

Coherent effects in backscattering of waves from a medium with random inhomogeneities

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The differential and total backscattering coefficients of the surface of a medium are found for arbitrary angles of incidence and emission of particles from the medium. These coefficients are obtained by solving the transport equation for the density matrix with account taken of multiple incoherent scattering as well as the refraction and reflection of waves by the interface between two media. It is shown that in the case of grazing angles of incidence a nonspecular peak can appear in the angular spectrum of the backreflected particles.

INTRODUCTION

When a particle or a photon moves in a medium, the wave function is formed as a result of interference between waves scattered by different atoms in a substance. Coherent or incoherent addition of waves may occur, depending on the positions of the scattering centers.

Well inside a scattering medium with a random distribution of atoms, when $n\lambda^3 \ll 1$ (n is the number of atoms per unit volume and λ is the wavelength of a particle), the waves add up incoherently and the cross section for the scattering by a small volume of the substance is proportional to the number of atoms contained in such a volume. The exception to this rule is only a small range of solid angles near the "backward" direction, where the coherence effects are manifested by waves that have traveled along the same paths in the scattering medium in the forward and reverse directions.¹⁻⁷

On the other hand, near the surface of the medium the situation is very different, since the very existence of an interface between a substance and vacuum alters the condition for the interference of scattered waves. If this interface is sufficiently abrupt compared with the mean free path l of the particles or photons in the substance, the condition of quasi-homogeneity of the wave field is no longer obeyed⁸ and it is generally not possible to go over from wave equations to the transport equation for intensities.⁹ In other words, near an abrupt vacuum-medium interface the mutual coherence function of the wave field of particles or photons

$$\rho(\mathbf{r}, \mathbf{r}') = \langle \psi(\mathbf{r}) \psi^*(\mathbf{r}') \rangle$$

cannot be represented in the form⁸

$$\rho(\mathbf{r}, \mathbf{r}') \equiv \Phi(\mathbf{r} - \mathbf{r}'; (\mathbf{r} + \mathbf{r}')/2),$$

where the characteristic scale of the change of Φ in respect of the difference variable $\mathbf{r} - \mathbf{r}'$ is considerably less than the scale of its variation along $(\mathbf{r} + \mathbf{r}')/2$ (Ref. 10). Consequently, the angular distribution of particles scattered in a randomly inhomogeneous medium with an abrupt boundary differs greatly from the solution of the corresponding problem in transport theory.

The presence of an abrupt boundary of a medium results in specular reflection and in refraction of the incident and scattered waves and, consequently, causes diffraction-induced deformation of the angular spectrum of incoherent scattered radiation emerging from the medium.

A theoretical analysis of the angular distribution of scattered particles, allowing for the reflection and refraction at the boundary of a substance, is of interest in studies of the interactions of neutrons with solids,¹¹ in electron spectroscopy with angular resolution,¹² and in x-ray and γ -ray optics of surfaces.¹³⁻¹⁵

We shall solve the transport equation for the density matrix (mutual coherence function) to find the angular spectrum of particles emerging from a medium. The solution obtained allows both for reflection and refraction of waves at the interface between the medium and vacuum, and for the usual incoherent multiple scattering. It is assumed that the wavelength of the incident particles (photons) is many times greater than the characteristic size of the scattering centers and that the differential cross section for single scattering is isotropic. The case under discussion is realized in practice in the interaction of neutrons with atomic nuclei, of electromagnetic waves with atoms and molecules as well as with small optical inhomogeneities of a medium, and of slow electrons with impurity centers.

1. TRANSPORT EQUATION FOR MULTIPLE SCATTERING OF WAVES IN A RANDOMLY INHOMOGENEOUS MEDIUM

We shall consider the motion of a nonrelativistic zero-spin particle in a substance with a random distribution of atoms (the results obtained below remain valid also in the case of scattering of electromagnetic waves in randomly inhomogeneous media). If we ignore the recoil of atoms colliding with an incident particle, we can reduce the problem of calculation of the angular distributions and other characteristics of the wave field of the scattered particles to a determination of the average (over the distribution of atoms) solution of the equation

$$\begin{aligned} & \left(\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \mathbf{r}^2} + E \right) \rho(\mathbf{r}, \mathbf{r}'; \mathbf{R}_1 \dots \mathbf{R}_N) \\ & - \left(\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \mathbf{r}'^2} + E \right) \rho(\mathbf{r}, \mathbf{r}'; \mathbf{R}_1 \dots \mathbf{R}_N) \\ & = \left(\sum_a U_a(\mathbf{r}) - \sum_{a'} U_{a'}(\mathbf{r}') \right) \rho(\mathbf{r}, \mathbf{r}'; \mathbf{R}_1 \dots \mathbf{R}_N), \end{aligned} \quad (1)$$

where the averaging operation represents integration of the density matrix from Eq. (1) using the coordinate function of the distribution of atoms in matter:

$$\rho(\mathbf{r}, \mathbf{r}') = \int d\mathbf{R}_1 \dots d\mathbf{R}_N \rho(\mathbf{r}, \mathbf{r}'; \mathbf{R}_1 \dots \mathbf{R}_N) F(\mathbf{R}_1 \dots \mathbf{R}_N). \quad (2)$$

