Symmetry properties of fields reflected by rough surfaces

A. V. Andreev

International Educational and Science Laser Center, M. V. Lomonosov Moscow State University, 119899 Moscow, Russia
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The symmetry properties of fields reflected by uneven surfaces are determined. The application of these symmetry properties yields a theory of the reflection and scattering of waves by regularly and randomly nonuniform surfaces that does not employ the Born approximation. The investigations made it possible to determine the limits of applicability of the standard theories of wave scattering by rough surfaces based on different variants of the Born approximation of the distorted-wave theory. Principles are proposed for developing algorithms for reconstructing from the angular reflection and scattering spectra the surface relief and the static characteristics of the protuberances.
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1. INTRODUCTION

The surfaces of real bodies and the interfaces between media are, as a rule, always uneven. The reflection of waves from an uneven surface leads to a number of new phenomena which do not occur in the case of an ideally smooth interface. These include the suppression of specular reflection in the visible[1] and x-ray[2] ranges, diffuse scattering of waves, anomalous reflection effects (Wood's anomaly,[3] Yoneda anomalous reflection,[4] backscattering[5]) and a host of other phenomena. The characteristic scale of surface protuberances is the product $\kappa_z h$ of the component of the wave vector of the incident wave in the direction normal to the interface and the rms height of the protuberances. Therefore, surfaces which are ideally smooth for optical radiation can be very rough for x-rays. Wave reflection phenomena at nonuniform surfaces are used to control the angular spectrum and polarization of reflected beams; they strongly influence the character of the interaction of intense radiation with solid surfaces, which results in structure formation on the surface or generation of harmonics of the radiation, and they form the basis of methods of surface spectroscopy based on the angular spectrum of the reflected radiation. For this reason, the problem of determining the fields reflected by regularly and randomly nonuniform surfaces is of interest from the standpoint of general physics and for the development of methods in the theory of waves, surface spectroscopy, the theory of the interaction of intense laser radiation with matter, the theory of solids (heterostructures, multilayered film structures), statistical optics, radio physics, and in other fields.

The methods for calculating the angular spectra of waves reflected by rough surfaces can be divided into two basic groups:[6–8] the geometric-optics approximation for large-scale nonuniformities and perturbation theory for small-scale nonuniformities. In the perturbation theory, first an average is performed over the protuberances and the concept of a transitional layer, describing either a smooth variation of the polarizability from zero in vacuum up to the value in the volume of the material, is introduced or a film model, in which the region of the protuberances is replaced by a film with an effective value of the polarizability, is used. The parameters of the transitional layer are chosen so as to obtain the best agreement with the experimental angular specular-reflection spectra. Fluctuations of the permittivity, i.e., the difference between its real and average values, are regarded as a perturbation which resulting in diffuse scattering. This scheme describes quite well the angular diffuse-scattering spectra for $\kappa_z h \ll 1$, when diffuse scattering is weak. However, as the parameter $\kappa_z h$ increases, the integrated intensity of diffuse scattering increases above the intensity of the incident wave even in first-order perturbation theory.

In the present paper a theory of the reflection and scattering of x-rays by nonuniform surfaces which is not based on perturbation theory is proposed. The symmetry properties of the fields reflected by an arbitrary rough surface are determined. These symmetry properties made it possible to obtain exact integral equations relating the angular spectra of the reflected and refracted waves to the angular spectra of the incident wave for arbitrary scalar fields. In the case of one-dimensional irregularities of the surface relief the theory developed is also applicable to vector fields. This approach has a number of advantages over different variants of the perturbation theory. First, the law of conservation of the energy flux holds. This means that the total energy flux of the waves scattered by both sides of an interface in nonabsorbing media equals the energy flux of the incident wave. Second, the formulas obtained describe simultaneously both diffuse scattering and broadening of the specularly reflected components, and since in this method the specularly reflected and diffusely scattered components are described in different orders of perturbation theory, the characteristic restrictions in the distorted-wave method on the correlation length of the protuberances are thereby removed. Third, the formulas proposed make it possible to develop algorithms for reconstructing the surface profile in the case of a regularly nonuniform surface or the distribution function of the height and gradient of the protuberances in the case of a randomly nonuniform surface.

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2. BOUNDARY CONDITIONS

The Helmholtz equation describing the propagation of radiation in a medium with permittivity $\varepsilon(\mathbf{r})$ for scalar fields has the form

$$\Delta E(\mathbf{r})+\kappa^2\varepsilon(\mathbf{r})E(\mathbf{r})=0. \tag{1}$$

Let us consider first the reflection from a layer with permittivity ε_2 in a medium with permittivity ε_1. We shall assume that the equations of the top and bottom interfaces $\xi(\rho)$ and $\eta(\rho)$, respectively, are smooth functions. Then the boundary conditions for Eq. (1) will be that the fields and their normal derivatives are continuous. We denote waves with positive projections of the wave vector on the z axis by $E_0(\mathbf{r})$ in medium 1 and $E_1(\mathbf{r})$ in medium 2 and waves with negative projections by $E_r(\mathbf{r})$ and $E_2(\mathbf{r})$, respectively. We denote by $E_t(\mathbf{r})$ the wave passing through the layer. Then the boundary conditions on the top boundary $\xi(\boldsymbol{\rho})$ and bottom boundary $\eta(\boldsymbol{\rho})$ of the layer have the form

$$[E_0(\mathbf{r})+E_r(\mathbf{r})]|_{z=\xi(\rho)}=[E_1(\mathbf{r})+E_2(\mathbf{r})]|_{z=\xi(\rho)},$$
$$\mathbf{n}_\xi\nabla[E_0(\mathbf{r})+E_r(\mathbf{r})]|_{z=\xi(\rho)}=\mathbf{n}_\xi\nabla[E_1(\mathbf{r})+E_2(\mathbf{r})]|_{z=\xi(\rho)}, \tag{2a}$$

$$[E_1(\mathbf{r})+E_2(\mathbf{r})]|_{z=\eta(\rho)}=E_t(\mathbf{r})|_{z=\eta(\rho)},$$
$$\mathbf{n}_\eta\nabla[E_1(\mathbf{r})+E_2(\mathbf{r})]|_{z=\eta(\rho)}=\mathbf{n}_\eta\nabla E_t(\mathbf{r})|_{z=\eta(\rho)}. \tag{2b}$$

Here $\mathbf{n}_\xi$ and $\mathbf{n}_\eta$ are the normals to the interfaces at the point ρ. So, $\mathbf{n}_\xi$ has the form

$$\mathbf{n}_\xi=\left\{-\frac{\xi_x}{\sqrt{1+\xi_x^2+\xi_y^2}},-\frac{\xi_y}{\sqrt{1+\xi_x^2+\xi_y^2}},\frac{1}{\sqrt{1+\xi_x^2+\xi_y^2}}\right\}, \tag{3}$$

where $\xi_x=\partial\xi/\partial x$. We expand the amplitudes of the fields $E_\alpha(\mathbf{r})$ in a two-dimensional Fourier integral of the following form:

$$E_\alpha=\int d\mathbf{k}_\parallel E_\alpha(\mathbf{k}_\parallel)\exp[i\Gamma_\alpha(\mathbf{k}_\parallel)z+i\mathbf{k}_\parallel\boldsymbol{\rho}], \tag{4}$$

where $\Gamma_0(\mathbf{k}_\parallel)=\sqrt{\kappa^2\varepsilon_1-\mathbf{k}_\parallel^2}$, $\Gamma_r(\mathbf{k}_\parallel)=-\sqrt{\kappa^2\varepsilon_1-\mathbf{k}_\parallel^2}$, and so on. After the expansions (4) are substituted into the boundary conditions (2), the following wave functions appear in them:

$$u_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi)=\exp[i\Gamma_1(\mathbf{k}_\parallel)\xi+i\mathbf{k}_\parallel\boldsymbol{\rho}],$$
$$w_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi)=\exp[i\Gamma_2(\mathbf{k}_\parallel)\xi+i\mathbf{k}_\parallel\boldsymbol{\rho}],$$
$$\bar{u}_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi)=\exp[-i\Gamma_1(\mathbf{k}_\parallel)\xi+i\mathbf{k}_\parallel\boldsymbol{\rho}],$$
$$\bar{w}_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi)=\exp[-i\Gamma_2(\mathbf{k}_\parallel)\xi+i\mathbf{k}_\parallel\boldsymbol{\rho}], \tag{5}$$

where $\Gamma_1(\mathbf{k}_\parallel)=\sqrt{\kappa^2\varepsilon_1-\mathbf{k}_\parallel^2}$ and $\Gamma_2(\mathbf{k}_\parallel)=\sqrt{\kappa^2\varepsilon_2-\mathbf{k}_\parallel^2}$. With the notations (5), the boundary conditions (2) can be written in the form

$$\int d\mathbf{k}_\parallel E_0(\mathbf{k}_\parallel)u_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi)+\int d\mathbf{k}_\parallel E_r(\mathbf{k}_\parallel)\bar{u}_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi)$$
$$=\int d\mathbf{k}_\parallel E_1(\mathbf{k}_\parallel)w_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi)+\int d\mathbf{k}_\parallel E_2(\mathbf{k}_\parallel)\bar{w}_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi),$$

