F_j(\mathbf{q}) \sum_{R_i R_j} e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)} \sum_{\alpha\beta} (\delta_{\alpha\beta} - e_\alpha e_\beta)\, \frac{1}{2\pi\hbar}$$

$$\times \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}(E_{\mathbf{p}'}-E_{\mathbf{p}})t} \{\langle S_{R_i}^\alpha(0)\, S_{R_j}^\beta(t)\rangle - \langle S_{R_i}^\alpha\rangle \langle S_{R_j}^\beta\rangle\}\, dt. \qquad (8.3)$$

We first consider the scattering in which the tran-
sition energy $E_{\mathbf{p}'} - E_{\mathbf{p}}$ is small compared with the
initial energy. In this case we can start from a static
approximation for the correlations, considering their
limiting values for $t = 0$. It is clear that such an ap-
proximation describes elastic scattering. Integrating
expression (8.3) for this case over $dE_{\mathbf{p}'}$, we express
the cross sections for critical scattering into unit
solid angle in the form

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{crit}} = (r_0\gamma)^2 \frac{kT}{g^2\mu_0^2} \sum_{ij} \sum_{\alpha\beta} F_i(\mathbf{q})\, F_j(\mathbf{q})\, \chi_{ij}^{\alpha\beta}(\mathbf{q})$$

$$\times (\delta_{\alpha\beta} - e_\alpha e_\beta)\, e^{i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)}, \qquad (8.4)$$

where

$$\chi_{ij}^{\alpha\beta}(\mathbf{q}) = \beta g^2\mu_0^2 \sum_{R_i R_j} e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{r}_i-\mathbf{R}_j+\mathbf{r}_j)} \{\langle S_{R_i}^\alpha S_{R_j}^\beta\rangle - \langle S_{R_i}^\alpha\rangle \langle S_{R_j}^\beta\rangle\} \qquad (8.5)$$

is the magnetic susceptibility tensor of the scatterer
describing the reaction of its magnetic system to an
inhomogeneous external magnetic field. In fact, if a
magnetic field $\mathbf{H}_{R_i}$ acts on a spin located at the
lattice point $\mathbf{R}_i$, it leads to a change in the equili-
brium value of the magnetic moment by an amount
$\delta\mu_{R_i}$. The average value of the magnetic moment in
the presence of an external inhomogeneous field is

$$\mu_{R_i} = \frac{g\mu_0\, \mathrm{Sp}\,[e^{-\beta\,(\mathcal{H}+\delta\mathcal{H})}\, S_{R_i}]}{\mathrm{Sp}\, e^{-\beta\,(\mathcal{H}+\delta\mathcal{H})}} \equiv \mu_{R_i}^0 + \delta\mu_{R_i}, \qquad (8.6)$$

where $\delta\mathcal{H} = -g\mu_0 \sum_{iR_i} (\mathbf{S}_{R_i}\cdot\mathbf{H}_{R_i})$. Expanding the traces

in powers of $\delta\mathcal{H}$, we get in first approximation

$$\delta\mu_{R_i}^\alpha \approx g^2\mu_0^2$$

$$\times \sum_{\beta R_j} \int_0^\beta d\beta_1\, [\langle S_{R_i}^\alpha(0)\, S_{R_j}^\beta(i\hbar\beta_1)\rangle - \langle S_{R_i}^\alpha(0)\rangle \langle S_{R_j}^\beta(0)\rangle]\, H_{R_j}^\beta. \qquad (8.7)$$

We shall be interested in the classical limit of the
spin properties of a system which is near the phase
transition point, so we shall neglect the non-commuta-
tivity of the spin operators, setting $S_{R_i}^\beta(i\hbar\beta_1) = S_{R_i}^\beta$.
In place of (8.7) we will have

$$\delta\mu_{R_i}^\alpha = \beta g^2\mu_0^2 \sum_\beta \sum_{jR_j} (\langle S_{R_i}^\alpha S_{R_j}^\beta\rangle - \langle S_{R_i}^\alpha\rangle \langle S_{R_j}^\beta\rangle)\, H_{R_j}^\beta. \qquad (8.8)$$

The equation for the Fourier component (8.8) has the
form

$$N\delta\mu_i^\alpha(\mathbf{k}) = \sum_j \sum_\beta \chi_{ij}^{\alpha\beta}(\mathbf{k})\, H_j^\beta(\mathbf{k}), \qquad (8.9)$$

where $H_j^\beta(\mathbf{k}) = \sum_{R_j} H_{R_j}^\beta\, e^{i\mathbf{k}\cdot(\mathbf{R}_j-\mathbf{r}_j)}$ is the Fourier

component of the external field and N is the number
of cells in the sample. The last relation shows that
$\chi_{ij}^{\alpha\beta}(\mathbf{k})$, given by expression (8.5), is the magnetic
susceptibility tensor. According to (8.4) the calcula-
tion of the cross section reduces to calculating the
magnetic susceptibility tensor, taking into account the
spatial dispersion. Its components can be expressed
in terms of the exchange integrals if we use the fact
that each spin is in equilibrium under the action of
the external field and the molecular field of its neigh-
bors.

Above the transition point ($T > T_0$) the local
equation for the magnetic moment at site $\mathbf{R}_i$ can ob-
viously be written in the form[35]

$$\mu_{R_i} = \frac{S_i(S_i+1)}{3kT}\left(g^2\mu_0^2\, \mathbf{H}_{R_i} + \sum_{jR_j} 2J_{R_i R_j}\mu_{R_j}\right). \qquad (8.10)$$

If we define the Hermitian matrix of rank n by the
equation

$$A_{ij}(\mathbf{k}) = \delta_{ij} \frac{3kT}{S_i(S_i+1)} - \sum_{R_j} 2J_{R_i R_j}\, e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j-\mathbf{r}_i+\mathbf{r}_j)}, \qquad (8.11)$$

then equation (8.10) in Fourier components can be easily written in the form

$$\sum_i A_{ij}(\mathbf{k})\,\mu_j^\alpha(\mathbf{k}) = g^2\mu_0^2 H_j^\alpha(\mathbf{k}). \qquad (8.12)$$

Going over to the inverse matrix A^{-1} and comparing with (8.9), we get

$$\chi_{ij}^{\alpha\beta}(\mathbf{k}) = Ng^2\mu_0^2\,[A^{-1}(\mathbf{k})]_{ij}\,\delta_{\alpha\beta}. \qquad (8.13)$$

Below the transition temperature ($T < T_0$) we should include the presence of spontaneous magnetization in the system. The equation for calculating the magnetic moment of the ion at point R_i in the direction of spontaneous magnetization (z axis) is written in the form

$$\mu_{R_i} = B_i(|\,\mathbf{F}_{R_i} + \mathbf{H}_{R_i}\,|), \qquad (8.14)$$

where

$$B_i(H) = \tfrac{1}{2}\,g\mu_0\left\{(2S_i + 1)\coth\left[\beta g\mu_0\left(S_i + \tfrac{1}{2}\right)H\right]\right.$$

$$\left.-\coth\left[\tfrac{1}{2}\,\beta g\mu_0 H\right]\right\} \qquad (8.15)$$

is the Brillouin function, $\mathbf{F}_{R_i}$ is the molecular field at point R_i. It is given by the expression

$$\mathbf{F}_{R_i} = \frac{1}{g^2\mu_0^2}\sum_{jR_j}' 2J_{R_iR_j}\mu_{R_j}. \qquad (8.16)$$