In Eq. (1), $E = \hbar^2 p_0^2 / 2m$ is the total energy of the incident particle, the summation over $a = 1, 2, \dots, N$ is carried out over all the atoms in the medium, and U_a is the operator of the interaction of a particle with an individual atom. In the case of uncorrelated positions of the scattering centers the distribution function of Eq. (2) is

$$F(\mathbf{R}_1 \dots \mathbf{R}_N) = V^{-N} \theta(\mathbf{R}_1) \dots \theta(\mathbf{R}_N), \quad (3)$$

where $\theta(\mathbf{R})$ is equal to unity within a volume V occupied by the scattering medium and vanishes outside this volume. When the condition $(N/V)\lambda^3 = n\lambda^3 \ll 1$, is satisfied and the reflection into a narrow range of angles $\Delta\vartheta \sim \lambda/l$ in the "backward" direction is ignored,¹⁻⁷ the averaging of Eq. (1) with the distribution function (3) yields for $\rho(\mathbf{r}, \mathbf{r}')$ a transport equation which has the following operator form^{16,17} [a bar is used for the operation of averaging of Eq. (2), which yields $\bar{\rho} = \rho(\mathbf{r}, \mathbf{r}')$]

$$\bar{\rho} = \rho_0 + \hat{G} \left(\sum_a \hat{\mathcal{T}}_a \bar{\rho} \hat{\mathcal{T}}_a^+ \right) \hat{G}^+, \quad (4)$$

where $\hat{\mathcal{T}}_a$ is the matrix representing the scattering by a single atom¹⁸:

$$\hat{\mathcal{T}}_a = \hat{U}_a + \hat{U}_a \frac{1}{E - \hat{K} + i0} \hat{\mathcal{T}}_a, \quad (5)$$

$\hat{K} = -(\hbar^2/2m)\partial^2/\partial\mathbf{r}^2$ is the kinetic energy operator, and \hat{G} represents the solution of the equation

$$(E - \hat{K} - \sum_a \hat{\mathcal{T}}_a) \hat{G} = \hat{1}. \quad (6)$$

The quantity ρ_0 in Eq. (4) describes the wave field of particles which do not undergo incoherent scattering:

$$(\hat{G}^{-1})\rho_0 - \rho_0(\hat{G}^{-1})^+ = 0. \quad (7)$$

At large distances from the boundary of the scattering medium the field ρ_0 is a superposition of the incident waves and of the waves reflected coherently from the surface of the substance.

In the operators \hat{G}^{-1} and $(\hat{G}^{-1})^+$ are applied on the left and right of Eq. (4), we obtain the differential form of the transport equation:

$$\begin{aligned} & (\hat{G}_0^{-1})\bar{\rho} - \bar{\rho}(\hat{G}_0^{-1})^+ \\ & = \sum_a \hat{\mathcal{T}}_a \bar{\rho} (1 + \hat{\mathcal{T}}_a \hat{G}^+) - \sum_a (1 + \hat{G} \hat{\mathcal{T}}_a) \bar{\rho} \hat{\mathcal{T}}_a^+, \end{aligned} \quad (8)$$

where $\hat{G}_0 = (E - \hat{K} + i0)^{-1}$.

If on the right-hand side of Eq. (8) we assume that $\hat{G} = \hat{G}_0$, we obtain the transport equation of Migdal and Polievktov-Nikoladze¹⁹ for fast particles. Physically, the change from Eq. (8) to the equation derived in Ref. 19 represents neglect of the influence of the medium on the propagation of the scattered wave.

Equations of the type (4) and (8) make it possible to describe multiple elastic scattering allowing for the influence of inelastic collisions. If we ignore the energy lost by the particles, the only inelastic scattering channel is the absorption.

In the s -scattering case a matrix element of the operator $\hat{\mathcal{T}}_a$ in the coordinate representation is

$$\langle \mathbf{r} | \hat{\mathcal{T}}_a | \mathbf{r}' \rangle = -\frac{2\pi\hbar^2}{m} f\delta(\mathbf{r} - \mathbf{R}_a) \delta(\mathbf{r}' - \mathbf{R}_a), \quad (9)$$

where f is the scattering amplitude. The total scattering cross section is $\sigma_{\text{tot}} = (4\pi/\rho_0) \text{Im} f$, the elastic cross section is $\sigma_{\text{el}} = 4\pi|f|^2$ and the difference between them $\sigma_{\text{in}} = \sigma_{\text{tot}} - \sigma_{\text{el}}$ is the cross section for the absorption of particles by a single center.

Substituting Eq. (9) into Eqs. (4) and (6), we obtain respectively an equation for the density matrix (2) averaged over the distribution of the atoms

$$\begin{aligned} & \rho(\mathbf{r}, \mathbf{r}') = \rho_0(\mathbf{r}, \mathbf{r}') + n(2\pi\hbar^2/m)^2 |f|^2 \\ & \times \int d\mathbf{r}'' \theta(\mathbf{r}'') G(\mathbf{r}, \mathbf{r}'') \rho(\mathbf{r}'', \mathbf{r}'') G^*(\mathbf{r}', \mathbf{r}'') \end{aligned} \quad (10)$$

and an equation for the Green function $G(\mathbf{r}, \mathbf{r}')$

$$\left(\frac{\partial^2}{\partial\mathbf{r}^2} + p_0^2 + 4\pi n f \theta(\mathbf{r}) \right) G(\mathbf{r}, \mathbf{r}') = \frac{2m}{\hbar^2} \delta(\mathbf{r} - \mathbf{r}'). \quad (11)$$

If the quantum-mechanical state of the particles incident on a medium is a pure state,²⁰ we can represent $\rho_0(\mathbf{r}, \mathbf{r}')$ by a product of wave functions

$$\rho_0(\mathbf{r}, \mathbf{r}') = \Psi_0(\mathbf{r}) \Psi_0^*(\mathbf{r}'), \quad (12)$$

each of which satisfies according to Eq. (7), the equation

$$\left(\frac{\partial^2}{\partial\mathbf{r}^2} + p_0^2 + 4\pi n f \theta(\mathbf{r}) \right) \Psi_0(\mathbf{r}) = 0. \quad (13)$$

For a plane wave $\exp(i\mathbf{p}_0 \cdot \mathbf{r})$ incident on a substance from $z = -\infty$ the boundary condition for Eq. (13) is of the form

$$\Psi_0(\mathbf{r})_{\text{inc}} |_{z=-\infty} = \exp(i\mathbf{p}_0 \cdot \mathbf{r}). \quad (14)$$

Equations (10), (11), and (13) together with the boundary condition (14) determine completely the density matrix $\rho(\mathbf{r}, \mathbf{r}')$ both inside the medium and outside it, and can be used to calculate the distribution of scattered particles for arbitrary angles of incidence and escape from the medium.