$$\int d\mathbf{k}_\parallel E_0(\mathbf{k}_\parallel)[\Gamma_1(\mathbf{k}_\parallel)-\mathbf{k}_\parallel\nabla\xi]u_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi)-\int d\mathbf{k}_\parallel E_r(\mathbf{k}_\parallel)$$
$$\times[\Gamma_1(\mathbf{k}_\parallel)+\mathbf{k}_\parallel\nabla\xi]\bar{u}_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi)$$
$$=\int d\mathbf{k}_\parallel E_1(\mathbf{k}_\parallel)[\Gamma_2(\mathbf{k}_\parallel)-\mathbf{k}_\parallel\nabla\xi]w_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi)$$
$$-\int d\mathbf{k}_\parallel E_2(\mathbf{k}_\parallel)[\Gamma_2(\mathbf{k}_\parallel)+\mathbf{k}_\parallel\nabla\xi]\bar{w}_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi), \tag{6}$$

$$\int d\mathbf{k}_\parallel E_1(\mathbf{k}_\parallel)w_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\eta)+\int d\mathbf{k}_\parallel E_2(\mathbf{k}_\parallel)\bar{w}_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\eta)$$
$$=\int d\mathbf{k}_\parallel E_t(\mathbf{k}_\parallel)u_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\eta),$$

$$\int d\mathbf{k}_\parallel E_1(\mathbf{k}_\parallel)[\Gamma_2(\mathbf{k}_\parallel)-\mathbf{k}_\parallel\nabla\eta]w_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\eta)-\int d\mathbf{k}_\parallel E_2(\mathbf{k}_\parallel)$$
$$\times[\Gamma_2(\mathbf{k}_\parallel)+\mathbf{k}_\parallel\nabla\eta]\bar{w}_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\eta)=\int d\mathbf{k}_\parallel E_t(\mathbf{k}_\parallel)$$
$$\times[\Gamma_1(\mathbf{k}_\parallel)-\mathbf{k}_\parallel\nabla\eta]u_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\eta).$$

3. SYMMETRY PROPERTIES OF THE WAVE FUNCTIONS

The boundary conditions (6) contain the product of the wave functions (5) and the cofactors $\Gamma_n(\mathbf{k}_\parallel)\pm\mathbf{k}_\parallel\nabla\xi$. We shall investigate the symmetry properties of matrix elements of the form $\int d\boldsymbol{\rho}\bar{u}_\nu(\boldsymbol{\rho},\xi)[\Gamma_n(\mathbf{k}_\parallel)\pm\mathbf{k}_\parallel\nabla\xi]u_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi)$. Integrating by parts according to the formula

$$\int_{-\infty}^{+\infty}uw'dx=uw\Big|_{-\infty}^{+\infty}-\int_{-\infty}^{+\infty}u'wdx,$$

it is easy to show that the matrix elements possess the following symmetry properties:

$$\int d\boldsymbol{\rho}\bar{u}_\nu^*(\boldsymbol{\rho},\xi)[\Gamma_1(\mathbf{k}_\parallel)-\mathbf{k}_\parallel\nabla\xi]u_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi)$$
$$=\int d\boldsymbol{\rho}\bar{u}_\nu^*(\boldsymbol{\rho},\xi)[\Gamma_1(\boldsymbol{\nu})+\boldsymbol{\nu}\nabla\xi]u_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi)+C_1,$$

$$\int d\boldsymbol{\rho}u_\nu^*(\boldsymbol{\rho},\xi)[\Gamma_1(\mathbf{k}_\parallel)+\mathbf{k}_\parallel\nabla\xi]\bar{u}_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi)$$
$$=\int d\boldsymbol{\rho}u_\nu^*(\boldsymbol{\rho},\xi)[\Gamma_1(\boldsymbol{\nu})-\boldsymbol{\nu}\nabla\xi]\bar{u}_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi)-C_2,$$

$$\int d\boldsymbol{\rho}\bar{w}_\nu^*(\boldsymbol{\rho},\xi)[\Gamma_2(\mathbf{k}_\parallel)-\mathbf{k}_\parallel\nabla\xi]w_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi)$$
$$=\int d\boldsymbol{\rho}\bar{w}_\nu^*(\boldsymbol{\rho},\xi)[\Gamma_2(\boldsymbol{\nu})+\boldsymbol{\nu}\nabla\xi]\rangle_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi)+C_3, \tag{7}$$

$$\int d\boldsymbol{\rho}w_\nu^*(\boldsymbol{\rho},\xi)[\Gamma_2(\mathbf{k}_\parallel)+\mathbf{k}_\parallel\nabla\xi]\bar{w}_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi)$$
$$=\int d\boldsymbol{\rho}w_\nu^*(\boldsymbol{\rho},\xi)[\Gamma_2(\boldsymbol{\nu})-\boldsymbol{\nu}\nabla\xi]\bar{w}_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi)-C_4,$$

where

$$C_\alpha = i\,\frac{k_x+\nu_x}{\Gamma^{(\alpha)}}\int dy\,\exp[i\Gamma^{(\alpha)}\xi + i(\mathbf{k}_\parallel-\boldsymbol{\nu})\boldsymbol{\rho}]\Big|_{x=-\infty}^{x=+\infty}$$

$$+ i\,\frac{k_y+\nu_y}{\Gamma^{(\alpha}}\int dx\,\exp[i\Gamma^{(\alpha)}\xi + i(\mathbf{k}_\parallel-\boldsymbol{\nu})\boldsymbol{\rho}]\Big|_{y=-\infty}^{y=+\infty}.$$

Here

$$\Gamma^{(1)} = \Gamma_1(\mathbf{k}_\parallel)+\Gamma_1(\boldsymbol{\nu}),\quad \Gamma^{(2)} = -\Gamma^{(1)},$$

$$\Gamma^{(3)} = \Gamma_2(\mathbf{k}_\parallel)+\Gamma_1(\boldsymbol{\nu}),\quad \Gamma^{(4)} = -\Gamma^{(3)}.$$

In the case when the equation for the interface $\zeta(\rho)$ satisfies the condition

$$\xi(\boldsymbol{\rho})|_{\rho\to\infty} = \xi(-\boldsymbol{\rho})|_{\rho\to\infty},$$

using the definition of the delta function it is easy to show that

$$C_\alpha = -(2\pi)^2\,\frac{k_\parallel^2-\nu^2}{\Gamma^{(\alpha)}}\,\delta(\mathbf{k}_\parallel-\boldsymbol{\nu}), \tag{8}$$

and therefore in this case we can set all $C_\alpha=0$. Using the properties (7), we can obtain from the boundary conditions (6) integral equations relating the Fourier components of the scattered and incident fields, the refracted and incident fields, and so on.

The equations (7) are invariant with respect to the substitutions $\mathbf{k}_\parallel \to -\boldsymbol{\nu}$ and $\boldsymbol{\nu}\to -\mathbf{k}_\parallel$. This invariance is an analog of the reciprocity theorem[9] and makes it possible to relate the angular spectra of the waves reflected and refracted by an uneven interface.

The physical meaning of the symmetry relations (7) is most simply explained for the case of a one-dimensional relief. Let $\xi = x\tan\theta$, i.e., the interface makes an angle θ with the x axis of the (x,z) coordinate system. In this case the first equation in Eq. (7) assumes the form

$$[\Gamma_1(k_\parallel) = k_\parallel\tan\theta]\delta(k_\parallel+\Gamma_1(k_\parallel)\tan\theta-\nu+\Gamma_1(\nu)\tan\theta)$$
$$= [\Gamma_1(\nu)-\nu\tan\theta]\delta(k_\parallel+\Gamma_1(k_\parallel)\tan\theta-\nu$$
$$+\Gamma_1(\nu)\tan\theta). \tag{9}$$

We now introduce the coordinate system (x', z') which is associated with the interface:

$$x' = x\cos\theta + z\sin\theta,\quad z' = z\cos\theta - x\sin\theta.$$

It is easy to see that the equality of the tangential

$$k'_\parallel = k_\parallel\cos\theta + \Gamma_1(k_\parallel)\sin\theta = \nu\cos\theta - \Gamma_1(\nu)\sin\theta = \nu'$$

and normal

$$\Gamma'_1(k_\parallel) = \Gamma_1(k_\parallel)\cos\theta = k_\parallel\sin\theta = -(-\Gamma_1(\nu)\cos\theta$$
$$+\nu\sin\theta) = |\Gamma'(\nu)|$$

components of the wave vectors of the incident and reflected waves relative to the interface x' follows from Eq. (9) (see Fig. 1). Therefore reflection from an ideal interface $\xi = x\tan\theta$ is governed by the laws of specular reflection.

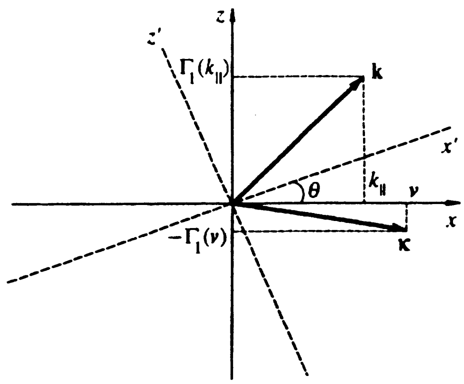

FIG. 1. For the interpretation of Eqs. (7). Here $\varkappa = \{\nu, -\Gamma_1(\nu)\}$.