Equation (8.14) leads to the following expression for the susceptibility tensor when $T < T_0$:

$$\chi_{ij}^{\alpha\beta}(\mathbf{k}) = Ng^2\mu_0^2\,[A^{\alpha-1}(\mathbf{k})]_{ij}\,\delta_{\alpha\beta}, \qquad (8.17)$$

where

$$A_{ij}^z(\mathbf{k}) = \delta_{ij}\,\frac{g^2\mu_0^2}{\left(\dfrac{\partial B_i}{\partial H}\right)_{F_i}} - \sum_{jR_j} 2J_{R_iR_j}\,e^{i\mathbf{k}\,(\mathbf{R}_i - \mathbf{R}_j - \mathbf{r}_i + \mathbf{r}_j)},$$

$$A_{ij}^x(\mathbf{k}) = A_{ij}^y(\mathbf{k}) = g^2\mu_0^2\frac{F_i}{\mu_i}\delta_{ij} - \sum_{jR_j} 2J_{R_iR_j}\,e^{i\mathbf{k}\,(\mathbf{R}_i - \mathbf{R}_j - \mathbf{r}_i + \mathbf{r}_j)}. \qquad (8.18)$$

In the last relations μ_i and $\mathbf{F}_i$ are the average values of the spin of the ion at position i and the molecular field acting on it in the absence of the external field.

Thus, in the molecular field approximation the critical scattering is described by formula (8.4), where the magnetic susceptibility tensor is expressed by (8.13) for $T > T_0$ and by (8.17) for $T < T_0$. The specific calculation of the cross section for critical scattering using the method described of de Gennes and Villain was recently done for magnetite [36] and hematite.[37]. The extension of the method to the case of antiferromagnetism was done by de Gennes in [38].

Now let us consider in detail the critical scattering in the simplest kind of ferromagnet consisting of one sublattice, for the paramagnetic region ($T > T_0$). Now it is more convenient not to use the method of de Gennes and Villain, but to start from the initial formulas (8.4) and (8.5) expressing the cross section in terms of the susceptibility $\chi^{\alpha\beta}(\mathbf{q})$. Since in the

paramagnetic region $\chi^{\alpha\beta}(\mathbf{q}) = \chi(\mathbf{q})\delta^{\alpha\beta}$; expression (8.4) takes the form

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{crit}} = N\,(r_0\gamma)^2\cdot\frac{2}{3}\,S\,(S + 1)\,F^2(q)\,\frac{\chi(q)}{\chi_0}, \qquad (8.19)$$

where $\chi_0 = N\dfrac{q^2\mu_0^2 S(S + 1)}{3kT}$ is the magnetic susceptibility in the absence of exchange interaction, $\chi(\mathbf{q})$ is the susceptibility describing the response of the system to the inhomogeneous magnetic field with wave vector q. According to (8.5), $\chi(\mathbf{q})$ is expressed as follows in terms of the spin correlator:

$$S\,(S + 1)\,\frac{\chi(q)}{\chi_0} = \sum_R \langle S_0 S_R\rangle\,e^{i\mathbf{qR}}. \qquad (8.20)$$

Here S_0 is the spin of the site chosen as the coordinate origin. Here we have first of all used the fact that $\langle S_R^\alpha S_{R'}^\beta\rangle$ depends only on the difference $\mathbf{R} - \mathbf{R}'$ and secondly that $\langle S_R^\alpha S_{R'}^\alpha\rangle$ is the same for all $\alpha = x, y, z$ above the Curie point.

The further calculation requires a knowledge of the correlator $\langle S_0 S_R\rangle$. At present there is no method for exact calculation of this quantity, but certain general properties of this quantity as a function of R can be understood from physical arguments. It is completely obvious that in the absence of spin interactions $\langle S_0 S_R\rangle \equiv 0$, since in this case the spin projections which refer to different sites are statistically independent, and so their average value is equal to zero. The presence of exchange interaction leads to a certain correlation of the spin projections at different sites which increases as we approach the Curie point. This correlation manifests itself in the development of fluctuations of the magnetization whose magnitude increases near the Curie point. The phenomenological analysis given by Van Hove [6] led to the following dependence of the correlations near the Curie point at large R (the long-range part of the correlation):

$$\langle S_0 S_R\rangle = \frac{V_0 S\,(S + 1)}{4\pi r_1^2 R}\,e^{-k_1 R}, \qquad (8.21)$$

where V_0 is the volume per magnetic atom and r_1 and k_1 are certain phenomenological constants depending on temperature; r_1 should change slowly with temperature and in order of magnitude should be several interatomic distances, while k_1 should behave completely differently. As we approach the Curie point, the correlations should increase, so k_1^{-1} reaches a macroscopic size at the Curie point and drops off with increasing temperature to a value of the order of r_1.

From relations (8.20) and (8.21) we quickly see that

$$(k_1 r_1)^2 = \frac{\chi_0}{\chi(0)}. \qquad (8.22)$$

Substituting (8.21) in (8.20) and summing over the whole crystal, we get $\chi(\mathbf{q})$. But we are not interested in the whole range of values of q, but only those which lie near vectors of the reciprocal lattice, i.e.,

we are interested in the critical state near the position of the Bragg peak. For this reason we write the right-hand side of (8.20) in the form $\sum_{R} \langle S_0 S_R \rangle$ $\times e^{i(q-\tau) \cdot R}$ and expand the exponential in a series in powers of $q - \tau$; we find after summation over lattice sites for small values of $|q - \tau|$ (in the case of a cubic crystal)

$$\frac{\chi(q)}{\chi_0} = \frac{1}{r_1^2(k_1^2 + |q - \tau|^2)} . \qquad (8.23)$$

The expression for the scattering cross section when $T > T_0$ takes the form

$$\left(\frac{d\sigma}{d\Omega}\right)_{crit} = \frac{2}{3} S(S+1)(\gamma r_0)^2 \frac{F^2(q)}{r_1^2[k_1^2 + |q - \tau|^2]} . \qquad (8.24)$$

Since k_1 drops off sharply as we approach the Curie point, it follows from formula (8.24) that near the Bragg peak the scattering intensity increases markedly with decreasing temperature, reaching a maximum value at the Curie point. For a fixed temperature the dependence of the intensity on the deviation of the scattering angle θ from the position of the Bragg peak θ_B corresponding to the reciprocal lattice vector τ, is given by the factor

$$[k_1^2 + \tau^2(\theta - \theta_B)^2]^{-1}, \qquad (8.24')$$

i.e., the distribution has a Lorentz shape with width $\sim k_1$.

Critical scattering for $\tau = 0$ corresponds to scattering at small angles. Critical scattering with $\tau \neq 0$ can actually be observed if the form factor $F(q)$ is not small for $q = \tau$. The occurrence of critical scattering with $\tau \neq 0$ is an important feature of critical magnetic scattering as compared, for example, with the critical scattering of light by a liquid, where it does not occur. The scattering with $\tau \neq 0$ necessarily shows that, despite the strong disordering fluctuations of the magnetization, the spin system preserves its ordered position in space because of the structure of the lattice of the crystal.

