

# Multiple Scattering of Waves in 3D Crystals (Natural or Photonic) Formed by Anisotropically Scattering Centers

Baryshevsky V.G., Gurnevich E.A.

Research Institute for Nuclear Problems, Belarusian State University,  
11 Bobruiskaya Str., Minsk 220050, Belarus;  
e-mail: bar@inp.bsu.by; genichgurn@gmail.com

## Abstract

This paper considers the refraction and diffraction of waves in three-dimensional crystals formed by anisotropically scattering centers. The partial wave expansion method is used to consider the effect of multiple rescattering of waves by centers composing a crystal. The expression for the refractive index of a crystal is derived. It is shown that instead of the diagonal elements of the scattering matrix  $\mathbf{T}$ , appearing in the expression for the refractive index of a chaotic medium, the derived expression includes the diagonal elements of the reaction matrix  $\mathbf{K}$ . This fact is taken into account in writing the equations describing the dynamical diffraction of waves in a crystal.

The results can be of interest for research into, e.g., diffraction of cold neutrons and photons in crystals, nanocrystalline materials, as well as for the description of parametric and diffraction radiation in electromagnetic crystals formed by anisotropically scattering centers.

## 1 Introduction

For waves of different nature (photons, neutrons, etc.), the index of refraction,  $n$ , in the medium composed of chaotically distributed identical centers can be expressed in terms of the amplitude of elastic scattering by a single center as follows [1, 2, 3, 4]:

$$n^2 = 1 + \frac{4\pi\rho}{k^2}f(0). \quad (1)$$

Here  $\rho$  is the density of scatterers (the number of scatters per 1 cm<sup>3</sup> of matter) and  $f(0)$  is the forward elastic scattering amplitude, which is a complex number.

According to the optical theorem [2, 3, 4], the imaginary part of the amplitude  $f(0)$  of coherent elastic scattering at zero angle is related to the total cross section  $\sigma$  of scattering by the center as

$$\text{Im } f(0) = \frac{k\sigma}{4\pi}, \quad (2)$$

where  $\sigma = \sigma_{el} + \sigma_r$  with  $\sigma_{el}$  being the elastic scattering cross section and  $\sigma_r$  is the reaction cross section. Thus, according to (1), even in the case of elastic scattering ( $\sigma_r = 0$ ) by individual centers, the refractive index  $n$  has an imaginary part describing the attenuation of waves in the medium. Such attenuation occurs because the waves scattered at nonzero angles acquire a random phase due to chaotic distribution of scatterers.

When the waves are scattered in crystals, the situation is quite different, because the scatterers in this case are periodically distributed in space [3, 6, 7], and the phases of rescattered waves are not random. As a result, in the case of purely elastic scattering of waves by the centers composing a crystal, the refractive index should not contain an imaginary part, i.e., it should be real. For example, according to [3, 7, 8], for isotropic scattering of neutrons by crystal nuclei (the scattering amplitude  $f$  in this case is independent of the scattering angle – this is true for thermal and cold neutrons, whose wavelength  $\lambda$  is much larger than the nuclear radius  $R_n$ ) multiple rescattering of waves by the centers (nuclei), composing the crystal, leads to the following expression for the refractive index:

$$n^2 = 1 + \frac{4\pi}{k^2\Omega_3} \frac{f}{1 + ikf}, \quad (3)$$

where  $\Omega_3$  is the unit cell volume of the crystal, i.e.,

$$n^2 = 1 + \frac{4\pi}{k^2\Omega_3} \frac{f(1 - ikf^*)}{|1 + ikf|^2} = 1 + \frac{4\pi}{k^2\Omega_3} \frac{\text{Re } f}{|1 + ikf|^2}. \quad (4)$$

In deriving (4) we used the optical theorem (2) and took into account that for isotropic elastic scattering  $\sigma = 4\pi|f|^2$ . As we can see from (4), multiple rescattering of waves in crystals causes the refractive index to become real.

Let us recall that (3) is derived under the assumption that the wave is isotropically scattered by the scattering center. This assumption is true, e.g., for thermal and cold neutrons, whose wavelength  $\lambda$  is much larger than the nuclear radius. However, various artificial crystals (metamaterials), which are currently being studied, are composed of the elements comparable in size with the wavelength of the incident radiation (photons, cold and ultra-cold neutrons). As a consequence, the amplitude of wave scattering by the center becomes dependent on the scattering angle. Moreover, the scattering amplitude can depend on the scattering angle even when the wavelength is large compared to the size of the scatterer; this is true, e.g., for scattering of electromagnetic waves. In this regard, one may wonder what the expression for the refractive index will look like in this case, and what equation will describe diffraction in crystals composed of such scatterers.

The refraction and diffraction of photons in artificial (electromagnetic, photonic) crystals built from metallic wires have been considered previously in [9, 10, 11, 12]. The characteristic feature of electromagnetic wave scattering by a wire is that the scattering amplitude is independent of the scattering angle if the wave has a polarization parallel to the wire and a wavelength  $\lambda$  much larger than the wire's radius, while for wave polarization orthogonal to the wire, the scattering amplitude  $f$  depends on the scattering angle even for the wavelengths  $\lambda$  much larger than the wire's radius [10, 11]

$$f = f_0 + f_1 \cos \theta. \quad (5)$$

A detailed analysis given in [10, 11] has shown that in the case of angular dependence (5), the following expression for the refractive index is valid:

$$n^2 = 1 + \frac{4\pi}{k^2\Omega_3} \left\{ \frac{f_0}{1 + ikf_0} + \frac{f_1}{1 + i\frac{k}{3}f_1} \right\}. \quad (6)$$

According to (6), in the case of purely elastic scattering, multiple rescattering of waves in crystals leads to the absence of an imaginary part in  $n^2$ .

The present paper considers the refraction and diffraction of waves in three-dimensional crystals built from the centers scattering the incident wave anisotropically. Here the results of [11] are generalized to the case of arbitrary angular dependence  $f(\theta)$ . We derive the expression for the refractive index and the equations describing dynamical diffraction of waves that generalize the equations of dynamical diffraction of X-rays and neutrons in crystals to this case.