4. REFLECTION FROM A REGULARLY NONUNIFORM SURFACE

We consider first reflection from a semi-infinite layer of material 2, i.e. from one interface of the materials with permittivities ε_1 and ε_2. Now let E_t denote the wave in layer 2. Then the boundary conditions assume the form

$$\int d\mathbf{k}_\parallel E_0(\mathbf{k}_\parallel) u_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi) + \int d\mathbf{k}_\parallel E_r(\mathbf{k}_\parallel)\bar{u}_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi)$$
$$= \int d\mathbf{k}_\parallel E_t(\mathbf{k}_\parallel) w_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi),$$
$$\int d\mathbf{k}_\parallel E_0(\mathbf{k}_\parallel)[\Gamma_1(\mathbf{k}_\parallel) - \mathbf{k}_\parallel\nabla\xi]u_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi) - \int d\mathbf{k}_\parallel E_r(\mathbf{k}_\parallel)$$
$$\times[\Gamma_1(\mathbf{k}_\parallel) + \mathbf{k}_\parallel\nabla\xi]\bar{u}_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi)$$
$$= \int d\mathbf{k}_\parallel E_t(\mathbf{k}_\parallel)[\Gamma_2(\mathbf{k}_\parallel) - \mathbf{k}_\parallel\nabla\xi]w_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi). \tag{10}$$

Using the properties (7) and (8) it is easy to obtain from Eq. (10)

$$\int d\mathbf{k}_\parallel E_0(\mathbf{k}_\parallel)\int d\boldsymbol{\rho}\bar{w}^*_{\boldsymbol{\nu}}$$
$$\times(\boldsymbol{\rho},\xi)[\Gamma_1(\mathbf{k}_\parallel) - \Gamma_2(\boldsymbol{\nu}) - (\mathbf{k}_\parallel+\boldsymbol{\nu})\nabla\xi]u_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi)$$
$$= \int d\mathbf{k}_\parallel E_r(\mathbf{k}_\parallel)\int d\boldsymbol{\rho}\bar{w}^*_{\boldsymbol{\nu}}(\boldsymbol{\rho},\xi)[\Gamma_1(\mathbf{k}_\parallel) + \Gamma_2(\boldsymbol{\nu}) + (\mathbf{k}_\parallel$$
$$+\boldsymbol{\nu})\nabla\xi]\bar{u}_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi), \tag{11a}$$

$$\int d\mathbf{k}_\parallel E_0(\mathbf{k}_\parallel)\int d\boldsymbol{\rho} u^*_{\boldsymbol{\nu}}(\boldsymbol{\rho},\xi)[\Gamma_1(\mathbf{k}_\parallel) + \Gamma_1(\boldsymbol{\nu}) - (\mathbf{k}_\parallel$$
$$+\boldsymbol{\nu})\nabla\xi]u_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi) = \int d\mathbf{k}_\parallel E_t(\mathbf{k}_\parallel)\int d\boldsymbol{\rho} u^*_{\boldsymbol{\nu}}(\boldsymbol{\rho},\xi)$$
$$\times[\Gamma_2(\mathbf{k}_\parallel) + \Gamma_2(\boldsymbol{\nu}) - (\mathbf{k}_\parallel+\boldsymbol{\nu})\nabla\xi]w_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi). \tag{11b}$$

The equations (11a) and (11b) are the desired integral equations relating the Fourier spectra of the reflected and refracted waves with the Fourier spectrum of the incident wave. It is easy to see that in the case of a smooth surface $\xi(\rho)=0$ the amplitudes of the reflected and refracted waves are related to the amplitude of the incident wave by the Fresnel reflection coefficient r and refraction coefficient t:

$$E_r(\boldsymbol{\nu})=E_0(\boldsymbol{\nu})\frac{\Gamma_1(\boldsymbol{\nu})-\Gamma_2(\boldsymbol{\nu})}{\Gamma_1(\boldsymbol{\nu})+\Gamma_2(\boldsymbol{\nu})}=E_0(\boldsymbol{\nu})r(\boldsymbol{\nu}), \tag{12a}$$

$$E_t(\boldsymbol{\nu})=E_0(\boldsymbol{\nu})\frac{2\Gamma_1(\boldsymbol{\nu})}{\Gamma_1(\boldsymbol{\nu})+\Gamma_2(\boldsymbol{\nu})}=E_0(\boldsymbol{\nu})t(\boldsymbol{\nu}). \tag{12b}$$

The gradients $\nabla\xi(\rho)$ of the relief take account of the local slopes of the interface, and factors of the form $\exp[i(\Gamma(\mathbf{k}_\parallel)+\Gamma_2(\boldsymbol{\nu}))\xi(\boldsymbol{\rho})]$ take account of the local phase increments on reflection.

The equations (11a and b) can be further simplified. Integrating by parts, as done in the derivation of the relations (7), it is easy to obtain from Eqs. (11a and b)

$$\begin{aligned}\int d\mathbf{k}_\parallel &\frac{E_0(\mathbf{k}_\parallel)}{\Gamma_1(\mathbf{k}_\parallel)+\Gamma_2(\boldsymbol{\nu})}\int d\boldsymbol{\rho}\exp[i(\Gamma_1(\mathbf{k}_\parallel)\\&+\Gamma_2(\boldsymbol{\nu}))\xi(\boldsymbol{\rho})+i(\mathbf{k}_\parallel-\boldsymbol{\nu})\boldsymbol{\rho}]\\&=\int d\mathbf{k}_\parallel\frac{E_r(\mathbf{k}_\parallel)}{\Gamma_1(\mathbf{k}_\parallel)-\Gamma_2(\boldsymbol{\nu})}\int d\boldsymbol{\rho}\exp[-i(\Gamma_1(\mathbf{k}_\parallel)\\&-\Gamma_2(\boldsymbol{\nu}))\xi(\boldsymbol{\rho})+i(\mathbf{k}_\parallel-\boldsymbol{\nu})\boldsymbol{\rho}],\end{aligned} \tag{13a}$$

$$\begin{aligned}E_0(\boldsymbol{\nu})&\frac{2\Gamma_1(\boldsymbol{\nu})}{\kappa^2(\varepsilon_2-\varepsilon_1)}\\&=\int d\mathbf{k}_\parallel\frac{E_t(\mathbf{k}_\parallel)}{\Gamma_2(\mathbf{k}_\parallel)-\Gamma_1(\boldsymbol{\nu})}\frac{1}{(2\pi)^2}\\&\times\int d\boldsymbol{\rho}\exp[i(\Gamma_2(\mathbf{k}_\parallel)-\Gamma_1(\boldsymbol{\nu}))\xi(\boldsymbol{\rho})+i(\mathbf{k}_\parallel-\boldsymbol{\nu})\boldsymbol{\rho}].\end{aligned} \tag{13b}$$

The equation (13a) is obtained directly from Eq. (11a) by integration by parts. In deriving Eq. (13b) we employed the following device:

$$\int_K d\mathbf{k}_\parallel E_0(\mathbf{k}_\parallel)P(\mathbf{k}_\parallel,\boldsymbol{\nu})=\int_{K_1} d\mathbf{k}_\parallel E_0(\mathbf{k}_\parallel)P(\mathbf{k}_\parallel,\boldsymbol{\nu})+\int_{k(\boldsymbol{\nu})} d\mathbf{k}_\parallel E_0(\mathbf{k}_\parallel)P(\mathbf{k}_\parallel,\boldsymbol{\nu}),$$

where

$$P(\mathbf{k}_\parallel,\boldsymbol{\nu})=\frac{1}{(2\pi)^2}\int d\boldsymbol{\rho}u^*_{\boldsymbol{\nu}}(\boldsymbol{\rho},\xi)[\Gamma_1(\mathbf{k}_\parallel)+\Gamma_1(\boldsymbol{\nu})-(\mathbf{k}_\parallel+\boldsymbol{\nu})\nabla\xi]u_{\mathbf{k}_\parallel}(\boldsymbol{\rho},\xi). \tag{14}$$

We divide the region of integration K into the region $k(\nu)$ near the point $\mathbf{k}_\parallel=\boldsymbol{\nu}$ and the region $K_1=K-k(\boldsymbol{\nu})$. In the region K_1 the integral (14) equals zero. Using the expansion $\Gamma(\mathbf{k}_\parallel)=\Gamma(\boldsymbol{\nu})-\boldsymbol{\nu}\cdot\mathbf{s}/\Gamma(\boldsymbol{\nu})$, where $\mathbf{s}=\mathbf{k}_\parallel-\boldsymbol{\nu}$, the integral (14) can be put into the form

$$\begin{aligned}P(\mathbf{k}_\parallel,\boldsymbol{\nu})&=2\Gamma_1(\boldsymbol{\nu})\frac{1}{(2\pi)^2}\int d\boldsymbol{\rho}\left[1-\frac{\boldsymbol{\nu}\nabla\xi}{\Gamma_1(\boldsymbol{\nu})}+o(\mathbf{s})\right]\exp\left\{i\left[\mathbf{s}\left(\boldsymbol{\rho}-\frac{\boldsymbol{\nu}\xi}{\Gamma_1(\boldsymbol{\nu})}\right)+o(\mathbf{s}^2)\right]\right\}\Bigg|_{s\to0}\\&=2\Gamma_1(\boldsymbol{\nu})\delta(\mathbf{k}_\parallel-\boldsymbol{\nu}).\end{aligned}$$

5. PROPERTIES OF THE ANGULAR REFLECTION SPECTRA

The methods of x-ray spectroscopy of surfaces and interfaces of multilayer nanostructures have undergone intense development in the last few years.[10,11] X-Rays with a wavelength of the order of 1 Å make it possible to determine the statistical characteristics of protuberances whose characteristic height is of the order of several angstroms. For this reason, when we speak about the properties of the angular reflection spectra, we shall have in mind x-rays.

