NEUTRON DIFFRACTION IN A POLARIZED CRYSTAL

V. G. BARYSHEVSKIĬ

Belorussian State University

Submitted to JETP editor June 17, 1966

J. Exptl. Theoret. Phys. (U.S.S.R.) 51, 1587–1591 (November, 1966)

The paper is devoted to the diffraction of slow polarized neutrons in a crystal with polarized nuclei. Owing to the energy difference between the state of a neutron with its spin directed along the target polarization and opposite to it, it is possible to obtain by means of an alternating magnetic field a resonance reorientation of the neutron spin. Several resonance frequencies are thus obtained, in contrast to the case when there are no diffracted waves in the crystal.

IT has been shown previously that the spin of a neutron wave passing through a target with polarized nuclei should precess.[1] The frequency of this precession is determined by the difference of the indices of refraction Δn of the neutron wave in the state with the spin directed along the polarization of the nuclei and in the state with the spin directed opposite to the polarization of the nuclei. The existence of two indices of refraction leads to the circumstance that for a given wavelength an energy difference ΔE^0 appears between these states of a neutron in the target. The energy difference is given by the expression

$$\Delta E^0 = \hbar k v \Delta n, \tag{1}$$

where k is the wave number of the neutron, and v its velocity. Therefore, if a magnetic field rotating about the direction of polarization is set up in the polarized target, then transitions will occur, in analogy with paramagnetic resonance, between the different states of polarization of the neutron at the frequency of the rotating field, $\Delta E^0/\hbar$.[1]

It is well known that when the Bragg conditions are fulfilled there appear in the crystal, in addition to the transmitted coherent wave, several coherent waves.[2,3] The magnitudes of the amplitudes and of the wave vectors of all the waves depend on the initial conditions, i.e., on the angle of incidence of the beam and on the orientation of the surface of the crystal relative to the crystallographic planes. The presence of a complex wave field leads to the circumstance that in this region one cannot, generally speaking, ascribe to the crystal a definite index of refraction.[2] The phenomenon of the precession of the neutron spin in a polarized target when the Bragg conditions are close to being fulfilled requires therefore additional consideration.

Let a flux of slow, polarized neutrons be incident on a crystal consisting of identical nuclei with a polarization vector **p**. The amplitude of the coherent scattering will then be of the form

$$a = \alpha + \beta \boldsymbol{\sigma} \mathbf{p}, \tag{2}$$

where $\boldsymbol{\sigma}$ is a vector composed of Pauli matrices.

It follows from [4] that the coherent neutron wave in the crystal is described by the following expression:[1)]

$$\psi(\mathbf{r}) = \begin{pmatrix} \psi_+(\mathbf{r}) \\ \psi_-(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} c_+ \\ c_- \end{pmatrix} e^{i\mathbf{kr}} + \sum_m \begin{pmatrix} c_+ A_m^+ \\ c_- A_m^- \end{pmatrix} \frac{\exp(ik|\mathbf{r}-\mathbf{R}_m|)}{|\mathbf{r}-\mathbf{R}_m|}, \tag{3}$$

where $\mathbf{R}_m$ is the radius vector of the m-th nucleus and $\begin{pmatrix} c_+ \\ c_- \end{pmatrix}$ is a wave function which describes the initial spin state of the neutron. The $A_m^\pm$ satisfy a system of equations of the form

$$A_m^\pm = (\alpha \pm \beta p) e^{i\mathbf{kR}_m} + (\alpha \pm \beta p) \sum_{k \neq i} A_k^\pm \frac{\exp[ik|\mathbf{R}_i - \mathbf{R}_k|]}{|\mathbf{R}_i - \mathbf{R}_k|} \tag{4}$$

and denote the effective scattering amplitudes of a neutron polarized along and opposite to the polarization of the nuclei respectively.

Relations (3) and (4) show that two coherent neutron waves propagate in a polarized crystal: with spin directed opposite to the polarization of the nuclei $\psi_-(\mathbf{r})$, and with spin directed along the polarization of the nuclei $\psi_+(\mathbf{r})$. If the target polar-

[1)]We choose the direction of the axis of quantization and of the z axis of the coordinate system along the polarization vector of the nuclei.

ization p is zero, then there is a single wave. It follows also from (3) and (4) that the equations which describe the propagation of each coherent wave are of the same form as the system of equations which describe the transmission of a coherent wave through an unpolarized target. In analyzing (3) and (4) one can, therefore, make use of the theory developed for the description of neutron diffraction in a crystal with unpolarized nuclei.[6, 7]

As was shown in [6] (see also [8]), if we seek a neutron wave $\varphi(\mathbf{r})$ of the form

$$\varphi(\mathbf{r}) = \chi(\mathbf{r}) e^{i\varkappa\mathbf{r}}, \tag{5}$$

where $\chi(\mathbf{r})$ is a periodic function in the crystal, then we obtain the following relation for $\boldsymbol{\kappa}$:

$$\lim_{\mathbf{r}\to\mathbf{r}_p} \left\{-\frac{4\pi}{V}\sum_{\tau}\frac{e^{i\varkappa\mathbf{r}}}{k^2-(\varkappa+\tau)^2}-\frac{1}{|\mathbf{r}-\mathbf{r}_p|}\right\}=\frac{1+ika}{a}. \tag{6}$$

In this expression $\boldsymbol{\tau}$ is a reciprocal lattice vector, and V the volume of a unit cell.

