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# Resonance Properties of Scattering and Generation of Waves on Cubically Polarisable Dielectric Layers

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## 1. Introduction

In this paper we investigate the problem of scattering and generation of waves on an isotropic, non-magnetic, linearly polarised (E-polarisation), non-linear, layered, cubically polarisable, dielectric structure, which is excited by a packet of plane waves, in the range of resonant frequencies. We consider wave packets consisting of both strong electromagnetic fields at the excitation frequency, leading to the generation of waves, and of weak fields at the multiple frequencies, which do not lead to the generation of harmonics but influence on the process of scattering and generation of waves. The analysis of the quasi-homogeneous electromagnetic fields of the non-linear dielectric layered structure made it possible to derive a condition of phase synchronism of waves. If the classical formulation of the mathematical model is supplemented by this condition of phase synchronism, we arrive at a rigorous formulation of a system of boundary-value problems with respect to the components of the scattered and generated fields (see Angermann & Yatsyk (2011)). This system is transformed to equivalent systems of non-linear problems, namely a system of one-dimensional non-linear Fredholm integral equations of the second kind and a system of non-linear boundary-value problems of Sturm-Liouville type. The numerical algorithms of the solution of the non-linear problems are based on iterative procedures which require the solution of a linearised system in each step. In this way the approximate solution of the non-linear problems is described by means of solutions of linearised problems with an induced dielectric permeability. The analytical continuation of these problems into the region of complex values of the frequency parameter allows us to switch to the analysis of spectral problems. The corresponding eigen-frequencies form a discrete, countable set of points, with the only possible accumulation point at infinity, and lie on a complex two-sheeted Riemann surface. In the frequency domain, the resonant scattering and generation properties of non-linear structures are determined by the proximity of the excitation frequencies of the non-linear structures to the complex eigen-frequencies of the corresponding homogeneous linear spectral problems with the induced non-linear dielectric permeability of the medium.

Results of calculations of characteristics of the scattered field of a plane wave are presented, taking into account the third harmonic generated by non-linear cubically polarisable layers with both negative as well as positive values of the cubic susceptibility of the medium.

Within the framework of the closed system, which is given by a system of self-consistent boundary-value problems, we show the following. The variation of the imaginary part of the permittivity of the layer at the excitation frequency can take both positive and negative values along the height of the non-linear layer. It is induced by the non-linear part of the permittivity and is caused by the loss of energy in the non-linear medium (at the frequency of the incident field), which is spent for the generation of the electromagnetic field of the third harmonic (at the triple frequency). The magnitude of this variation is determined by the amplitude and phase characteristics of the fields which are scattered and generated by the non-linear layer.

It is shown that layers with negative and positive values of the coefficient of cubic susceptibility of the non-linear medium have fundamentally different scattering and generation properties in the range of resonance. For instance, in the case of negative values of the susceptibility, a decanalisation of the electromagnetic field can be detected. With the increase of intensity of the incident field, the maximal variations of the reflection and transmission coefficients can be observed in the vicinity of the normal incidence of the plane wave. A previously transparent structure becomes semi-transparent, and the reflection and transmission coefficients become comparable. For the layer considered here, the maximal portion of the total energy generated in the third harmonic is observed in the direction normal to the structure and amounts to 3.9% of the total dissipated energy. For a layer with a positive value of the susceptibility an effect of energy canalisation is observed. The increase of intensity of the incident field leads to an increase of the angle of transparency which increasingly deviates from the direction normal to the layer and which is responsible for a reflection coefficient close to zero. In this case, the maximal portion of energy generated in the third harmonic is observed near the angle of transparency of the non-linear layer. In the numerical experiments there have been reached intensities of the excitation field of the layer such that the relative portion of the total energy generated in the third harmonic is 36%. The paper also presents results of numerical calculations that describe properties of the non-linear dielectric permeabilities of the layers as well as their scattering and generation characteristics. The tests are illustrated by figures showing the dependence on the amplitudes and the angles of incidence of the plane wave for layers with negative and positive values of the coefficient of the cubic susceptibility of the non-linear medium.