## 2 Scattering by a single center

### 2.1 Method of partial waves

For concreteness, let us consider scattering of a scalar wave by a spherically symmetric potential. Because the angular momentum in a spherically symmetric field is conserved, it appears reasonable to present the initial plane wave  $\Psi_0(\vec{r}) = e^{i\vec{k}\vec{r}}$  as a superposition of spherical waves with different angular momenta (partial waves) and consider scattering of each of these waves separately. Let us recall here that the wave function of a state with angular momentum  $l$  and the projection thereof  $m$  can be expressed as [4]

$$\psi_{klm} = R_{kl}(r)Y_{lm}(\theta, \varphi),$$

where  $Y_{lm}$  are the spherical functions, and the radial function  $R_{kl}$  has the form

$$R_{kl}(r) = 2kj_l(kr), \quad (7)$$

where  $j_l$  are the so-called spherical Bessel functions. Knowing the asymptotic behavior of the Bessel functions, we find  $R_{kl} \approx \frac{2}{r} \sin(kr - \frac{\pi l}{2})$  far from and  $R_{kl} \approx \frac{2k^{l+1}}{(2l+1)!!} r^l$  near the origin of coordinates.

In place of the functions  $R_{kl}$ , the scattering theory often uses the functions  $R_{kl}^\pm(r) = \pm ikh_l^{(1,2)}(kr)$  corresponding to spherical waves converging towards (the minus sign and the spherical Hankel function of the second kind) and diverging from the center (the plus sign and the Hankel function of the first kind). The limiting expressions for the functions  $R_{kl}^\pm$  at  $kr \gg 1$  and near the origin of coordinates have the form

$$R_{kl}^\pm \approx \frac{1}{r} e^{\pm i(kr - \pi l/2)}, \quad kr \gg 1; \quad (8)$$

$$R_{kl}^\pm \approx \frac{(2l-1)!!}{k^l} r^{-l-1}, \quad r \rightarrow 0, \quad (9)$$

where  $(2l-1)!! = 1 \cdot 3 \cdot 5 \cdot \dots \cdot (2l-1)$ .

Let an initial plane wave propagate along the  $z$ -axis in the Cartesian coordinate system:  $\Psi_0(\vec{r}) = e^{i\vec{k}\vec{r}} \equiv e^{ikz}$ . The scatterer is located at the origin of coordinates. Because the function  $e^{ikz}$  is axially symmetric about the  $z$ -axis, its partial-wave expansion contains only spherical functions that are independent of the angle  $\varphi$  (i.e.,  $m=0$ ) and has the form (as shown, for example, in [4]):

$$e^{ikz} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos \theta) = -\frac{i}{2k} \sum_{l=0}^{\infty} (2l+1) i^l (R_{kl}^+ - R_{kl}^-) P_l(\cos \theta), \quad (10)$$

where  $P_l$  are the Legendre polynomials. In view of (8), we can easily see that far from the center, each partial wave in (10) is a sum of two spherical waves: diverging from and converging towards the center.

The solution of the scattering problem for  $\Psi(\vec{r})$  can be sought in a similar form as in (10):

$$\Psi(\vec{r}) = -\frac{i}{2k} \sum_{l=0}^{\infty} (2l+1) i^l P_l(\cos \theta) R_l^*(r), \quad (11)$$

where  $R_l^*(r)$  is the function of interest. Since the interaction between the incident wave (incident particle flow) and the scattering potential will affect only the amplitude of spherical waves diverging from the center, the asymptotic expression for  $R_l^*(r)$  at  $kr \gg 1$  can be written in the form [13]

$$-\frac{i}{2k} R_l^*(r) = -\frac{i}{2k} (S_l R_{kl}^+ - R_{kl}^-) = j_l(kr) - \frac{i}{2k} (S_l - 1) R_{kl}^+ \approx \frac{1}{kr} \sin(kr - l\pi/2) + \frac{i}{2} (1 - S_l) \frac{e^{i(kr - l\pi/2)}}{kr}. \quad (12)$$

The coefficient  $S_l$  is the diagonal matrix element of the scattering matrix  $S$  and corresponds to the orbital angular momentum  $l$  [4, 13].

Thus the wave function  $\Psi(\vec{r})$  at  $kr \gg 1$  can finally be presented as a sum of the incident plane wave and the scattered spherical wave diverging from the center

$$\Psi(\vec{r}) = \Psi_0(\vec{r}) + \Psi_{sc}(\vec{r}) = \Psi_0 + f(\theta) \frac{e^{ikr}}{r}. \quad (13)$$

Using (10) and (12)-(13), one can easily find that the scattering amplitude  $f(\theta)$  is expressed in terms of the matrix elements of the scattering matrix as<sup>1</sup>

$$f(\theta) = \frac{i}{2k} \sum_{l=0}^{\infty} (2l+1)(1-S_l)P_l(\cos\theta) \equiv \sum_{l=0}^{\infty} f_l P_l(\cos\theta), \quad (14)$$

where the notation  $f_l = \frac{i}{2k}(2l+1)(1-S_l)$  is introduced. The scattered wave at  $kr \gg 1$  has the form

$$\Psi_{sc}(\vec{r}) = -\frac{i}{2k} \sum_{l=0}^{\infty} (2l+1)i^l(S_l-1)R_{kl}^+(r)P_l(\cos\theta) = \sum_{l=0}^{\infty} i^l f_l R_{kl}^+(r)P_l(\cos\theta) \approx f(\theta) \frac{e^{ikr}}{r}. \quad (15)$$

For further consideration it is convenient to establish how the amplitude of a partial wave, which acts directly on the scatterer, relates to the amplitude of the resulting scattered wave. This can easily be done by term-by-term comparison of the expressions (15) for the scattered wave and (10) for the incident wave with the limiting values of  $j_l(kr)$  as  $r \rightarrow 0$  (i.e., near the scatterer) substituted for the functions  $j_l(kr)$ . As a result, we have that if the partial wave  $\Psi_l^0 = i^l k^l r^l P_l(\cos\theta)$  acts on the scatterer, then the scattered wave far from it has the form

$$\Psi_l^{sc} = (2l-1)!! i^l f_l R_{kl}^+(r)P_l(\cos\theta) \approx (2l-1)!! f_l \frac{e^{ikr}}{r} P_l(\cos\theta). \quad (16)$$