2. COHERENT WAVE FIELD AND GREEN FUNCTION

Before we solve the equation for the density matrix (10), we must calculate the Green function G and find the coherent wave field.

We shall consider the case when the scattering medium occupies the region in space where $z > 0$. Then Eq. (13) can be rewritten in the form of the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial\mathbf{r}^2} + U_0 \theta(\mathbf{r}) \right) \Psi_0(\mathbf{r}) = E \Psi_0(\mathbf{r}) \quad (15)$$

using the optical potential

$$U_0 = -\frac{2\pi\hbar^2 n f}{m}, \quad f = f_1 + i f_2. \quad (16)$$

The imaginary part of U_0 is related to the total scattering cross section of a single atom by the optical theorem

$$\text{Im} U_0 = -(n\hbar^2 p_0 / 2m) \sigma_{\text{tot}}.$$

Allowing for the continuity of $\Psi_0(\mathbf{r})$ and its derivatives at $z = 0$, and also using the boundary condition (14), we readily obtain

$$\begin{aligned}\psi_0(\mathbf{r}) &= \varphi_0(z) \exp(i\mathbf{p}_0 \cdot \mathbf{r}_\perp), \quad \mathbf{r}_\perp = (x, y), \\ \varphi_0(z) &= \exp(ik_0 z) + \frac{k_0 - \kappa_0}{k_0 + \kappa_0} \exp(-ik_0 z), \quad z < 0, \quad (17) \\ \varphi_0(z) &= \frac{2k_0}{k_0 + \kappa_0} \exp(i\kappa_0 z), \quad z > 0,\end{aligned}$$

where $k_0 = (\mathbf{p}_0)_z = p_0 \mu_0$ and $\kappa_0 = (k_0^2 + 4\pi n f)^{1/2}$. The second term in Eq. (17) in the $z < 0$ case describes a wave reflected specularly by the surface of the scattering medium.

The solution of Eq. (11) for the Green function can be found using the Fourier transform with respect to coordinates parallel to the surface:

$$G(\mathbf{r}, \mathbf{r}') = \int (2\pi)^{-2} d\mathbf{q} \exp\{i\mathbf{q} \cdot (\mathbf{r}_\perp - \mathbf{r}'_\perp)\} g_{\mathbf{q}}(z, z').$$

The function $g_{\mathbf{q}}(z, z')$ satisfies the equation

$$\left(\frac{\partial^2}{\partial z^2} + p_0^2 - q^2 + 4\pi n f \theta(z) \right) g_{\mathbf{q}}(z, z') = \frac{2m}{\hbar^2} \delta(z - z'), \quad z' > 0. \quad (18)$$

The conditions of continuity at $z = 0$ yield⁹

$$g_{\mathbf{q}}(z, z') = -\frac{2im}{\hbar^2} \frac{1}{k + \kappa} \exp(i\kappa z' - ikz), \quad z < 0, \quad (19)$$

$$g_{\mathbf{q}}(z, z') = \frac{im}{\hbar^2 \kappa} \left\{ \frac{k - \kappa}{k + \kappa} \exp(i\kappa(z + z')) - \exp(i\kappa|z - z'|) \right\}, \quad z > 0,$$

where

$$k = (p_0^2 - q^2)^{1/2}, \quad \kappa = (k^2 + 4\pi n f)^{1/2}, \quad \text{Re } \kappa > 0.$$

Comparing Eq. (19) with the Green function of an infinite medium

$$G_{\text{inf}}(\mathbf{r} - \mathbf{r}') = -\frac{m}{2\pi\hbar^2} \frac{1}{|\mathbf{r} - \mathbf{r}'|} \exp(i(p_0^2 + 4\pi n f)^{1/2} |\mathbf{r} - \mathbf{r}'|),$$

we can easily show that the presence of a surface has a strong influence on the motion of a particle at depths

$$z \lesssim (4\pi n |f|)^{-1/2} \quad (20)$$

only at grazing angles of incidence or emission from a medium when

$$|\mu|, \mu_0 \lesssim (4\pi n |f|)^{1/2} / p_0 \ll 1. \quad (21)$$

In Eq. (21) we have $\mu_0 = \cos \vartheta_0$ and $\mu = \cos \vartheta$, where ϑ_0 and ϑ are, respectively, the angles between the inward normal to the surface and the angles of incidence and emission of the particles.

3. ANGULAR SPECTRUM OF BACKSCATTERED PARTICLES AND TOTAL REFLECTION COEFFICIENT

The angular and energy distributions of particles emerging from a medium are described in quantum mechanics by the diagonal elements of the density matrix in the momentum representation²⁰:

$$\rho(\mathbf{p}, \mathbf{p}') = \int d\mathbf{r} d\mathbf{r}' \exp\{-i\mathbf{p}\mathbf{r} + i\mathbf{p}'\mathbf{r}'\} \rho(\mathbf{r}, \mathbf{r}'). \quad (22)$$