In our case we can thus seek for the coherent waves in the crystal an expression of the form

$$\psi_\pm(\mathbf{r}) = \chi_\pm(\mathbf{r}) e^{i\varkappa_\pm\mathbf{r}}. \tag{7}$$

The wave vectors $\boldsymbol{\kappa}_\pm$ satisfy then a relation analogous to (5) with the substitution of $(\alpha \pm \beta p)$ for α.

Assume now that a Bragg reflection is possible. For simplicity we consider the case when two reciprocal lattice points ($\boldsymbol{\tau} = 0$ and $\boldsymbol{\tau} = \boldsymbol{\tau}_1$) lie close to the sphere of reflection. This means that the values of $\boldsymbol{\kappa}_\pm$ and $|\boldsymbol{\kappa}_\pm + \boldsymbol{\tau}_1|$ are close to the value of the wave vector k of the neutron outside the crystal. It follows hence[6] that in an equation of the type (5) the main contribution is due to the two corresponding terms of the sum, i.e., one can write approximately

$$\frac{4\pi}{V}\left(\frac{1}{\varkappa_\pm^2-k^2}+\frac{1}{(\varkappa_\pm+\tau_1)^2-k^2}\right)=\frac{1+ik(\alpha\pm\beta p)}{\alpha\pm\beta p}. \tag{8}$$

Let us set

$$\varkappa_\pm = k(1+\varepsilon_0^\pm), \qquad |\varkappa_\pm+\tau_1| = k(1+\varepsilon_1^\pm). \tag{9}$$

Then, accurate to terms quadratic in ϵ, Eq. (8) can be presented in the form

$$1/\varepsilon_0^\pm + 1/\varepsilon_1^\pm = \Omega_\pm, \tag{10}$$

where

$$\Omega_\pm = \frac{k^2V}{2\pi}\frac{1+ik(\alpha\pm\beta p)}{\alpha\pm\beta p}.$$

If we introduce the quantities

$$\xi_0^\pm = k(1+\varepsilon_0^\pm) - k(1+1/\Omega_\pm) = k(\varepsilon_0^\pm - 1/\Omega_\pm),$$

$$\xi_1^\pm = k(1+\varepsilon_1^\pm) - k(1+1/\Omega_\pm) = k(\varepsilon_1^\pm - 1/\Omega_\pm), \tag{11}$$

then the dispersion equation (10) can be written in the form

$$\xi_0^\pm\xi_1^\pm = k^2\Omega_\pm. \tag{12}$$

Equations (12) are equations of parabolas analogous to the equation obtained from the dynamical theory of x-ray diffraction[2)].[2, 3] In particular, it follows from (12) that the two systems of parabolas whose vertices lie on a straight line located in the reflecting crystallographic plane correspond to the two states of polarization of the neutron. Four values of $\xi_0^\pm = \xi_1^\pm$, equal to $k/\Omega_\pm$ and $-k/\Omega_\pm$ correspond to these four vertices.

One can readily show that the vertices corresponding to the values $\xi_0^\pm = \xi_1^\pm = -k/\Omega_\pm$ coincide. The wave vectors of the waves at that point of the dispersion surface are equal to k, and consequently these vertices coincide with the Laue point L.

Let us now return to the problem of the coherent wave in the crystal. As is well known,[2, 3] the center of propagation of the waves should lie on the intersection of the normal to the surface of the crystal upon which the wave is incident, and the dispersion surface. It follows hence, for example, that when the surface of the crystal is perpendicular to the reflecting plane the normal to the surface of the crystal will, generally speaking, intersect all four branches of the hyperbolas (this situation is analogous to the Laue case in the diffraction of x rays[2, 3]). It is thus possible to excite at a corresponding angle of incidence of the primary beam eight coherent waves (two for each center of propagation). Just as in the case of the transmission of neutrons through an unpolarized target,[6, 7] two coupled, coherent waves of the form

$$\psi_\pm(\mathbf{r}) = B_1^\pm \exp[i\varkappa_\pm\mathbf{r}] + B_2^\pm \exp[i(\varkappa_\pm+\tau_1)\mathbf{r}], \tag{13}$$

correspond to each center of propagation. Hence the amplitudes $B_{1,2}^\pm$ are determined by the location of the center of propagation on the dispersion surface and by the boundary conditions.[6, 7]

The wave vectors of these waves take on the following values:

[2)]In general the right-hand side of (12) is complex. The wave vectors of the waves in the crystal are consequently also complex: $\kappa = \kappa' + i\kappa''$. However, in the case of neutrons the inequality $\kappa''/\kappa' \ll 1$ is fulfilled to an even greater degree than for x rays. If we are not interested in problems connected with the absorption of waves in a crystal, then the imaginary part in the right-hand side of (12) can be neglected. [3] Below we shall consider the dispersion equation and the wave vectors to be real.

$$\varkappa_{\pm} = k\left(1 + \frac{1}{\Omega_{\pm}} + \frac{\xi_0^{\pm}}{k}\right),$$

$$|\varkappa_{\pm} + \tau_1| = k\left(1 + \frac{1}{\Omega_{\pm}} + \frac{\xi_1^{\pm}}{k}\right). \qquad (14)$$

The values of ξ can be both positive and negative. The same sign of ξ_0 and ξ_1 corresponds to a given center of propagation.