## 2. Maxwell equations and wave propagation in non-linear media with cubic polarisability

In this section we give a short overview on the derivation of the mathematical model. A more detailed explanation can be found in Angermann & Yatsyk (2011). Electrodynamical wave phenomena in charge- and current-free media can be described by the Maxwell equations

$$\nabla \times \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t}, \quad \nabla \times \mathbf{H} = \frac{1}{c} \frac{\partial \mathbf{D}}{\partial t}, \quad \nabla \cdot \mathbf{D} = 0, \quad \nabla \cdot \mathbf{B} = 0. \quad (1)$$

Here  $\mathbf{E} = \mathbf{E}(\mathbf{r}, t)$ ,  $\mathbf{H} = \mathbf{H}(\mathbf{r}, t)$ ,  $\mathbf{D} = \mathbf{D}(\mathbf{r}, t)$  and  $\mathbf{B} = \mathbf{B}(\mathbf{r}, t)$  denote the vectors of electric and magnetic field intensities, electric displacement, and magnetic induction, respectively, and  $(\mathbf{r}, t) \in \mathbb{R}^3 \times (0, \infty)$ . The symbol  $\nabla$  represents the formal vector of partial derivatives w.r.t. the spatial variables, i.e.  $\nabla := (\partial/\partial x, \partial/\partial y, \partial/\partial z)^\top$ , where the symbol  $\cdot^\top$  denotes the

transposition. In addition, the system (1) is completed by the material equations

$$\mathbf{D} = \mathbf{E} + 4\pi\mathbf{P}, \quad \mathbf{B} = \mathbf{H} + 4\pi\mathbf{M}, \quad (2)$$

where  $\mathbf{P}$  and  $\mathbf{M}$  are the vectors of the polarisation and magnetic moment, respectively. In the present paper, the non-linear medium under consideration is located in an infinite plate of thickness  $4\pi\delta$ , where  $\delta > 0$  is a given parameter:  $\{\mathbf{r} = (x, y, z)^\top \in \mathbb{R}^3 : |z| \leq 2\pi\delta\}$ . As in the books Akhmediev & Ankevich (2003), Kivshar & Agrawal (2005) and Miloslavsky (2008), the investigations will be restricted to non-linear media without dispersion (cf. Agranovich & Ginzburg (1966)), i.e. we use the following expansion of the polarisation vector in terms of the electric field intensity:

$$\mathbf{P} = \chi^{(1)}\mathbf{E} + (\chi^{(2)}\mathbf{E})\mathbf{E} + ((\chi^{(3)}\mathbf{E})\mathbf{E})\mathbf{E} + \dots, \quad (3)$$

where  $\chi^{(1)}$ ,  $\chi^{(2)}$ ,  $\chi^{(3)}$  are the media susceptibility tensors of rank one, two and three, with components  $\{\chi_{ij}^{(1)}\}_{i,j=1}^3$ ,  $\{\chi_{ijk}^{(2)}\}_{i,j,k=1}^3$  and  $\{\chi_{ijkl}^{(3)}\}_{i,j,k,l=1}^3$ , respectively (see Butcher (1965)). In the case of media which are invariant under the operations of inversion, reflection and rotation, in particular of isotropic media, the quadratic term disappears.

It is convenient to split  $\mathbf{P}$  into its linear and non-linear parts as  $\mathbf{P} = \mathbf{P}^{(L)} + \mathbf{P}^{(NL)} := \chi^{(1)}\mathbf{E} + \mathbf{P}^{(NL)}$ . Similarly, with  $\varepsilon := \mathbf{I} + 4\pi\chi^{(1)}$  and  $\mathbf{D}^{(L)} := \varepsilon\mathbf{E}$ , where  $\mathbf{I}$  denotes the identity in  $\mathbb{C}^3$ , the displacement field in (2) can be decomposed as