It is useful to note that the same sort of expression for the susceptibility $\chi(q)$ as (8.23) can be obtained by the method of de Gennes and Villain if we start from relations (8.13) and (8.11). In fact, writing (8.11) for $i = j = 1$ and expanding the exponential in series in powers of $|q - \tau|$ we immediately get, by using (8.13), the relation (8.23), where the parameters r_1 and k_1 are equal to

$$r_1^2 = \frac{a^2}{z} \frac{T_0}{T} , \qquad k_1^2 = \frac{z}{a^2} \frac{T - T_0}{T_0} . \qquad (8.25)$$

Here a is the lattice constant, z is the number of nearest neighbors, $T_0 = 2zJS(S + 1)/3k$ is the Curie temperature. We see that r_1 and k_1 have the properties predicted by Van Hove's phenomenological theory. The length r_1 has microscopic dimensions and depends very slightly on temperature in the vicinity of the Curie point. The quantity k_1^{-1} increases sharply as one approaches the Curie point, but far from it coincides with r_1. Thus the method of de Gennes and

Villain allows one to calculate the values of r_1 and k_1 and to find their temperature dependence. Furthermore it permits us to generalize the expressions for the scattering cross section (8.24) to the case of several ferromagnetic sublattices. One can show[35] that, in the general case, near Bragg maxima the critical scattering is equal to

$$\left(\frac{d\sigma}{d\Omega}\right)_{crit} = \frac{2}{3}(r_0\gamma)^2 \frac{1}{n} \sum_{i=1}^{n} S_i(S_i+1) \frac{F_i^2(q)}{r_1^2(\tau)[k_1^2 + |q - \tau|^2]} , \qquad (8.26)$$

where

$$k_1^2 = \frac{\sum_i \chi_0^i}{r_1^2(0) \sum_{ij} \chi_{ij}(0)} , \qquad (8.27)$$

$$r_1^2(\tau) = \frac{\sum_i S_i(S_i+1)}{18kT \sum_{ij} \tilde{A}_{ij}(\tau) e^{i\tau(r_i - r_j)}} \sum_\alpha \left(\frac{\partial^2\Delta}{\partial k_\alpha^2}\right)_{\substack{T=T_0 \\ k=0}} , \qquad (8.28)$$

in which $\tilde{A}_{ij}(k)$ is the minor of the matrix $A_{ij}(k)$ and $\Delta(k)$ is its determinant, so that $[A^{-1}(k)]_{ij} = \tilde{A}_{ij}(k)/\Delta(k)$.

In the general case, expression (8.22) is replaced by the following:

$$[k_1 r_1(0)]^2 = \frac{\sum_i \chi_0^i}{\sum_{ij} \chi_{ij}(0)} . \qquad (8.29)$$

Expression (8.26), like (8.24), is valid near the Curie point when $T - T_0 \ll T_0$. Below the Curie point, when $T_0 - T \ll T_0$ the critical scattering is described by formula (8.4), taking into account (8.17).

For the case where the ferromagnet has a single sublattice, the expression for the cross section takes the simple form

$$\left(\frac{d\sigma}{d\Omega}\right)_{crit} = N(r_0\gamma)^2 \frac{kT}{g^2\mu_0^2} F^2(q) \{\chi_{||}(q)(1 - e_z^2) + \chi_\perp(q)(1 + e_z^2)\}, \qquad (8.30)$$

where $\chi_{||}$ and $\chi_\perp$ are the longitudinal and transverse components of the magnetic susceptibility tensor. Using expression (8.18) for the scattering vectors near the Bragg peaks, we can represent the cross section (8.30) in the form

$$\left(\frac{d\sigma}{d\Omega}\right)_{crit} = N(r_0\gamma)^2 F^2(q) \frac{1}{3} S(S+1)$$
$$\times \left\{\frac{1 - e_z^2}{r_1^2[k_{||}^2 + |q - \tau|^2]} + \frac{1 + e_z^2}{r_1^2[k_\perp^2 + |q - \tau|^2]}\right\} . \qquad (8.31)$$

Here $r_1^2 = \frac{a^2}{z} \frac{T_0}{T}$ is a parameter which coincides formally with that which appeared in the paramagnetic region, while the parameters $k_{||}^2$ and $k_\perp^2$ are equal to

$$k_{||}^2 = \frac{g^2\mu_0^2 \left(\frac{\partial B}{\partial H}\right)_F^{-1} - 2zJ}{2Ja^2} , \qquad k_\perp^2 = \frac{g^2\mu_0^2 \frac{F}{\mu} - 2zJ}{2Ja^2} . \qquad (8.32)$$

The parameters $k_{||}$ and $k_\perp$ drop off rapidly as we approach the Curie point, so the scattering intensity,

according to (8.31) increases rapidly, reaching its maximum value at the Curie point. Furthermore, with increasing temperature the intensity also drops sharply and is again described by formula (8.24); thus the scattering of neutrons in the neighborhood of Bragg reflections in the vicinity of the Curie point gives peaks in the temperature dependence of the intensity.

An important difference between the critical scattering in the ferromagnetic region and the scattering above the Curie point consists in the fact that in the first case the intensity depends on the position of the scattering vector relative to the direction of the spontaneous magnetic moment of the crystal. The scattering described by the two terms in curly brackets in expression (8.31), which are related to the correlations of the longitudinal or transverse components of the spin, can be separated if we measure the scattering in two directions: when the vector q is perpendicular and when it is parallel to the vector m. Since at the Curie point $k_{||}$ and $k_{\perp}$ are equal to zero, the intensity of the scattering given by formula (8.31) can easily be seen to agree with the value of the intensity at the Curie point as given by formula (8.24); thus both these formulas coalesce at the Curie point.

It is also interesting to note that, from a comparison of (8.31) and (8.24), it follows that below the Curie point the long-range part of the correlations changes with distance according to the same law as in the paramagnetic domain (cf. (8.21)), with the single difference that the rate of drop-off of the correlations will be different for the longitudinal and transverse components of the spins. It will be given by factors $k_{||}$ and $k_{\perp}$ respectively in place of k_1. Right up to the Curie point $k_{\perp} \gg k_{||}$, so the correlation of the perpendicular components drops off more rapidly. This has the consequence that the contribution to the cross section from the second term in (8.31) is small compared to the contribution of the first term which is associated with longitudinal correlations (except, of course, for the case where q is close to m).

In conclusion we note that the distribution of intensity of critical scattering of neutrons with angle is determined by the long-range part of the spin correlations as given by expression (8.2). These correlation functions determine the scattering not only for neutrons, but also, for example, for electrons in a ferromagnetic metal which also leads to anomalies in electrical conductivity and other kinetic coefficients in the vicinity of the Curie point. Thus the computation of such correlation functions is of general theoretical interest.

The method of de Gennes and Villain which is described here consists in using the relation of these correlation functions to the magnetic susceptibility which is calculated using the molecular field approximation. Another possibility for calculating was proposed earlier by Elliott and Marshall,[39] who de-

veloped an equation for the correlation functions using the cluster method of Bethe and Peierls,[40] i.e., again in the molecular field approximation which is appropriate in the vicinity of the Curie point.

A more general procedure for calculating correlation functions on the Heisenberg model of a ferromagnet consists in using the two-time Green's functions. Bogolyubov and Tyablikov[26] in this way developed the correlation function for spin $s = \frac{1}{2}$. A generalization of their method to arbitrary spin has been given recently.[41] The expression obtained by this method for the correlation function in the form of a Fourier series is valid approximately for the whole range of temperatures in which the ferromagnetic state exists, but the summation of the Fourier series in the intermediate temperature range can be done only numerically.

