Specular reflection of neutrons from targets with polarized nuclei

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(Submitted October 3, 1975)

Zh. Eksp. Teor. Fiz. **70**, 430–434 (February 1976)

An analysis is made of the specular reflection of neutrons from targets with polarized nuclei. It is found that a crystalline polarized target can have several critical reflection angles. It is shown that the specular reflection of neutrons from targets with polarized nuclei can be used in studies of the spin components of the amplitudes of neutron scattering by nuclei.

PACS numbers: 25.40.−h, 24.70.+s

Investigations of the spin-dependent part of the amplitude of the scattering of a neutron by a nucleus give information on the nature of the interaction of neutrons with nuclei (for example, of the properties of levels of complex nuclei).

Unfortunately, information on the spin parts of the scattering amplitudes is not available for the majority of the nuclei because it is not sufficient to measure the total and coherent neutron cross sections to find these parts. A direct method for the determination of the spin parts of the scattering amplitudes involves the use of polarized neutron beams and polarized targets.[1] In this connection one should mention particularly the methods based on the refraction and diffraction of neutrons in polarized nuclear targets[2–7] which can improve the sensitivity of the experiments carried out on polarized neutrons and nuclei.

The present paper is concerned with some aspects of the specular reflection of neutrons from polarized targets.

Specular reflection is one of the main methods for the determination of the amplitude of the coherent scattering of neutrons by nuclei.[8] The critical glancing angle θ, at which a neutron beam is totally reflected, is governed by the refractive index of the target n, i.e., by the amplitude of the elastic coherent scattering through zero angle $f(0)$. If the target nuclei are polarized, the scattering amplitude of a neutron with a spin parallel to the polarization vector of the nuclei, $f_+(0)$, is not equal to the scattering amplitude of a neutron with the opposite spin direction, $f_-(0)$. Consequently, the specular reflection from a polarized target is governed by two refractive indices $n_\pm$ and is generally characterized by two critical glancing angles $\theta_\pm$,[9] which may be used in measuring the spin-dependent part of the amplitude of the elastic coherent scattering of a neutron by a nucleus.

Since the critical glancing angle θ is governed by the amplitude $f(0)$, it follows that (see, for example,[8]) the specular reflection of neutrons is independent of the aggregate state of the target (with the exception of the scattering in the presence of very narrow resonances[10]).

On the other hand, it is clear from physical considerations that a wave reflected specularly from a planar boundary of a target becomes a coherent superposition of waves scattered by nuclei in the direction θ. If this wave is reflected from a crystal surface, a consequence of the periodic distribution of the nuclei is that a coherent wave scattered under diffraction conditions may be propagated not only near zero scattering angle but also near angles governed by the Bragg condition. Consequently, in contrast to the specular reflection by an amorphous boundary, the tangential component of the wave vector of the reflected wave $\mathbf{k}'_{t0}$ may differ from the tangential component of the wave vector of the incident wave $\mathbf{k}'_{t0}$, i.e., $\mathbf{k}'_{t0}=\mathbf{k}_{t0}+2\pi\boldsymbol{\tau}_t$, where $2\pi\boldsymbol{\tau}_t$ is the component of the reciprocal lattice vector of the crystal parallel to its surface. Consequently, a superposition of two plane waves with momenta $\mathbf{k}_{t0}$ and $\mathbf{k}_{t0}+2\pi\boldsymbol{\tau}_t$ travels along the surface of a crystal "mirror" and this alters the nature of the interaction of the waves with the mirror. For example, we shall show later that in the case of two-wave diffraction by a crystalline mirror with unpolarized nuclei there are two critical reflection angles, whereas in the case of a mirror with polarized nuclei, the number of such critical angles reaches four.

We shall first consider this phenomenon in the case of reflection of neutrons from a target with unpolarized nuclei.

Following the above treatment, a neutron wave outside the mirror surface can be described by

$$\psi_I(\mathbf{r})=\exp\{i(\mathbf{k}_{t0}\mathbf{r}_\perp+k_{0z}z)\}+A\exp\{i(\mathbf{k}_{t0}\mathbf{r}_\perp-k_{0z}z)\}+B\exp\{i(\mathbf{k}_{t0}'\mathbf{r}_\perp-k_{z0}'z)\}, \tag{1}$$

where the z axis of the coordinate system is directed into the target, the target occupies the half-space $z>0$, and $\mathbf{k}'_{z0}$ is given by $\mathbf{k}'_{z0}=(\mathbf{k}_0^2-\mathbf{k}'^2_{t0})^{1/2}$, which follows from the constancy of energy under elastic scattering conditions.