## 2.2 Scattering matrix

In the general case, it is convenient for describing the scattering process to introduce the operator  $\hat{T}$  (the so-called  $T$ -operator or  $T$ -matrix), whose matrix elements on the energy surface are related to the matrix elements of the scattering matrix  $S$  as [13]

$$S_{ba} = \delta_{ba} - 2\pi i T_{ba} \delta(E_b - E_a), \quad (17)$$

where  $E_b$  and  $E_a$  are the total energy of the final  $b$  and the initial  $a$  states, respectively. Let us recall here that the matrix elements of the  $T$  matrix are proportional to the scattering amplitude (or the reaction amplitude, if a reaction takes place). Particularly, partial amplitudes  $f_l$  can be expressed in terms of matrix elements  $T_l$  in a rather simple way

$$f_l = -\frac{\pi}{k}(2l+1)T_l. \quad (18)$$

Sometimes it is more convenient to define the asymptotic behavior of the wave function at infinity in the form of standing waves [14], rather than in the form of a superposition of converging and diverging waves as is done in (12)

$$R_l \sim \sin(kr - \frac{l\pi}{2}) + K_l \cos(kr - \frac{l\pi}{2}). \quad (19)$$

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<sup>1</sup>The convergence conditions for this series, see in [4].

In the standing-wave representation, a new operator  $\hat{K}$  acts as a scattering operator (the corresponding matrix is usually called the reaction matrix). Like the operator  $\hat{T}$ , this operator allows one to solve any scattering problem [14, 15].

Let us note that in contrast to  $T$  and  $S$ , the reaction matrix  $K$ , introduced here, is Hermitian ( $K^\dagger = K$ ), and so its eigenvalues are real. Matrix elements of the operator  $\hat{K}$  on the energy surface are related to the matrix elements of the  $T$ -matrix by the so-called Heitler equations [2, 15]

$$K_{ba} = T_{ba} + i\pi \sum_c K_{bc} T_{ca} \delta(E_c - E_a). \quad (20)$$

Relation (20) takes rather a simple form if the matrices  $K$  and  $T$  are diagonal – for example, when the orbital angular momentum is conserved, then for every partial wave having the moment  $l$  we have

$$K_l = \frac{T_l}{1 - i\pi T_l}. \quad (21)$$

### 3 Propagation of waves in crystals

Let us proceed to the consideration of wave scattering in crystals. To begin with, we shall consider the case when the diffraction conditions are not fulfilled, and a single refracted wave propagates in the crystal. Following [11], we assume that the amplitude of scattering by a single center is small,  $k|f(\theta)| \ll 1$ , and the refractive index is close to unity,<sup>2</sup>  $|n^2 - 1| \ll 1$ .

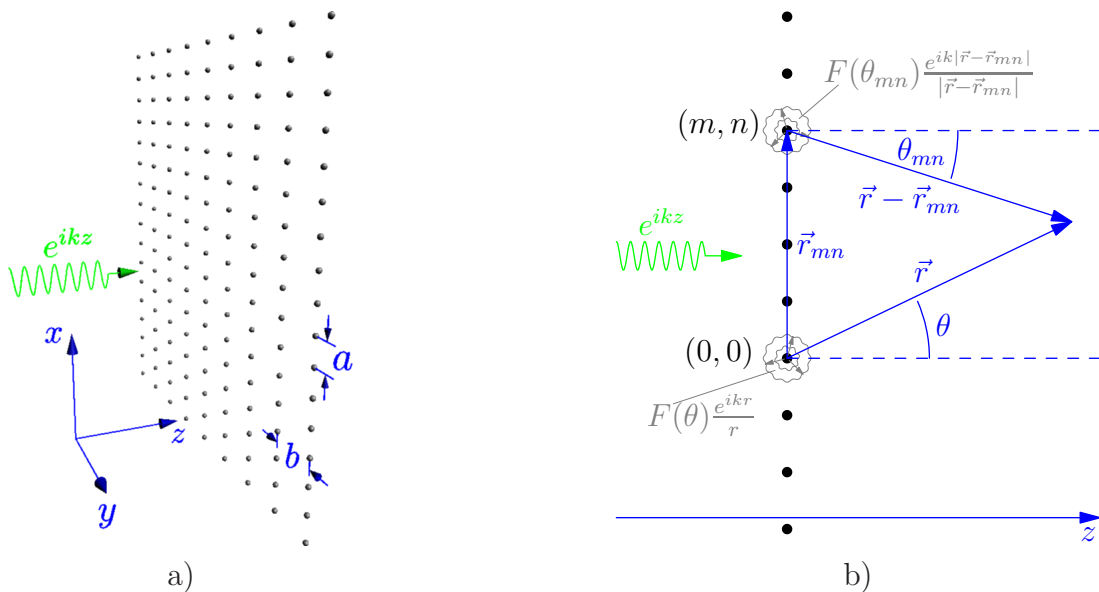


Figure 1: Plane-wave scattering by a two-dimensional grating: a) 3D view; b) relation between the polar angles  $\theta$  and  $\theta_{m,n}$ .

We shall first analyze scattering by one crystal plane. Let a plane wave  $\Psi_0 = e^{ikz}$  be normally incident on a two-dimensional grating composed of scattering centers (see Fig. 1). Let us specify

<sup>2</sup>In the general case, the denominator of the expression for the effective scattering amplitude in (3) should have the form  $1 + iC_1(k)A + C_2(k)A$ , where  $C_1(k)$  and  $C_2(k)$  are the real coefficients (see e.g. [7]). If  $|n^2 - 1| \ll 1$ , then multiple rescattering of waves by the centers composing the crystal has a significant influence only on the imaginary part of the refractive index, having practically no effect on its real part, and we only need to find  $C_1(k)$ . If  $n$  differs significantly from unity, we need to calculate both  $C_1(k)$  and  $C_2(k)$ . The relevant example can also be found in [9, 16] that discuss a two-dimensional crystal built from metallic threads (wires). In a long-wave approximation, the refractive index of such a crystal can be appreciably different from unity. In the present paper we shall focus only on calculating  $C_1(k)$ .