Now let us turn to the critical scattering. Up to now we have studied only the static approximation for the critical scattering, in which we neglected the change in energy of the neutron $\hbar\omega = E_p - E_{p'}$ on scattering. The energy distribution of the scattered neutrons is related to the dependence of the spin operators or spin correlations on the time. It is simplest to get the qualitative features of this dependence using a phenomenological method. Let us assume that the dependence of the correlations on time is given in the vicinity of the Curie point (for $T > T_0$) by a damping of the magnetization fluctuations, which in turn are described by a phenomenological equation for irreversible processes in a spin system, for example, by the diffusion equation

$$\frac{\partial M}{\partial t} = \Lambda_1 \Delta M, \qquad (8.33)$$

where Λ_1 is the diffusion coefficient, which is inversely proportional to the magnetic susceptibility. From this the Fourier component of the magnetization $M_q \sim e^{-\Lambda_1 q^2 t}$, so that we can write for the time correlation

$$\sum_R \langle S_0 S_R(t) \rangle e^{iqR} = \sum_R \langle S_0 S_R \rangle e^{iqR} e^{-\Lambda_1 q^2 t}. \qquad (8.34)$$

Substituting this expression in (8.3) for the case $i = j = 1$, and integrating over the time, we find in place of (8.24)

$$\left(\frac{d^2\sigma}{d\Omega \, dE_{p'}}\right)_{crit} = \frac{2}{3}(r_0\gamma)^2 S(S+1)$$

$$\times \frac{F^2(q)}{r_1^2[k_1^2 + |q - \tau|^2]} \frac{1}{\pi} \frac{\Lambda_1 \hbar |q - \tau|^2}{(\Lambda_1 \hbar)^2 |q - \tau|^4 + [E_{p'} - E_p]^2}. \qquad (8.35)$$

The energy distribution of the neutrons in the vicinity of the Bragg peak is described by a Lorentz-shaped line with width $\Lambda_1 \hbar |q - \tau|^2$. Since as we approach the Curie point $\Lambda_1 \to 0$, the energy distribution function in (8.35) tends toward $\delta(E_p - E_{p'})$. This means that near the Curie point the critical scattering of neutrons is quasi-elastic. Upon integrating expres-

sion (8.35) over $dE_{p'}$, we get the angular distribution (8.24), multiplied by a factor which is close to unity.

From these statements we see that the experimental study of critical scattering near the phase transition point should give valuable information about the behavior of the fluctuations of the magnetization.

At present critical scattering has been studied most completely for magnetite.[36] The incompleteness of the spin wave theory of the scattering of neutrons in the vicinity of the Curie point was shown experimentally for magnetite in [42]. Later Riste [36] carried out a careful study of critical scattering and a comparison of the experimental results with the theory of de Gennes and Villain. The general picture of the scattering turned out to be that proposed by Van Hove, while quantitatively the results were in good agreement with the predictions of de Gennes and Villain for magnetitie. The critical scattering has also been studied carefully for hematite.[37]

V. SCATTERING OF POLARIZED NEUTRONS

9. Differential Cross Section for Scattering of Polarized Neutrons

In the scattering of polarized neutrons we have an interference of nuclear and magnetic scattering which was absent when the neutrons were not polarized. Consequently, in the expression for the differential scattering cross section

$$\frac{d^2\sigma}{d\Omega\,dE_{p'}} = \frac{m^2}{(2\pi)^3\hbar^5}\frac{p'}{p}\int_{-\infty}^{+\infty} dt\, e^{\frac{i}{\hbar}(E_{p'}-E_p)t}\,\mathrm{Sp}\,[\varrho_\sigma\langle V_{p',p}^+V_{p',p}(t)\rangle]$$
(9.1)

we should include both of the interactions of the neutron with the crystal, nuclear and magnetic, so that the quantity $V_{p',p}$ takes the form

$$V_{p',p} = \sum_l \left[A_l + \frac{1}{2}B_l(\sigma \mathbf{I}_l)\right]$$

$$\times e^{i\mathbf{q}\mathbf{R}_l} - \frac{4\pi\hbar^2}{m}r_0\gamma\frac{1}{2}\sum_j F_j(\mathbf{q})\,e^{i\mathbf{q}\mathbf{R}_j}(\mathbf{S}_j, \sigma - (\mathbf{e}\sigma)\,\mathbf{e}).$$
(9.2)

The polarization state of the incident neutron beam is given by the spin density matrix

$$\varrho_\sigma = \frac{1}{2}(1 + \mathbf{p}_0\sigma),$$
(9.3)

where $\frac{1}{2}\sigma$ is the spin operator of the neutron and $\mathbf{p}_0 = \mathrm{Tr}\,\rho_\sigma\sigma$ is the polarization vector, equal to twice the average value of the neutron spin in the beam. The individual components of the vector σ are the Pauli matrices which satisfy the commutation relations

$$\sigma_\alpha\sigma_\beta - \sigma_\beta\sigma_\alpha = 2i\varepsilon_{\alpha\beta\gamma}\sigma_\gamma, \quad \sigma_\alpha\sigma_\beta + \sigma_\beta\sigma_\alpha = 2\delta_{\alpha\beta}.$$
(9.4)

It should be emphasized that expression (9.1) has the most general form possible for a beam of particles with spin $\frac{1}{2}$, this following directly from the properties of the Pauli matrices.

It is clear that in calculating the scattering cross

section we require expressions for the traces of various products of Pauli matrices. From the commutation relations (9.4) one can easily obtain the following relations:

$$\frac{1}{2}\mathrm{Sp}\,1 = 1, \quad \frac{1}{2}\mathrm{Sp}\,\sigma_\alpha = 0, \quad \frac{1}{2}\mathrm{Sp}\,(\sigma_\alpha\sigma_\beta) = \delta_{\alpha\beta},$$

$$\frac{1}{2}\mathrm{Sp}\,(\sigma_\alpha\sigma_\beta\sigma_\gamma) = i\varepsilon_{\alpha\beta\gamma},$$

$$\frac{1}{2}\mathrm{Sp}\,(\sigma_\alpha\sigma_\beta\sigma_\gamma\sigma_\delta) = \delta_{\alpha\beta}\delta_{\gamma\delta} - \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}.$$
(9.5)

As we easily see from relations (9.1) and (9.2), all problems concerning the scattering of polarized neutrons in a magnetic material require the calculation of traces of the operators

$$L_j = (\mathbf{S}_j, \sigma - (\mathbf{e}\sigma)\,\mathbf{e})$$
(9.6)

in products with other such operators and with the Pauli matrices. The results of such computations are given in the following table (9.8), in which the vector $\mathfrak{M}_j$ denotes

$$\mathfrak{M}_j = \mathbf{S}_j - (\mathbf{e}\mathbf{S}_j)\,\mathbf{e}.$$
(9.7)

Thus we have

$$\left.\begin{aligned}
\frac{1}{2}\mathrm{Sp}\,\{\sigma L\} &= \mathfrak{M}, \\
\frac{1}{2}\mathrm{Sp}\,\{(\mathbf{p}\sigma)\,L\} &= (\mathfrak{M}\mathbf{p}), \\
\frac{1}{2}\mathrm{Sp}\,\{(\mathbf{p}\sigma)\,\sigma L\} &= i\,[\mathfrak{M}\times\mathbf{p}], \\
\frac{1}{2}\mathrm{Sp}\,\{(\mathbf{p}\sigma)\,L\sigma\} &= -i\,[\mathfrak{M}\times\mathbf{p}], \\
\frac{1}{2}\mathrm{Sp}\,\{L_1 L_2\} &= (\mathfrak{M}_1\mathfrak{M}_2), \\
\frac{1}{2}\mathrm{Sp}\,\{L_1\sigma L_2\} &= -i\,[\mathfrak{M}_1\times\mathfrak{M}_2], \\
\frac{1}{2}\mathrm{Sp}\,\{(\mathbf{p}\sigma)\,L_1 L_2\} &= i\,[\mathfrak{M}_1\times\mathfrak{M}_2]\,\mathbf{p}, \\
\frac{1}{2}\mathrm{Sp}\,\{(\mathbf{p}\sigma)\,L_1\sigma L_2\} &= \mathfrak{M}_1\,(\mathfrak{M}_2\mathbf{p}) + (\mathfrak{M}_1\mathbf{p})\,\mathfrak{M}_2 - \mathbf{p}\,(\mathfrak{M}_1\mathfrak{M}_2).
\end{aligned}\right\}$$
(9.8)