Inside the crystal target the neutron wave is a superposition of Bloch waves satisfying, in the two-wave approximation, the usual system of dynamic equations[11,12]:

$$(k_0^2-u_{00}-k^2)\varphi(\mathbf{k})-u_{01}\varphi(\mathbf{k}+2\pi\boldsymbol{\tau})=0,$$
$$-u_{10}\varphi(\mathbf{k})+[k_0^2-u_{11}-(\mathbf{k}+2\pi\boldsymbol{\tau})^2]\varphi(\mathbf{k}+2\pi\boldsymbol{\tau})=0, \tag{2}$$

where the quantities $u_{\alpha\beta}=u(\mathbf{k}^\alpha,\mathbf{k}^\beta)$ ($\alpha,\beta=0,\ 1;\ \mathbf{k}^0=\mathbf{k}$, $\mathbf{k}^1=\mathbf{k}+2\pi\boldsymbol{\tau}$) are of the form

$$u_{\alpha\beta}=-\frac{4\pi}{\Omega}\sum_j f_j(\mathbf{k}^\alpha,\mathbf{k}^\beta)\exp\{i(\mathbf{k}^\alpha-\mathbf{k}^\beta)\boldsymbol{\rho}_j\};$$

f_j is the amplitude of the coherent scattering by a j-th nucleus in a unit cell (the contribution to the total cross section due to the elastic coherent scattering is excluded from the imaginary part f_j), Ω is the volume of a unit cell, k is the wave number of the wave in the target, ρ_j is the coordinate of a j-th nucleus in a unit cell, and summation is carried out over all the nuclei in a unit cell.

The condition of solvability of the system (2) subject to the equality of the tangential components of the wave vectors $\mathbf{k}_0$ and $\mathbf{k}$ leads to the following expression for the z component of the wave vector of a neutron in a target when the vector $\boldsymbol{\tau}$ is parallel to the target surface:

$$k_{z1(2)}=\left\{k_{0z}^2-\frac{u_{00}+u_{11}+k_{t0}^2\alpha}{2}\pm\frac{1}{2}\left[(u_{00}-u_{11}-k_{t0}^2\alpha)^2+4u_{01}u_{10}\right]^{1/2}\right\}^{1/2},$$
$$\alpha=(2\mathbf{k}_{t0}+2\pi\boldsymbol{\tau})\cdot 2\pi\boldsymbol{\tau}/k_{t0}^2. \qquad (3)$$

The general solution describing a wave traveling into a crystal can be expressed in the form

$$\psi_{II}(\mathbf{r})=\varphi(\mathbf{k}_1)\exp\{i\mathbf{k}_{0t}\mathbf{r}_\perp+ik_{1z}z\}+\varphi(\mathbf{k}_1+2\pi\boldsymbol{\tau})\exp\{i\mathbf{k}_{0t}'\mathbf{r}_\perp+ik_{1z}z\}$$
$$+\varphi(\mathbf{k}_2)\exp\{i\mathbf{k}_{0t}\mathbf{r}_\perp+ik_{2z}z\}+\varphi(\mathbf{k}_2+2\pi\boldsymbol{\tau})\exp\{i\mathbf{k}_{0t}'\mathbf{r}_\perp+ik_{2z}z\}. \qquad (4)$$

Applying the condition of continuity of the wave at the boundary, we obtain

$$1+A=\varphi(\mathbf{k}_1)+\varphi(\mathbf{k}_2),\qquad B=\varphi(\mathbf{k}_1+2\pi\boldsymbol{\tau})+\varphi(\mathbf{k}_2+2\pi\boldsymbol{\tau}),$$
$$k_{0z}-k_{0z}A=k_{1z}\varphi(\mathbf{k}_1)+k_{2z}\varphi(\mathbf{k}_2),\qquad -k_{z0}'B=k_{1z}\varphi(\mathbf{k}_1+2\pi\boldsymbol{\tau})+k_{2z}\varphi(\mathbf{k}_2+2\pi\boldsymbol{\tau}). \qquad (5)$$

Solving the system (5) subject to the relationship between $\varphi(\mathbf{k})$ and $\varphi(\mathbf{k}+2\pi\boldsymbol{\tau})$ which follows from Eq. (2), we find the amplitude of the specularly reflected wave A and of the wave B diffracted in the plane of the mirror:

$$A=\frac{(k_{1z}-k_{0z})(k_{z0}'+k_{2z})c_2-(k_{2z}-k_{0z})(k_{0z}'+k_{1z})c_1}{(k_{0z}+k_{2z})(k_{z0}'+k_{1z})c_1-(k_{0z}+k_{1z})(k_{0z}'+k_{2z})c_2}, \qquad (6)$$

$$B=\frac{2(k_{1z}-k_{2z})k_{0z}c_1c_2}{(k_{0z}+k_{2z})(k_{0z}'+k_{1z})c_1-(k_{0z}+k_{1z})(k_{0z}'+k_{2z})c_2}, \qquad (7)$$

$$c_{1(2)}=-\frac{2u_{10}}{u_{11}+k_{0t}^2\alpha-u_{00}\pm[(u_{11}+k_{0t}^2\alpha-u_{00})^2+4u_{01}u_{10}]^{1/2}}. \qquad (8)$$