$$\mathbf{D} = \mathbf{D}^{(L)} + 4\pi\mathbf{P}^{(NL)}. \quad (4)$$

$\varepsilon$  is the linear term of the permittivity tensor. Furthermore we assume that the media are non-magnetic, i.e.  $\mathbf{M} = \mathbf{0}$ , so that

$$\mathbf{B} = \mathbf{H} \quad (5)$$

by (2). Resolving the equations (1), (4) and (5) w.r.t.  $\mathbf{H}$ , a single vector-valued equation results:

$$\nabla^2\mathbf{E} - \nabla(\nabla \cdot \mathbf{E}) - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{D}^{(L)} - \frac{4\pi}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{P}^{(NL)} = \mathbf{0}. \quad (6)$$

In addition, if the media under consideration are isotropic and transversely inhomogeneous w.r.t.  $z$ , i.e.  $\varepsilon = \varepsilon^{(L)}\mathbf{I}$  with a scalar, possibly complex-valued function  $\varepsilon^{(L)} = \varepsilon^{(L)}(z)$ , if the wave is linearly E-polarised, i.e.  $\mathbf{E} = (E_1, 0, 0)^\top$ ,  $\mathbf{H} = (0, H_2, H_3)^\top$ , and if the electric field  $\mathbf{E}$  is homogeneous w.r.t. the coordinate  $x$ , i.e.  $\mathbf{E}(\mathbf{r}, t) = (E_1(t; y, z), 0, 0)^\top$ , then equation (6) simplifies to

$$\nabla^2\mathbf{E} - \frac{\varepsilon^{(L)}}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{E} - \frac{4\pi}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{P}^{(NL)} = \mathbf{0}, \quad (7)$$

where  $\nabla^2$  reduces to the Laplacian w.r.t.  $y$  and  $z$ , i.e.  $\nabla^2 := \partial^2/\partial y^2 + \partial^2/\partial z^2$ .

The stationary problem of the diffraction of a plane electromagnetic wave (with oscillation frequency  $\omega > 0$ ) on a transversely inhomogeneous, isotropic, non-magnetic, linearly polarised, dielectric layer filled with a cubically polarisable medium (see Fig. 1) is studied in the frequency domain (i.e. in the space of the Fourier amplitudes of the electromagnetic field), taking into account the multiple frequencies  $s\omega$ ,  $s \in \mathbb{N}$ , of the excitation frequency generated by non-linear structure, where a time-dependence of the form  $\exp(-is\omega t)$  is assumed. The transition between the time domain and the frequency domain is performed by means of

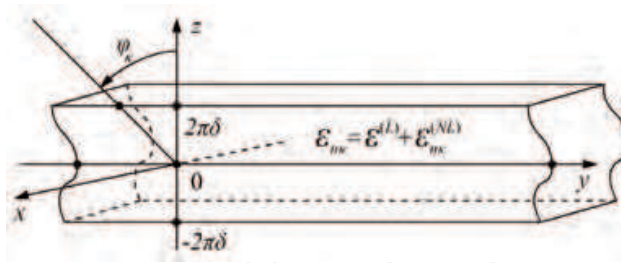


Fig. 1. The non-linear dielectric layered structure

direct and inverse Fourier transforms:

$$\hat{\mathbf{F}}(\mathbf{r}, \hat{\omega}) = \int_{\mathbb{R}} \mathbf{F}(\mathbf{r}, t) e^{i\hat{\omega}t} dt, \quad \mathbf{F}(\mathbf{r}, t) = \frac{1}{2\pi} \int_{\mathbb{R}} \hat{\mathbf{F}}(\mathbf{r}, \hat{\omega}) e^{-i\hat{\omega}t} d\hat{\omega},$$

where  $\mathbf{F}$  is one of the vector fields  $\mathbf{E}$  or  $\mathbf{P}^{(NL)}$ . Applying formally the Fourier transform to equation (7), we obtain the following representation in the frequency domain:

$$\nabla^2 \hat{\mathbf{E}}(\mathbf{r}, \hat{\omega}) + \frac{\varepsilon^{(L)} \hat{\omega}^2}{c^2} \hat{\mathbf{E}}(\mathbf{r}, \hat{\omega}) + \frac{4\pi \hat{\omega}^2}{c^2} \hat{\mathbf{P}}^{(NL)}(\mathbf{r}, \hat{\omega}) = 0. \quad (8)$$