the coordinates of the scatterers in the form  $\vec{r}_{m,n} = (x_{m,n}, y_{m,n}, z_{m,n}) = (ma, nb, 0)$ , where  $m, n$  are the integers, while  $a$  and  $b$  are the grating periods. Multiple scattering is (for the moment) ignored. Then the wave  $\Psi(\vec{r})$  that has passed through the grating can be written as a sum of the incident plane wave and spherical waves scattered with the amplitude  $f(\theta)$

$$\Psi(\vec{r}) = e^{ikz} + ik \sum_{m,n,l} i^l f_l h_l(k|\vec{r} - \vec{r}_{m,n}|) P_l(\cos \theta_{m,n}), \quad (22)$$

where  $\theta_{m,n}$  is the angle between vectors  $\vec{k}$  and  $\vec{r} - \vec{r}_{m,n}$ . This sum can be transformed using the Poisson summation formula. Particularly, at  $l = 0$  the summation over  $m$  and  $n$  yields

$$ik \sum_{m,n} h_0(k|\vec{r} - \vec{r}_{m,n}|) = \sum_{m,n} \frac{e^{ik|\vec{r} - \vec{r}_{m,n}|}}{|\vec{r} - \vec{r}_{m,n}|} = \frac{2i\pi}{kab} e^{ik|z|} + \frac{1}{ab} \sum_{m,n \neq (0,0)} \Phi\left(\frac{2\pi m}{a}, \frac{2\pi n}{b}\right), \quad (23)$$

where the function  $\Phi(\alpha, \beta)$  is defined as follows

$$\Phi(\alpha, \beta) = \begin{cases} \frac{2i\pi e^{-i(\alpha x + \beta y)}}{\sqrt{k^2 - \alpha^2 - \beta^2}} e^{i\sqrt{k^2 - \alpha^2 - \beta^2}|z|}, & \text{when } k^2 > \alpha^2 + \beta^2; \\ \frac{2\pi e^{-i(\alpha x + \beta y)}}{\sqrt{\alpha^2 + \beta^2 - k^2}} e^{-\sqrt{\alpha^2 + \beta^2 - k^2}|z|}, & \text{when } k^2 < \alpha^2 + \beta^2. \end{cases} \quad (24)$$

For simplicity, let us assume that the conditions  $ka < 2\pi$  and  $kb < 2\pi$  are fulfilled. Then the second term in (23) appears to be a strongly attenuating wave, and at large values of  $z$  (as a rule, when  $z$  becomes  $z \sim a, b$ ), we obtain that a plane wave with the amplitude  $A = (1 + \frac{2i\pi f_0}{kab})$  is produced through the interaction between a plane wave with unit amplitude  $e^{ikz}$  and a plane grating.

Let us note that at large values of  $k$ , instead of one plane wave produced through scattering, several plane waves with wave vectors pointing in different directions may appear. When, for example,  $2\pi < ka < 4\pi$  and  $kb < 2\pi$ , it follows from (23)-(24) that the resulting field, induced through scattering by a plane grating, is a superposition of three plane waves with wave vectors  $k\vec{e}_z$ ,  $\frac{2\pi}{a}\vec{e}_x + \sqrt{k^2 - (2\pi/a)^2}\vec{e}_z$ , and  $-\frac{2\pi}{a}\vec{e}_x + \sqrt{k^2 - (2\pi/a)^2}\vec{e}_z$  ( $\vec{e}_x$  and  $\vec{e}_z$  are the versors of a Cartesian coordinate system). However, by means of simple but cumbersome calculations (step-by-step consideration of the cases  $2\pi < ka < 4\pi$ ,  $4\pi < ka < 6\pi$ ,  $2\pi < kb < 4\pi$ , etc.) we can rigorously show that taking account of additional waves has no influence on the final result for the crystal refractive index and it remains valid for any values of  $k$  beyond the conditions of diffraction.

Knowing the value of the sum over  $m$  and  $n$  at  $l = 0$  in (22), we can calculate the sums for  $l \neq 0$  using the well-known recurrent relations for Legendre polynomials and spherical Hankel functions [17, 18]. We can readily show that taking sums over  $m$  and  $n$  for all  $l$  gives the already known result  $\frac{2i\pi}{kab} e^{ikz}$ ; then we finally obtain the following expression for the wave that has passed through the grating:

$$\Psi(\vec{r}) \approx e^{ikz} + \frac{2i\pi}{kab} e^{ikz} \sum_l f_l = \left(1 + \frac{2i\pi}{kab} f(0)\right) e^{ikz}, \quad (25)$$

where  $f(0)$  is the zero-angle scattering amplitude. Analyzing the successive scattering of waves by several ( $m$  number) gratings spaced a distance  $c$  apart, we obtain the following expression for the transmitted wave:

$$\Psi(\vec{r}) = \left(1 + \frac{2i\pi}{kab} f(0)\right)^m e^{ikz}.$$

It can be presented in the form  $\Psi(\vec{r}) = e^{iknz}$ , where the refractive index  $n$  is defined by the equality (valid when  $|n - 1| \ll 1$ )

$$n \approx 1 + \frac{2\pi}{k^2 \Omega_3} f(0), \quad (26)$$

where  $\Omega_3 = abc$  is the unit cell volume of the crystal. This equality coincides with the expression for  $n$  in the case of chaotically distributed scatterers [3].

In the above analysis we ignored the influence of multiple rescattering of waves on the scattering process. In actuality, each center scatters not only the initial plane wave, but also spherical waves, which have been scattered by all other centers. Let us take into consideration this multiple rescattering of waves by the centers composing a crystal. Let us first analyze the process of rescattering by one crystal plane. Obviously, in the general case the wave is the sum of the initial incident wave and spherical waves, which diverge from each center. But, unlike the case described in (22), their amplitudes will differ from the amplitude  $f(\theta)$  of scattering by a single center.

Let  $F(\theta)$  denote the amplitude of scattering by the center that is a part of a crystal plane. In a similar manner as we considered the amplitude  $f(\theta)$ , we can expand the amplitude  $F(\theta)$  using Legendre polynomials and write  $F(\theta)$  in the form  $F(\theta) = \sum_l F_l P_l(\cos \theta)$ . Since the grating is infinite and periodic in the  $(x, y)$  plane, the scattering amplitude  $F(\theta)$  is independent of the position of the scatterer  $(m, n)$  in this plane. As a consequence, we only need to find the value of  $F(\theta)$  for the scatterer located at the origin of coordinates (for brevity's sake it will be termed "reference scatterer").