In the case $(\Gamma_1-\Gamma_2)\xi\ll1$ and an incident plane wave, $E_0(\mathbf{k}_\parallel)=E_0\delta(\mathbf{k}_\parallel-\boldsymbol{\kappa}_\parallel)$, Eq. (13a) assumes the form

$$E_r(\boldsymbol{\nu})=E_0\frac{\Gamma_1(\boldsymbol{\nu})-\Gamma_2(\boldsymbol{\nu})}{\Gamma_1(\boldsymbol{\kappa}_\parallel)+\Gamma_2(\boldsymbol{\nu})}\frac{1}{(2\pi)^2}\int d\boldsymbol{\rho}\exp[i(\Gamma_1(\boldsymbol{\kappa}_\parallel)+\Gamma_2(\boldsymbol{\nu}))\xi(\boldsymbol{\rho})+i(\boldsymbol{\kappa}_\parallel-\boldsymbol{\nu})\boldsymbol{\rho}]. \tag{15}$$

For $(\boldsymbol{\kappa}_\parallel-\boldsymbol{\nu})\boldsymbol{\kappa}_\parallel\xi\ll\Gamma_1(\boldsymbol{\kappa}_\parallel)$, in turn, we obtain from the last expression

$$\exp[i(\Gamma_1(\boldsymbol{\kappa}_\parallel)+\Gamma_2(\boldsymbol{\kappa}_\parallel))\xi(\boldsymbol{\rho})]=\int d\boldsymbol{\nu}\frac{E_r(\boldsymbol{\nu})}{E_0}\frac{\Gamma_1(\boldsymbol{\kappa}_\parallel)+\Gamma_2(\boldsymbol{\nu})}{\Gamma_1(\boldsymbol{\nu})-\Gamma_2(\boldsymbol{\nu})}\exp[i(\boldsymbol{\nu}-\boldsymbol{\kappa}_\parallel)\boldsymbol{\rho}]. \tag{16}$$

Therefore, with these approximations, the angular spectrum of the reflected wave makes it possible to reconstruct the surface relief.

The problem of reconstructing the surface relief from the angular reflection spectrum can also be solved in the general case. The equation (13a) can be rewritten as

$$\begin{aligned}\sum_{n=0}^{N}\int d\mathbf{k}_\parallel E_0(\mathbf{k}_\parallel)&\frac{i^n(\Gamma_1(\mathbf{k}_\parallel)+\Gamma_2(\boldsymbol{\nu}))^{n-1}}{n!}\xi_n(\boldsymbol{\nu}-\mathbf{k}_\parallel)\\&=\sum_{n=0}^{N}\int d\mathbf{k}_\parallel E_r(\mathbf{k}_\parallel)\frac{(-i)^n(\Gamma_1(\mathbf{k}_\parallel)-\Gamma_2(\boldsymbol{\nu}))^{n-1}}{n!}\\&\times\xi_n(\boldsymbol{\nu}-\mathbf{k}_\parallel).\end{aligned} \tag{17}$$

where

$$\xi_n(\boldsymbol{\nu}-\mathbf{k}_\parallel)=\frac{1}{(2\pi)^2}\int d\boldsymbol{\rho}\xi^n(\boldsymbol{\rho})\exp[-i(\boldsymbol{\nu}-\mathbf{k}_\parallel)\boldsymbol{\rho}].$$

For known $E_r(\mathbf{k}_\parallel)$ and $E_0(\mathbf{k}_\parallel)$ the system of equations (17) is to be solved for $\xi_n(\boldsymbol{\nu}-\mathbf{k}_\parallel)$. The number of data in the angular reflection spectrum determines the number of Fourier components of the relief harmonics that can be determined. The number N of relief harmonics that can be reconstructed is determined by the number of values of the angle of incidence. For example, if only the Fourier components from the relief $\xi(\boldsymbol{\nu})=\xi_1(\boldsymbol{\nu})$ are used, then they can be reconstructed from the data on the angular scattering spectrum at one angle of incidence:

$$\begin{aligned}E_r(\boldsymbol{\nu})-E_0(\boldsymbol{\nu})r(\boldsymbol{\nu})=i\int d\mathbf{k}_\parallel&\left[E_0(\mathbf{k}_\parallel)\frac{\Gamma_1(\boldsymbol{\nu})-\Gamma_2(\boldsymbol{\nu})}{\Gamma_1(\mathbf{k}_\parallel)+\Gamma_2(\boldsymbol{\nu})}+E_r(\mathbf{k}_\parallel)\frac{\Gamma_1(\boldsymbol{\nu})-\Gamma_2(\boldsymbol{\nu})}{\Gamma_1(\mathbf{k}_\parallel)-\Gamma_2(\boldsymbol{\nu})}\right]\\&\times\xi(\boldsymbol{\nu}-\mathbf{k}_\parallel).\end{aligned}$$

In the case of a sufficiently smooth relief the equations (13a and b) can be reduced to Fredholm integral equations of the second kind. Indeed, using in Eqs. (13a and b) the identity

$$e^{i\Gamma\xi}=1+(e^{i\Gamma\xi}-1),$$

we obtain from Eq. (13a)

$$E_r(\boldsymbol{\nu})+\int d\mathbf{k}_\parallel F_-(\mathbf{k}_\parallel,\boldsymbol{\nu})E_r(\mathbf{k}_\parallel)=E_0(\boldsymbol{\nu})r(\boldsymbol{\nu})$$
$$+\int d\mathbf{k}_\parallel F_+(\mathbf{k}_\parallel,\boldsymbol{\nu})E_0(\mathbf{k}_\parallel). \tag{18}$$

where

$$F_\pm(\mathbf{k}_\parallel,\boldsymbol{\nu})=\frac{\Gamma_-(\boldsymbol{\nu})}{\Gamma_\pm(\mathbf{k}_\parallel)}\frac{1}{(2\pi)^2}\int d\boldsymbol{\rho}[\exp[\pm i\Gamma_\pm\xi(\boldsymbol{\rho})]$$
$$-1]\exp[i(\mathbf{k}_\parallel-\boldsymbol{\nu})\boldsymbol{\rho}],$$

$$\Gamma_\pm(\mathbf{k}_\parallel)=\Gamma_1(\mathbf{k}_\parallel)\pm\Gamma_2(\boldsymbol{\nu}).$$

The equation (18) can be solved iteratively:[12]

$$E_r(\boldsymbol{\nu})=E_0(\boldsymbol{\nu})r(\boldsymbol{\nu})+\int d\mathbf{k}_\parallel F(\mathbf{k}_\parallel,\boldsymbol{\nu})E_0(\mathbf{k}_\parallel)$$
$$-\int d\mathbf{k}_\parallel\int d\mathbf{k}_\parallel' F(\mathbf{k}_\parallel,\mathbf{k}_\parallel')F_-(\mathbf{k}_\parallel',\boldsymbol{\nu})E_0(\mathbf{k}_\parallel)$$
$$+\int d\mathbf{k}_\parallel\int d\mathbf{k}_\parallel'\int d\mathbf{k}_\parallel'' F(\mathbf{k}_\parallel,\mathbf{k}_\parallel')F_-(\mathbf{k}_\parallel',\mathbf{k}_\parallel'')F_-$$
$$\times(\mathbf{k}_\parallel'',\boldsymbol{\nu})E_0(\mathbf{k}_\parallel)+\ldots, \tag{19}$$

where

$$F(\mathbf{k}_\parallel,\boldsymbol{\nu})=F_+(\mathbf{k}_\parallel,\boldsymbol{\nu})-F_-(\mathbf{k}_\parallel,\boldsymbol{\nu})r(\mathbf{k}_\parallel)$$
$$=\frac{\Gamma_-(\boldsymbol{\nu})}{\Gamma_-(\mathbf{k}_\parallel)}\frac{1}{(2\pi)^2}\int d\boldsymbol{\rho}[r_1(\mathbf{k}_\parallel,\boldsymbol{\nu})\exp[i\Gamma_+\xi(\boldsymbol{\rho})]$$
$$-r(\mathbf{k}_\parallel)\exp[-i\Gamma_-\xi(\boldsymbol{\rho})]]\exp[i(\mathbf{k}_\parallel-\boldsymbol{\nu})\boldsymbol{\rho}]$$
$$=\Gamma_-(\boldsymbol{\nu})\sum_{n=1}^{\infty}\frac{i^n\Gamma_+^{n-1}(\mathbf{k}_\parallel)}{n!}(1$$
$$-r_1^{n-1}(\mathbf{k}_\parallel,\boldsymbol{\nu})r(\mathbf{k}_\parallel))\frac{1}{(2\pi)^2}\int d\boldsymbol{\rho}\xi^n(\boldsymbol{\rho})$$
$$\times\exp[i(\mathbf{k}_\parallel-\boldsymbol{\nu})\boldsymbol{\rho}]. \tag{20}$$