A stationary (i.e.  $\sim \exp(-i\hat{\omega}t)$ ) electromagnetic wave propagating in a weakly non-linear dielectric structure gives rise to a field containing all frequency harmonics (see Sukhorukov (1988), Vinogradova et al. (1990)). Therefore, the quantities describing the electromagnetic field in the time domain subject to equation (7) can be represented by means of the Fourier series

$$\mathbf{F}(\mathbf{r}, t) = \frac{1}{2} \sum_{n \in \mathbb{Z}} \mathbf{F}(\mathbf{r}, n\omega) e^{-in\omega t}, \quad \mathbf{F} \in \{\mathbf{E}, \mathbf{P}^{(NL)}\}. \quad (9)$$

Applying to (9) the Fourier transform, we obtain

$$\hat{\mathbf{F}}(\mathbf{r}, \hat{\omega}) = \frac{1}{2} \int_{\mathbb{R}} \sum_{n \in \mathbb{Z}} \mathbf{F}(\mathbf{r}, n\omega) e^{-in\omega t} e^{i\hat{\omega}t} dt = \frac{\sqrt{2\pi}}{2} \mathbf{F}(\mathbf{r}, n\omega) \delta(\hat{\omega}, n\omega), \quad \mathbf{F} \in \{\mathbf{E}, \mathbf{P}^{(NL)}\}, \quad (10)$$

where  $\delta(s, s_0) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{i(s-s_0)t} dt$  is the Dirac delta-function located at  $s = s_0$ .

Substituting (10) into (8), we obtain an infinite system of coupled equations w.r.t. the Fourier amplitudes of the electric field intensities of the non-linear structure in the frequency domain:

$$\nabla^2 \mathbf{E}(\mathbf{r}, s\omega) + \frac{\varepsilon^{(L)} (s\omega)^2}{c^2} \mathbf{E}(\mathbf{r}, s\omega) + \frac{4\pi (s\omega)^2}{c^2} \mathbf{P}^{(NL)}(\mathbf{r}, s\omega) = 0, \quad s \in \mathbb{Z}. \quad (11)$$

In the case of a three-component  $E$ -polarised electromagnetic field

$$\mathbf{E}(\mathbf{r}, s\omega) = (E_1(s\omega; y, z), 0, 0)^\top, \quad \mathbf{H}(\mathbf{r}, s\omega) = (0; H_2(s\omega; y, z), H_3(s\omega; y, z))^\top, \quad (12)$$

the system (11) reduces to a system of scalar equations w.r.t.  $E_1$ :

$$\nabla^2 E_1(\mathbf{r}, s\omega) + \frac{\varepsilon^{(L)} (s\omega)^2}{c^2} E_1(\mathbf{r}, s\omega) + \frac{4\pi (s\omega)^2}{c^2} P_1^{(NL)}(\mathbf{r}, s\omega) = 0, \quad s \in \mathbb{N}. \quad (13)$$

In writing equation (13), the property  $E_1(\mathbf{r}; j\omega) = \bar{E}_1(\mathbf{r}; -j\omega)$  of the Fourier coefficients and the lack of influence of the static electric field  $E_1(\mathbf{r}, s\omega)|_{s=0} = 0$  on the non-linear structure were taken into consideration.

