Quantum kinetic equation without the Born approximation for inelastic scattering of particles in crystals

S. L. Dudarev

Moscow Engineering-Physics Institute
(Submitted 4 May 1988)
Zh. Eksp. Teor. Fiz. **94**, 289–306 (November 1988)

A quantum kinetic equation that describes inelastic collisions without the use of the Born approximation is derived for the particle density matrix, for scattering by an individual atom or nucleus in a crystal. The problem of spin incoherent scattering and depolarization of neutrons in a thick crystal is solved. Analytic expressions are obtained for the intensity distribution in the Kossel patterns produced upon diffraction of particles emitted from the crystal. Resonance singularities are observed in the backscattering angular spectrum and are similar to those known in the problem of weak localization of waves in a randomly inhomogeneous medium.

1. INTRODUCTION

A quantum-mechanical description of inelastic scattering of a particle in matter, under conditions when the time of collision with an individual atom is many times shorter than the free path time between successive collisions, yields a kinetic equation for the density matrix. The first to formulate a quantum kinetic equation for a particle in a medium with random disposition of the scatterers was Migdal.[1] His derivation of the kinetic equation is based on the use of the Born approximation in the problem of particle scattering by an atom. A generalization of the approach proposed in Ref. 1 permits the collision integral in this equation to be expressed in term of the exact one-center scattering amplitude,[2] and allows account to be taken of the short-range correlations in the disposition of the atoms.[3,4]

A quantum kinetic equation that describes the motion of a fast charged particle in a crystal was derived by Kagan and Kononets[5-7] in an approximation quadratic in the inelastic-interaction operator. This equation made possible, for the first time, a consistent explanation of a large group of phenomena observed in experiments on the scattering of fast nonrelativistic protons[6,7] and electrons[8] in crystals thicker than the particle mean free path for excitation of the electron and phonon subsystems. At the same time, a number of workers[9-13] pointed out the limitations of the Born approximation for the description of the scattering of nonrelativistic electrons in matter, and particularly that the Born series does not converge for atoms of heavy elements ($Z \gtrsim 40$). The possibility of a simple replacement of the Born scattering amplitude by its exact value in the problem of dynamic diffraction of particles in a crystal was pointed out by Hoerni.[9] Kagan and Afanas'ev[14] have shown that the effective potential of the interaction of resonant neutrons with crystal nuclei is proportional to the renormalized scattering amplitude in which the elastic part is excluded from the resonance width. Under conditions of strong incoherent spin and thermal scattering, the resonance width is restored to a value corresponding to a disordered disposition of the resonant nuclei.[15] The authors of the cited papers confined themselves to consideration of the equation for the wave function of the coherent field, in the framework of which the influence of the inelastic scattering reduces to effective absorption of the particles. This makes it impossible to use the methods developed in Refs. 14 and 15 for the analysis of recently observed diffraction singularities in the angular distribution of thermal neutrons inelastically scattered in thick single crystals.[16-18]

Thus, to solve a number of problems of particle scattering in crystals, it is of interest to develop a method of simultaneously taking into account diffraction and inelastic collisions under conditions when there is no convergent series for the potential of the interaction between the particle and an individual scattering center. It is shown below that in certain cases the effective elastic-interaction potential and the inelastic-collision integral in the quantum kinetic equation can be calculated by using the pair-collision approximation.[19,20] In this approximation the expansion parameter is not the interaction potential but the matrix for scattering by an individual center. The resultant series, which differs in structure from the Born series, makes it possible to carry out summation in the case of uncorrelated excitations and to obtain an equation in closed form. In the problem of scattering of thermal neutrons, the smallness of the amplitude f compared with the particle wavelength λ makes it possible to confine oneself in the inelastic-collision integral to an approximation linear in f/λ and to take into account the correlations of the motions of the crystalatom nuclei. For fast charged particles, an expansion in a Born series reduces the obtained kinetic equation to a known form.[5-8] The use of a quantum kinetic equation in the problem of spin incoherent scattering of thermal neutrons in a single crystal explains the mechanism whereby the Kossel patterns are produced in the angular distribution of the scatterd particles and makes it possible to analyze the ensuing polarization phenomena. Under Laue diffraction conditions, resonant backscattering-amplification is observed, similar to the one known in weak-localization theory[21,22]

2. KINETIC EQUATION FOR INELASTIC COLLISIONS OF PARTICLES IN CRYSTALS

A formally exact solution of the Schrödinger equation for particle scattering by N bound centers is provided by the two-equation system[20]

$$\Psi=\chi+\mathcal{G}_0\sum_a\hat{\mathcal{T}}_a\Psi_a,\quad \Psi_a=\chi+\mathcal{G}_0\sum_{b\neq a}\hat{\mathcal{T}}_b\Psi_b, \tag{1}$$

where χ is the wave function of the particle system prior to the collision, $\mathcal{G}_0=(E_0-\hat{K}-\hat{H}+i0)^{-1}$, is the free-motion Green's function, $\hat{K}$ is the particle kinetic-energy opera-

 0038-5646/88/112338-10$04.00

tor, $\hat{H}$ is the crystal Hamiltonian, and E_0 is the sum of the particle energies in the crystal. The summation in (1) is over all the scattering centers $a = 1 \ldots N$. If the quasifree scattering condition

$$\tau_0 \ll \omega_{ph}^{-1} \tag{2}$$

is met, where τ_0 is the collision time and ω_{ph} is the characteristic frequency of the oscillations of the nucleus in the binding potential about the equilibrium condition, the operator $\hat{\mathcal{T}}_a$ coincides with the matrix for scattering by a free particle. For resonance interaction, condition (2) is equivalent to the case of a broad resonance line $\Gamma \gg \omega_{ph}$.[15]

A kinetic equation for the density matrix of a particle can be obtained by summing the bilinear combination of the wave functions $\Psi\Psi^+$ from (1) over the quantum numbers of the internal degrees of freedom of the crystal[6,8]:

$$\rho = \mathrm{Sp}_0(\Psi\Psi^+). \tag{3}$$

Before we proceed to derive the relation satisfied by the density matrix (3), we obtain the wave function φ of the elastically scattering particle (the coherent wave field). In the substance, the function φ satisfies the homogeneous equation

$$G^{-1}\varphi = 0, \tag{4}$$

where $\hat{G} = \mathrm{Sp}_0(\rho_0 \mathcal{G})$ [$\mathrm{Sp} \equiv \mathrm{Tr}$] denotes the Green's function of the elastic-scattering problem, and ρ_0 is the equilibrium thermodynamic density matrix of the crystal. The function $\mathcal{G}$ is the solution of the system of equations [cf. (1)]

$$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 \sum_a \hat{\mathcal{T}}_a \mathcal{G}_a, \qquad \mathcal{G}_a = \mathcal{G}_0 + \mathcal{G}_0 \sum_{b \neq a} \hat{\mathcal{T}}_b \mathcal{G}_b. \tag{5}$$

To continue the analysis, it is convenient to separate from the matrix $\hat{\mathcal{T}}_a$ the averaged part which is diagonal in the quantum numbers of the internal degrees of freedom of the crystal

$$\hat{T}_a = \mathrm{Sp}_0(\rho_0 \hat{\mathcal{T}}_a), \tag{6}$$

and the fluctuation term that describes inelastic scattering by the center a:

$$\hat{t}_a = \hat{\mathcal{T}}_a - \hat{T}_a. \tag{7}$$

Substitution of (6) and (7) in (5) makes it possible to express the Green's function by the series

$$G = G_0 + G_0 \sum_a \hat{T}_a G_0 + G_0 \sum_a \hat{T}_a G_0 \sum_{b \neq a} \hat{T}_b G_0$$

$$\ldots + G_0 \sum_a \mathrm{Sp}_0 \left[\rho_0 \left\{ \hat{t}_a \mathcal{G}_0 \sum_{b \neq a} \hat{t}_b + \hat{t}_a \mathcal{G}_0 \sum_{b \neq a} \hat{T}_b \mathcal{G}_0 \sum_{c \neq b} \hat{t}_c + \ldots \right\} \right]$$

$$\times G_0 + \ldots, \tag{8}$$

where $G_0 = (E - \hat{K} + i0)^{-1}$ and E is the particle energy. It must be emphasized that the structure of the series in pair collisions (8) differs from the structure of the usual Born expansion in the potential, since the number of the preceding scatterer is excluded from the sum over the atoms in each term of the series (8).