We shall now make allowance for the fact that, with the exception of very rare cases of very narrow neutron resonances of width less than the characteristic phonon frequencies, the forward scattering amplitude of a neutron interacting with a nucleus is independent of the structure of a crystal.[8] Consequently, $u_{00}=u_{11}$. If the Bragg conditions are satisfied exactly ($\alpha=0$) and $u_{01}=u_{10}$, then

$$A=-\frac{1}{2}\left(\frac{k_{1z}-k_{0z}}{k_{1z}+k_{0z}}+\frac{k_{2z}-k_{0z}}{k_{2z}+k_{0z}}\right),$$
$$B=\frac{(k_{1z}-k_{2z})k_{0z}}{(k_{1z}+k_{0z})(k_{2z}+k_{0z})}. \qquad (9)$$

According to Eq. (9) the amplitude of the specularly reflected wave A can be represented as a superposition of the amplitudes describing the specular reflection from a substance with refractive indices $n_1=k_{1z}/k_{0z}$ and $n_2=k_{2z}/k_{0z}$. Consequently, there are two reflection thresholds ($k_{1z}=0$ and $k_{2z}=0$), i.e., there are two glancing angles at which the intensity of the reflected wave changes abruptly. When the glancing angle is reduced, i.e., in the limit $k_{0z}\to 0$, the values of $k_{1(2)z}$ given by Eq. (3) generally tend to a constant different from zero. It then follows from Eqs. (6) and (7) that in the limit $k_{0z}\to 0$ the amplitude A approaches -1 whereas the amplitude B exhibits two peaks and tends to zero. However, in the special case of a rigid lattice, when $u_{00}=u_{11}=u_{01}=u_{10}$, and for exact fulfillment of the Bragg conditions, the values of A and B tend to $-1/2$. Then, without allowance for the diffraction the reflection threshold is given by $k_{0z}^2=u_{00}$, whereas in the presence of diffraction the threshold condition is $k_{0z}^2=2u_{00}$, i.e., in the latter case the critical angle rises by a factor of $\sqrt{2}$ compared with the former case.

The appearance of two reflection thresholds is due to the fact that, under diffraction conditions, superposition of two plane waves gives rise to a standing wave whose nodes are located at the nuclei or between them. Consequently, there is a corresponding change in the energy of the interaction of the neutron wave with the crystal. Since the reflection occurs whenever the kinetic energy of a particle corresponding to the normal (relative to the surface of the crystal) velocity component becomes less than the potential energy of the interaction with the crystal, the change in this energy under diffraction conditions affects the critical angle.

We shall now analyze the total reflection from a target with polarized nuclei. Since, in general, electrons can also be polarized, we shall allow for the magnetic $n-e$ interaction. In this case the reflection from a target can be analyzed if the quantities ψ and φ occurring in Eqs. (1) and (2) are understood to be spinors and if allowance is made for the fact that f_j depends on the neutron spin:

$$\hat f_j(\mathbf{k}^\alpha,\mathbf{k}^\beta)=\hat f_{j\,\mathrm{nucl}}(\mathbf{k}^\alpha,\mathbf{k}^\beta)+\hat f_{j\,\mathrm{magn}}(\mathbf{k}^\alpha,\mathbf{k}^\beta)=(\alpha_j+\beta_j\boldsymbol{\sigma}\mathbf{p}_j)\exp\{-w(\mathbf{k}^\alpha-\mathbf{k}^\beta)\}$$
$$-4\pi\mu_n\left[\frac{(\boldsymbol{\sigma}(\mathbf{k}^\alpha-\mathbf{k}^\beta))((\mathbf{k}^\alpha-\mathbf{k}^\beta)\boldsymbol{\mu}_j)}{(\mathbf{k}^\alpha-\mathbf{k}^\beta)^2}-\boldsymbol{\sigma}\boldsymbol{\mu}_j\right]F_j(\mathbf{k}^\alpha-\mathbf{k}^\beta)\exp\{-w(\mathbf{k}^\alpha-\mathbf{k}^\beta)\}, \qquad (10)$$

where $\mathbf{p}_j$ is the polarization vector of a j-th nucleus in a unit cell, $\exp[-w(\mathbf{k}^\alpha-\mathbf{k}^\beta)]$ is the Debye–Waller factor, μ_n is the magnetic moment of a neutron, μ_j is the magnetic moment of a j-th atom in a unit cell, and $F_j(\mathbf{k}^\alpha-\mathbf{k}^\beta)$ is the atomic form factor.