To obtain the equation for  $F(\theta)$ , let us note that there are two waves scattered by the reference center: the initial plane wave  $\Psi_0 = e^{ikz}$  and the wave

$$\Psi_{sc,0} = ik \sum_{(m,n) \neq (0,0), l} i^l F_l h_l(k|\vec{r} - \vec{r}_{m,n}|) P_l(\cos \theta_{m,n}),$$

coming from all other centers. As a result of scattering of these two waves, a diverging spherical wave of amplitude  $F(\theta)$  is produced.

To analyze the scattering process using the method described in section 2, we only need to properly perform the partial-wave expansion of the wave  $\Psi_{sc,0}$ . Let us consider a wave scattered by the center  $(m, n)$ :

$$\Psi_{sc}^{(m,n)} = ik \sum_{l=0}^{\infty} i^l F_l h_l(k|\vec{r} - \vec{r}_{m,n}|) P_l(\cos \theta_{m,n}).$$

We can see that for the angles  $\theta_{m,n}$  and  $\theta$ , the following relation holds (see Fig. 1, b)):

$$\cos \theta_{m,n} = \frac{r}{|\vec{r} - \vec{r}_{m,n}|} \cos \theta. \quad (27)$$

Then in the vicinity of the reference scatterer ( $r \rightarrow 0$ ), the wave  $\Psi_{sc}^{(m,n)}$  has the form

$$\Psi_{sc}^{(m,n)} = ik \sum_{j=0}^{\infty} i^j F_j h_j(kr_{m,n}) P_j \left( \frac{r}{r_{m,n}} \cos \theta \right). \quad (28)$$

Legendre polynomials of argument  $\cos \theta \cdot r/r_{m,n}$  can be expanded in Legendre polynomials of argument  $\cos \theta$

$$P_j \left( \frac{r}{r_{m,n}} \cos \theta \right) = \sum_{l=0}^{\infty} \frac{1}{2} \alpha_{lj} P_l(\cos \theta), \quad (29)$$

where

$$\alpha_{lj} = (2l + 1) \int_0^{\pi} P_j \left( \frac{r}{r_{m,n}} \cos \theta \right) P_l(\cos \theta) \sin \theta d\theta. \quad (30)$$

Upon evaluating the integrals (30) and substituting the obtained values into (28) and (29), we get the following expression for the wave  $\Psi_{sc}^{(m,n)}$ , which holds true when  $r \rightarrow 0$  (for details, see Appendix A):

$$\Psi_{sc}^{(m,n)} \approx ik \sum_{l=0}^{\infty} i^l r^l P_l(\cos \theta) \frac{1}{2^l} \frac{1}{(2l-1)!!} \left\{ \frac{1}{r_{m,n}^l} \sum_{j=0}^{\infty} F_{l+2j} h_{l+2j}(kr_{m,n}) \frac{1}{2^{2j}} \frac{(2(l+j))!}{j!(l+j)!} \right\}. \quad (31)$$

Now we only need to perform the summation of (31) over all  $m$  and  $n$  but  $(m,n) = (0,0)$ . Since we are interested in the correction to the imaginary part of the scattering amplitude, it suffices to find only the real parts of the sums  $\sum_{m,n} h_{l+2j}(kr_{m,n}) r_{m,n}^{-l}$  (as one can see in what follows). After quite a cumbersome summation procedure (see Appendix A), we finally have

$$\Psi_{sc,0} = \sum_{(m,n) \neq (0,0)} \Psi_{sc}^{(m,n)} \approx ik \sum_{l=0}^{\infty} i^l r^l k^l P_l(\cos \theta) \frac{1}{(2l-1)!!} \left\{ -\frac{1}{2l+1} F_l + \frac{2\pi}{k^2 ab} \sum_{j=0}^{\infty} F_{l+2j} \right\}. \quad (32)$$

In view of (10) and (32), the wave acting on the reference scatterer has the form

$$\Psi_{inc} = e^{ikz} + \Psi_{sc,0} = \sum_{l=0}^{\infty} \frac{1}{(2l-1)!!} i^l r^l k^l P_l(\cos \theta) \left\{ 1 - ik \frac{F_l}{2l+1} + \frac{2\pi i}{kab} \sum_{j=0}^{\infty} F_{l+2j} \right\}. \quad (33)$$

The interaction between this wave and the scatterer results in the formation of a scattered wave, which, according to (16), can be written as follows:

$$\Psi_{sc}^{(0,0)} = \sum_{l=0}^{\infty} i^l f_l R_{kl}^+(r) P_l(\cos \theta) \left\{ 1 - ik \frac{F_l}{2l+1} + \frac{2\pi i}{kab} \sum_{j=0}^{\infty} F_{l+2j} \right\}. \quad (34)$$

On the other hand, the wave scattered by the reference center is just a diverging spherical wave of amplitude  $F(\theta)$

$$\Psi_{sc}^{(0,0)} = \sum_{l=0}^{\infty} i^l F_l R_{kl}^+(r) P_l(\cos \theta). \quad (35)$$

Setting (34) equal to (35), we can obtain the following set of equations for partial amplitudes  $F_l$ :

$$F_l = f_l - \frac{ik}{2l+1} f_l F_l + \frac{2i\pi}{kab} f_l F_l + \frac{2i\pi}{kab} f_l \sum_{j=1}^{\infty} F_{l+2j}. \quad (36)$$

Assuming that the scattering amplitude is small ( $kf_l \ll 1$ ), we can solve the equations and obtain the following expressions for the amplitudes  $F_l$ :

$$F_l \approx \frac{f_l}{1 + \frac{ik}{2l+1} f_l - \frac{2i\pi}{kab} f_l}. \quad (37)$$

Thus when the wave  $\Psi_0(\vec{r}) = e^{ikz}$  is scattered by a plane grating of scattering centers, a plane wave is produced (at  $z > 0$ ), whose amplitude can be described by the expression that follows rather than by (25)

$$\Psi(\vec{r}) = e^{ikz} + \frac{2i\pi}{kab} e^{ikz} \sum_{l=0}^{\infty} F_l. \quad (38)$$



When  $z < 0$ , the wave field induced through scattering is a sum of the incoming wave incident on the grating and the wave reflected from it

$$\Psi(\vec{r}) = e^{ikz} + \frac{2i\pi}{kab} e^{-ikz} \sum_{l=0}^{\infty} (-1)^l F_l. \quad (39)$$