If the excitations in the system of scattering centers are independent for $a \neq b$ (an example is the Einstein model of thermal motion of the atoms or the subsystem of nuclear spins), we have

$$\mathrm{Sp}_{a \neq b}\{\rho_0 \hat{t}_a \hat{t}_b\} = 0$$

and the following estimate holds

$$G = G_1 + G_0 \sum_a \mathrm{Sp}_0\{\rho_0 \hat{t}_a (\mathcal{G}_a - \mathcal{G}_0) \hat{t}_a\} G_0, \tag{9}$$

where G_1 is the sum of those terms of the series (8) which contain only the elastic-scattering operator $\hat{T}$. The result of the summation, which is in fact the formal solution of the backscattering problem for the operator $\hat{T}$, is[23]

$$G_1 = \left(E - \hat{K} - \sum_a \hat{V}_a + i0 \right)^{-1}, \tag{10}$$

where $\hat{V}_a = \hat{T}_a (1 + G_0 \hat{T}_a)^{-1}$. The ratio of the second term in the right-hand side of (9) to the first is of the order of $\xi = \max\{R, \lambda\}/l \ll 1$, where R is the effective radius of the scattering-center potential, λ is the particle wavelength, and l is the characteristic scale, connected with the scattering, of the change of the particle wave function in the medium.

The Green's function G in (10) describes particle motion in an effective non-Hermitian (see below) potential $\hat{V} = \Sigma_a \hat{V}_a$. In the absence of inelastic excitations, when $\hat{t}_a = 0$, the operator $\hat{V}_a$ coincides with the usual scattering-center potential $\hat{U}_a$ connected with the matrix $\hat{\mathcal{T}}_a$ by the relation (Ref. 20, p. 76 of Russian translation)

$$\hat{\mathcal{T}}_a = \hat{U}_a + \hat{U}_a \frac{1}{E - \hat{K} - \hat{U}_a + i0} \hat{U}_a. \tag{11}$$

In the case of a random disposition of the atoms, the elasticscattering operator $\hat{T}_a$ is obtained by averaging $\hat{\mathcal{T}}_a$ over the volume occupied by the scattering medium. $\hat{T}_a$ is then independent of the atom number a and is macroscopically small, $\hat{T}_a \sim 1/\Omega$. Substitution of this value of $\hat{T}$ in (10) leads, accurate to terms of order $1/\Omega$, to the known expression for $\hat{V} = N\hat{T}$ for the optical potential.[24]

In the presence of collective excitations in the crystal, $\mathrm{Sp}_0\{\rho_0 \hat{t}_a \hat{t}_b\} = 0$ the effective potential V can be calculated by expanding (10) in a series and comparing term-by-term with (8). Accurate to terms quadratic in the scattering amplitude, we obtain easily

$$\hat{V} = \sum_a (\hat{T}_a - \hat{T}_a G_0 \hat{T}_a) + \sum_a \sum_{b \neq a} \mathrm{Sp}_0\{\rho_0 \hat{t}_a \mathcal{G}_0 \hat{t}_b\}. \tag{12}$$

In the particular case of resonance interaction with the scattering center, Eq. (12) coincides with Eq. (3.16) of the paper by Afanas'ev and Kagan[15] (see Appendix 1).

We consider two examples of the calculation of the effective potential $\hat{V}$ in (10), using the known elastic-collision operator (6).

I. In the case of s-scattering, the element of elastic transition between states with momenta $\mathbf{p}_0$ and $\mathbf{p}_1$ in a rigid lattice takes the form (here and below, $\hbar = 1$)

$$\langle \mathbf{p}_1 | \hat{T}_a | \mathbf{p}_0 \rangle = -\frac{2\pi}{m} f.$$

The calculation of the corresponding potential $\hat{V}_a$ of (10) reduces to summation of a geometric progression

$$\langle \mathbf{p}_1|\hat{V}_a|\mathbf{p}_0\rangle = -\frac{2\pi}{m}f-\left(\frac{2\pi}{m}f\right)^2\int\frac{d^3q_1}{(2\pi)^3}\frac{1}{E-\varepsilon_{\mathbf{q}_1}+i0}$$
$$-\left(\frac{2\pi}{m}f\right)^3\int\frac{d^3q_1\,d^3q_2}{(2\pi)^6}\frac{1}{E-\varepsilon_{\mathbf{q}_1}+i0}\frac{1}{E-\varepsilon_{\mathbf{q}_2}+i0}-\ldots.$$

The calculation result can be written in the form

$$\langle \mathbf{p}_1|\hat{V}_a|\mathbf{p}_0\rangle = -\frac{2\pi}{m}f\frac{1}{1+ip_0f+r(E)}, \tag{13}$$

where

$$r(E)=-\frac{f}{m}\,\text{v.p.}\int\frac{d^3q_1}{E-\varepsilon_{\mathbf{q}}}(2\pi)^{-3}.$$

Note that the parameter of the expansion in (13) is the ratio of the scattering amplitude to the particle wavelength, $f/\lambda \ll 1$. Substitution in (13) of the resonance scattering amplitude

$$f=-\frac{1}{2p}\frac{\Gamma_e}{E-E_0+i\Gamma/2}$$

transforms this equation into

$$\langle \mathbf{p}_1|\hat{V}_a|\mathbf{p}_0\rangle = \frac{2\pi}{m}\frac{1}{2p}\frac{\Gamma_e}{E-E_0'+i(\Gamma-\Gamma_e)/2}. \tag{14}$$

The width of the resonance singularity in the effective potential (14) and its position on the energy scale do not agree with the corresponding parameters of the cross section for scattering by an isolated center. In crystals, the cause of the narrowing and shift of the resonance is the periodic character of the atom disposition, which excludes an elastic channel for scattering by an individual center.[14]

II. If the condition $R/\lambda \gg 1$ is met, the matrix (11) for scattering of a fast electron by an atom can be calculated in the eikonal approximation[20]

$$\langle \mathbf{r}|\hat{\mathcal{T}}_a|\mathbf{r}'\rangle = U_a(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')-\frac{i}{v}\theta(z-z')$$
$$\times\exp[ip(z-z')]\delta(\boldsymbol{\rho}-\boldsymbol{\rho}')U_a(\boldsymbol{\rho},z)$$
$$\times U_a(\boldsymbol{\rho},z')\exp\left[-\frac{i}{v}\int_{z'}^{z}U_a(\boldsymbol{\rho},\zeta)\,d\zeta\right], \tag{15}$$

where $\boldsymbol{\rho}=(x,y)$, and the z axis is directed along the momentum $\mathbf{p}=m\mathbf{v}$ of the incident particles. The matrix element (6) with zero longitudinal-momentum transfer is in this case

$$\langle \boldsymbol{\rho},p|\hat{T}_a|\boldsymbol{\rho},p\rangle$$
$$=iv\delta(\boldsymbol{\rho}-\boldsymbol{\rho}')\left[\left\langle\exp\left(-\frac{i}{v}\int_{-\infty}^{\infty}U_a(\boldsymbol{\rho},\zeta)\,d\zeta\right)\right\rangle-1\right]. \tag{16}$$

Here $\langle\ldots\rangle$ denotes averaging over the ground state of the electronic subsystem and over the thermal motion of the atomic nucleus. Comparison of (16) with (10) yields for the matrix element of the effective potential

$$\overline{V}_a(\boldsymbol{\rho})=\int_{-\infty}^{\infty}d\zeta\,V_a(\boldsymbol{\rho},\zeta)$$
$$=iv\ln\left\{\left\langle\exp\left(-\frac{i}{v}\int_{-\infty}^{\infty}U_a(\boldsymbol{\rho},\zeta)\,d\zeta\right)\right\rangle\right\}. \tag{17}$$

This relation has a simple meaning: the phase advance of the wave function on passage of the particle through the potential $V_a(\boldsymbol{\rho},\zeta)$ coincides with the phase advance for elastic scattering (16).

In the theory of the channeling effect, frequent use is made of the concept of an atomic-plane or atomic-axis potential U directed along the particle-motion direction.[25] This quantity is connected with the potential (17) by the relation

$$U_\perp(\boldsymbol{\rho})=\frac{1}{c_\parallel}\sum_a{}'\overline{V}_a(\boldsymbol{\rho}), \tag{18}$$

where $a_\parallel$ is the crystal-lattice period along $\mathbf{p}$, and the summation is over the atoms in a plane paerpendicular to the particle-motion direction. In the Born limit, series expansion of the exponential and of the logarithm in (17) leads to a known result.[5-7] The use of the parabolic model

$$\int_{-\infty}^{\infty}U_a(\boldsymbol{\rho},\zeta)\,d\zeta=k(\boldsymbol{\rho}-\mathbf{u})^2/2,$$

where $\mathbf{u}$ is the transverse thermal displacement, permits an analytic calculation of the integral (17) and we can write for the channel potential

$$\begin{aligned}\operatorname{Re}U_\perp(\boldsymbol{\rho})&=\frac{k\rho^2}{2a_\parallel}\frac{1}{1+\varkappa^2}+\frac{v}{a_\parallel}\operatorname{arctg}\varkappa,\\ \operatorname{Im}U_\perp(\boldsymbol{\rho})&=-\frac{k\rho^2}{2a_\parallel}\frac{\varkappa}{1+\varkappa^2}-\frac{v}{2a_\parallel}\ln(1+\varkappa^2),\end{aligned} \tag{19}$$

where $\varkappa=k\langle\mathbf{u}^2\rangle/v$. The imaginary part of the effective potential is the result of thermal inelastic scattering of the electrons. In accord with the law that the wave function of a coherent field decreases with the depth in the crystal, the imaginary part of the channel potential (19) is negative.