Using this table, it is not difficult to get the following general expression for the trace, which determines the differential cross section (9.1):

$$\mathrm{Sp}\,[\varrho_\sigma\langle V_{p',p}^+V_{p',p}(t)\rangle] = \sum_{ll'}\left[A_l A_{l'} + \frac{1}{4}B_l^2 I_l\,(I_l+1)\,\delta_{ll'}\right]$$

$$\times \langle e^{-i\mathbf{q}\mathbf{R}_l}e^{i\mathbf{q}\mathbf{R}_{l'}(t)}\rangle + \left(\frac{4\pi\hbar^2}{m}r_0\gamma\right)^2\frac{1}{4}\sum_{jj'}F_j(\mathbf{q})\,F_{j'}(\mathbf{q})$$

$$\times \langle e^{-i\mathbf{q}\mathbf{R}_j}e^{i\mathbf{q}\mathbf{R}_{j'}(t)}\rangle\,\langle(\mathfrak{M}_j\mathfrak{M}_{j'}(t))\rangle - \frac{4\pi\hbar^2}{m}r_0\gamma\frac{1}{2}\sum_{lj}A_l F_j(\mathbf{q})$$

$$\times \langle e^{-i\mathbf{q}\mathbf{R}_l}e^{i\mathbf{q}\mathbf{R}_j(t)}\rangle\,\langle(\mathfrak{M}_j(t))\,\mathbf{p}_0\rangle - \frac{4\pi\hbar^2}{m}r_0\gamma\frac{1}{2}\sum_{lj}A_l F_j(\mathbf{q})$$

$$\times \langle e^{-i\mathbf{q}\mathbf{R}_j}e^{i\mathbf{q}\mathbf{R}_l(t)}\rangle\,\langle(\mathfrak{M}_j)\,\mathbf{p}_0\rangle + \left(\frac{4\pi\hbar^2}{m}r_0\gamma\right)^2\frac{1}{4}\sum_{jj'}F_j(\mathbf{q})\,F_{j'}(\mathbf{q})$$

$$\times \langle e^{-i\mathbf{q}\mathbf{R}_j}e^{i\mathbf{q}\mathbf{R}_{j'}(t)}\rangle\,i\,\langle[\mathfrak{M}_j\times\mathfrak{M}_{j'}(t)]\rangle\,\mathbf{p}_0.$$
(9.9)

In getting this expression we have made an approxima-

tion: we have neglected the interaction of the spin system with the lattice, as a result of which it was possible to split the average of the product into a product of the averages over the states of the magnetic system and the lattice.

The scattering cross section is gotten by integrating (9.9) with respect to the time so that, as one easily sees, the first two terms describe the scattering of unpolarized neutrons. The additional term in the cross section arising as a result of polarization of the neutrons is proportional to the initial polarization vector p_0. The third and fourth terms in (9.9) come from interference of nuclear and magnetic scattering.

It is of particular interest to consider (9.9) in two special cases: when the scatterer is a ferromagnet and when it is an antiferromagnet. For simplicity we shall assume that in both cases the crystal consists of atoms of only one type. From expression (9.9) we should separate out first the parts corresponding to elastic and inelastic scattering. For this purpose we express the operator of the spin vector S_j in a coordinate system where the z axis is directed along the spontaneous magnetic moment. (If the crystal consisted of several sublattices, we should have to choose a separate coordinate system for each of them with the z axis along the magnetization vector of the sublattice.)

In the case of one sublattice

$$S_j = S_j^z \mathbf{m} + \frac{1}{2} S_j^- \mathbf{m}^- + \frac{1}{2} S_j^+ \mathbf{m}^+, \qquad (9.10)$$

where $\mathbf{m}^\pm = \mathbf{m}^x \pm i\mathbf{m}^y$, $\mathbf{m}^x$, $\mathbf{m}^y$ are unit vectors the x and y axes. According to (9.10), the vector $\mathfrak{M}_j$ (9.7) breaks up into components:

$$\mathfrak{M}_j = S_j^z \mathbf{M} + \frac{1}{2} S_j^+ \mathbf{M}^- + \frac{1}{2} S_j^- \mathbf{M}^+, \qquad (9.11)$$

where

$$\mathbf{M} = \mathbf{m} - (\mathbf{em})\,\mathbf{e}, \quad \mathbf{M}^\pm = \mathbf{m}^\pm - (\mathbf{em}^\pm)\,\mathbf{e}. \qquad (9.12)$$

Thus the whole expression (9.9) can be broken up into a "longitudinal" part associated with the projections S_j^z and leading to elastic scattering, and a "transverse" part associated with the operators $S_j^\pm$ and leading to inelastic scattering. In this way we get for a ferromagnet

$$\frac{1}{2} \mathrm{Sp} \{\varrho_\sigma \langle V_{\mathbf{p'p}}^+ V_{\mathbf{p'p}}(t)\rangle\} = N \left\{ \overline{A^2} - \overline{A}^2 + \frac{1}{4} \overline{B^2 I(I+1)} \right\} e^{-2W_q}$$

$$+ \left\{ \overline{A}^2 + \left(\frac{4\pi\hbar^2}{m}\right)^2 (r_0\gamma)^2 F^2(\mathbf{q}) S^2(T) \frac{1}{4} M^2 \right.$$

$$\left. - \frac{4\pi\hbar^2}{m} r_0\gamma F(\mathbf{q}) S(T) \overline{A}(\mathbf{Mp_0}) \right\} \left| \sum_j e^{i\mathbf{qR}_j} \right|^2 e^{-2W_q}$$

$$+ \left(\frac{4\pi\hbar^2}{m} r_0\gamma\right)^2 e^{-2W_q} F^2(\mathbf{q}) \frac{1}{16} \sum_{jj'} e^{-i\mathbf{q}(\mathbf{R}_j - \mathbf{R}_{j'})}$$

$$\times \{\langle S_j^- S_{j'}^+(t)\rangle [1 + (\mathbf{em})^2 + 2(\mathbf{em})(\mathbf{ep_0})]$$

$$+ \langle S_j^+ S_{j'}^-(t)\rangle [1 + (\mathbf{em})^2 - 2(\mathbf{em})(\mathbf{ep_0})]\}, \qquad (9.13)$$

and for an antiferromagnet (two sublattices)

$$\frac{1}{2} \mathrm{Sp} \{\varrho_\sigma \langle V_{\mathbf{p'p}}^+ V_{\mathbf{p'p}}(t)\rangle\} = N \left\{ \overline{A^2} - \overline{A}^2 + \frac{1}{4} \overline{B^2 I(I+1)} \right\} e^{-2W_q}$$

$$+ \overline{A}^2 \left| \sum_l e^{i\mathbf{qR}_l} \right|^2 e^{-2W_q} + \left(\frac{4\pi\hbar^2}{m} r_0\gamma\right)^2 F^2(\mathbf{q}) S^2(T) \cdot \frac{1}{2}$$

$$\times (1 - \cos(\mathbf{qr}_{12})) M^2 \left| \sum_j e^{i\mathbf{qR}_j} \right|^2 \times e^{-2W_q} + \left(\frac{4\pi\hbar^2}{m} r_0\gamma\right)^2$$

$$\times F^2(\mathbf{q}) e^{-2W_q} \frac{1}{16} \sum_{jj'} e^{-i\mathbf{q}(\mathbf{R}_j - \mathbf{R}_{j'})} \sum_{vv'} e^{-i\mathbf{q}(\mathbf{r}_v - \mathbf{r}_{v'})} \langle S_{jv}^+ S_{j'v'}^-(t)$$

$$+ S_{jv}^- S_{j'v'}^+(t)\rangle [1 + (\mathbf{em})^2]. \qquad (9.14)$$

In the last expression m is a unit vector in the direction of magnetization of either sublattice. As we see, this expression is invariant with respect to the choice of the sublattices. This is completely natural since the sublattices are equivalent.