All possible special cases (for example, polarized electrons and unpolarized nuclei and vice versa) are obtained from Eq. (10).

It should be noted that $\hat f_{j\mathrm{magn}}$ is not single-valued when $\mathbf{k}^\alpha-\mathbf{k}^\beta\to 0$. The multivalued nature of this function is due to the long range of the magnetic dipole–dipole interaction. An appropriate analysis shows that the magnetic contribution to u_{00} can be expressed in terms of the macroscopic magnetic field and it is of the form

$$\hat u_{00\mathrm{magn}}=-(2m\mu_n/\hbar^2)\boldsymbol{\sigma}\mathbf{B}. \qquad (11)$$

In subsequent analysis we must draw attention to the fact that the operator system of equations obtained in this way simplifies considerably in the following important cases.

1. Only the nuclei are polarized and their spins are collinear. In this case the selection of the quantization axis along the polarization vector splits the operator system into two independent systems of equations for the two components of the neutron spin, one of which is parallel (φ_+) and the other antiparallel (φ_-) to the quantization axis.

2. The electron spins are also ordered but neutrons are diffracted by a system of planes satisfying the condition $\tau \perp \mu_j$, where **p**, μ, and **B** are collinear.

3. The splitting of the operator system into equations for the components φ_+ and φ_- occurs also for $\boldsymbol{\tau} \parallel \boldsymbol{\mu}_j$ and collinear **p** and **B**. It follows from Eq. (10) that in this case the magnetic contribution to $u_{01(10)}$ is generally equal to zero.

We shall assume that the conditions 1, 2, or 3 are satisfied.

We shall investigate next the specific case of specular reflection by a target with spins parallel to the surface. As pointed out earlier, in cases 1–3 the system of the operator equations separates into two independent systems of equations for $\varphi_\pm$. These quantities satisfy an equation such as Eq. (2) subject to the replacement of $f_j(\mathbf{k}^\alpha, \mathbf{k}^\beta)$ by

$$f_{j\pm}(\mathbf{k}^\alpha, \mathbf{k}^\beta) = (\alpha_j \pm \beta_j p_j) \exp[-w_j(\mathbf{k}^\alpha - \mathbf{k}^\beta)]$$

in case 1 and by

$$f_{j\pm}(\mathbf{k}^\alpha, \mathbf{k}^\beta) = (\alpha_j \pm \beta_j p_j) \exp[-w_j(\mathbf{k}^\alpha - \mathbf{k}^\beta)] \mp 4\pi\mu_n\mu_j F_j(\mathbf{k}^\alpha - \mathbf{k}^\beta) \exp[-w_j(\mathbf{k}^\alpha - \mathbf{k}^\beta)]$$

in case 2. In case 3, the quantity $u_{\alpha\beta(\pm)}$ is identical with $u_{\alpha\beta(\pm)}$ for case 1 and $u_{00\pm}$ includes the contribution (11).

Solving the equations for each component of the neutron spin in the same way as for an unpolarized target, we find that the amplitudes A and B are described by expressions analogous to Eqs. (6) and (7), where k and c are replaced with $k_\pm$ and $c_\pm$. Hence, it follows directly that in general the reflection of neutrons by a polarized crystal is characterized by four critical reflection angles (two angles for each spin component).

We shall conclude by pointing out that the different reflection coefficients of the different spin components (as in the case of the ordinary diffraction in a polarized target[13]) appear even in the case of a mirror with an antiferromagnetic ordering of the spins of the nuclei (electrons). Since in this case we have $u_{00(+)} = u_{00(-)}$, it follows that $A_+ \neq A_-$ and $B_+ \neq B_-$ only for $u_{01(+)}u_{10(+)} \neq u_{01(-)}u_{10(-)}$, which occurs in the case of interference between independent and spin-dependent parts of the structure amplitude.

The investigated anomalies of the specular reflection of neutrons are of more general application and they appear, for example, in the case of specular reflection of light (sound) from liquid crystals and magnetically ordered crystals with canted structures, and also in the specular reflection of x rays and resonant γ quanta. In the case of x rays (and also γ rays, if the nuclear levels are unsplit) polarized parallel (or perpendicular) to the surface of a crystal the problem of reflection is fully analogous to the case of neutrons discussed above and it is described by formulas analogous to Eqs. (6)–(8).

The author is deeply grateful to I. I. Gurevich and M. I. Podgoretskiĭ for valuable discussions.

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Translated by A. Tybulewicz