In the last expression we introduced the notation

$$r_1(\mathbf{k}_\parallel,\boldsymbol{\nu})=\frac{\Gamma_-(\mathbf{k}_\parallel)}{\Gamma_+(\mathbf{k}_\parallel)}=\frac{\Gamma_1(\mathbf{k}_\parallel)-\Gamma_2(\boldsymbol{\nu})}{\Gamma_1(\mathbf{k}_\parallel)+\Gamma_2(\boldsymbol{\nu})}.$$

A number of conclusions about the angular reflection spectrum for x-rays can be drawn on the basis of the structure of the expressions (19) and (20). We introduce the scattering angle $\theta_s=\cos^{-1}(\nu/\kappa)$. It follows from the last expression that $|r_1(\mathbf{k}_\parallel,\boldsymbol{\nu})|^2\approx 1$, when the scattering angle is less than the critical angle for total external reflection $\theta_s<\theta_c$, and $|r_1(\mathbf{k}_\parallel,\boldsymbol{\nu})|^2\ll 1$ for $\theta_s>\theta_c$. On the other hand, the reflection coefficient $r(\mathbf{k}_\parallel)$ depends only on the angle of incidence $\theta_0=\cos^{-1}(k_\parallel/\kappa)$ and satisfies similar properties: $|r(\mathbf{k}_\parallel)|^2\approx 1$ for $\theta_0<\theta_c$ and $|r(\mathbf{k}_\parallel)|^2\ll 1$ for $\theta_0>\theta_c$. Therefore, for a large angle of incidence and a small scattering angle, the term $F_+(\mathbf{k}_\parallel,\boldsymbol{\nu})$ makes the main contribution to $F(\mathbf{k}_\parallel,\boldsymbol{\nu})$, and for a small angle of incidence and a large scattering angle the term $F_-(\mathbf{k}_\parallel,\boldsymbol{\nu})$ makes the main contribution. In the region of total external reflection the amplitude of the scattered field is sensitive to the phase of the coefficients $r_1(\mathbf{k}_\parallel,\boldsymbol{\nu})$ and $r(\mathbf{k}_\parallel)$; this can lead to oscillations in the angular spectrum of the intensity of the reflected waves. These features of the angular spectra could be helpful in developing methods for reconstructing the surface profile from the angular reflection spectra of x-rays.

6. REFLECTION FROM A FLAT LAYER

Recurrence methods are very effective for calculating the angular reflection spectra of multilayer structures. In principle, a recurrence procedure can be constructed on the basis of Eqs. (11a and b). However, it is more convenient to construct the procedure on the basis of equations for the waves reflected and refracted by a layer of finite thickness.

We introduce the notation

$$I_\xi(\bar{w}_\nu\,u_\mathbf{k})=\frac{1}{(2\pi)^2}\int d\boldsymbol{\rho}\bar{w}_\nu^*(\boldsymbol{\rho},\xi)u_\mathbf{k}(\boldsymbol{\rho},\xi),$$

and so on. From the boundary conditions (6) and the symmetry properties of the wave functions (7) for a flat layer, it is easy to obtain the following integral equations relating the amplitudes of the reflected and refracted waves to the amplitude of the incident wave:

$$\int d\mathbf{k}E_0(\mathbf{k})\int d\mathbf{k}'\left\{\frac{I_\xi(\bar{w}_{\mathbf{k}'},u_\mathbf{k})}{\Gamma_1(\mathbf{k})+\Gamma_2(\mathbf{k}')}\frac{I_\eta(\bar{u}_\nu,\bar{w}_{\mathbf{k}'})}{\Gamma_2(\mathbf{k}')-\Gamma_1(\boldsymbol{\nu})}\right.$$
$$\left.+\frac{I_\xi(w_{\mathbf{k}'},u_\mathbf{k})}{\Gamma_1(\mathbf{k})-\Gamma_2(\mathbf{k}')}\frac{I_\eta(\bar{u}_\nu,w_{\mathbf{k}'})}{\Gamma_2(\mathbf{k}')-\Gamma_1(\boldsymbol{\nu})}\right\}$$
$$=\int d\mathbf{k}E_r(\mathbf{k})\int d\mathbf{k}'\left\{\frac{I_\xi(\bar{w}_{\mathbf{k}'},\bar{u}_\mathbf{k})}{\Gamma_1(\mathbf{k})-\Gamma_2(\mathbf{k}')}\frac{I_\eta(\bar{u}_\nu,\bar{w}_{\mathbf{k}'})}{\Gamma_2(\mathbf{k}')-\Gamma_1(\boldsymbol{\nu})}\right.$$
$$\left.+\frac{I_\xi(w_{\mathbf{k}'},\bar{u}_\mathbf{k})}{\Gamma_1(\mathbf{k})+\Gamma_2(\mathbf{k}')}\frac{I_\eta(\bar{u}_\nu,w_{\mathbf{k}'})}{\Gamma_2(\mathbf{k}')+\Gamma_1(\boldsymbol{\nu})}\right\},$$
$$E_0(\boldsymbol{\nu})\frac{4\Gamma_1(\boldsymbol{\nu})}{\kappa^2(\varepsilon_1-\varepsilon_2)}=\int d\mathbf{k}E_t(\mathbf{k})\int d\mathbf{k}'\frac{\kappa^2(\varepsilon_2-\varepsilon_1)}{\Gamma_2(\mathbf{k}')}$$
$$\times\left\{\frac{I_\xi(u_\nu,w_{\mathbf{k}'})}{\Gamma_2(\mathbf{k}')-\Gamma_1(\boldsymbol{\nu})}\frac{I_\eta(w_{\mathbf{k}'},u_\mathbf{k})}{\Gamma_1(\mathbf{k})-\Gamma_2(\mathbf{k}')}\right.$$
$$\left.+\frac{I_\xi(u_\nu,\bar{w}_{\mathbf{k}'})}{\Gamma_2(\mathbf{k}')+\Gamma_1(\boldsymbol{\nu})}\frac{I_\eta(\bar{w}_{\mathbf{k}'},u_\mathbf{k})}{\Gamma_1(\mathbf{k})+\Gamma_2(\mathbf{k}')}\right\}. \tag{21}$$

Recurrence methods based on Eqs. (21) make it possible to calculate the angular reflection spectra of arbitrary multilayer structures.

7. SCATTERING BY A ROUGH SURFACE

Now let $\xi(\rho)$ be a random function. If the surface protuberances are statistically homogeneous, then the correlation function has the form

$$\langle \xi(\boldsymbol{\rho}')\xi(\boldsymbol{\rho}'')\rangle = \sigma^2 R(\boldsymbol{\rho}''-\boldsymbol{\rho}'), \tag{22}$$

where σ is the rms height of the protuberances. The integral equation relating the angular spectrum of the scattered wave to the angular spectrum of the incident wave has the form (11a). Squaring the absolute values of both parts of Eqs. (11a), we obtain for the statistically homogeneous protuberances

$$\int d\mathbf{k}_\parallel |E_0(\mathbf{k}_\parallel)|^2 \int d\boldsymbol{\rho} K_0(\mathbf{k}_\parallel,\boldsymbol{\nu},\boldsymbol{\rho})\exp[-i(\mathbf{k}_\parallel-\boldsymbol{\nu})\boldsymbol{\rho}] = \int d\mathbf{k}_\parallel |E_r(\mathbf{k}_\parallel)|^2 \int d\boldsymbol{\rho} K_r(\mathbf{k}_\parallel,\boldsymbol{\nu},\boldsymbol{\rho})\exp[-i(\mathbf{k}_\parallel-\boldsymbol{\nu})\boldsymbol{\rho}], \tag{23}$$

where

$$K_0(\mathbf{k}_\parallel,\boldsymbol{\nu},\boldsymbol{\rho}) = \langle[\Gamma_- - \mathbf{m}\nabla\xi(\boldsymbol{\rho}')][\Gamma_-^* - \mathbf{m}\nabla\xi(\boldsymbol{\rho}'')]\exp[i\Gamma_+\xi(\boldsymbol{\rho}') - i\Gamma_+^*\xi(\boldsymbol{\rho}'')]\rangle,$$

$$K_r(\mathbf{k}_\parallel,\boldsymbol{\nu},\boldsymbol{\rho}) = \langle[\Gamma_+ + \mathbf{m}\nabla\xi(\boldsymbol{\rho}')][\Gamma_+^* + \mathbf{m}\nabla\xi(\boldsymbol{\rho}'')] \times\exp[-i\Gamma_-\xi(\boldsymbol{\rho}') + i\Gamma_-^*\xi(\boldsymbol{\rho}'')]\rangle.$$

Here

$$\Gamma_\pm(\mathbf{k}_\parallel) = \Gamma_1(\mathbf{k}_\parallel) \pm \Gamma_2(\boldsymbol{\nu}), \quad \mathbf{m} = \mathbf{k}_\parallel + \boldsymbol{\nu}.$$