We proceed now to derive a kinetic equation for the particle density matrix (3). It is easiest to obtain this equation in the case (9), (10) of uncorrelated excitations. To this end, each of the wave functions Ψ and Ψ^+ under the trace symbol in (3) must be represented by the series (1) in the collisions. A graphic illustration of the subsequent summation over the quantum numbers of the internal degrees of freedom of the crystal is shown in Fig. 1. The solid lines in

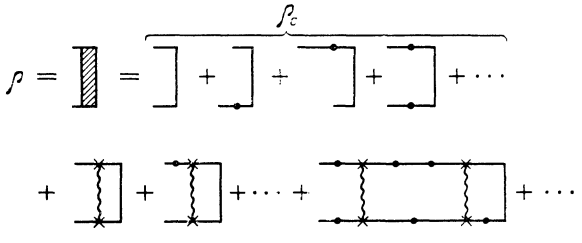

FIG. 1.

this figure correspond to the free Green's functions G_0, the points to the elastic-scattering operators T, and the crosses to the inelastic-collision operators. Joining the crosses by wavy lines means equality of the numbers of atoms from which inelastic scattering takes place. In accordance with the estimate (9), diagrams combining joinings of operators t located on one (upper or lower) straight line have the smallness $\xi \ll 1$. The sum of all the diagrams without inelastic collision is equal to the density matrix $\rho_c = \varphi\varphi^+$ of the coherent field, where φ is the solution of Eq. (4). Allowance for all the diagrams without intersecting wavy lines yields the sought kinetic equation

$$\rho=\rho_c+G\sum_a \mathrm{Sp}_0\left\{\hat{t}_a\frac{1}{1+G_0\hat{T}_a}\rho\rho_0\frac{1}{1+\hat{T}_a{}^+G_0{}^+}\hat{t}_a{}^+\right\}G^+, \quad (20)$$

in which account is taken of the connection of the wave $\rho_{aa} = \mathrm{Sp}_0(\Psi_a\Psi_a^+)$ incident on the center a with the exact solution (3):

$$\rho_{aa}=\frac{1}{1+G_0\hat{T}_a}\rho\frac{1}{1+\hat{T}_a{}^+G_0{}^+}$$

and $G_a \approx G$ at large distances from the scatterer a. The collision integral of the kinetic equation (20) is connected with the imaginary part of the effective potential $\hat{V}$ of (10) by the optical theorem and satisfies the total-probability conservation condition (Appendix 2).

In the derivation of the collision integral in the case of correlated excitations the required $(\sim\hat{\mathscr{T}})^2$ accuracy is ensured even by the first nonvanishing approximation with respect to the inelastic-scattering operator:

$$\rho=\rho_c+G\sum_{a,b}\mathrm{Sp}_0\{\hat{t}_a\rho\rho_0\hat{t}_b{}^+\}G^+. \quad (21)$$

The expression corresponding to (21) for the effective potential $\hat{V}$ in the Green's function (10) has the form (12).

Equation (20) under the condition $\max\{R,\lambda\}/l \ll 1$, Eq. (9), and Eq. (21) provide under the condition $f/\lambda \ll 1$ a complete description of a quantum particle in a crystal under conditions of strong elastic and inelastic scattering by atoms or atomic nuclei. Using these equations, we obtain below a solution of the problem of spin incoherent scattering of thermal neutrons in a single crystal in a geometry with backscattering a semi-infinite sample. Many regularities observed in the analysis of this solution can be of interest also for inelastic scattering of x-ray photons and electrons in crystals, or of light in layered structures.

3. KOSSEL-PATTERN FORMATION IN SPIN INCOHERENT NEUTRON SCATTERING IN A SINGLE CRYSTAL

Neutron diffraction by the effective periodic potential (12) leads to singularities in the angular distribution of inelastically scattered particles near the Bragg directions. These singularities are sometimes called Kossel patterns.[18] The intensity distributions in these patterns were analysed in Refs 16 and 17 by using the single inelastic (incoherent) scattering approximation which is valid for thin crystals with $L \ll (n\sigma_{\mathrm{tot}})^{-1}$. The results of Refs. 16 and 17 are not valid in thick crystals or in strongly absorbing substances, and it is necessary to use a more general approach based on a solution of the kinetic equation (21).

Incoherent scattering of thermal neutrons in crystals at low temperatures is known to be the result of a random distribution of nuclei of different isotopes in the lattice (isotopic incoherence) and of the absence of correlations in the orientations of the nuclear spins (spin incoherence).[26,27] We consider below the physically more interesting case of isotopic incoherent scattering accompanied simultaneously by depolarization of the particles. A generalization of the resultant equation to include the case of isotopic incoherence entails no difficulties (see, e.g., Ref. 27, p.334).

The matrix for neutron scattering by a nucleus bound at a point $\mathbf{R}_a$ and having a spin $\mathbf{I}$ is (Ref. 27, p. 12)

$$\langle\mathbf{r}|\hat{\mathscr{T}}_a|\mathbf{r}'\rangle=\frac{2\pi}{m}(A+B(\mathbf{sI}))\delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{r}-\mathbf{R}_a), \quad (22)$$

where s is the neutron spin. Averaging in (22) over the quantum numbers of the internal degrees of freedom reduces to summation over the projections of the nuclear spin

$$\begin{aligned}\langle\mathbf{r}|\hat{T}_a|\mathbf{r}'\rangle&=\frac{2\pi}{m}A\delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{r}-\mathbf{R}_a),\\ \langle\mathbf{r}|\hat{t}_a|\mathbf{r}'\rangle&=\frac{2\pi}{m}B(\mathbf{sI})\delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{r}-\mathbf{R}_a).\end{aligned} \quad (23)$$

The imaginary part of the scattering length A is connected with the total nuclear collision cross section by the optical theorem

$$\mathrm{Im}\,A=-\frac{p_0}{4\pi}(\sigma_{coh}+\sigma_{in}+\sigma_a), \quad (24)$$

where $\sigma_{\mathrm{coh}} = 4\pi|A|^2$, $\sigma_{\mathrm{in}} = \pi|B|^2I(I+1)$, and σ_a is the nuclear cross section for neutron absorption. In accord with Eq. (24), the imaginary part of the effective potential (13)

$$\begin{aligned}\langle\mathbf{r}|\hat{V}_a|\mathbf{r}'\rangle&=\frac{2\pi}{m}(A+ip_0A^2)\delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{r}-\mathbf{R}_a)\\ &\approx\frac{2\pi}{m}(A+ip_0|A|^2)\delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{r}-\mathbf{R}_a)\end{aligned} \quad (25)$$

is proportional to the sum of the cross sections for incoherent scattering and absorption. Substitution of expressions (23) in (21) leads to a system of equations for the coordinate dependences of the neutron spin density-matrix elements (the subscripts + and − pertain to the signs of the particle spin projection):

$$\rho_{++}(\mathbf{r},\mathbf{r}')=\rho_{++}^{(c)}(\mathbf{r},\mathbf{r}')+\frac{\pi\sigma_{in}}{m^2}\sum_a G(\mathbf{r},\mathbf{R}_a)G^*(\mathbf{r}',\mathbf{R}_a)\times\left\{\frac{1}{3}\rho_{++}(\mathbf{R}_a,\mathbf{R}_a)+\frac{2}{3}\rho_{--}(\mathbf{R}_a,\mathbf{R}_a)\right\}, \quad (26)$$

$$\rho_{--}(\mathbf{r},\mathbf{r}')=\rho_{--}^{(c)}(\mathbf{r},\mathbf{r}')+\frac{\pi\sigma_{in}}{m^2}\sum_a G(\mathbf{r},\mathbf{R}_a)\times G^*(\mathbf{r}',\mathbf{R}_a)\left\{\frac{1}{3}\rho_{--}(\mathbf{R}_a,\mathbf{R}_a)+\frac{2}{3}\rho_{++}(\mathbf{R}_a,\mathbf{R}_a)\right\}, \quad (27)$$

$$\rho_{+-}(\mathbf{r},\mathbf{r}')=\rho_{+-}^{(c)}(\mathbf{r},\mathbf{r}')+\frac{\pi\sigma_{in}}{3m^2}\times\sum_a G(\mathbf{r},\mathbf{R}_a)G^*(\mathbf{r}',\mathbf{R}_a)\rho_{+-}(\mathbf{R}_a,\mathbf{R}_a). \quad (28)$$