We assume that the main contribution to the non-linearity is introduced by the term  $\mathbf{P}^{(NL)}(\mathbf{r}, s\omega)$  (cf. Yatsyk (2007), Shestopalov & Yatsyk (2007), Kravchenko & Yatsyk (2007), Angermann & Yatsyk (2008), Yatsyk (2006), Schürmann et al. (2001), Smirnov et al. (2005), Serov et al. (2004)), and we take only the lowest-order terms in the Taylor series expansion of the non-linear part  $\mathbf{P}^{(NL)}(\mathbf{r}, s\omega) = \left( P_1^{(NL)}(\mathbf{r}, s\omega), 0, 0 \right)^\top$  of the polarisation vector in the vicinity of the zero value of the electric field intensity, cf. (3). In this case, the only non-trivial component of the polarisation vector is determined by susceptibility tensor of the third order  $\chi^{(3)}$ . In the time domain, this component can be represented in the form (cf. (3) and (9)):

$$P_1^{(NL)}(\mathbf{r}, t) \doteq \frac{1}{8} \sum_{\substack{n, m, p, s \in \mathbb{Z} \setminus \{0\} \\ n+m+p=s}} \chi_{1111}^{(3)}(s\omega; n\omega, m\omega, p\omega) E_1(\mathbf{r}, n\omega) E_1(\mathbf{r}, m\omega) E_1(\mathbf{r}, p\omega) e^{-is\omega t}, \quad (14)$$

where the symbol  $\doteq$  means that higher-order terms are neglected. Applying to (14) the Fourier transform w.r.t. time, we obtain an expansion in the frequency domain:

$$P_1^{(NL)}(\mathbf{r}, s\omega) = \frac{1}{4} \sum_{j \in \mathbb{N}} 3\chi_{1111}^{(3)}(s\omega; j\omega, -j\omega, s\omega) |E_1(\mathbf{r}, j\omega)|^2 E_1(\mathbf{r}, s\omega) + \frac{1}{4} \sum_{\substack{n, m, p \in \mathbb{Z} \setminus \{0\} \\ n \neq -m, p=s \\ m \neq -p, n=s \\ n \neq -p, m=s \\ n+m+p=s}} \chi_{1111}^{(3)}(s\omega; n\omega, m\omega, p\omega) E_1(\mathbf{r}, n\omega) E_1(\mathbf{r}, m\omega) E_1(\mathbf{r}, p\omega). \quad (15)$$

We see that, under the above assumptions, the electromagnetic waves in a non-linear medium with a cubic polarisability are described by an infinite system (13)&(15) of coupled non-linear equations (Yatsyk (2007), Shestopalov & Yatsyk (2007), Kravchenko & Yatsyk (2007), Angermann & Yatsyk (2010)). In what follows we will consider the equations in the frequency space taking into account the relation  $\kappa = \frac{\omega}{c}$ .

Here we study non-linear effects involving the waves at the first three frequency components of  $E_1$  only. That is, we further neglect the influence of harmonics of order higher than 3. Then it is possible to restrict the examination of the system (13)&(15) to three equations, and also to leave particular terms in the representation of the polarisation coefficients. Taking into account only the non-trivial terms in the expansion of the polarisation coefficients and using the so-called *Kleinman's rule* (i.e. the equality of all the coefficients  $\chi_{1111}^{(3)}$  at the multiple frequencies, Kleinman (1962), Miloslavsky (2008)), we arrive at the following system:

$$\begin{cases} \nabla^2 E_1(\mathbf{r}, \kappa) + \varepsilon^{(L)} \kappa^2 E_1(\mathbf{r}, \kappa) + 4\pi \kappa^2 \left( P_1^{(PSM)}(\mathbf{r}, \kappa) + P_1^{(GC)}(\mathbf{r}, \kappa) \right) = -4\pi \kappa^2 P_1^{(G)}(\mathbf{r}, \kappa), \\ \nabla^2 E_1(\mathbf{r}, 2\kappa) + \varepsilon^{(L)} (2\kappa)^2 E_1(\mathbf{r}, 2\kappa) + 4\pi (2\kappa)^2 \left( P_1^{(PSM)}(\mathbf{r}, 2\kappa) + P_1^{(GC)}(\mathbf{r}, 2\kappa) \right) = 0, \\ \nabla^2 E_1(\mathbf{r}, 3\kappa) + \varepsilon^{(L)} (3\kappa)^2 E_1(\mathbf{r}, 3\kappa) + 4\pi (3\kappa)^2 P_1^{(PSM)}(\mathbf{r}, 3\kappa) = -4\pi (3\kappa)^2 P_1^{(G)}(\mathbf{r}, 3\kappa), \end{cases} \quad (16)$$