Calculation of these elements generally requires integration of Eq. (2) over all three spatial coordinates. However, in the

adopted formulation of the problem, when all the particles emerging from a medium have the same energy E , the angular distribution can be determined if we know the distribution of particles between the components of the momentum parallel to the surface $\mathbf{q} = (q_x, q_y)$ in the limit $z \rightarrow -0$:

$$\rho(\mathbf{q}, z; \mathbf{q}, z) |_{z \rightarrow -0}$$

$$= \int d\mathbf{r}_\perp d\mathbf{r}'_\perp \exp(i\mathbf{q} \cdot (\mathbf{r}_\perp' - \mathbf{r}_\perp)) \rho(\mathbf{r}_\perp, z; \mathbf{r}'_\perp, z) |_{z \rightarrow -0}. \quad (23)$$

The diagonal elements of Eq. (23) are related simply to the angular spectrum of the backscattered particles:

$$\rho(\mathbf{q}, 0; \mathbf{q}, 0) \frac{d\mathbf{q}}{(2\pi)^2} = S(\mu, \varphi) d|\mu| d\varphi \Sigma \quad (24)$$

or

$$S(\mu) = \int_0^{2\pi} S(\mu, \varphi) d\varphi = \frac{p_0^2 |\mu|}{2\pi \Sigma} \rho(q, 0; q, 0), \quad (25)$$

where

$$|\mu| = |\cos \vartheta| = (1 - q^2/p_0^2)^{1/2} \quad (q < p_0),$$

$S(\mu)$ is the density of the flux of particles reaching an element of a solid angle $2\pi d|\mu|$, and Σ is a surface area.

Integrating Eq. (10) in accordance with Eq. (23), we find that

$$\begin{aligned}\rho(\mathbf{q}, 0; \mathbf{q}', 0) &= \Psi_0(\mathbf{q}, 0) \Psi_0^*(\mathbf{q}', 0) \\ &+ |f|^2 (2\pi)^2 \delta(\mathbf{q} - \mathbf{q}') n (2\pi\hbar^2/m)^2 \int_0^\infty dz \\ &\times g_{\mathbf{q}}(0, z) \rho(z, z) g_{\mathbf{q}'}^*(0, z).\end{aligned} \quad (26)$$

Equation (26) readily yields the distribution of incoherently scattered particles:

$$\rho_{\text{in}}(\mathbf{q}, 0; \mathbf{q}, 0) = n (2\pi\hbar^2/m)^2 \Sigma |f|^2 \int_0^\infty dz |g_{\mathbf{q}}(0, z)|^2 \rho(z, z). \quad (27)$$

It follows from Eq. (27) that to calculate the angular distribution of particles emerging from a medium it is necessary to find first the density of the particles $\rho(z, z) = \rho(z)$ in the scattering medium for $z > 0$. A closed equation for the density $\rho(z)$ can be obtained by substituting $\mathbf{r} = \mathbf{r}'$ in Eq. (10):

$$\rho(z) = |\Psi_0(z)|^2 + n \left(\frac{2\pi\hbar^2}{m} \right)^2 |f|^2 \int_0^\infty dz' A(z, z') \rho(z'), \quad (28)$$

where

$$A(z, z') = \int \frac{d\mathbf{q}}{(2\pi)^2} |g_{\mathbf{q}}(z, z')|^2. \quad (29)$$

An explicit expression for the kernel $A(z, z')$ is readily obtained by substituting Eq. (19) into the integral (29).

An analysis shows that an allowance for the refraction and reflection of noncoherently scattered waves [i.e., the first term in Eq. (19) for $g_{\mathbf{q}}(z, z')$ when $z > 0$] changes little the solution of Eq. (28). The corresponding corrections are of the order of the ratio of the width of the angular region where the diffraction effects are important [Eq. (21)] to 4π :

$$\Delta\vartheta/4\pi \sim (n|f|\lambda^2)^{1/2} \ll 1.$$

Consequently, the solution of Eq. (28) can be found in

the form of an expansion in terms of a small parameter $\xi = (n|f|\lambda^2)^{1/2}$:

$$\rho(z) = \rho^{(0)}(z) + \xi \rho^{(1)}(z) + \dots \quad (30)$$

The expression for the angular spectrum of the backscattered waves given by Eq. (27) is also in the form of a series in terms of the parameter ξ . Then, in the leading (in respect to ξ) approximation, the angular spectrum is simply expressed in terms of $\rho^{(0)}(z)$.

Neglecting in the calculation of the integral (29) terms of the order of $(n|f|\lambda^2)^{1/2} \ll 1$, we find that the kernel of Eq. (28) becomes

$$A(z, z') \approx \left(\frac{m}{\hbar^2}\right)^2 \int_{q < p_0} \frac{dq}{(2\pi)^2} \exp\left\{-n\sigma_{tot} \frac{|z-z'|}{(1-q^2/p_0^2)^{1/2}}\right\} \times (p_0^2 - q^2)^{-1} = \frac{1}{2\pi} \left(\frac{m}{\hbar^2}\right)^2 E_1(n\sigma_{tot}|z-z'|), \quad (31)$$

where

$$E_1(x) = \int_1^\infty (dt/t) \exp(-xt)$$

is the exponential integral.²¹

Using Eq. (31), we can reduce Eq. (28) to

$$\rho^{(0)}(z) = |\psi_0(z)|^2 + \frac{n\sigma_{el}}{2} \int_0^\infty dz' E_1(n\sigma_{tot}|z-z'|) \rho^{(0)}(z'), \quad (32)$$

where

$$|\psi_0(z)|^2 = \frac{4k_0^2}{|k_0 + \kappa_0|^2} \exp\left\{-\frac{n\sigma_{tot}z p_0}{\text{Re } \kappa_0}\right\}. \quad (33)$$

Equation (32) differs from the equation for the density of particles in the usual transport theory²² only by the source function $|\psi_0(z)|^2$.