To determine K_0 and K_v it is necessary to know the six-dimensional distribution function of $w(\xi(\rho'),\ \xi(\rho''),\ \xi_x(\rho'),\ \xi_x(\rho''),\ \xi_y(\rho'),\ \xi_y(\rho''))$. We shall assume that the distribution function is Gaussian:

$$w(x_1,\dots,x_6,\boldsymbol{\rho}) = \frac{1}{\sigma_1\dots\sigma_6\sqrt{D}}\exp\left\{-\frac{1}{2D}\sum_{n,m=1}^{6} D_{nm} \times\frac{x_n-a_n}{\sigma_n}\frac{x_m-a_m}{\sigma_m}\right\}, \tag{24}$$

where $a_n = \langle x_n\rangle$ and $\sigma_n^2 = \langle (x_n-a_n)^2\rangle$. Calculating the averages of the products of the function ξ and its derivatives, we obtain for the correlation matrix D_{nm}

$$D_{nm} = \begin{vmatrix} 1 & R & 0 & R_x & 0 & R_y \\ R & 1 & -R_x & 0 & -R_y & 0 \\ 0 & -R_x & \gamma_1^2 & -R_{xx} & \gamma_{12}^2 & -R_{xy} \\ R_x & 0 & -R_{xx} & \gamma_1^2 & -R_{xy} & \gamma_{12}^2 \\ 0 & -R_y & \gamma_{12}^2 & -R_{xy} & \gamma_2^2 & -R_{yy} \\ R_y & 0 & -R_{xy} & \gamma_{12}^2 & -R_{yy} & \gamma_2^2 \end{vmatrix}, \tag{25}$$

where $R_x = \partial R(\rho)/\partial x$, $R_{xy} = \partial^2 R(\rho)/\partial x\partial y$, $\gamma_1^2 = -R_{xx}(0)$, $\gamma_2^2 = -R_{yy}(0)$, and $\gamma_{12}^2 = -R_{xy}(0)$. The averages of interest to us can be easily calculated with the aid of the characteristic function

$$\theta(p_1,\dots,p_6) = \langle \exp[i(p_1x_1+\dots+p_6x_6)]\rangle,$$

which for the distribution (24) has the form[13]

$$\theta(p_1,\dots,p_6) = \exp\left[i\sum_{n=1}^{6} a_n p_n - \frac{1}{2}\sum_{n,m=1}^{6}\sigma_n\sigma_m R_{nm}p_n p_m\right]. \tag{26}$$

Using the formula (26) and the correlation matrix (25), it is easy to obtain

$$K_0(\mathbf{k}_\parallel,\boldsymbol{\nu},\boldsymbol{\rho}) = \left[|\Gamma_-|^2 - i\sigma^2\mathbf{m}\nabla R(\Gamma_+\Gamma_- + \Gamma_+^*\Gamma_-^*) - \sigma^2\sum_{\alpha,\beta} m_\alpha m_\beta (R_{\alpha\beta} + \sigma^2|\Gamma_+|^2 R_\alpha R_\beta)\right]\exp\left[-\frac{\sigma^2}{2}(\Gamma_+^2 + \Gamma_+^{*2} - 2|\Gamma_+|^2 R)\right],$$

$$K_r(\mathbf{k}_\parallel,\boldsymbol{\nu},\boldsymbol{\rho}) = \left[|\Gamma_+|^2 + i\sigma^2\mathbf{m}\nabla R(\Gamma_+\Gamma_- + \Gamma_+^*\Gamma_-^*) - \sigma^2\sum_{\alpha,\beta} m_\alpha m_\beta (R_{\alpha\beta} + \sigma^2|\Gamma_-|^2 R_\alpha R_\beta)\right]\exp\left[-\frac{\sigma^2}{2}(\Gamma_-^2 + \Gamma_-^{*2} - 2|\Gamma_-|^2 R)\right],$$

where $\alpha,\ \beta = x,\ y$.

Integrating by parts, as discussed in Sec. 3, we can put Eq. (23) in the form

$$\int d\mathbf{k}_\parallel |E_0(\mathbf{k}_\parallel)|^2 \frac{\exp[-\sigma^2(\Gamma_+^2+\Gamma_+^{*2})/2]}{|\Gamma_+|^2}\int d\boldsymbol{\rho} \times\exp[\sigma^2|\Gamma_+|^2 R(\boldsymbol{\rho}) - i(\mathbf{k}_\parallel-\boldsymbol{\nu})-\boldsymbol{\rho}] = \int d\mathbf{k}_\parallel |E_r(\mathbf{k}_\parallel)|^2 \frac{\exp[-\sigma^2(\Gamma_-^2+\Gamma_-^{*2})/2]}{|\Gamma_+|^2}\int d\boldsymbol{\rho} \times\exp[\sigma^2|\Gamma_-|^2 R(\boldsymbol{\rho}) - i(\mathbf{k}_\parallel-\boldsymbol{\nu})-\boldsymbol{\rho}]. \tag{27}$$

Equation (27) makes it possible to calculate the angular spectrum of the scattering intensity if the correlation function of the protuberances is known.

8. PROPERTIES OF THE ANGULAR SCATTERING SPECTRA

In the case $\delta^2|\Gamma|^2 \ll 1$, when only the first two terms need be retained in the expansion of the exponential in Eq. (27), we obtain

$$|E_r(\boldsymbol{\nu})|^2 - |E_0(\boldsymbol{\nu})|^2|\bar{r}(\boldsymbol{\nu})|^2 = \sigma^2\int d\mathbf{k}_\parallel\left[|E_0(\mathbf{k}_\parallel)|^2\frac{|\Gamma_-(\boldsymbol{\nu})|^2}{|\Gamma_+(\mathbf{k}_\parallel)|^2}\frac{f_+(\mathbf{k}_\parallel)}{f_-(\boldsymbol{\nu})} - |E_r(\mathbf{k}_\parallel)|^2\frac{|\Gamma_-(\boldsymbol{\nu})|^2}{|\Gamma_-(\mathbf{k}_\parallel)|^2}\frac{f_-(\mathbf{k}_\parallel)}{f_-(\boldsymbol{\nu})}\right]R(\mathbf{k}_\parallel-\boldsymbol{\nu}), \tag{28}$$

where

$$f_{\pm}(\mathbf{k}_{\|})=\exp\left[-\frac{\sigma^2}{2}(\Gamma_{\pm}^2(\mathbf{k}_{\|})+\Gamma_{\pm}^{*2}(\mathbf{k}_{\|}))\right],$$

$$\bar{r}(\boldsymbol{\nu})=r(\boldsymbol{\nu})\exp[-2\sigma^2\Gamma_1(\boldsymbol{\nu})\Gamma_2(\boldsymbol{\nu})]. \quad (29)$$

We note that the expression for the reflection coefficient $\bar{r}(\nu)$ is identical to the expression obtained previously in Ref. 14 and later generalized in Ref. 15. One can see from Eq. (28) that this expression is only the zeroth approximation in the series expansion in the small parameter $\sigma^2|\Gamma|^2$. We shall now determine the difference of the angular scattering spectrum calculated according to the exact formula (27) and by the distorted-wave method.

The equation (27) can be put in the form

$$\begin{aligned}|E_r(\boldsymbol{\nu})|^2&+\int d\mathbf{k}_{\|}|E_r(\mathbf{k}_{\|})|^2\frac{f_-(\mathbf{k}_{\|})}{f_-(\boldsymbol{\nu})}\left|\frac{\Gamma_-(\boldsymbol{\nu})}{\Gamma_-(\mathbf{k}_{\|})}\right|^2\frac{1}{(2\pi)^2}\int d\boldsymbol{\rho}\\&\times\{\exp[\sigma^2|\Gamma_-(\mathbf{k}_{\|})|^2R(\boldsymbol{\rho})]-1\}\exp[-i(\mathbf{k}_{\|}-\boldsymbol{\nu})\boldsymbol{\rho}]\\&=|E_0(\boldsymbol{\nu})|^2|\bar{r}(\boldsymbol{\nu})|^2+\int d\mathbf{k}_{\|}|E_0(\mathbf{k}_{\|})|^2\frac{f_+(\mathbf{k}_{\|})}{f_-(\boldsymbol{\nu})}\left|\frac{\Gamma_-(\boldsymbol{\nu})}{\Gamma_+(\mathbf{k}_{\|})}\right|^2\\&\times\frac{1}{(2\pi)^2}\int d\boldsymbol{\rho}\{\exp[\sigma^2|\Gamma_+(\mathbf{k}_{\|})|^2R(\boldsymbol{\rho})]-1\}\\&\times\exp[-i(\mathbf{k}_{\|}-\boldsymbol{\nu})\boldsymbol{\rho}].\end{aligned} \quad (30)$$