Substituting (9.13) and (9.14) in formula (9.1), we can get an explicit expression for the scattering cross section for polarized neutrons,[43] but it is not worth writing it since all of its features are easily seen from the last two expressions.

It is interesting to note that for an antiferromagnet with two sublattices the cross section for scattering of polarized neutrons differs in no way from the cross section for scattering of unpolarized neutrons. This is exactly what should be the case. In fact, as follows from (9.1) and (9.3), the cross section is a linear function of the polarization vector p_0. Since p_0 is a pseudovector and the cross section is a scalar, p_0 can enter into the expression for the cross section only in a product with some pseudovector characterizing the scatterer. An antiferromagnet is not described by any magnetic pseudovector (the sublattices give only the axis of antiferromagnetism, but not its direction) so that in the cross section there is also no term containing the polarization vector.

On the other hand, a ferromagnet is characterized by a pseudovector—the direction of the spontaneous magnetic moment. For this reason in the scattering cross section obtained from (9.13) there are terms depending on the polarization. These terms change the intensity of the Bragg peaks because of interference between nuclear and magnetic scattering, and also change the intensity of inelastic magnetic scattering.

10. Change in Polarization on Scattering in Ferro- and Antiferromagnets

In scattering of polarized neutrons in magnetic materials, most of the information about the properties of the magnetic system can be obtained by studying not the scattering cross section, but the change in the polarization vector of the neutrons scattered in a given direction. The polarization vector of the neutrons after the scattering is given by the formula

$$p = \frac{\mathrm{Sp}\{\varrho_\sigma \langle V^+_{\mathbf{p'p}} \sigma V_{\mathbf{p'p}}\rangle\}}{\mathrm{Sp}\{\varrho_\sigma \langle V^+_{\mathbf{p'p}} V_{\mathbf{p'p}}\rangle\}} , \qquad (10.1)$$

by means of which we can easily calculate the polarization vector of the neutrons scattered in a given direction as a result of different processes: nuclear and magnetic, elastic and inelastic. Let us consider the scattering for two cases.

1. Ferromagnet. In purely nuclear scattering the polarization vector obviously can not change its direction, but as a result of the scattering one can get a partial depolarization of the beam. Calculations using

formula (10.1) lead to the following expression for the polarization vector of the neutrons scattered incoherently and elastically:

$$p_{\mathrm{incoh}} = \frac{\overline{A^2} - \overline{A}^2 - \frac{1}{12} B^2 I (I+1)}{\overline{A^2} - \overline{A}^2 + \frac{1}{4} B^2 I (I+1)} p_0. \qquad (10.2)$$

The polarization vector of neutrons which suffer a scattering without change in the magnetic state of the scatterer (without absorption or emission of spin waves) is [44]

$$p_{nm} = \frac{\overline{A}^2 p_0 + \left(\frac{4\pi\hbar^2}{m} r_0\gamma\right)^2 F^2(\mathbf{q}) S^2(T) \cdot \frac{1}{4} [2\mathbf{M}(\mathbf{M}p_0) - M^2 p_0] - \frac{4\pi\hbar^2}{m} r_0\gamma \overline{A}F(\mathbf{q}) S(T) \mathbf{M}}{\overline{A}^2 + \left(\frac{4\pi\hbar^2}{m} r_0\gamma\right)^2 F^2(\mathbf{q}) S^2(T) \frac{1}{4} M^2 - \frac{4\pi\hbar^2}{m} r_0\gamma \overline{A}F(\mathbf{q}) S(T) (\mathbf{M}p_0)} . \qquad (10.3)$$

The polarization vector p^+_m (p^-_m) due to scattering with emission (absorption) of one spin wave or, more precisely, processes of scattering in which the number of spin waves increases (decreases) by unity, has the form [44]

$$p^\pm_m = \frac{\pm 2(\mathbf{em})\,\mathbf{e} + 2M_x(\mathbf{M}_x p_0) + 2M_y(\mathbf{M}_y p_0) - (M^2_x + M^2_y)\,p_0}{1 + (\mathbf{em})^2 \mp 2(\mathbf{em})(\mathbf{e}p_0)} . \qquad (10.4)$$

It is easy to see that this expression is independent of rotation of the coordinate axes about the vector $\mathbf{m}$,

i.e., it is independent of the choice of the x and y axes.

The average polarization vector of neutrons scattered in a given direction n is obviously

$$p = \frac{p_{\mathrm{incoh}}\sigma_{\mathrm{incoh}}(\mathbf{n}) + p_{nm}\sigma_{nm}(\mathbf{n}, p_0) + p^+_m \sigma^+_m(\mathbf{n}, p_0) + p^-_m \sigma^-_m(\mathbf{n}, p_0)}{\sigma_{\mathrm{incoh}}(\mathbf{n}) + \sigma_{nm}(\mathbf{n}, p_0) + \sigma^+_m(\mathbf{n}, p_0) + \sigma^-_m(\mathbf{n}, p_0)} . \qquad (10.5)$$

Here $\sigma_{\mathrm{incoh}}(\mathbf{n})$ is the cross section for incoherent nuclear scattering

$$\sigma_{nm}(\mathbf{n}, p_0) = \left[1 + \frac{\left(\frac{4\pi\hbar^2}{m} r_0\gamma\right)^2 F^2(\mathbf{q}) S^2(T) \cdot \frac{1}{4} M^2 - \frac{4\pi\hbar^2}{m} r_0\gamma F(\mathbf{q}) S(T) \overline{A}(\mathbf{M}p_0)}{\overline{A}^2}\right] \sigma_n(\mathbf{n}). \qquad (10.6)$$

$$\sigma^\pm_m(\mathbf{n}, p_0) = \left[1 \mp \frac{2(\mathbf{e}\cdot\mathbf{m})(\mathbf{e}p_0)}{1 + (\mathbf{e}\cdot\mathbf{m})^2}\right] \sigma^\pm_m(\mathbf{n}), \qquad (10.7)$$

where $\sigma_n(\mathbf{n})$ is the cross section for nuclear scattering of unpolarized neutrons and $\sigma^\pm_m(\mathbf{n})$ is the cross section for magnetic scattering of unpolarized neutrons with increase or decrease in the number of spin waves by one.