The solution of Eq. (32) $\rho_0(z, \mu_0)$ with the source function

$$I_0(z) = \exp[-n\sigma_{tot}z/\mu_0]$$

is well known.²² The angular spectrum of backscattered particles is then given by the expression²³

$$S_0(|\mu|, \mu_0) = \frac{n\sigma_{el}}{2} \frac{1}{|\mu|} \int_0^\infty dz \exp\left\{-\frac{n\sigma_{tot}z}{|\mu|}\right\} \rho_0(z, \mu_0) = \frac{1}{2} \frac{\sigma_{el}}{\sigma_{tot}} \frac{\mu_0}{|\mu| + \mu_0} H\left(|\mu|, \frac{\sigma_{el}}{\sigma_{tot}}\right) H\left(\mu_0, \frac{\sigma_{el}}{\sigma_{tot}}\right), \quad (35)$$

and the total reflection coefficient (ratio of the number of the backscattered particles to the number of the incident particles) is

$$R_0(\mu_0) = \frac{1}{\mu_0} \int_0^1 d|\mu| |\mu| S_0(|\mu|) = 1 - \left(1 - \frac{\sigma_{el}}{\sigma_{tot}}\right)^{1/2} H\left(\mu_0, \frac{\sigma_{el}}{\sigma_{tot}}\right). \quad (36)$$

In Eqs. (35) and (36) the quantity $H(\mu, \omega)$ is the Chandrasekhar function (Ref. 23).¹⁾ In the classical transport theory the coherent reflection of radiation from the surface is ignored. Therefore, Eqs. (34) and (35) describe the angular spectrum and the backscattering coefficient of an incoherent

wave field under conditions when the refraction and reflection effects can be ignored.

The solution of Eq. (32) with the source function (33) can easily be expressed in terms of the solution $\rho_0(z, \mu_0)$ of the transport theory:

$$\rho^{(0)}(z) = \frac{4k_0^2}{|k_0 + \kappa_0|^2} \rho_0\left(z, \frac{\kappa_0}{p_0}\right). \quad (37)$$

Substituting now Eq. (37) into Eq. (27) for the angular spectrum of backscattered particles, we find that

$$S(|\mu|) = \frac{32p_0 n |f|^2 k_1 k_0^2}{|k_0 + \kappa_0|^2 |k_1 + \kappa_1|^2} \int_0^\infty dz \exp\left[-\frac{n\sigma_{tot}z p_0}{\text{Re } \kappa_0}\right] \times \rho_0\left(z, \frac{\text{Re } \kappa_0}{p_0}\right). \quad (38)$$

The integral (38) is readily calculated using the equality (35). Consequently, the angular distribution of incoherently scattered particles is given by the expression

$$S(\mu) = \frac{1}{2} \frac{\sigma_{el}}{\sigma_{tot}} \frac{4k_0^2}{|k_0 + \kappa_0|^2} \frac{4k_1}{|k_1 + \kappa_1|^2} \frac{\text{Re } \kappa_0 \text{Re } \kappa_1}{\text{Re } \kappa_0 + \text{Re } \kappa_1} \times H\left(\frac{\text{Re } \kappa_0}{p_0}; \frac{\sigma_{el}}{\sigma_{tot}}\right) H\left(\frac{\text{Re } \kappa_1}{p_0}; \frac{\sigma_{el}}{\sigma_{tot}}\right), \quad (39)$$

where the indices 0 and 1 represent, respectively, the incident and emitted (by the medium) particles

$$k_0 = p_0 \mu_0, \quad k_1 = p_0 |\mu|, \quad \kappa_i = (k_i^2 + 4\pi n f_i)^{1/2},$$

$$\text{Re } \frac{\kappa_i}{p_0} = \frac{1}{2^{1/2}} \left[\left(\mu_i^2 + \frac{4\pi n f_i}{p_0^2} \right) + \left\{ \left(\mu_i^2 + \frac{4\pi n f_i}{p_0^2} \right)^2 + \left(\frac{4\pi n f_i}{p_0^2} \right)^2 \right\}^{1/2} \right]^{1/2},$$

$$\frac{|\kappa_i|}{p_0} = \left[\left(\mu_i^2 + \frac{4\pi n f_i}{p_0^2} \right)^2 + \left(\frac{4\pi n f_i}{p_0^2} \right)^2 \right]^{1/2}.$$

At large incidence and emission angles [$\mu_0, |\mu| \gg (n|f|\lambda^2)^{1/2}$] Eq. (39) reduces to the classical result of Eq. (35). At grazing angles ($\mu_0 \ll 1$ or $|\mu| \ll 1$) the difference between $S(\mu)$ and $S_0(\mu)$ is of the order of the quantity $S_0(\mu)$ itself.

If Eq. (39) is integrated with respect to the angles, allowance for the inequality $(n|f|\lambda^2)^{1/2} \ll 1$ yields the following expression for the total incoherent-reflection coefficient

$$R_{in} = \frac{4k_0 \text{Re } \kappa_0}{|k_0 + \kappa_0|^2} \left[1 - \left(1 - \frac{\sigma_{el}}{\sigma_{tot}}\right)^{1/2} H\left(\frac{\text{Re } \kappa_0}{p_0}, \frac{\sigma_{el}}{\sigma_{tot}}\right) \right]. \quad (40)$$

Bearing in mind also that the coherent reflection coefficient of a surface is [see Eq. (17)]

$$R_{coh} = \left| \frac{k_0 - \kappa_0}{k_0 + \kappa_0} \right|^2, \quad (41)$$

we can readily find the total reflection coefficient of particles:

$$R_{tot} = R_{coh} + R_{in} = 1 - 4 \frac{k_0 \text{Re } \kappa_0}{|k_0 + \kappa_0|^2} \left(1 - \frac{\sigma_{el}}{\sigma_{tot}}\right)^{1/2} H\left(\frac{\text{Re } \kappa_0}{p_0}, \frac{\sigma_{el}}{\sigma_{tot}}\right). \quad (42)$$

If the scattering in the medium is purely elastic ($\sigma_{el} = \sigma_{tot}$), the number of backscattered particles is simply

equal to the number of incident particles and we have $R_{\text{tot}} = 1$.