An equation in closed form for the spin-independent

neutron density matrix

$$\rho(\mathbf{r},\mathbf{r}')=\rho_{++}(\mathbf{r},\mathbf{r}')+\rho_{--}(\mathbf{r},\mathbf{r}') \tag{29}$$

is obtained by adding (26) and (27):

$$\rho(\mathbf{r},\mathbf{r}')=\rho^{(c)}(\mathbf{r},\mathbf{r}')+\frac{\pi\sigma_{in}}{m^2}\sum_a G(\mathbf{r},\mathbf{R}_a)G^*(\mathbf{r}',\mathbf{R}_a)\rho(\mathbf{R}_a,\mathbf{R}_a). \tag{30}$$

The difference of the same equations describes the depolarization in incoherent scattering:

$$P(\mathbf{r},\mathbf{r}')=P^{(c)}(\mathbf{r},\mathbf{r}')-\frac{\pi\sigma_{in}}{3m^2}\sum_a G(\mathbf{r},\mathbf{R}_a)G^*(\mathbf{r}',\mathbf{R}_a)P(\mathbf{R}_a,\mathbf{R}_a), \tag{31}$$

where $P(\mathbf{r},\mathbf{r}')=\rho_{++}(\mathbf{r},\mathbf{r}')-\rho_{--}(\mathbf{r},\mathbf{r}')$.

The scalar form of the Green's function $G(\mathbf{r},\mathbf{R})$ in (26)–(28) is due to the absence of a spin dependence of the elastic scattering operator $\hat{T}_a$ of (23). For the same reason, the coherent-field polarization is independent of the coordinates:

$$\rho^{(c)}_{\sigma\sigma'}(\mathbf{r},\mathbf{r}')=\rho^{(0)}_{\sigma\sigma'}\varphi(\mathbf{r})\varphi^*(\mathbf{r}'). \tag{32}$$

The wave function $\varphi(\mathbf{r})$ from (32) satisfies a Schrodinger equation with an effective potential (25):

$$-\frac{1}{2m}\frac{\partial^2\varphi}{\partial\mathbf{r}^2}+\frac{2\pi}{m}(A+ip_0|A|^2)\sum_a\delta(\mathbf{r}-\mathbf{R}_a)\varphi(\mathbf{r})=\frac{p_0^2}{2m}\varphi(\mathbf{r}). \tag{33}$$

The boundary condition for (33) is

$$\varphi(\mathbf{r})|_{in}=\exp(i\mathbf{p}_0\mathbf{r}),\quad (\mathbf{p}_0)_z>0, \tag{34}$$

where $\mathbf{p}_0$ is the momentum of the neutrons incident on the crystal. The Green's function $G(\mathbf{r},\mathbf{R})$ in (26)–(28) is a solution, which attenuates at infinity, of the inhomogeneous equation (33)

$$\left[\frac{1}{2m}\frac{\partial^2}{\partial\mathbf{r}^2}+\frac{p_0^2}{2m}-\frac{2\pi}{m}(A+ip_0|A|^2)\sum_a\delta(\mathbf{r}-\mathbf{R}_a)\right]G(\mathbf{r},\mathbf{R})=\delta(\mathbf{r}-\mathbf{R}). \tag{35}$$

The weakness of the effective neutron-crystal interaction potential (the characteristic scale of the potential in (33), averaged over the volume of the unit cell, is 10^{-7} eV) makes it possible to solve Eqs. (33) and (35) by using the two-wave approximation of the dynamic theory of diffraction.[28] This approximation corresponds to replacement of the exact expression for the effective potential in (33) and (35) by

$$V(\mathbf{r})=\theta(z)\left(\Lambda-\frac{i}{2}\Gamma\right)(1+2\cos\mathbf{G}\mathbf{r}), \tag{36}$$

where $\mathbf{G}$ is the reciprocal lattice vector closest to the Bragg condition. The theta function introduced in (36) means that the crystal atoms occupy the half-space $z>0$. The choice of the phase of the potential (36) corresponds to the case of a simple cubic lattice one atom of which is located at the origin. Comparison of (36) with (33) yields for the Fourier component of the effective polarization (36)

$$V=V(\mathbf{G})=\Lambda-\frac{i}{2}\Gamma=\frac{2\pi n}{m}(A+ip_0|A|^2), \tag{37}$$

where n is the number of atoms per unit volume. In accordance with (24), the imaginary part of (37) is

$$\Gamma=nv(\sigma_{in}+\sigma_a)=nv\sigma_r, \tag{38}$$

where $v=p_0/m$ is the particle velocity. Note that the inequality $\Gamma\ll|\Lambda|$ usually holds for thermal neutrons.[29]

Depending on the orientation of the reciprocal-lattice vector $\mathbf{G}$ relative to the crystal surface $z=0$, a distinction is made betwen two diffraction geometries: the Laue case for $(\mathbf{p}_0+\mathbf{G})_z=0$ and the Bragg case for $(\mathbf{p}_0+\mathbf{G})_z<0$. The solution of Eqs. (26)–(28) is obtained below for the Laue case if the vector $\mathbf{G}$ is parallel to the crystal surface and for the Bragg case if $\mathbf{G}$ is directed opposite to the z axis. In both cases the solution of (33) with the potential (36) is

$$\varphi(\mathbf{r})=\alpha(z)e^{i\mathbf{p}_0\mathbf{r}}+\beta(z)e^{i(\mathbf{p}_0+\mathbf{G})\mathbf{r}}, \tag{39}$$

where the characteristic spatial scale of variation of the functions $\alpha(z)$ and $\beta(z)$ is many times larger than the lattice constant $2\pi/G$. Before solving the equations that follow for $\alpha(z)$ and $\beta(z)$ from (33), we note an important feature of relations (30) and (31). According to these equations, the density matrix $\rho(\mathbf{r},\mathbf{r}')$ for all values of $\mathbf{r}$ and $\mathbf{r}'$ can be determined from the known values of the neutron density $\rho(\mathbf{R}_a)=\rho(\mathbf{R}_a,\mathbf{R}_a)$ at the crystal lattice sites this is valid also for the $P(\mathbf{r}\,\mathbf{r}')$]. It is easy to obtain from (30) for the coordinate density of the particles the closed expression

$$\rho(\mathbf{R}_b)=|\varphi(\mathbf{R}_b)|^2+\frac{\pi\sigma_{in}}{m^2}\sum_a|G(\mathbf{R}_a,\mathbf{R}_b)|^2\rho(\mathbf{R}_b). \tag{40}$$

Since diffraction effects in the distribution of neutrons scattered from the weak potential (36) are manifested only in a narrow region of solid angle of width $\Delta\vartheta\sim m|\Lambda|/Gp_0\ll1$ near the Bragg directions (for a discussion of an analogous situation for electrons see Ref. 8), we can solve (40) by using as the squared Green's function the expression obtained without allowance for the Fourier coefficient of the potential with $\mathbf{G}\neq0$:

$$|G(\mathbf{R}_a,\mathbf{R}_b)|^2=\left(\frac{m}{2\pi}\right)^2\frac{1}{|\mathbf{R}_a-\mathbf{R}_b|^2}\exp(-n\sigma_r|\mathbf{R}_a-\mathbf{R}_b|). \tag{41}$$

This approximation has a simple meaning: when the inequality $m|\Lambda|/Gp_0\ll1$ holds, only a small fraction of the possible wave-propagation trajectories from the nucleus a to the nucleus b satisfy the Bragg condition. Substituting (41) in (40) and taking into account the homogeneity of the boundary condition (34) with respect to x and y, we can obtain for the z-dependent density of the particles at the lattice sites the relation

$$\rho(z)=|\alpha(z)+\beta(z)|^2+\frac{n\sigma_{in}}{2}\int_0^\infty dz'E_1(n\sigma_r|z-z'|)\rho(z'), \tag{42}$$

in which, in view of the slow variation of the functions $\rho(z_a)$ and $|\alpha(z_a)+\beta(z_a)|^2$, the summation over the lattice sites is replaced by integration, and E_1 is the integral exponential function.[30]