Since a neutron wave with spin directed along the polarization of the nuclei has a wave vector κ_+ not equal to the wave vector κ_- of the wave with spin directed opposite to the polarization of the nuclei, there appears in the crystal in accordance with the result of [1] precession of the neutron spin. Precession of the spin will also take place in the wave diffracted at the Bragg angle. It is important to note that as a result of the existence of several centers of propagation lying on various branches of the hyperbolas, the spin of the neutrons precesses, unlike in the case of transmission of neutrons through a polarized crystal without diffraction, with a number of frequencies. In other words, the energy difference ΔE between the two states of neutron polarization in a crystal at a given wavelength can have several values, the value of the difference ΔE depending on the initial conditions. In the case under consideration when four centers of propagation which belong to different branches of hyperbolas are excited we have for waves propagating in the initial direction:

$$\Delta E_1 = \hbar kv\left(\frac{1}{\Omega_+} + \frac{|\xi_0^+|}{k} - \frac{1}{\Omega_-} - \frac{|\xi_0^-|}{k}\right)$$

$$= \Delta E^0 + \hbar v(|\xi_0^+| - |\xi_0^-|),$$

$$\Delta E_2 = \Delta E^0 + \hbar v(|\xi_0^+| + |\xi_0^-|),$$
$$\Delta E_3 = \Delta E^0 - \hbar v(|\xi_0^+| + |\xi_0^-|),$$
$$\Delta E_4 = \Delta E^0 - \hbar v(|\xi_0^+| - |\xi_0^-|). \qquad (15)$$

The energy differences $\Delta E'$ of the diffracted waves can be obtained from the above by replacing ξ_0 by ξ_1.

In the general case ΔE and $\Delta E'$ do not coincide. However, when the boundary conditions are chosen such that $\xi_0 = \xi_1$ (i.e., the centers of propagation are located at the vertices of the hyperbolas) the differences ΔE and $\Delta E'$ become correspondingly equal and take on the following values:

$$\Delta E_1 = 2\Delta E^0, \quad \Delta E_2 = \frac{2\hbar kv}{\Omega_+}, \quad \Delta E_3 = -\frac{2\hbar kv}{\Omega_-},$$

$$\Delta E_4 = 0. \qquad (16)$$

As has already been indicated, the presence of energy differences leads to the possibility of using a rotating magnetic field of the corresponding frequency $\omega = \Delta E/\hbar$ to excite resonance transitions between neutron states with different polarization. For instance, when $\xi_0 = \xi_1$ there are three resonance frequencies. As is seen from (16), they all differ considerably from the energy difference between the two neutron polarization states in the crystal in the absence of diffraction ΔE^0. In the general case the number of resonance frequencies becomes even larger.[3)]

So far we have discussed the case when the centers of propagation located on various branches of the hyperbolas are excited simultaneously. In principle one can choose the initial conditions in such a way that only centers of propagation belonging to any one branch of the hyperbolas are excited (Bragg case[2,3]). Each branch corresponds to a certain definite state of polarization of the neutron (along or opposite to the direction of the polarization vector of the nuclei). It follows from this that, depending on which branch is chosen, waves with spin directed along or opposite to the polarization of the nuclei will also undergo diffraction.

The author expresses his deep gratitude to V. L. Lyuboshitz and M. I. Podgoretskiĭ for useful remarks.

[1] V. G. Baryshevskiĭ and M. I. Podgoretskiĭ, JETP **47**, 1050 (1964), Soviet Phys. JETP **20**, 704 (1965).

[2] R. W. James, Optical Principles of the Diffraction of X-rays, Russian transl. IIL, 1950.

[3] B. Batterman and H. Cole, Rev. Modern Phys. **36**, 681 (1964).

[4] V. G. Baryshevskiĭ, V. L. Lyuboshitz, and M. I. Podgoretskiĭ, JINR Preprint R-2111, 1965.

[5] V. G. Baryshevskiĭ, V. L. Lyuboshitz, and M. I. Podgoretskiĭ, JINR Preprint R-2230, 1965.

[6] M. Goldberger and F. Seitz, Phys. Rev. **71**, 294 (1947).

[7] Yu. Kagan and A. M. Afanas'ev, JETP **49**, 1504 (1965), Soviet Phys. JETP **22**, 1032 (1966).

[8] Yu. Kagan and A. M. Afanas'ev, JETP **50**, 271 (1966), Soviet Phys. JETP **23**, 178 (1966).

Translated by Z. Barnea
191

[3)] The conclusion concerning the existence of several frequencies of the precession of the spin is in principle also valid for neutrons diffracted by a magnetic lattice with polarized atoms.