Since Eqs. (39) and (40) are derived including only the first term of the expansion (30), we are essentially assuming that the refraction and reflection effects influence only the transmission of the incident and backscattered particles by the boundary of the medium and do not affect multiple scattering inside the medium. This assumption is based on the inequality $(n|f|\lambda^2)^{1/2} \ll 1$. A correct calculation of the next term of the expansion (30) in powers of $(n|f|\lambda^2)^{1/2}$ and of the corresponding corrections in Eqs. (39) and (40) will generally be outside the framework of the initial transport equation (4) [i.e., it is then necessary to include in Eq. (4) additional terms of higher degree in $(n|f|\lambda^2)^{1/2} \ll 1$].

4. DISCUSSION OF RESULTS

Equations (39) and (42) obtained above represent, respectively, differential distribution of incoherently scattered particles over the angles of emission and the total backscattering coefficient for arbitrary angles of incidence of the initial flux on the surface of a medium and for any ratio of the cross sections of the elastic and inelastic interactions with single atoms.

The dependences (39) and (42) are of the greatest interest at the grazing angles of incidence and emission when $|\mu_i| \sim (4\pi n|f_i|)^{1/2}/p_0$, and when the refraction and reflection effects alter radically the angular spectrum of the backscattered radiation.

We shall begin with an analysis of Eq. (42) for the total backscattering coefficient. At very low grazing angles of incidence when $\mu_0 \ll (4\pi n|f_i|)^{1/2}/p_0$ we find from Eq. (42) that $R_{\text{tot}} = 1$, which is identical with the familiar results obtained in electrodynamics of continuous media.²⁵ The value of R reaches unity because at very low grazing angles practically all the particles are reflected coherently and the coherent reflection coefficient itself tends to unity. The corresponding value found from the classical theory of radiative transfer²³ ignores completely coherent reflection and, therefore, does not give an expression which is correct in the limit $\mu_0 \rightarrow 0$ (Ref. 23):

$$R_{\text{tot}}^0|_{\mu_0 \rightarrow 0} = 1 - (1 - \sigma_{el}/\sigma_{\text{tot}})^{1/2} < 1.$$

If $\mu_0 \gg (4\pi n|f_i|)^{1/2}/p_0$, Eq. (42) becomes identical with Eq. (36) obtained earlier by solving the transport equation. The dependence (42) of the total backscattering coefficient of particles on the angle of incidence $\mu_0 = \cos\vartheta_0$ is plotted in Fig. 1. It follows from the above discussion that the value of R_{tot} found by solving the transport equation (4) for the range of low values of μ_0 is several times greater than the corresponding result obtained from the classical theory of radiative transport. It is also clear from Fig. 1 that the backscattering is stronger for $f_1 < 0$ than for $f_1 > 0$. This behavior of $R_{\text{tot}}(\mu_0)$ follows clearly from Eqs. (15) and (16). In the case when $f_1 < 0$, the scattering medium is optically less dense than vacuum [$\text{Re } U_0 > 0$ is a potential "wall"] and the specular reflection coefficient of waves incident on a surface [Eq. (41)] is higher than in the $f_1 > 0$ case.

We shall now consider the differential angular spectrum of particles leaving a medium as a result of multiple collisions with atoms.

An analysis of the differential angular distribution is

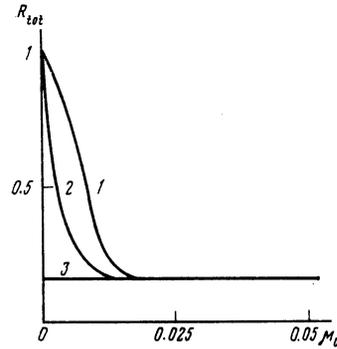


FIG. 1. Dependences of the total reflection coefficient on the direction of incidence of particles on the surface of a substance. The parameters of the scattering medium are $n|f_1|\lambda^2/\pi = 10^{-4}$, $n|f_2|\lambda^2/\pi = 3 \times 10^{-5}$, $\sigma_{el}/\sigma_{\text{tot}} = 0.3$; curves 1 and 2 are calculated on the basis of Eq. (42) for $f_1 < 0$ (curve 1) and $f_2 > 0$ (curve 2); curve 3 is calculated using the theory of radiative transfer.²³

important because of the discovery in 1963 of the anomalous reflection of x rays,²⁶ the onset of an additional nonspecular peak in the angular distribution of radiation scattered at grazing angles from substances with a disturbed surface layer. As pointed out in Refs. 14 and 15, this effect has not yet been explained consistently.

The expression for the reflection function (or the number of particles crossing a unit surface area per unit time in the direction μ) $J(\mu) = |\mu|S(\mu)$ can be deduced from Eq. (39), which gives

$$J(\mu) = \frac{4k_0^2}{|k_0 + \kappa_0|^2} \frac{4k_1^2}{|k_1 + \kappa_1|^2} \frac{1}{4\pi} \frac{\sigma_{el}}{\sigma_{\text{tot}}} \frac{\text{Re}(\kappa_0/p_0) \text{Re}(\kappa_1/p_0)}{\text{Re}(\kappa_0/p_0) + \text{Re}(\kappa_1/p_0)} \times H\left(\text{Re} \frac{\kappa_0}{p_0}, \frac{\sigma_{el}}{\sigma_{\text{tot}}}\right) H\left(\text{Re} \frac{\kappa_1}{p_0}, \frac{\sigma_{el}}{\sigma_{\text{tot}}}\right). \quad (43)$$