The squared modulus of the wave function of the coher-

ent field at the crystal lattice sites takes in the Laue-diffraction case the form (see, e.g., Ref. 31)

$$|\alpha(z)+\beta(z)|^2=(D_0^{(0)})^2\exp(-\mu_0^{(0)}z)+(D_1^{(0)})^2\exp(-\mu_1^{(0)}z)$$
$$+2D_0^{(0)}D_1^{(0)}\cos(\omega^{(0)}z)\exp\left(-\frac{\mu_0^{(0)}+\mu_1^{(0)}}{2}z\right), \quad (43)$$

where

$$D_{0,1}^{(0)}=\frac{1}{2}\left\{1\mp\frac{\Lambda}{|\Lambda|}\left[\frac{y_0-1}{(1+y_0^2)^{1/2}}\right]\right\},$$
$$\omega^{(0)}=\frac{2\Lambda}{\cos\theta_0}(1+y_0^2)^{1/2},$$
$$\mu_{0,1}^{(0)}=\frac{n\sigma_r}{\cos\theta_0}\left\{1\pm\frac{\Lambda}{|\Lambda|}\frac{1}{(1+y_0^2)^{1/2}}\right\},$$
$$y_0=\varepsilon_0/2\Lambda=[(\mathbf{p}_0+\mathbf{G})^2-\mathbf{p}_0^2]/4m\Lambda.$$

Solution of (33) in the Bragg geometry yields

$$|\alpha(z)+\beta(z)|^2=\left|\left\{\frac{\varepsilon_0}{2V}\left[\left(1+\frac{4V}{\varepsilon_0}\right)^{1/2}-1\right]\right\}\right|^2$$
$$\times\exp\left[\frac{\varepsilon_0 z}{v\cos\theta_0}\operatorname{Im}\left(1+\frac{4V}{\varepsilon_0}\right)^{1/2}\right]. \quad (44)$$

In the two equations above $\cos\theta_0=(\mathbf{p}_0)_z/p_0$ is the cosine of the angle of neutron diffraction by the crystal surface.

Of interest to us is the angular distribution $S(\vartheta_1,\varphi_1)$ of the neutrons emitted from the crystal, where ϑ_1 is the angle betwen the direction of particle motion and the inward normal to the surface. Since all neutrons have in our problem one and the same energy $E=\mathbf{p}_0^2/2m$, to calculate the angular distribution it suffices to know the Fourier transform of the density matrix

$$\rho(\mathbf{q},\mathbf{q};z,z')=\int dx\,dy e^{-i\mathbf{q}(\mathbf{r}_\perp-\mathbf{r}_\perp')}\rho(\mathbf{r},\mathbf{r}')$$

near the crystal surface as $z\to 0$ and $z'\to 0$ (Ref. 24):

$$S(\vartheta_1,\varphi_1)\sin\vartheta_1\,d\vartheta_1\,d\varphi_1=\frac{1}{\Sigma}\rho(\mathbf{q},\mathbf{q};0,0)\frac{d^2q}{(2\pi)^2}, \quad (45)$$

where Σ is the surface area. Integration of (30) with respect to x and y yields for $\rho(\mathbf{q},\mathbf{q},0)$ the expression

$$\rho(\mathbf{q},\mathbf{q},0)=|\varphi(\mathbf{q},0)|^2+\frac{\pi\sigma_{in}}{m^2}\Sigma n\int_0^\infty dz'|g_q(0,z')|^2\rho(z'), \quad (46)$$

in which $g_q(z,z')$ is the Fourier component of the Green's function (35), and the integration, just as in (42), is over the crystal-lattice sites. Substitution of the Green's function $g_q(z,z')$ in the form (39) in Eq. (35) allows us to write in the Laue case

$$|g_q(0,z)|^2=\left(\frac{m}{p_0|\cos\vartheta_1|}\right)^2\left[(D_0^{(1)})^2\exp(-\mu_0^{(1)}z)\right.$$
$$+(D_1^{(1)})^2\exp(-\mu_1^{(1)}z)$$
$$\left.+2D_0^{(1)}D_1^{(1)}\cos(\omega^{(1)}z)\exp\left(-\frac{\mu_1^{(1)}+\mu_0^{(1)}}{2}z\right)\right]. \quad (47)$$

In the Bragg case the calculation result is

$$|g_q(0,z)|^2=\left(\frac{m}{p_0|\cos\vartheta_1|}\right)^2\left|\frac{\varepsilon_1}{2V}\left[\left(1+\frac{4V}{\varepsilon_1}\right)^{1/2}-1\right]\right|^2$$
$$\times\exp\left[\frac{\varepsilon_1 z}{v|\cos\vartheta_1|}\operatorname{Im}\left(1+\frac{4V}{\varepsilon_1}\right)^{1/2}\right]. \quad (48)$$

The notation in (47) and (48) is the same as in (43) and (44), apart from replacement of the momentum $\mathbf{p}_0$ in all the equations by the momentum $\mathbf{p}_1$ of the emitted particles, taken with a minus sign. (In this case $\cos\vartheta_0$ must be replaced by $|\cos\vartheta_1|$.) The similarity of (47) and (48) to (43) and (44) is an obvious consequence of the reciprocity theorem.

Equations (42) and (46) can be solved by using the known result of radiation transport,[32,33] according to which the solution of the equation

$$\rho_0(z)=e^{-n\sigma_2 z/\mu_0}+\frac{n\sigma_1}{2}\int_0^\infty dz' E_1(n\sigma_2|z-z'|)\rho_0(z') \quad (49)$$

satisfies the integral equation

$$\frac{n\sigma_1}{2}\int_0^\infty dz e^{-n\sigma_2 z/\mu}\rho_0(z)=\frac{\sigma_1}{2\sigma_2}\frac{\mu\mu_0}{\mu+\mu_0}H\left(\mu,\frac{\sigma_1}{\sigma_2}\right)H\left(\mu_0,\frac{\sigma_1}{\sigma_2}\right), \quad (50)$$

in which $\operatorname{Re}\mu>0$, $\operatorname{Re}\mu_0>0$; $\sigma_1/\sigma_2\leqslant 1$, and

$$H(\mu,\omega)=1+\frac{\omega}{2}\mu\ln\left(1+\frac{1}{\mu}\right)+\frac{\omega^2}{4}\left\{\mu\int_0^1\frac{\mu\,d\mu'}{\mu+\mu'}\ln\left(1+\frac{1}{\mu'}\right)\right.$$
$$\left.+\left[\mu\ln\left(1+\frac{1}{\mu}\right)\right]^2\right\}+\ldots \quad (51)$$

is the Chandrasekhar function.[32,34] Comparison of (49) and (50) with (42) and (46) yields directly a result for the flux density of the backscattered particles $J(\vartheta_1,\varphi_1)=|\cos\vartheta_1|S(\vartheta_1,\varphi_1)$. In the Laue case

$$J(\vartheta_1,\varphi_1)=\frac{\sigma_{in}}{4\pi\sigma_r}\sum_{j,j'=0,1}D_j^{(0)}D_{j'}^{(1)}\frac{\nu_j^{(0)}\nu_{j'}^{(1)}}{\nu_j^{(0)}+\nu_{j'}^{(1)}}H\left(\nu_j^{(0)},\frac{\sigma_{in}}{\sigma_r}\right)H\left(\nu_{j'}^{(1)}\frac{\sigma_{in}}{\sigma_r}\right)$$
$$+\frac{\sigma_{in}}{4\pi\sigma_r}\frac{y_0y_1}{(1+y_0^2)(1+y_1^2)}\frac{(\sec\vartheta_0+|\sec\vartheta_1|)}{(\sec\vartheta_0+|\sec\vartheta_1|)^2+(4\Lambda^2/\Gamma^2)[\sec\vartheta_0(1+y_0^2)^{1/2}-|\sec\vartheta_1|(1+y_1^2)^{1/2}]^2} \quad (52)$$

where

$$\nu_{0,1}^{(i)}=|\cos\vartheta_i|\Big/\left[1\pm\frac{\Lambda}{|\Lambda|}\frac{1}{(1+y_i^2)^{1/2}}\right]$$

and account is taken of the smallness of the ratio $\Gamma/|\Lambda| \ll 1$. In the Bragg case

$$J(\vartheta_1, \varphi_1) = \frac{\sigma_{in}}{4\pi\sigma_r} \frac{|(\varepsilon_0/2V[(1+4V/\varepsilon_0)^{1/2}-1]|^2 |(\varepsilon_1/2V)[(1+4V/\varepsilon_1)^{1/2}-1]|^2}{[\cos\vartheta_0 \operatorname{Re}(1+4V/\varepsilon_0)^{1/2}]^{-1}+[|\cos\vartheta_1| \operatorname{Re}(1+4V/\varepsilon_1)^{1/2}]^{-1}}$$
$$\times H\left(\cos\vartheta_0 \operatorname{Re}\left(1+\frac{4V}{\varepsilon_0}\right)^{1/2}; \frac{\sigma_{in}}{\sigma_r}\right) H\left(|\cos\vartheta_1| \operatorname{Re}\left(1+\frac{4V}{\varepsilon_1}\right)^{1/2}; \frac{\sigma_{in}}{\sigma_r}\right). \quad (53)$$

Equations (52) and (53) solve completely the problem of calculating the angular distribution of neutrons reflected from a single crystal in spin incoherent scattering, for arbitrary direction of particle entry into and exit from the substance. The angular dependence (31) of the polarization of the scattered particles agrees with (52) and (53) apart from replacement of σ_{in} by $-\sigma_{in}/3$.