The equation (30) is a Fredholm equation of the second kind whose solution can be obtained by iteration:

$$\begin{aligned}|E_r(\boldsymbol{\nu})|^2&=|E_0(\boldsymbol{\nu})|^2|r(\boldsymbol{\nu})|^2+\int d\mathbf{k}_{\|}G(\mathbf{k}_{\|},\boldsymbol{\nu})|E_0(\mathbf{k}_{\|})|^2\\&-\int d\mathbf{k}_{\|}\int d\mathbf{k}_{\|}'G(\mathbf{k}_{\|},\mathbf{k}_{\|}')G_-(\mathbf{k}_{\|}',\mathbf{k}_{\|}'')G_-(\mathbf{k}_{\|}'',\boldsymbol{\nu})\\&\times|E_0(\mathbf{k}_{\|})|^2+\int d\mathbf{k}_{\|}\int d\mathbf{k}_{\|}'\int d\mathbf{k}_{\|}''G(\mathbf{k}_{\|},\mathbf{k}_{\|}')\\&\times G_-(\mathbf{k}_{\|}',\mathbf{k}_{\|}'')G_-(\mathbf{k}_{\|}'',\boldsymbol{\nu})|E_0(\mathbf{k}_{\|})|^2\ldots,\end{aligned} \quad (31)$$

where

$$\begin{aligned}G_{\pm}(\mathbf{k}_{\|},\boldsymbol{\nu})&=\left|\frac{\Gamma_-(\boldsymbol{\nu})}{\Gamma_{\pm}(\mathbf{k}_{\|})}\right|^2\frac{f_{\pm}(\mathbf{k}_{\|})}{f_-(\boldsymbol{\nu})}\frac{1}{(2\pi)^2}\\&\times\int d\boldsymbol{\rho}\{\exp[\sigma^2|\Gamma_{\pm}(\mathbf{k}_{\|})|^2R(\boldsymbol{\rho})]-1\}\\&\times\exp[-i(\mathbf{k}_{\|}-\boldsymbol{\nu})\boldsymbol{\rho}],\end{aligned} \quad (32)$$

$$\begin{aligned}G(\mathbf{k}_{\|},\boldsymbol{\nu})&=G_+(\mathbf{k}_{\|},\boldsymbol{\nu})-G_-(\mathbf{k}_{\|},\boldsymbol{\nu})|\bar{r}(\mathbf{k}_{\|})|^2\\&=\left|\frac{\Gamma_-(\boldsymbol{\nu})}{\Gamma_-(\mathbf{k}_{\|})}\right|^2\frac{f_-(\mathbf{k}_{\|})}{f_-(\boldsymbol{\nu})}\frac{1}{(2\pi)^2}\int d\boldsymbol{\rho}\,\exp[-i(\mathbf{k}_{\|}\\&-\boldsymbol{\nu})\boldsymbol{\rho}]\{|\bar{r}_1(\mathbf{k}_{\|},\boldsymbol{\nu})|^2\exp[\sigma^2|\Gamma_+(\mathbf{k}_{\|})|^2R(\boldsymbol{\rho})]\\&-|\bar{r}(\mathbf{k}_{\|})|^2\exp[\sigma^2|\Gamma_-(\mathbf{k}_{\|})|^2R(\boldsymbol{\rho})]\}.\end{aligned} \quad (33)$$

In Eq. (33) we introduce the variable

$$\begin{aligned}\bar{r}(\mathbf{k}_{\|},\boldsymbol{\nu})&=r_1(\mathbf{k}_{\|},\boldsymbol{\nu})\exp[-2\sigma^2\Gamma_1(\mathbf{k}_{\|})\Gamma_2(\boldsymbol{\nu})]\\&=\frac{\Gamma_1(\mathbf{k}_{\|})-\Gamma_2(\boldsymbol{\nu})}{\Gamma_1(\mathbf{k}_{\|})+\Gamma_2(\boldsymbol{\nu})}\exp[-2\sigma^2\Gamma_1(\mathbf{k}_{\|})\Gamma_2(\boldsymbol{\nu})].\end{aligned} \quad (34)$$

We note that $\bar{r}(\nu)=\bar{r}_1(\nu,\nu)$. Introducing the scattering angle $\theta_s=\cos^{-1}(\nu/\kappa)$ and the angle of incidence $\theta_0=\cos^{-1}(k_{\|}/\kappa)$ by analogy to Sec. 5, we can easily show that $\Gamma_{\pm}(\mathbf{k}_{\|})$, $\bar{r}_1(\mathbf{k}_{\|},\boldsymbol{\nu})$, and $\bar{r}(\mathbf{k}_{\|})$ have the following properties:

$$|\Gamma_+(\mathbf{k}_{\|})|^2\approx|\Gamma_-(\mathbf{k}_{\|})|^2,\quad|\bar{r}_1(\mathbf{k}_{\|},\boldsymbol{\nu})|^2\approx1\quad\text{for }\theta_s<\theta_c,$$

$$|\Gamma_+(\mathbf{k}_{\|})|^2>|\Gamma_-(\mathbf{k}_{\|})|^2,\quad|\bar{r}_1(\mathbf{k}_{\|},\boldsymbol{\nu})|^2\ll1\quad\text{for }\theta_s>\theta_c,$$

$$|\bar{r}(\mathbf{k}_{\|})|^2\approx1\ \text{for }\theta_0<\theta_c\ \text{and}\ |\bar{r}(\mathbf{k}_{\|})|^2\ll1\ \text{for }\theta_0>\theta_c.$$

It follows from Eq. (33) that for $\theta_0<\theta_c$ we have $G(\nu,\nu)\approx0$. Therefore the expression (29) determines the specular reflection coefficient to a good degree of accuracy. For $\theta_0>\theta_c$, as follows from Eq. (31), the reflection coefficient can differ substantially from the formula (29).

The factor $f_-(\mathbf{k}_{\|})/f_-(\nu)$ determines the angular dependence of the function $G(\mathbf{k}_{\|},\boldsymbol{\nu})$ on the scattering angle. It has the form

$$\begin{aligned}\frac{f_-(\mathbf{k}_{\|})}{f_-(\boldsymbol{\nu})}&=\exp\left\{-\frac{\sigma^2}{2}[\Gamma_1^2(\mathbf{k}_{\|})-\Gamma_1^2(\boldsymbol{\nu})-2(\Gamma_1(\mathbf{k}_{\|})\right.\\&\left.-\Gamma_2(\boldsymbol{\nu}))\Gamma_2(\boldsymbol{\nu})+\text{c.c.}]\right\}.\end{aligned}$$

If medium 1 is a vacuum, we have

$$\frac{f_-(\mathbf{k}_{\|})}{f_-(\boldsymbol{\nu})}=\exp\left\{\frac{\sigma^2}{2}\Gamma_1^2(\boldsymbol{\nu})-\sigma^2\Gamma_1(\boldsymbol{\nu})(\Gamma_2(\boldsymbol{\nu})+\Gamma_2^*(\boldsymbol{\nu}))\right\}, \quad (35)$$

and so this cofactor as a function of the wave vector ν possesses a maximum at $\theta_s\approx\theta_c$. For $\theta_0<\theta_c$ this maximum becomes sharper, since the term in the braces in Eq. (3) vanishes for $\theta_s<\theta_c$ and is different from zero for $\theta_s>\theta_c$. Therefore, the angular width of the maximum of the Yoneda anomalous scattering[4] depends on the angle of incidence. For $\theta_0<\theta_c$ the maximum is narrow and for $\theta_0>\theta_c$ the maximum of the Yoneda anomalous scattering broadens and is mainly determined by the function (35).

For a wide class of correlation functions, for example, of the form $R(\rho)=\exp[-(\rho/l)^{2h}]$, the following asymptotic formula is found to be helpful:

$$e^{AR(\rho)}\approx1+(e^A-1)R^{\sqrt{1+A^2}}. \quad (36)$$

In Figs. 2a, b, and c the solid curve is a plot of the function

$$f_1(\rho)=\exp\{A[(-(\rho/l)^{2h})-1]\}$$

and the dashed curve represents the function

$$f_2(\rho)=e^{-A}+(1-e^{-A})\exp[-\sqrt{1+A^2}(\rho/l)^{2h}]$$

where $A=1$ and $h=0.5$ (a), 0.75 (b), and 1 (c). Figure 2d displays the difference $\Delta f(\rho)=f_1(\rho)-f_2(\rho)$ of the functions $f_1(\rho)$ and $f_2(\rho)$ for $h=1$ and $A=0.1$ (1), 1 (2) and 10