The symmetry of Eq. (43) under transposition of μ_0 and μ_1 is a consequence of the reciprocity theorem. Comparing Eq. (43) with $J_0(\mu) = |\mu|S_0(\mu)$ of Eq. (35), we note that (apart from a factor) the formula for the angular spectrum of Eq. (43) can be obtained from the classical expression (35) if we replace the arguments of μ_0 and μ by $\text{Re}(\kappa_i/p_0)$ ($i = 0, 1$). Such a transformation in the $f_2 = 0$ case can be explained quite simply: along the direction $|\mu| = |\cos\vartheta|$ we observe waves in vacuum which had traveled in a medium in the direction $\mu = \kappa_1/p_0$ and were refracted on crossing the boundary of a substance. If $f_1 < 0$ (when the medium is optically less dense than vacuum) the waves incident on the interface from inside along the direction $\cos\vartheta \rightarrow 0$ emerge from the investigated substance at a finite angle $[|\mu_c| = |\cos\vartheta_c| = (4\pi n|f_1|)^{1/2}/p_0]$. Since inside the medium the flux density of backscattered particles always has a peak in the direction $\mu = 0$ if $\mu_0 \ll 1$ [Eq. (35)], the refraction shifts this peak by an amount equal to the critical angle $\vartheta_c = \cos^{-1}\mu_c$. Consequently, in the case of the grazing incidence of particles on a surface optically less dense than vacuum the scattering medium exhibits not only a specular peak in the angular distribution of incoherently scattered radiation, but also a maximum near the critical angle ϑ_c (see the Appendix).

On the other hand, if $f_1 > 0$, this peak does not appear because particles moving inside the medium along the direction $\mu = 0$ may not leave the investigated medium because of

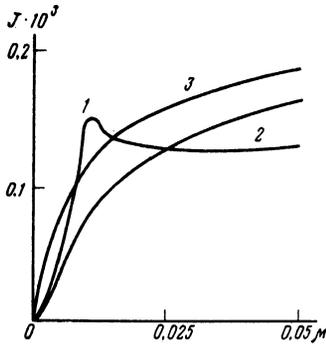


FIG. 2. Dependence of the reflection function on the direction of emission of particles from a medium. Parameters of the scattering medium: $n|f_1|\lambda^2/\pi = 10^{-4}$, $n|f_2|\lambda^2/\pi = 3 \times 10^{-5}$, $\sigma_{el}/\sigma_{tot} = 0.3$. The direction of incidence of particles when the medium is $\mu_0 = 0.009$; curves 1 and 2 are calculated on the basis of Eq. (43) for $f_1 < 0$ (curve 1) and $f_1 > 0$ (curve 2); curve 3 is calculated using the radiative transfer theory.²³

reflection by its boundary. Therefore, the angular spectrum of incoherently scattered radiation depends monotonically on the emission angle μ if $f_1 > 0$.

The angular spectra of scattered particles calculated from Eqs. (39) and (43), confirming the pattern described above, are shown in Fig. 2. In particular, the $J(\mu)$ curve corresponding to $f_1 < 0$ shows clearly a peak near

$$\mu_c = (4\pi n |f_1|)^{1/2} / p_0.$$

In spite of the fact that the model of isotropic scattering discussed above is unsuitable for the description of the interaction of x rays with a disturbed layer of matter, the angular distribution of the scattered particles described by Eq. (43) for the case $f_1 < 0$ is similar to that found experimentally.^{26, 13-15} It is quite possible that the anomalous reflection of

x rays and γ photons^{26, 13-15} is due to the refraction and reflection of incoherently scattered waves on transition from a material medium into vacuum.

It should be pointed out that the nature of the anomalous reflection is an analog of the formation of the Kikuchi patterns formed as a result of diffraction of inelastically scattered electrons in thick crystals¹⁰ or of the Kossel lines formed as a result of diffraction of γ photons and neutrons.²⁷

It follows from the above analysis that the anomalous reflection effect is associated with the refraction and reflection of scattered waves at the interface between media and it occurs quite commonly. Clearly, this effect can be observed for radiations of any type (for example photons, neutrons, and charged particles) in the case of grazing incidence on a surface separating "transparent" and scattering media.

CONCLUSIONS

We found the solution of the transport equation for multiple scattering in a disordered substance allowing for the reflection and refraction of waves at the boundary of a substance. In the isotropic scattering case we calculated the dependence of the total reflection coefficient on the angle of incidence of radiation on the surface of a substance and the angular spectrum of particles emitted by the substance. The solution obtained demonstrates the possibility of anomalous reflection of radiations of any type, for example, photons or neutrons. In particular, we can expect the angular resolution of the existing neutron spectrometers^{28, 29} to be sufficient for the observation of this effect.

APPENDIX

We shall analyze in detail Eq. (43). We consider first the simplest case when $f_2 = 0$. The relationship (43) then becomes

$$J(\mu) = \frac{\sigma_{el}}{4\pi\sigma_{tot}} \frac{4\mu_0^2}{(\mu_0 + (\mu_0^2 - \mu_c^2)^{1/2})^2} \frac{4\mu^2}{(|\mu| + (\mu^2 - \mu_c^2)^{1/2})^2} \frac{(\mu_0^2 - \mu_c^2)^{1/2} (\mu^2 - \mu_c^2)^{1/2}}{(\mu_0^2 - \mu_c^2)^{1/2} + (\mu^2 - \mu_c^2)^{1/2}} H\left(\frac{\mu_0^2 - \mu_c^2}{\mu_0^2 - \mu_c^2}, \frac{\sigma_{el}}{\sigma_{tot}}\right) H\left(\frac{\mu^2 - \mu_c^2}{\mu^2 - \mu_c^2}, \frac{\sigma_{el}}{\sigma_{tot}}\right), \quad (A.1)$$

where

$$(\mu_0^2 - \mu_c^2)^{1/2} = \text{Re}(\kappa_0/p_0)|_{f_2=0}, \quad (\mu^2 - \mu_c^2)^{1/2} = \text{Re}(\kappa_l/p_0)|_{f_2=0}.$$

From the physical point of view the limit $f_2 \rightarrow 0$ corresponds to ignoring the processes of scattering during the passage of waves or particles across the medium-vacuum interface.