4. DISCUSSION OF RESULTS

It is simplest to begin the analysis of the above equations with the dependence of the neutron backscattering coefficient, integrated over the emission angles,

$$R_{tot} = \int\limits_{\cos\vartheta_1<0} d\vartheta_1\, d\varphi_1 \sin\vartheta_1 J(\vartheta_1, \varphi_1) + R_{coh} \quad (54)$$

on the orientation of the flux of the incident particles relative to the atomic planes of the crystal. In the integration of (52) and (53) over the angles and it is convenient to use the equality[32]

$$\frac{\sigma_1}{2\sigma_2}\int_0^1 \frac{\mu\, d\mu}{\mu+\mu_0} H\left(\mu, \frac{\sigma_1}{\sigma_2}\right) H\left(\mu_0, \frac{\sigma_1}{\sigma_2}\right)$$
$$= 1-\left(1-\frac{\sigma_1}{\sigma_2}\right)^{1/2} H\left(\mu_0, \frac{\sigma_1}{\sigma_2}\right). \quad (55)$$

In the Laue case (52) there is no wave coherently reflected in the half-space $z<0$, and the only nonzero term in the sum (54) is the first:

$$R(\vartheta_0, \varphi_0) = \sum_{j=0,1} (D_j^{(0)})^2 \nu_j^{(0)} \left[1-\left(1-\frac{\sigma_{in}}{\sigma_r}\right)^{1/2} H\left(\nu_j^{(0)}, \frac{\sigma_{in}}{\sigma_r}\right)\right]. \quad (56)$$

The dependence calculated with Eq. (56) is shown in Fig.2a. The sign of $\Lambda<0$ and the cross-section ratio σ_{in}/σ_r agree with the corresponding values for vanadium.[28] In the plot we have used for the Chandrasekhar function the approximate expression

$$H(\mu, \omega) = \frac{1+3^{1/2}\mu}{1+[3(1-\omega)]^{1/2}\mu}, \quad 0\leqslant\mu\leqslant\infty, \quad \omega\leqslant 1,$$

which is accurate to 5% in the region $0\leqslant\omega\leqslant 1$, $0\leqslant\mu\leqslant 1$ (Ref. 24), and which yields the correct limit as $\mu\to\infty$ (Ref.34).

The minimum of the coefficient R_{tot} at $y_0 \sim 0.5$ is due to the anomalous passage of the neutrons. In particular, at $y_0 = 0$ one of the components of the wave field (43) is not scattered by nuclei, $\mu_0^{(0)} = 0$, and makes no contribution to (56). Under real conditions the thermal motion disturbs the strict periodicity of the arrangement of the nuclei and decreases the amplitude of the diffraction effect shown in Fig. 2a.

In the Bragg case (Fig. 2b) the intensity of the coherently scattered wave is appreciable

$$R_{coh} = \cos\vartheta_0 |\beta(0)|^2 = \cos\vartheta_0 \left|\frac{\varepsilon_0}{2V}\left[\left(1+\frac{4V}{\varepsilon_0}\right)^{1/2}-1\right]-1\right|^2 \quad (57)$$

and the total backscattering coefficient (54) is

$$R_{tot}/\cos\vartheta_0 = 1-\operatorname{Re}\left(1+\frac{4V}{\varepsilon_0}\right)^{1/2} \left|\frac{\varepsilon_0}{2V}\left[\left(1+\frac{4V}{\varepsilon_0}\right)^{1/2}-1\right]\right|^2$$
$$\times\left(1-\frac{\sigma_{in}}{\sigma_r}\right)^{1/2} H\left(\cos\vartheta_0 \operatorname{Re}\left(1+\frac{4V}{\varepsilon_0}\right)^{1/2}; \frac{\sigma_{in}}{\sigma_r}\right). \quad (58)$$

If $\sigma_{in} = 0$, Eq. (58) coincides with (57). (Note that in the Laue case (56) the backscattering coefficient for $\sigma_{in} = 0$ is exactly zero.) As seen from Fig. 2b, in the "total" reflection region $-2\leqslant y_0\leqslant 0$ the main contribution to (58) is made by the coherent wave. Far from the Bragg condition $(\mathbf{p}_0+\mathbf{G})^2 = \mathbf{p}_0^2$ the backscattering flux consists almost completely of the incoherent component.

We turn now to the analysis of the differential angular distrbution and to the polarization of the scattered neutrons. We assume the incident particles (32) to be totally polarized: $\rho_{++}^{(0)} = 1$ and $\rho_{--}^{(0)} = 0$. In the Bragg case it is easy to

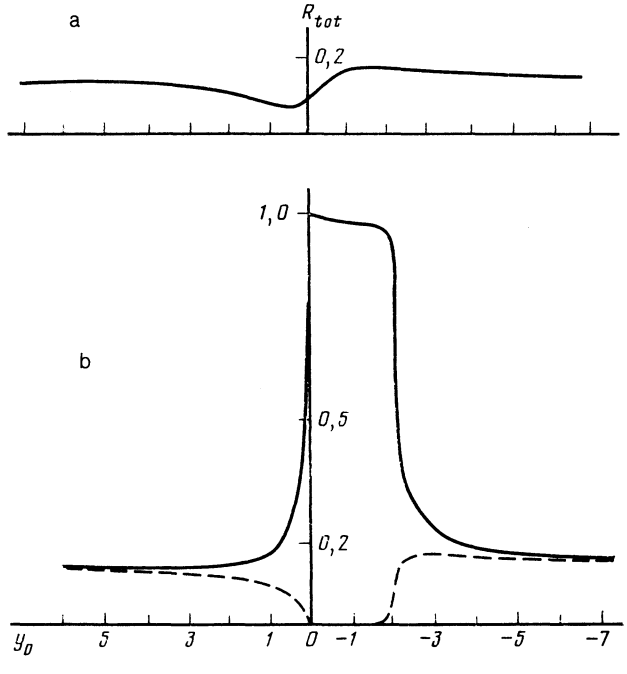

FIG. 2. Thermal-neutron backscattering coefficient, integrated over the emission angles, vs the angle between the incident particle flux and the atomic planes of the crystal ($\Lambda<0$, $\sigma_{in}/\sigma_r = 0.47$; $|\cos\vartheta_1| = 0.707$): a—Laue case; b—Bragg case, the dashed line shows the incoherent-scattering coefficient.

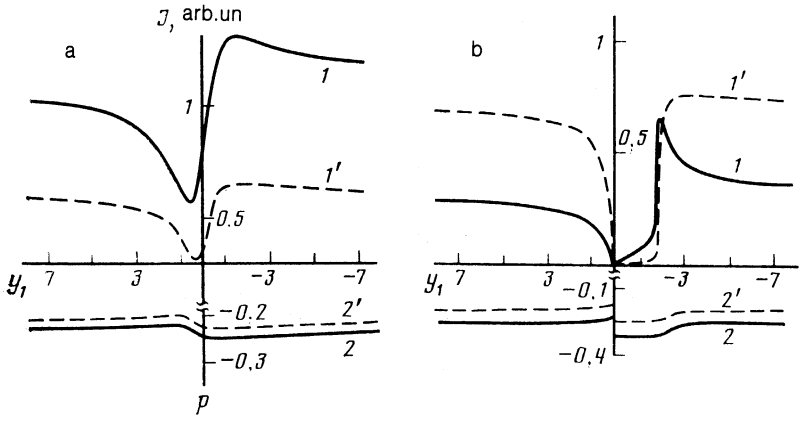

FIG. 3. Dependence of the differential backscattering coefficient (1, 1') and of the degree of polarization (2,2') $p(y') = (J_{++}(y_1) - J_{--}(y_1)/J(y_1)$, on the angle of neutron emission from a single crystal ($|\Lambda < 0$; $\sigma_{in}/\sigma_r = 0.47$, $|\cos\vartheta_0 = \cos\vartheta_1 = 0.707$); a) Laue case; solid line—$y_0 = 0$, dashed—$y_0 = 1$; b) Bragg case, solid line—$y_0 = -2$, dashed—$y_0 = 1$.