It is interesting to note the following fact: When $\sigma_{\mathrm{incoh}}(\mathbf{n}) = 0$, which occurs for a lattice consisting of atoms of a single isotope not having a spin, the polarization vector of the neutrons scattered in a given direction is expressed as a linear combination of the three, in general non-coplanar, vectors p_{nm}, p^+_m and p^-_m. These vectors are given by equations (10.3) and (10.4). From these equations one can see that we can calculate them beforehand if we know the nuclear scattering amplitude and also $F(\mathbf{q})$, $S(T)$, $\mathbf{e}$ and p_0. Thus, by measuring the polarization vector $\mathbf{p}$ of neutrons scattered in direction $\mathbf{n}$, and also the total cross section in that direction

$$\sigma(\mathbf{n}, p_0) = \sigma_{nm}(\mathbf{n}, p_0) + \sigma^+_m(\mathbf{n}, p_0) + \sigma^-_m(\mathbf{n}, p_0), \qquad (10.8)$$

we obviously can determine separately $\sigma_{nm}(\mathbf{n}, p_0)$, $\sigma^-_m(\mathbf{n}, p_0)$, and consequently $\sigma_n(\mathbf{n})$ and $\sigma^\pm_m(\mathbf{n})$. $\sigma^+_m(\mathbf{n}, p_0)$ and $\sigma^-_m(\mathbf{n}, p_0)$, and consequently $\sigma_n(\mathbf{n})$ and $\sigma^\pm_m(\mathbf{n})$.

Expressions (10.3)–(10.5) allow us to treat the case of scattering of unpolarized neutrons in a ferromagnet (Maleev[45]). Setting $p_0 = 0$, we get

$$p_{nm} = \frac{-\frac{4\pi\hbar^2}{m} r_0\gamma \overline{A}F(\mathbf{q}) S(T) \mathbf{M}}{\overline{A}^2 + \left(\frac{4\pi\hbar^2}{m} r_0\gamma\right)^2 F^2(\mathbf{q}) S^2(T) \frac{1}{4} [1 - (\mathbf{e}\cdot\mathbf{m})^2]} , \qquad (10.9)$$

$$p^\pm_m = \pm \frac{2(\mathbf{e}\cdot\mathbf{m})\,\mathbf{e}}{1 + (\mathbf{e}\cdot\mathbf{m})^2}, \qquad (10.10)$$

$$p = \frac{p_{nm}\sigma_{nm}(\mathbf{n}, 0) + p^+_m [\sigma^+_m(\mathbf{n}) - \sigma^-_m(\mathbf{n})]}{\sigma_{nm}(\mathbf{n}, 0) + \sigma^+_m(\mathbf{n}) + \sigma^-_m(\mathbf{n})} . \qquad (10.11)$$

Thus from the last relations it follows that initially unpolarized neutrons, when scattered in a ferromagnet in direction $\mathbf{n}$, become polarized, and the polarization vector (10.13) consists of two components. One of these (p_{nm}) is due to interference of the nuclear and the elastic magnetic scattering: the corresponding polarization is directed along the vector $\mathbf{M} = \mathbf{m} - (\mathbf{e}\cdot\mathbf{m})\mathbf{e}$. The other component, which appears because of inelastic magnetic scattering is directed along the vector $\mathbf{e}$. The components are perpendicular to one another so that they are easily separated. Thus, magnetizing a crystal perpendicular to the scattering vector $\mathbf{e}$, we separate out the part of the polarization due to interference of nuclear and

magnetic scattering. Magnetizing the crystal along the vector e, we get the part of the vector p due to inelastic magnetic scattering. This permits us to separate the inelastic magnetic scattering from the elastic.

2. Antiferromagnet. In the scattering of unpolarized neutrons by an antiferromagnet, polarization obviously cannot occur. This is related again to the fact that an antiferromagnet is not characterized by any pseudovector along which the polarization of the scattered neutrons could be directed. Nevertheless, in the scattering of polarized neutrons by an antiferromagnet one can have a rotation of the polarization vector. Just as in the case of a ferromagnet, we shall write the polarization vector of the neutrons scattered in a given direction as the result of various scattering processes.

For incoherent nuclear scattering, the polarization is proportional to the polarization of the incident beam

$$p_{incoh} = \alpha p_0, \qquad (10.12)$$

where the coefficient $\alpha \leq 1$ has a quite complicated form and can be calculated individually for each specific case.

For coherent nuclear scattering the polarization does not change. The polarization vector due to scattering without change in the magnetic state of the scatterer (elastic magnetic scattering) has the form [44]

$$p_{m0} = \frac{2(Mp_0)M}{M^2} - p_0, \qquad (10.13)$$

where $M = m - (e \cdot m)e$, and m is the direction of the magnetization vector of either sublattice. This formula describes in particular the polarization of neutrons scattered in the directions of the three Bragg peaks due to magnetic scattering which do not coincide with the nuclear Bragg peaks, since in these directions we can neglect all scattering processes except for the magnetic elastic scattering. It is not difficult to see that in absolute value the vector p_{m0} is equal to p_0. Breaking up the vector p_{m0} into two components, parallel and perpendicular to the vector M, and substituting this expansion in (10.13), one can verify that the vector p_{m0} is obtained from the vector p_0 by a rotation through $180°$ around the direction of m.

Thus, if p_0 is parallel to M, then as a result of magnetic reflection the polarization is unchanged, and this result is obviously valid for any Bragg peak. If, however, p_0 is perpendicular to M, then for magnetic Bragg peaks which do not coincide with nuclear peaks, the polarization is equal to

$$p = \frac{\sigma_n - \sigma_m}{\sigma_n + \sigma_m} p_0, \qquad (10.14)$$

where σ_n and σ_m are the cross sections for nuclear and magnetic scattering into the direction of the Bragg peak.

Now we write the polarization vector for inelastic magnetic scattering [44]

$$p_{mi} = 2 \frac{M_x(M_x p_0) + M_y(M_y p_0)}{M_x^2 + M_y^2} - p_0. \qquad (10.15)$$

This expression can be rewritten in invariant form

$$p_{mi} = 2 \frac{p_{0\perp} - e_\perp(p_0 \cdot e) + e(e \cdot m)(M \cdot p_0)}{1 + (e \cdot m)^2} - p_0, \qquad (10.16)$$

where $p_{0\perp}$ and $e_\perp$ are the components of the vectors p_0 and e perpendicular to the vector m. Thus, for example, $p_\perp = p - (p \cdot m)m$.

Now using (10.12), (10.13) and (10.15), we can write the average polarization of the neutrons scattered in a given direction in the form

$$p = \frac{\alpha \sigma_n(n) p_0 + \sigma_{m0}(n) p_{m0} + \sigma_{mi}(n) p_{mi}}{\sigma_n(n) + \sigma_{m0}(n) + \sigma_{mi}(n)}. \qquad (10.17)$$

Here $\sigma_n(n)$ is the cross section for nuclear scattering in the direction n, $\sigma_{m0}(n)$ is the cross section for magnetic scattering in which the number of spin waves does not change, and finally $\sigma_{mi}(n)$ is the cross section for scattering in which the total number of spin waves changes by unity. Obviously formula (10.17) allows one to determine α, $\sigma_{m0}(n)$ and $\sigma_{mi}(n)$, if one knows the polarization p and the total cross section for scattering in the given direction:

$$\sigma(n) = \sigma_n(n) + \sigma_{m0}(n) + \sigma_{mi}(n).$$

We note that in similar fashion one can treat the effects of polarization in scattering of neutrons in crystals with more complex magnetic structure, such as ferri- and antiferromagnets, weak ferromagnets with non-collinear sublattices, etc.

Particularly interesting effects associated with polarization of the neutrons should appear in crystals with helicoidal magnetic structure.[47,48]

[1] A. I. Akhiezer and I. Ya. Pomeranchuk, Nekotorye Voprosy Teorii Yadra (Some Problems of Nuclear Theory), Moscow, Gostekhizdat, 1950.

[2] G. E. Bacon, Neutron Diffraction, Oxford University Press, 1954.