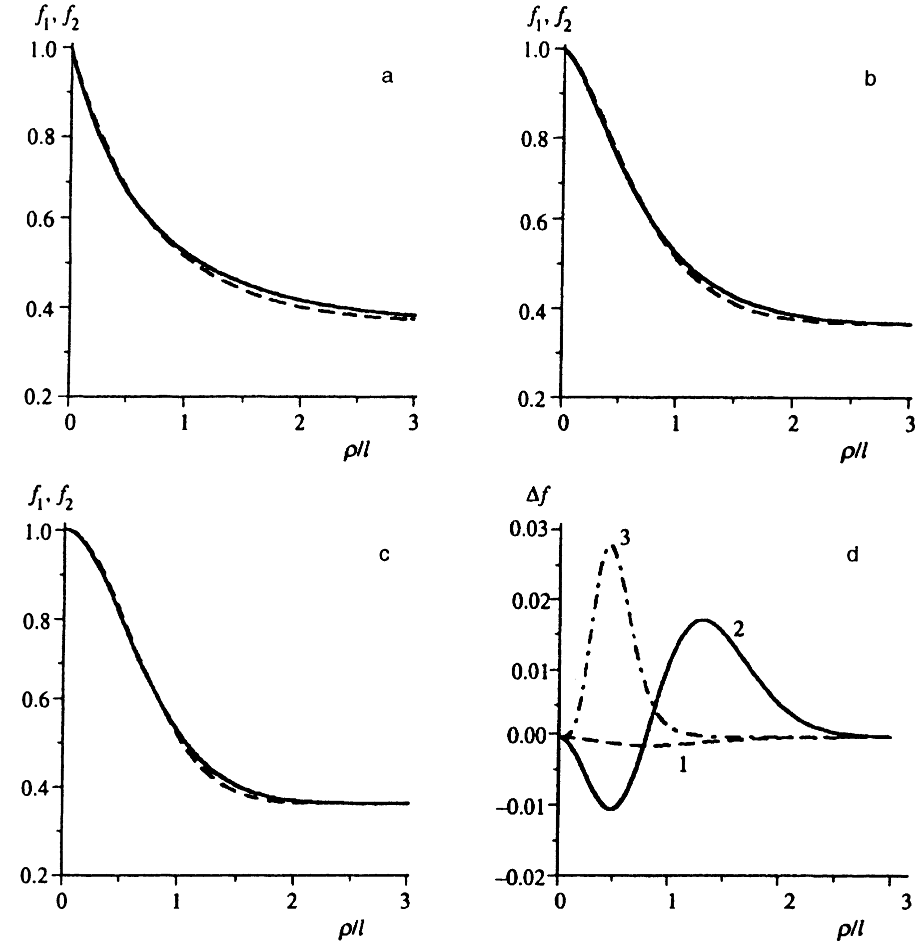

FIG. 2. For the interpretation of Eq. (36).

(3). As one can see from Fig. 2d, the maximum deviation of the function $f_2(\rho)$ from the function $f_1(\rho)$ is less than 3%. Using the formula (36), it is easy to estimate the angular width of the nonspecular scattering spectrum. Thus, for a Gaussian distribution function $R(\rho)=\exp[-(\rho/l)^2]$ the functions $G_\pm(\mathbf{k}_\parallel,\boldsymbol{\nu})$ have the form

$$G_\pm(\mathbf{k}_\parallel,\boldsymbol{\nu})=\left|\frac{\Gamma_-(\boldsymbol{\nu})}{\Gamma_\pm(\mathbf{k}_\parallel)}\right|^2\frac{f_\pm(\mathbf{k}_\parallel)}{f_-(\boldsymbol{\nu})}\{\exp[\sigma^2|\Gamma_\pm(\mathbf{k}_\parallel)|^2]-1\}\frac{L_\pm^2(\mathbf{k}_\parallel)}{4\pi}\exp\left[-\frac{1}{4}(\mathbf{k}_\parallel-\boldsymbol{\nu})^2L_\pm^2(\mathbf{k}_\parallel)\right], \quad (37)$$

where

$$L_\pm^2(\mathbf{k}_\parallel)=\frac{l^2}{\sqrt{1+\sigma^4|\Gamma_\pm(\mathbf{k}_\parallel)|^4}}. \quad (38)$$

Therefore, for $\sigma^2|\Gamma|^2\ll 1$ the angular width of the nonspecular scattering spectrum is determined by the longitudinal correlation length of the protuberances. For $\sigma^2|\Gamma|^2>1$, when the phase increment on the transitional layer of the interphase becomes equal to 2π, the angular width of the nonspecular scattering spectrum starts to depend on the characteristic slope angle σ/l of the protuberances.

The correlation function of the protuberances can be reconstructed from the angular scattering spectra. Expanding in a series the exponential of the correlation function in Eq. (27), we obtain

$$|E_r(\boldsymbol{\nu})|^2-|E_0(\boldsymbol{\nu})|^2|\bar{r}(\boldsymbol{\nu})|^2=\int d\mathbf{k}_\parallel\frac{|\Gamma_-(\boldsymbol{\nu})|^2}{|\Gamma_+(\mathbf{k}_\parallel)|^2}\frac{f-(\mathbf{k}_\parallel)}{f_-(\boldsymbol{\nu})}\sum_{n=1}^{N}\frac{\sigma^{2n}}{n!}\times[|E_0(\boldsymbol{\nu})|^2|\bar{r}_1(\mathbf{k}_\parallel,\boldsymbol{\nu})|^2|\Gamma_+(\mathbf{k}_\parallel)|^{2n}-|E_r(\mathbf{k}_\parallel)|^2|\Gamma_-(\mathbf{k}_\parallel)|^{2n}]\frac{1}{(2\pi)^2}\int d\boldsymbol{\rho}R^n(\boldsymbol{\rho})\times\exp[-i(\mathbf{k}_\parallel-\boldsymbol{\nu})\boldsymbol{\rho}]. \quad (39)$$

Replacing the integral over $\mathbf{k}_\parallel$ in Eq. (39) by a sum with a step equal to the step of the experimental data in the angular scattering spectrum, we obtain a system of algebraic equations for $R_n(\mathbf{k}_\parallel-\boldsymbol{\nu})$. The accuracy with which $R_n(\mathbf{k}_\parallel-\boldsymbol{\nu})$ is determined and the number of harmonics of the relief depend on the size of the array of experimental data.

As noted above, the formula (36), which greatly simplifies the problem of reconstructing the correlation function, especially if $\sigma^2|\Gamma_\pm|^2<1$, can be used for a wide class of correlation functions. In this case, we obtain from Eq. (27), using Eq. (36),

$$|E_r(\boldsymbol{\nu})|^2-|E_0(\boldsymbol{\nu})|^2|\bar{r}(\boldsymbol{\nu})|^2$$
$$=\int d\mathbf{k}_\parallel \frac{|\Gamma_-(\boldsymbol{\nu})|^2}{|\Gamma_+(\mathbf{k}_\parallel)|^2}\frac{f_-(\mathbf{k}_\parallel)}{f_-(\boldsymbol{\nu})}[|E_0(\mathbf{k}_\parallel)|^2|\bar{r}_1(\mathbf{k}_\parallel,\boldsymbol{\nu})|^2$$
$$\times[\exp(\sigma^2|\Gamma_+(\mathbf{k}_\parallel)|^2)-1]$$
$$-|E_r(\mathbf{k}_\parallel)|^2[\exp(\sigma^2|\Gamma_-(\mathbf{k}_\parallel)|^2)$$
$$-1]]\frac{1}{(2\pi)^2}\int d\boldsymbol{\rho}R(\boldsymbol{\rho})\exp[-i(\mathbf{k}_\parallel-\boldsymbol{\nu})\boldsymbol{\rho}].$$

For an incident plane wave $|E_0(\mathbf{k}_\parallel)|^2=I_0\delta(\mathbf{k}_\parallel-\boldsymbol{\kappa}_\parallel)$ and $|\Gamma_-|^2<|\Gamma_+|^2$ the formula (39) simplifies substantially and assumes the form

$$|E_r(\boldsymbol{\nu})|^2-I_0|\bar{r}(\boldsymbol{\nu})|^2\delta(\boldsymbol{\kappa}_\parallel-\boldsymbol{\nu})$$
$$=I_0\frac{|\Gamma_-(\boldsymbol{\nu})|^2}{|\Gamma_+(\boldsymbol{\kappa}_\parallel)|^2}\frac{f_-(\boldsymbol{\kappa}_\parallel)}{f_-(\boldsymbol{\nu})}|\bar{r}_1(\boldsymbol{\kappa}_\parallel,\boldsymbol{\nu})|^2[\exp(\sigma^2|\Gamma_+(\boldsymbol{\kappa}_\parallel)|^2)$$
$$-1]\frac{1}{(2\pi)^2}\int d\boldsymbol{\rho}R(\boldsymbol{\rho})\exp[-i(\boldsymbol{\kappa}_\parallel-\boldsymbol{\nu})\boldsymbol{\rho}].$$

We can see that in this case the correlation function of the protuberances is determined from the measured angular dependences of the scattering intensity by means of a two-dimensional Fourier transform.

9. CONCLUSIONS

The incident, reflected, and transmitted wave fields can be represented as expansions in terms of the wave functions (5). These wave functions satisfy the symmetry properties (7), which are the analog of the reciprocity theorem for the propagation of electromagnetic radiation in an inhomogeneous medium.[9] The indicated symmetry properties make it possible to obtain integral equations relating the angular spectra of the reflected and refracted waves with the angular spectrum of the incident wave. A substantial difference of the obtained equations from other perturbation theory equations the (distorted-wave method) is that here the law of conservation of the energy flux holds. In the case when the interface is sufficiently smooth, these integral equations can be reduced to Fredholm integral equations of the second kind, which can be solved by the method of iterations. The rate of convergence of the iteration series depends on the form of the two-dimensional Fourier spectrum of the interface and increases with the angles of incidence and scattering.

The investigations performed made it possible to determine the limits of applicability of the standard expressions, which are widely used for determining the statistical characteristics of protuberances, for the reflection coefficients of rough surfaces. Algorithms were developed for reconstructing the surface profile from the angular reflection spectra and the correlation functions of the protuberances from the angular scattering spectra. In contrast to the distorted-wave theory, the expressions which we have obtained do not contain any limits on the correlation length and the amplitude of the protuberances.

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