obtain for the degree of polarization

$$\frac{J_{++}(\vartheta_1,\varphi_1)-J_{--}(\vartheta_1,\varphi_1)}{J(\vartheta_1,\varphi_1)} = -\frac{1}{3}\frac{H(\cos\vartheta_0\,\mathrm{Re}(1+4V/\varepsilon_0)^{1/2};\,-\sigma_{in}/3\sigma_r)}{H(\cos\vartheta_0\,\mathrm{Re}(1+4V/\varepsilon_0)^{1/2};\,\sigma_{in}/\sigma_r)} \times\frac{H(|\cos\vartheta_1|\,\mathrm{Re}(1+4V/\varepsilon_1)^{1/2};\,-\sigma_{in}/3\sigma_r)}{\times H(|\cos\vartheta_1|\,\mathrm{Re}(1+4V/\varepsilon_1)^{1/2};\,\sigma_{in}/\sigma_r)}. \quad (59)$$

In the single incoherent scattering case, Eq. (59) goes over into the known result (Ref. 27, p. 334):

$$\frac{J_{++}(\vartheta_1,\varphi_1)-J_{--}(\vartheta_1,\varphi_1)}{J(\vartheta_1,\varphi_1)} = -\frac{1}{3}. \quad (60)$$

The difference between the degree of polarization of the neutrons emitted from the crystal and $-1/3$ is the result of multiple depolarizing collisions, the contribution of which corresponds to the succeeding expansion terms in (51).

The differential angular distribution and the degree of particle polarization, calculated using Eqs. (53) and (59) for two different orientations of the neutron flux incident on the crystal, are shown in Fig. 3b. It can be seen that the number of particles scattered in a solid-angle element do_1 in the region $-2 \leqslant y_1 \leqslant 0$ of the variation of the relative-energy-deviation parameter is very insignificant. By comparison with Fig. 2b, this phenomenon can be interpreted as a consequence of the reciprocity theorem. In fact, in this range of y_0 the incident wave undergoes almost total Bragg reflection and penetrates into the crystal to a depth many times smaller thin the mean free path $(n\sigma_r)^{-1}$. The almost exclusively incoherent single scattering character of the neutrons from that entering the reflected flux in the region $-2 < y_1 < 0$ is also attested to by the behavior of the degree of polarization of the emitted particles, which is close to $-1/3$ in the indicated range of y_1.

The equation for the degree of particle polarization in the Laue geometry, obtained by replacing σ_{in} in (52) by $-(1/3)\sigma_{in}$, is very unwieldy. It is convenient therefore to confine oneself to the graphic illustration of this diffraction case, shown in Fig. 3a.

As seen from Figs. 3a and 3b, the particle angular distributions obtained in different diffraction geometries are characterized by a number of common peculiarities. In particular, the number of particles backscattered into the angle region $y_1 \lesssim -1$ is as a rule larger than the number corresponding to $y_1 > 0$. These peculiarities are due to the spatial structure of the neutron wave field produced by dynamic diffraction in a crystal.[35] The region $y_1 \lesssim -1$ (recall that $\Lambda < 0$) corresponds to periodic modulation of the squared modulus of the wave function, under which the neutron density reaches a maximum in the vicinity of the atomic nuclei. This leads to an overall enhancement of the incoherent backscattering (Fig. 2) and to an increase of the amplitude of the diffraction effect (Fig. 3). Corresponding to the opposite sign of the parameter characterizing the deviation from the Bragg condition $y_1 \gtrsim 0$, on the contrary, is a pattern of a wave field localized in the space between the nuclei. In particular, the value $y_1 = 0$ in the Bragg geometry corresponds to zero neutron density in the crystal lattice sites Eq. (44)]. Under these conditions the intensity of the incoherent scattering weakens and the amplitude of the diffraction effects decreases in the angular distribution of the particles emitted from the crystal.

Noteworthy in the analysis of the angular distribution of neutrons backscattered in Laue geometry is the presence of resonance anomalies in this distribution [second term of Eq. (52)]. In view of their small angular width and of the integrated intensity of these resonances, they cannot be drawn to required scale in Fig. 3a. The resonances in the distribution (52) are caused by oscillatory terms in expressions (43) and (47). It must be emphasized that in the angular spectrum of the emitted particles these resonances are shifted relative to the diffraction anomalies shown in Fig. 3 and are not conected with the direction of the incident particles by some Bragg reflection. The resonances are the result of the equality of the oscillation periods of the coherent-field density at the lattice sites (43) and of the squared modulus of the Green's function (47) that describes the particle propagation from the scattering center to the crystal surface. The analog of these resonances in a disordered medium is the enhancement of the scattering "backward," an effect thoroughly investigated in the theory of wave propagation in randomly inhomogeneous media[36] and in the weak-localization problem.[21,22] It is interesting to note that in the contrast to the case of random disposition of the atoms, the cause of the resonances here is diffraction by the periodic potential (25), which can lead not only to amplification (if $y_0 y_1 > 0$) but also to resonant attenuation (if $y_0 y_1 < 0$) of the backscattering. It appears that these effects can be observed not only in the distribution of the scattered neutrons, but also in

experiments on electron diffraction in crystals or of optical photons in layered structures.

5. CONCLUSIONS

A kinetic equation was formulated above for the particle density in a crystal; the equation describes inelastic collisions without using the Born approximation in the problem of scattering by an individual atom or nucleus. The analytic solution obtained for the problem of spin incoherent scattering and depolarization of neutrons in a thick crystal points to the possibility of using this equation to describe collisions of strongly interacting particles whose scattering is not easily analyzed by the known methods.[5-8]

The author is indebted to E. E. Gorodnichev, D. B. Rogozkin, and M. I. Ryazanov for a discussion of the work and for helpful remarks.

APPENDIX 1

To prove the equivalence of expression (12) and Eq. (3.16) of Ref. 15, we rewrite the latter in our notation:

$$\hat{V}=\sum_a \hat{T}_a+\sum_a{\sum_{b\neq a}}' \mathrm{Sp}_0\{\rho_0\hat{\mathscr{T}}_a\mathscr{G}_0\hat{\mathscr{T}}_b\}, \qquad (A.1.)$$

where the prime in the second term denotes that it is necessary to exclude from the sum over the intermediate momenta in $\mathscr{G}_0$ all the vectors that differ from the incident-particle momentum $\mathbf{p}_0$ by one of the reciprocal-lattice vectors. Consider the second term of (A.1.1):

$$\sum_a{\sum_{b\neq a}}' \mathrm{Sp}_0\{\rho_0(\hat{T}_a+\hat{t}_a)\mathscr{G}_0(\hat{T}_b+\hat{t}_b)\}$$
$$={\sum_{a,b}}' \mathrm{Sp}_0\{\rho_0(\hat{T}_a+\hat{t}_a)\mathscr{G}_0(\hat{T}_b+\hat{t}_b)\}$$
$$-\mathrm{Sp}_0\{\rho_0(\hat{T}_a+\hat{t}_a)\mathscr{G}_0(\hat{T}_a+\hat{t}_a)\}. \qquad (A.1.2)$$

Since the operator $\Sigma_a\hat{T}_a$ has nonzero matrix elements only with a momentum shift equal to the reciprocal lattice vector, and $\mathrm{Sp}_0\{\rho_0\hat{t}_a\}=0$, we readily obtain from (A.1.2)

$${\sum_{a,b}}' \mathrm{Sp}_0\{\rho_0\hat{t}_a\mathscr{G}_0\hat{t}_b\}-\hat{T}_aG_0\hat{T}_a-\mathrm{Sp}_0\{\rho_0\hat{t}_a\mathscr{G}_0\hat{t}_a\}$$
$$=\sum_a{\sum_{b\neq a}}' \mathrm{Sp}_0\{\rho_0\hat{t}_a\mathscr{G}_0\hat{t}_b\}-\hat{T}_aG_0\hat{T}_a. \qquad (A.1.3)$$

Since most momenta that differ from $\mathbf{p}_0$ by the reciprocal-lattice vector in all of momentum space have zero measure, and the operator $\mathrm{Sp}_0\{\rho_0\hat{t}_a\mathscr{G}_0\hat{t}_b\}$ is not singular at the points of this set, the prime of the last sum in (A.1.3) can be omitted). Substitution of the resultant expression in (A.1.1) reduces it to the form (12).