The further analysis is performed in a similar manner as in [11]. It is convenient to introduce the following notation:  $F_0^* \equiv \sum_{l=0}^{\infty} F_{2l}$ ,  $F_1^* \equiv \sum_{l=0}^{\infty} F_{2l+1}$ . Then (38)-(39) can be written in a more compact form

$$\Psi(\vec{r}) = e^{ikz} + \frac{2i\pi}{kab} (F_0^* \pm F_1^*) e^{ik|z|}, \quad (40)$$

where the plus sign refers to the case  $z > 0$ , while the minus sign refers to  $z < 0$  (forward and backward scattering, respectively)

Worthy of mention is that (40) has the same form as in the analysis of the simplest case of anisotropic scattering ( $l = 0, 1$ ) with the amplitude  $F^*(\theta) = F_0^* + F_1^* \cos \theta$ . The quantities  $\frac{2i\pi}{kab} (F_0^* \pm F_1^*)$  can be interpreted as the ‘‘amplitudes of forward (backward) scattering’’ of a plane wave by a two-dimensional grating (crystal plane) composed of scattering centers.

Let us consider a crystal composed of a set of above-discussed plane two-dimensional gratings placed at a distance  $c$  apart. The wave incident on the grating placed at the origin of coordinates is a sum of waves scattered by all other gratings. Following [11], let us assume that these waves have the amplitude  $\Phi = (\Phi_0 \pm \Phi_1) e^{iqcm}$ , where  $q$  is the wave number in the crystal,  $m$  is the integer (the number of the grating), and neither  $\Phi_0$  nor  $\Phi_1$  depends on  $m$ , owing to the periodicity of the crystal lattice. Because all these waves are scattered by this grating with the known amplitude  $\frac{2i\pi}{kab} (F_0^* \pm F_1^*)$  and produce a plane wave of amplitude  $(\Phi_0 \pm \Phi_1)$ , we can write the following set of equations for the amplitudes  $\Phi_0$  and  $\Phi_1$  (for details see [11]):

$$\Phi_0 = F_0^* \left\{ \frac{2\pi i}{kab} \Phi_0 S_3 + \frac{2\pi i}{kab} \Phi_1 S_4 \right\}, \quad (41)$$

$$\Phi_1 = F_1^* \left\{ \frac{2\pi i}{kab} \Phi_0 S_4 + \frac{2\pi i}{kab} \Phi_1 S_3 \right\}, \quad (42)$$

where the sums  $S_3$  and  $S_4$  are

$$S_3 = \sum_{m \neq 0} e^{iqcm} e^{ikc|m|} = -1 - i \frac{\sin kc}{\cos kc - \cos qc} \simeq -1 - \frac{2i}{kc} \cdot \frac{1}{n^2 - 1},$$

$$S_4 = \sum_{m=1}^{\infty} (e^{-iqcm} - e^{iqcm}) e^{ikcm} = -i \frac{\sin qc}{\cos kc - \cos qc} \simeq -\frac{2i}{kc} \cdot \frac{1}{n^2 - 1}.$$

By setting the determinant of (41)-(42) equal to zero, we obtain the dispersion equation for the wave number  $q$ . The solution of this dispersion equation has the form

$$n^2 = \frac{q^2}{k^2} = 1 + \frac{4\pi}{k^2 \Omega_3} \sum_l \frac{f_l}{1 + \frac{ik}{2l+1} f_l}, \quad (43)$$

where  $\Omega_3$  is the unit cell volume of the crystal.

As is seen, in the case of isotropic scattering (only  $l = 0$  is considered), this equation reduces to a well-known formula for the crystal refractive index:  $n^2 = 1 + \frac{4\pi}{k^2\Omega_3} \frac{f_0}{1 + ikf_0}$  [3, 8], while in the simplest anisotropic case ( $l = 0, 1$ ) we arrive at equation (6), first derived in [11].

Remembering the relationship (18) between the partial amplitudes  $f_l$  and the matrix elements  $T_l$ , we can present (43) in the form

$$n^2 = 1 - \frac{4\pi^2}{k^3\Omega_3} \sum_l (2l + 1) \frac{T_l}{1 - i\pi T_l}, \quad (44)$$

It follows from (21) that the expression for  $n^2$  can be recast as

$$n^2 = 1 - \frac{4\pi^2}{k^3\Omega_3} \sum_l (2l + 1) K_l. \quad (45)$$

Let us recall that if the scatterers make up a chaotic medium, then

$$n^2 = 1 + \frac{4\pi\rho}{k^2} f(0) = 1 - \frac{4\pi^2\rho}{k^3} \sum_l (2l + 1) T_l, \quad (46)$$

where  $\rho$  is the density of scatterers in the medium (in crystals  $\rho = \frac{1}{\Omega_3}$ ).

As we see, what differs (45), defining the crystal refractive index, from (46) is the reaction matrix  $K_l = \frac{T_l}{1 - i\pi T_l}$  that appears in (45) instead of the scattering matrix  $T_l$  in (46). This means that at a large distance from the center located inside the crystal, multiple coherent rescattering of waves in crystals changes the asymptotic behavior of a wave function according to (19). But at a large distance from the crystal, the asymptotic behavior of a wave function still has the form

$$\mathcal{F} \frac{e^{ikr}}{r}, \quad (47)$$

where  $\mathcal{F}$  is the scattering amplitude as a whole.

The basic difference between (45) and (46) is that in the case of elastic scattering by a single center, equation (45) is purely real, while (46) has both real and imaginary parts (the wave attenuates in the medium). Equation (45) is real because in the case of elastic scattering, the matrix  $K$  is Hermitian and diagonal in  $l$ . Thus, wave attenuation in crystals may come only from inelastic scattering by the centers composing the crystal, while in a chaotic medium, both inelastic scattering by individual centers and purely elastic scattering contribute to the attenuation of waves.