[3] R. P. Ozerov, UFN 45, 481 (1951), 47, 445 (1952).

[4] C. G. Shull and E. O. Wollan, Solid State Physics 2, 138 (1956).

[5] L. Van Hove, Phys. Rev. 95, 249 (1954).

[6] L. Van Hove, Phys. Rev. 95, 1374 (1954).

[7] Y. Toyazawa, Progr. Theoret. Phys. (Kyoto) 20, 53 (1958); Yu. A. Izyumov, FMM 11, 801 (1961).

[8] L. Landau and E. Lifshitz, Quantum Mechanics, Addison-Wesley, 1958.

[9] E. Condon and G. Shortley, Theory of Atomic Spectra, Cambridge University Press, 1935.

[10] O. Halpern and M. H. Johnson, Phys. Rev. 55, 898 (1939).

[11] G. T. Trammell, Phys. Rev. 92, 1387 (1953).

[12] P. Debye, Ann. Physik 43, 49 (1914); I. Waller, Z. Physik 17, 398 (1923).

[13] M. A. Krivoglaz and A. A. Smirnov, Teoriya Uporyadochivayushchikhsya Splavov (Theory of Ordered Alloys) Moscow, Gostekhizdat, 1958.

[14] S. V. Maleev, Doctoral Dissertation, Leningrad, 1958.

[15] Yu. Kagan and V. A. Maslov, JETP 41, 1296 (1961); Soviet Phys. JETP 14, 922 (1962); Yu. Kagan, JETP 41, 659 (1961), Soviet Phys. JETP 14, 472 (1962).

[16] V. G. Bar'yakhtar and S. V. Maleev, JETP 39, 1430 (1960), Soviet Phys. JETP 12, 995 (1961).

[17] S. V. Maleev, JETP 33, 1010 (1957), Soviet Phys. JETP 6, 776 (1958).

[18] A. Sjölander, Arkiv. Fysik 14, 315 (1958).

[19] G. Placzek and L. Van Hove, Phys. Rev. 93, 1207 (1954).

[20] V. S. Oskot-skiĭ, FTT 2, 701 (1960), Soviet Phys. Solid State 2, 647 (1960).

[21] Yu. Kagan, JETP 40, 312 (1961), Soviet Phys. JETP 13, 211 (1961).

[22] L. Van Hove, Phys. Rev. 89, 1189 (1953).

[23] Yu. Kagan, JETP 42, 1375 (1962), Soviet Phys. JETP 15, 954 (1962).

[24] T. Holstein and H. Primakoff, Phys. Rev. 58, 1098 (1940).

[25] S. V. Maleev, JETP 34, 1518 (1958), Soviet Phys. JETP 7, 1048 (1958).

[26] N. N. Bogolyubov and S. V. Tyablikov, DAN 126, 53 (1959), Soviet Phys. Doklady 4, 604 (1959).

[27] V. N. Kashcheev and M. A. Krivoglaz, FTT 3, 1541 (1961), Soviet Phys. Solid State 3, 1117 (1961).

[28] Yu. A. Izyumov, FMM 12, 480 (1961).

[29] M. A. Krivoglaz, JETP 40, 567 (1961), Soviet Phys. JETP 13, 397 (1961); V. N. Kashcheev and M. A. Krivoglaz, FTT 3, 1528 (1961), Soviet Phys. Solid State 3, 1107 (1961); M. A. Krivoglaz, FTT 3, 2761 (1961), Soviet Phys. Solid State 3, 2015 (1961).

[30] G. Baym, Phys. Rev. 121, 741 (1961).

[31] R. J. Elliott and R. D. Lowde, Proc. Roy. Soc. (London) A230, 46 (1955).

[32] H. Palevsky and D. J. Hughes, Phys. Rev. 92, 202 (1953); G. L. Squires, Proc. Phys. Soc. (London), A67, 248 (1954); M. K. Wilkinson and C. G. Shull, Phys. Rev. 103, 516 (1956); R. D. Lowde, Proc. Roy. Soc. (London), A235, 305 (1956); R. D. Lowde, Revs. Modern Phys. 30, 69 (1956); M. Ericson and B. Jacrot, J. Phys. Chem. Solids, 13, 235 (1960).

[33] A. W. McReynolds and T. Riste, Bull. Am. Phys. Soc. 1, 133 (1956); T. Riste, Congres de magnetisme, Grenoble, 1958; A. W. McReynolds and T. Riste, Phys. Rev. 95, 1161 (1954); Riste, Blinowski, and Janik, J. Phys. Chem. Solids 9, 153 (1959).

[34] M. A. Krivoglaz, DAN 118, 51 (1958), Soviet Phys.

Doklady 3, 61 (1958).

[35] P. G. de Gennes and J. Villain, J. Phys. Chem. Solids 13, 10 (1960).

[36] T. Riste, J. Phys. Chem. Solids, 17, 308 (1961).

[37] T. Riste and A. Wanic, J. Phys. Chem. Solids 17, 318 (1961).

[38] P. G. de Gennes, J. Phys. Chem. Solids 6, 43 (1958).

[39] R. J. Elliott and W. Marshall, Revs. Modern Phys. 30, 75 (1958).

[40] U. Firgau, Ann. Physik, 40, 295 (1941).

[41] R. A. Tahir-Kheli and D. ter Haar, Phys. Rev. 127, 88 (1962).

[42] Riste, Blinowski, and Janik, J. Phys. Chem. Solids 9, 153 (1959).

[43] A. W. Saenz, Phys. Rev. 119, 1542 (1960).

[44] Yu. A. Izyumov and S. V. Maleev, JETP 41, 1644 (1961), Soviet Phys. JETP 14, 1168 (1962).

[45] S. V. Maleev, JETP 40, 1224 (1961), Soviet Phys. JETP 13, 860 (1961).

[46] G. S. Zhdanov and R. P. Ozerov, UFN 76, 239 (1962), Soviet Phys. Uspekhi 5, 104 (1962).

[47] Yu. A. Izyumov, JETP 42, 1673 (1962), Soviet Phys. JETP 15, 1162 (1962).

[48] Maleev, Bar'yakhtar, and Suris, FTT (in press).

[49] R. Ericksson, unpublished, cf. [50].

[50] A. Yoshimore, J. Phys. Soc. Japan 14, 807 (1959).

[51] W. C. Koehler, Acta Cryst. 14, 535 (1961).

[52] T. A. Kaplan, Phys. Rev. 119, 1460 (1960).

[53] K. Yosida and H. Miwa, J. Appl. Phys., 32S, 8 (1961).

[54] B. N. Brockhouse, J. Appl. Phys. Suppl. 33 (1) (1962). Inelastic Scattering of Neutrons in Solids and Liquids, I.A.E.A., Vienna, 1961.

[55] B. N. Brockhouse, Phys. Rev. 106, 859 (1957); 111, 1273 (1958).

[56] R. D. Lowde and N. Umakantha, Phys. Rev. Letters 4, 452 (1960).

[57] R. N. Sinclair and B. N. Brockhouse, Phys. Rev. 120, 1638 (1960).

[58] Murasik, Ruta-Wala, and Wanic, Physica 27, 883 (1961).

[59] B. N. Brockhouse and H. Watanabe, Conference on Inelastic Scattering of Neutrons in Solids and Liquids, Chalk River, 1962.

[60] H. Mori and K. Kawasaki, Progr. Theoret. Phys. (Kyoto) 27, 529 (1962).

[61] Yu. A. Izyumov, FTT 5, 717 (1963), Soviet Phys. Solid State (in press).

Translated by M. Hamermesh