where

$$\begin{aligned} P_1^{(PSM)}(\mathbf{r}, n\kappa) &:= \frac{3}{4}\chi_{1111}^{(3)}(|E_1(\mathbf{r}, \kappa)|^2 + |E_1(\mathbf{r}, 2\kappa)|^2 + |E_1(\mathbf{r}, 3\kappa)|^2)E_1(\mathbf{r}, n\kappa), \quad n = 1, 2, 3, \\ P_1^{(GC)}(\mathbf{r}, \kappa) &:= \frac{3}{4}\chi_{1111}^{(3)} \frac{[\bar{E}_1(\mathbf{r}, \kappa)]^2}{E_1(\mathbf{r}, \kappa)} E_1(\mathbf{r}, 3\kappa)E_1(\mathbf{r}, \kappa), \quad P_1^{(G)}(\mathbf{r}, \kappa) := \frac{3}{4}\chi_{1111}^{(3)} E_1^2(\mathbf{r}, 2\kappa)\bar{E}_1(\mathbf{r}, 3\kappa), \\ P_1^{(GC)}(\mathbf{r}, 2\kappa) &:= \frac{3}{4}\chi_{1111}^{(3)} \frac{\bar{E}_1(\mathbf{r}, 2\kappa)}{E_1(\mathbf{r}, 2\kappa)} E_1(\mathbf{r}, \kappa)E_1(\mathbf{r}, 3\kappa)E_1(\mathbf{r}, 2\kappa), \\ P_1^{(G)}(\mathbf{r}, 3\kappa) &:= \frac{3}{4}\chi_{1111}^{(3)} \left\{ \frac{1}{3}E_1^3(\mathbf{r}, \kappa) + E_1^2(\mathbf{r}, 2\kappa)\bar{E}_1(\mathbf{r}, \kappa) \right\}. \end{aligned}$$

The terms  $P_1^{(PSM)}(\mathbf{r}, n\omega)$  are usually called *phase self-modulation (PSM)* terms (cf. Akhmediev & Ankevich (2003)). The permittivity of the non-linear medium filling a layer (see Fig. 1) can be represented as

$$\varepsilon_{n\kappa} = \varepsilon^{(L)} + \varepsilon_{n\kappa}^{(NL)} \quad \text{for } |z| \leq 2\pi\delta. \quad (17)$$

Outside the layer, i.e. for  $|z| > 2\pi\delta$ ,  $\varepsilon_{n\kappa} = 1$ . The linear and non-linear terms of the permittivity of the layer are given by the coefficients at  $(n\kappa)^2 E_1(\mathbf{r}, n\kappa)$  in the second and third addends in each of the equations of the system, respectively. Thus  $\varepsilon^{(L)} = D_1^{(L)}(\mathbf{r}, n\kappa)/E_1(\mathbf{r}, n\kappa) = 1 + 4\pi\chi_{11}^{(1)}$ , where the representations for the linear part of the complex components of the electric displacement  $D_1^{(L)}(\mathbf{r}, n\kappa) = E_1(\mathbf{r}, n\kappa) + 4\pi P_1^{(L)}(\mathbf{r}, n\kappa) = \varepsilon^{(L)} E_1(\mathbf{r}, n\kappa)$  and the polarisation  $P_1^{(L)}(\mathbf{r}, n\kappa) = \chi_{11}^{(1)} E_1(\mathbf{r}, n\kappa)$  are taken into account. Similarly, the third term of each equation of the system makes it possible to write the non-linear component of  $\varepsilon_{n\kappa}$  in the form