Let us take as an example the electromagnetic crystal built from parallel metallic wires (see [9, 10, 11]). As shown in [10], the Vavilov-Cherenkov effect in such crystals can be observed because the refractive index of a wave with orthogonal polarization is greater than unity. Let the wire spacing in the crystal be  $d_x = d_y = 0.1$  cm and the wire radius  $R = 25 \mu$  m. Using well-known expressions for the amplitude of electromagnetic wave scattering by a wire [9], we can show that, e.g., at a frequency  $f = 1$  THz, the refractive index of a crystal is  $n^2 \approx 1.002$ , while for a chaotic medium of the same density  $n^2 \approx 1.002 + 1.3 \cdot 10^{-3}i$ . Let a crystal (or a chaotic medium) have a thickness  $z = 10$  cm. We can readily obtain that in a chaotic medium of such thickness, the amplitude of a transmitted electromagnetic wave of frequency 1 THz will reduce by a factor of  $\exp(kz\text{Im}n) \approx 3.9$  (i.e., the reduction is significant), while in a crystal it will remain practically the same. It can be seen that the use of (46) for calculating the refractive index of crystals could lead to the erroneous conclusion that the generated Cherenkov radiation rapidly decays in crystals.

These results (the fact that scattering by the center belonging to the crystal is described by  $\frac{T_l}{1 - i\pi T_l}$  rather than by the matrix elements  $T_l$ ) should necessarily be taken into account in considering diffraction in crystals. Dynamical diffraction of X-rays and neutrons in crystals can be described by the following set of equations [3, 6, 19, 20]:

$$\left(1 - \frac{k^2}{k_0^2}\right) \varphi(\vec{k}) + \sum_{\vec{\tau}} g(\vec{\tau}) \varphi(\vec{k} - \vec{\tau}) = 0, \quad (48)$$

$$\Psi(\vec{r}) = \sum_{\vec{\tau}} \varphi(\vec{k} + \vec{\tau}) e^{i(\vec{k} + \vec{\tau})\vec{r}}, \quad (49)$$

where  $g(\vec{\tau}) = \frac{4\pi}{k^2 \Omega_3} f(\vec{k}, \vec{k} + \vec{\tau})$  is the structure amplitude and  $\vec{\tau}$  is the reciprocal lattice vector of the crystal.

The elements of the scattering matrix  $T_l$  in (48)-(49) appear only in expression for the structure amplitude  $g(\vec{\tau})$  (because they enter into the scattering amplitude  $f(\vec{k}, \vec{k} + \vec{\tau}) \equiv f(\theta_\tau)$ ). Replacing the amplitude  $T_l$  by  $\frac{T_l}{1 - i\pi T_l}$  gives the following expression for the structure amplitude:

$$g(\vec{\tau}) = \frac{4\pi}{k^2 \Omega_3} \sum_l \frac{f_l}{1 + \frac{ik}{2l+1} f_l} P_l(\cos(\vec{k}, \vec{k} + \vec{\tau})) = -\frac{4\pi^2}{k^3 \Omega_3} \sum_l (2l+1) \frac{T_l}{1 - i\pi T_l} P_l(\cos(\vec{k}, \vec{k} + \vec{\tau})). \quad (50)$$

The analysis shows that equations (48)-(49) together with (50) fully describe the dynamical diffraction of waves in a crystal.

## 4 Conclusion

This paper considers the influence of multiple rescattering on the propagation of waves in crystals composed of anisotropically scattering centers. We used the partial wave expansion method to generalize the results of [11], valid only in a particular case when the amplitude of scattering by a single center depends on the angle as  $f(\theta) = f_0 + f_1 \cos \theta$  ( $s$ - and  $p$ -scattering), to the case of arbitrary scattering anisotropy (with orbital quantum numbers  $l > 1$ ). What is more, we analyzed a general three-dimensional problem instead of a two-dimensional one, considered in [11]. It was shown for the first time that the expression for the refractive index of a three-dimensional crystal must include the quantities  $\frac{T_l}{1 - i\pi T_l}$  (in the case of elastic scattering, they coincide with the diagonal elements of the reaction matrix  $\mathbf{K}$  [see (21)]) instead of the diagonal elements of the scattering matrix  $T_l$ , which enter into the equation in the case of a chaotic medium. As a consequence, the structure amplitude in equations (48)-(49) describing the dynamical diffraction of waves in a crystal must be calculated by formula (50).

Because a general approach is applied to the description of the scattering process, the results thus obtained are valid for a wide range of problems and beneficial for many applications. These results can be of interest for research into, e.g., diffraction of cold neutrons and photons in crystals, nanocrystalline materials, as well as for the description of parametric and diffraction radiation in electromagnetic crystals formed by anisotropically scattering centers.

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## A Partial-Wave Expansion of $\Psi_{sc,0}$

Using (29)-(30), let us transform (28) for the wave  $\Psi_{sc}^{(m,n)}$  scattered by the center  $(m, n)$ . First, we find the coefficients  $\alpha_{lj}$

$$\alpha_{lj} = (2l + 1) \int_{-1}^1 P_j\left(\frac{r}{r_{m,n}}x\right) P_l(x) dx. \quad (51)$$

Because  $P_j(rx/r_{m,n})$  is the  $j$ -th degree polynomial of argument  $rx/r_{m,n}$

$$P_j\left(\frac{r}{r_{m,n}}x\right) = \sum_{k=0}^j a_k^{(j)} \left(\frac{r}{r_{m,n}}\right)^k x^k,$$

the quantities  $\alpha_{lj}$  [according to (51)] in the general case are the  $j$ -th degree polynomials of argument  $r/r_{m,n}$

$$\alpha_{lj} = \sum_{k=0}^j c_k \left(\frac{r}{r_{m,n}}\right)^k.$$

Since we are concerned with the behavior of the wave  $\Psi_{sc}^{(m,n)}$  in the vicinity of the reference scatterer, i.e., as  $r \rightarrow 0$ , we shall keep only the first nonzero term in the power series expansion of  $\alpha_{lj}$  over  $r/r_{m,n}$ . We shall also take into account that the integral

$$\int_{-1}^1 P_l(x) x^m = 0$$

at all  $m < l$  (see [21]). Then we have that  $\alpha_{lj} \equiv 0$  at  $j < l$ , and

$$\lim_{r \rightarrow 0} \alpha_{lj} = a_l^{(j)} \left(\frac{r}{r_{m,n}}\right)^l (2l + 1) \int_{-1}^1 P_l(x) x^l dx \quad (52)$$