APPENDIX 2

To prove the validity of the total-probability conservation law, we rewrite the kinetic equation in differential form. To this end we apply to the left and right sides of this equation the operators G^{-1} and $(G^{-1})^+$ and subtract the obtained relations from one another:

$$(G_0^{-1})\rho-\sum_a\hat{T}_a(1+G_0\hat{T}_a)^{-1}\rho-\rho(G_0^{-1})^+$$
$$-\rho\sum_a(1+T_a^+G_0^+)^{-1}\hat{T}_a^+$$
$$=\sum_a\mathrm{Sp}_0\{\hat{t}_a(1+G_0\hat{T}_a)^{-1}\rho_0\rho(1+\hat{T}_a^+G_0^+)^{-1}\hat{t}_a^+\}G^+$$
$$-G\sum_a\mathrm{Sp}_0\{\hat{t}_a(1+G_0\hat{T}_a)^{-1}\rho_0\rho(1+\hat{T}_a^+G_0^+)^{-1}\hat{t}_a^+\}. \qquad (A.2.1)$$

We sum the diagonal elements of this equation over the momentum and spin projection of the particle:

$$\mathrm{Sp}\Big[\rho\sum_a(1+\hat{T}_a^+G_0^+)^{-1}\hat{T}_a^+-\sum_a\hat{T}_a(1+G_0\hat{T}_a)^{-1}\rho\Big]$$
$$=\mathrm{Sp}\Big[\sum_a\mathrm{Sp}_0\{\hat{t}_a(1+G_0\hat{T}_a)^{-1}\rho\rho_0(1+\hat{T}_a^+G_0^+)^{-1}\hat{t}_a^+\}G^+$$
$$-G\sum_a\mathrm{Sp}_0\{\hat{t}_a(1+G_0\hat{T}_a)^{-1}\rho\rho_0(1+\hat{T}_a^+G_0^+)^{-1}\hat{t}_a^+\}\Big]. \qquad (A.2.2)$$

The use of cyclic permutation under the trace sign, and also of the estimate (9), shows that the sufficient condition for satisfying (A.2.2) is

$$\frac{1}{1+\hat{T}_a^+G_0^+}\hat{T}_a^+-\hat{T}_a\frac{1}{1+G_0\hat{T}_a}$$
$$=\frac{1}{1+\hat{T}_a^+G_0^+}\mathrm{Sp}_0\{\rho_0\hat{t}_a^+(G_0^+-G_0)\hat{t}_a\}\frac{1}{1+G_0\hat{T}_a}. \qquad (A.2.3)$$

Substitution of the definitions (6) in (7) reduces (A.2.3) to the form

$$\hat{T}_a^+-\hat{T}_a=\mathrm{Sp}_0\{\rho_0\hat{\mathscr{T}}_a^+(G_0^+-G_0)\hat{\mathscr{T}}_a\}. \qquad (A.2.4)$$

It is easy to verify the validity of the last relation by comparing (A.2.4) with the unitarity condition for the scattering matrix (Ref. 20, p. 199 of the Russian translation):

$$\hat{\mathscr{T}}_a^+-\hat{\mathscr{T}}_a=2\pi i\hat{\mathscr{T}}_a^+\delta(E-\hat{K})\hat{\mathscr{T}}_a=\hat{\mathscr{T}}_a^+(G_0^+-G_0)\hat{\mathscr{T}}_a.$$

An equation similar to (A.2.2), accurate to terms of order $\hat{\mathscr{T}}^2$, holds also for Eq. (21).

[1] A. B. Migdal, Dokl. Akad.Nauk SSSR, **105**, 77 (1955).
[2] A. B. Migdal and N. M. Poluevktov-Nikoladze, *ibid.* **105**, 233 (1955).
[3] V. M. Finkel'berg, Zh. Eksp. Teor. Fiz. **53**, 401 (1967) [Sov. Phys. JETP **26**, 268 (1968)].
[4] Yu. N. Barabanenkov, Usp. Fiz. Nauk **117**, 49 (1975) [Sov. Phys. Usp. 673 (1975).
[5] Y. Kagan and Yu. V. Kononets, Zh. Eksp. Teor. Fiz. **58**, 226 (1970) [Sov. Phys. JETP **31**, 124 (1970)].
[6] Yu. Kagan and Yu. V. Kononets, *ibid.* **64**, 1042 (1973) [**37**, 530 (1973)].
[7] Yu. Kagan and Yu. V. Kononets, *ibid.* **66**, 1693 (1974) [**39**, 832 (1974)].
[8] S. L. Dudarev and M. Ryazanov, Acta Cryst. **A44**, 52 (1988). Zh. Eksp. Teor. Fiz. **88**, 631 (1985) [Sov. Phys. JETP **61**, 370 (1985)].
[9] J. A. Hoerni, Phys. Rev. **102**, 1534 (1956).
[10] A. Owie and R. M. Stern, Z. Naturforsch. **B27a**, 382 (1972).
[11] S. K. Andersen and A. Howie, Surf. Sci. **50**, 197 (1975).
[12] J. M. Cowley, Diffraction Physics [Russ. transl.], Mir, 1979, p. 90 [Possibly: Crystal Structure Determination by Electron Diffraction, Pergamon].
[13] L. Reimer, *Transmission Electron Microscopy*, Springer, 1984, p. 140.
[14] Yu. Kagan and A. M. Afanas'ev, Zh. Eksp. Teor. Fiz. **50**, 271 (1966) [Sov. Phys. JETP **23**, 178 (1966)].
[15] A. M. Afanas'ev and Yu. Kagan, ibid. **52**, 191 (1967) [**25**, 124 (1967)].

[16]D. Petrascheck, Phys. Rev. **B31**, 4043 (1985).
[17]D. Petrascheck, *ibid.* p. 7466.
[18]V. P. Glazkov, A. V. Irodova, V. A. Somenkov, and S. Sh. Shil'shtein, Pis'ma Zh. Eksp. Teor. Fiz. **44**, 169 (1986) [JETP Lett. **44**, 216 (1986).
[19]Yu. N. Gnedin and A. Z. Dolginov, Zh. Eksp. Teor. Fiz. **45**, 1136 (1963) [Sov. Phys. JETP **18**, 784 (1964)].
[20]M. L. Goldberger and K. M. Watson, *Collision Theory*, Wiley, 1964.
[21]D. E. Khmel'nitskii, Physica **B+C126**, 235 (1984).
[22]A. A. Golubentsev, Zh. Eksp. Teor. Fiz. **86**, 47 (1984) [Sov. Phys. JETP **59**, 26 (1984)].
[23]R. T. Prosser, J. Math. Phys. **17**, 1775 (1976).
[24]E. E. Gorodnichev, S. L. Dudarev, D. B. Rogozkin, and M. I. Ryazanov, Zh. Eksp. Teor. Fiz. **93**, 1642 (1987) [Sov. Phys. JETP **66**, 938 (1987)].
[25]V. A. Bazylev and N. K. Zhevago, Emission of Fast Particles in Matter and in External Fields [in Russian], Nauka, 1987, Chap. 6.
[26]I. I. Gurevich and L. V. Tarasov, eds., *Low-Energy Neutron Physics* Am. Elsevier, 1968.
[27]W. Marshall and S. W. Lovsey, *Theory of Thermal Neutron Scattering*, Oxford, 1971.
[28]H. Rauch and D. Petrascheck, *Neutron Diffraction*, Springer, 1978, p. 303.
[29]Neutron Cross sections, Vol. 1, Pàrts A. and B, Academic, 1981.
[30]M. Abramowitz and I. A. Stegun, *Handbook of Special Functions*, Dover, 1964.
[31]Z. G. Pinsker, X-Ray Crystal Optics [in Russian] Nauka, 1982.
[32]S. Chandrashekar, *Radiative Transfer*, Dover, 1960.
[33]E. M. Case and P. F. Zweifel, *Linear Transport Theory*, Addison-Wesley, 1967.
[34]V. V. Ivanov, Radiative Transfer and Spectra of Celestial Bodies [in Russian], Nauka, 1969, §5.4.
[35]Y. Kagan and A. M. Afanas'ev, Zh. Eksp. Teor. Fiz. **49**, 1504 (1965) [Sov. Phys. JETP **22**, 1032 (1966)].
[36]Yu. A. Kravtsov and A. I. Saichev, Usp. Fiz. Nauk **137**, 501 (1982) [Sov. Phys. Usp. **25**, 494 (1982)].

Translated by J. G. Adashko