The quantities

$$D_0 = 4\mu_0(\mu_0^2 - \mu_c^2)^{1/2} / (\mu_0 + (\mu_0^2 - \mu_c^2)^{1/2})^2,$$

$$D_1 = 4|\mu|(\mu^2 - \mu_c^2)^{1/2} / (|\mu| + (\mu^2 - \mu_c^2)^{1/2})^2$$

in Eq. (A.1) represent the transmission coefficients of a surface for incident and backscattered waves. The quantity

$$S_{in}(\mu) = \frac{\sigma_{el}}{4\pi\sigma_{tot}} \frac{4\mu_0^2}{(\mu_0 + (\mu_0^2 - \mu_c^2)^{1/2})^2} \frac{(\mu_0^2 - \mu_c^2)^{1/2}}{(\mu_0^2 - \mu_c^2)^{1/2} + (\mu^2 - \mu_c^2)^{1/2}} \times H\left(\frac{\mu_0^2 - \mu_c^2}{\mu_0^2 - \mu_c^2}, \frac{\sigma_{el}}{\sigma_{tot}}\right) H\left(\frac{\mu^2 - \mu_c^2}{\mu^2 - \mu_c^2}, \frac{\sigma_{el}}{\sigma_{tot}}\right) \quad (A.2)$$

is the density of the particle flux incident on a surface from the interior of a scattering medium, but before refraction at

the boundary. An allowance is made in Eq. (A.2) for the fact that not all the incident particles penetrate the medium and some are reflected coherently.

At grazing angles of incidence and scattering $\mu_0, |\mu| \ll 1$ the Chandrasekhar functions in Eq. (A.2) for S_{in} can be assumed to be approximately unity.^{23, 24} Then,

$$S_{in}(\mu) \approx \frac{\sigma_{el}}{4\pi\sigma_{tot}} \frac{(\mu_0^2 - \mu_c^2)^{1/2}}{(\mu_0^2 - \mu_c^2)^{1/2} + (\mu^2 - \mu_c^2)^{1/2}}. \quad (A.3)$$

If $|\mu_0 - \mu_c| \ll \mu_c$ the particle density flux S_{in} governed by Eq. (A.3) has a sharp maximum at $|\mu| = \mu_c$. The appearance of a second maximum is due to a large number of particles which travel practically parallel to the surface before they cross the boundary between the investigated medium and vacuum.

The existence of a maximum of the reflection function $J(\mu)$ of Eq. (A.1) is due to competition between two factors: a fall of the quantity $S_{in}(\mu)$ and an increase in the transmission coefficient $D_1(\mu)$ on increase in $(\mu^2 - \mu_c^2)^{1/2}$ [$D_1(\mu)$ is a square-root singularity and $|\mu| = \mu_c$: $D_1(\mu) \approx (\mu^2 - \mu_c^2)^{1/2}$]. It is then found that $J(\mu)$ has a

maximum only if $|\mu_0 - \mu_c| \ll \mu_c [|\mu|_{\max} = \mu_0 + 1/4(\mu_0^2 - \mu_c^2)^{1/2}]$. For example, if $\mu_0 = 1.03\mu_c$, then $|\mu|_{\max} \approx 1.055\mu_c$.

Inclusion in Eq. (43) of the imaginary part of the scattering amplitude does not alter the physical meaning of the factors occurring in Eq. (43). In particular, the factor $D_1 = 4k_1 \operatorname{Re}(\kappa_1/p_0)/|k_1 + \kappa_1|^2$ represents the transmission coefficient of scattered waves crossing the boundary of the investigated medium. In contrast to the above case, when $f_2 \neq 0$ the transmission coefficient D_1 does not vanish abruptly at $|\mu| = \mu_c$ and the square-root singularity disappears [$D_1(\mu_c) \neq 0$]. Consequently, the behavior of the reflection function is governed mainly by the behavior of the function S_{in} at $|\mu| \sim \mu_c$. Consequently, the anomalous reflection peak is sharper than for $f_2 = 0$. As f_2 is increased, the peak broadens and it disappears for $f_2 \gtrsim |f_1|$.

It should be pointed out that if $f_2 \neq 0$, the reflection function $J(\mu)$ does not vanish also if $|\mu|, \mu_0 \lesssim \mu_c$. With decrease of μ_0 ($\mu_0 < \mu_c$), the value of $|\mu|_{\max}$ tends to μ_c .

The nonzero value of the reflection function in the $f_2 = 0$ case for $|\mu|, \mu_0 \lesssim \mu_c$ is associated with the contribution to $J(\mu)$ made by barrier processes of crossing the boundary of a medium by particles which have been scattered at distances of the order of λ/μ_c from the surface.

¹⁾For $H(\mu, \omega)$ in a square defined by $0 \leq \mu < 1, 0 \leq \omega < 1$ we find that the following approximate formula²⁴ is accurate to within 1%:

$$H(\mu, \omega) = \frac{1 + 3^{1/2}\mu}{1 + (3(1-\omega))^{1/2}\mu} \times \left[1 - \frac{\omega}{4} (1 + \omega^3)\mu (\ln \mu + 1.33 - 1.458\mu^{0.82}) \right].$$

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