at  $j \geq l$ . Moreover, we can easily show that  $\alpha_{lj} \equiv 0$  when  $j > l$  and  $j - l = 1, 3, 5, \dots$  (i.e., when the parities of  $j$  and  $l$  do not coincide), because the corresponding coefficients  $a_l^{(j)}$  equal zero. Using the known values of the coefficients  $a_l^{(j)}$  of the  $j$ -th degree Legendre polynomial and the integral in (52) (see [21, 22]), we obtain the expression

$$\lim_{r \rightarrow 0} \alpha_{lj} = (2l + 1) \cdot \left(\frac{r}{r_{m,n}}\right)^l \cdot \frac{2 \cdot l!}{(2l + 1)!!} \cdot \frac{1}{2^j} \cdot (-1)^{(j-l)/2} \frac{j!}{\left(\frac{j-l}{2}\right)! \left(\frac{j+l}{2}\right)!} \frac{(j+l)!}{j!l!},$$

that holds true if  $(j - l)$  is a nonnegative even number. In all other cases, the coefficients  $\alpha_{lj}$  are identically zero. The introduction of a new index  $j'$  using the relation  $j = l + 2j'$  enables writing this expression in a more convenient form (the prime in the new index is dropped):

$$\lim_{r \rightarrow 0} \alpha_{l,l+2j} = \left(\frac{r}{r_{m,n}}\right)^l \frac{1}{2^{l+2j-1}} \frac{(-1)^j}{(2l - 1)!!} \frac{(2(l + j))!}{j!(l + j)!}. \quad (53)$$

Substitution of (53) into (28)-(29) gives

$$\begin{aligned} \Psi_{sc}^{(m,n)} &= ik \sum_{j=0}^{\infty} i^j F_j h_j(kr_{m,n}) P_j\left(\frac{r}{r_{m,n}} \cos \theta\right) = ik \sum_{l=0}^{\infty} P_l(\cos \theta) \left\{ \sum_{j=0}^{\infty} i^j F_j h_j(kr_{m,n}) \frac{\alpha_{lj}}{2} \right\} = \\ &= ik \sum_{l=0}^{\infty} i^l r^l P_l(\cos \theta) \frac{1}{2^l} \frac{1}{(2l - 1)!!} \left\{ \frac{1}{r_{m,n}^l} \sum_{j=0}^{\infty} F_{l+2j} h_{l+2j}(kr_{m,n}) \frac{1}{2^{2j}} \frac{(2(l + j))!}{j!(l + j)!} \right\}, \quad (54) \end{aligned}$$

i.e., we have the expression identical to (31).

For partial-wave expansion of  $\Psi_{sc,0}$ , we need to perform summation of (54) over all  $m, n$  but  $(m, n) = (0, 0)$ . To do this, it suffices to find the values of the sums  $\sum_{m,n} h_{l+2j}(kr_{m,n})r_{m,n}^{-l}$ , where  $r_{m,n} = \sqrt{(am)^2 + (bn)^2}$ . As stated in section 3, we are interested only in the real parts of these sums. For convenience, let us introduce the notation

$$\Sigma_{lj} \equiv \text{Re} \sum_{(m,n) \neq (0,0)} \frac{h_{l+2j}(kr_{m,n})}{r_{m,n}^l}.$$

The first sum can be found using, for example, the Poisson summation formula:

$$\Sigma_{00} = \frac{2\pi}{k^2 ab} - 1. \quad (55)$$

The following formula for the spherical Hankel functions is helpful in seeking  $\Sigma_{l0}$  at  $l > 0$  [18]:

$$\frac{h_{l+1}(kr)}{r^{l+1}} = \frac{1}{k^{l+2}} \int_0^k k^{l+2} \frac{h_l(kr)}{r^l} dk. \quad (56)$$

Using the mathematical induction method and (56), we can readily prove that

$$\Sigma_{l0} = k^l \frac{1}{(2l-1)!!} \left\{ \frac{2\pi}{k^2 ab} - \frac{1}{2l+1} \right\} \quad (57)$$

for all  $l$ .

To find the values of  $\Sigma_{lj}$  at  $j > 0$ , let us make use of the the recurrent relation between the Hankel functions in the form [18]

$$h_{l+2j}(kr) = \frac{2l+4j-1}{kr} h_{l+2j-1}(kr) - h_{l+2j-2}(kr). \quad (58)$$

Substitution of  $j = 1, 2, \dots$  into (58) gives the following values for the first few sums

$$\begin{aligned} \Sigma_{l1} &= k^l \frac{2\pi}{k^2 ab} \frac{2}{(2l+1)!!}, \\ \Sigma_{l2} &= k^l \frac{2\pi}{k^2 ab} \frac{8}{(2l+3)!!}, \\ \Sigma_{l3} &= k^l \frac{2\pi}{k^2 ab} \frac{48}{(2l+5)!!}, \\ &\dots \end{aligned}$$

One can see that the general expression for  $\Sigma_{lj}$  at  $j > 0$  will have the form

$$\Sigma_{lj} = k^l \frac{2\pi}{k^2 ab} \frac{2^j j!}{(2l+2j-1)!!}. \quad (59)$$

The equality (59) can be rigorously proved using the mathematical induction method.

Transform the double factorials in (57) and (59) by formula  $(2n+1)!! = \frac{(2n+1)!}{2^n \cdot n!}$  and thus obtain the final expressions for  $\Sigma_{lj}$

$$\Sigma_{lj} = k^l \cdot 2^l \cdot \frac{2^{2j-1}(l+j-1)!j!}{(2l+2j-1)!} \cdot \frac{2\pi}{k^2 ab}, \quad j > 0, \quad (60)$$

$$\Sigma_{l0} = k^l \cdot 2^l \cdot \frac{2^{-1}(l-1)!}{(2l-1)!} \left\{ -\frac{1}{2l+1} + \frac{2\pi}{k^2 ab} \right\}. \quad (61)$$

Simple transformations of (54) and (60)-(61) give the sought expansion for the wave  $\Psi_{sc,0}$  when  $r \rightarrow 0$

$$\Psi_{sc,0} = \sum_{(m,n) \neq (0,0)} \Psi_{sc}^{(m,n)} \approx ik \sum_{l=0}^{\infty} i^l r^l k^l P_l(\cos \theta) \frac{1}{(2l-1)!!} \left\{ -\frac{1}{2l+1} F_l + \frac{2\pi}{k^2 ab} \sum_{j=0}^{\infty} F_{l+2j} \right\}.$$