$$\begin{aligned} \varepsilon_{n\kappa}^{(NL)} &= \alpha(z) [|E_1(\mathbf{r}, \kappa)|^2 + |E_1(\mathbf{r}, 2\kappa)|^2 + |E_1(\mathbf{r}, 3\kappa)|^2 \\ &\quad + \delta_{n1} \frac{[\bar{E}_1(\mathbf{r}, \kappa)]^2}{E_1(\mathbf{r}, \kappa)} E_1(\mathbf{r}, 3\kappa) + \delta_{n2} \frac{\bar{E}_1(\mathbf{r}, 2\kappa)}{E_1(\mathbf{r}, 2\kappa)} E_1(\mathbf{r}, \kappa)E_1(\mathbf{r}, 3\kappa)], \end{aligned} \quad (18)$$

where  $\alpha(z) := 3\pi\chi_{1111}^{(3)}(z)$  is the so-called *function of cubic susceptibility*. For transversely inhomogeneous media (a layer or a layered structure), the linear part  $\varepsilon^{(L)} = \varepsilon^{(L)}(z) = 1 + 4\pi\chi_{11}^{(1)}(z)$  of the permittivity is described by a piecewise smooth or even a piecewise constant function. Similarly, the function of the cubic susceptibility  $\alpha = \alpha(z)$  is also a piecewise smooth or even a piecewise constant function. This assumption allows us to investigate the diffraction characteristics of a non-linear layer and of a layered structure (consisting of a finite number of non-linear dielectric layers) within one and the same mathematical model.

Here and in what follows we use the following notation:  $(\mathbf{r}, t)$  are dimensionless spatial-temporal coordinates such that the thickness of the layer is equal to  $4\pi\delta$ . The time-dependence is determined by the factors  $\exp(-i\omega t)$ , where  $\omega := \kappa c$  is the dimensionless circular frequency and  $\kappa$  is a dimensionless frequency parameter such that  $\kappa = \omega/c := 2\pi/\lambda$ . This parameter characterises the ratio of the true thickness  $h$  of the layer to the free-space wavelength  $\lambda$ , i.e.  $h/\lambda = 2\kappa\delta$ .  $c = (\varepsilon_0\mu_0)^{-1/2}$  denotes a dimensionless parameter, equal to the absolute value of the speed of light in the medium containing the layer ( $\Im c = 0$ ).  $\varepsilon_0$  and  $\mu_0$  are the material parameters of the medium. The absolute values of the true variables  $\mathbf{r}', t', \omega'$  are given by the formulas  $\mathbf{r}' = h\mathbf{r}/4\pi\delta$ ,  $t' = th/4\pi\delta$ ,  $\omega' = \omega 4\pi\delta/h$ .

### 3. Quasi-homogeneous electromagnetic fields in a transversely inhomogeneous non-linear dielectric layered structure and the excitation by wave packets

The scattered and generated field in a transversely inhomogeneous, non-linear dielectric layer excited by a plane wave is *quasi-homogeneous* along the coordinate  $y$ , hence it can be represented as

$$(C1) \quad E_1(\mathbf{r}, n\kappa) =: E_1(n\kappa; y, z) := U(n\kappa; z) \exp(i\phi_{n\kappa}y), \quad n = 1, 2, 3.$$

Here  $U(n\kappa; z)$  and  $\phi_{n\kappa} := n\kappa \sin \varphi_{n\kappa}$  denote the complex-valued transverse component of the Fourier amplitude of the electric field and the value of the longitudinal propagation constant (longitudinal wave-number) at the frequency  $n\kappa$ , respectively, where  $\varphi_{n\kappa}$  is the given angle of incidence of the exciting field of frequency  $n\kappa$  (cf. Fig. 1).

Furthermore we require that the following *condition of the phase synchronism of waves* is satisfied:

$$(C2) \quad \phi_{n\kappa} = n\phi_\kappa, \quad n = 1, 2, 3.$$

Then the permittivity of the non-linear layer can be expressed as

$$\begin{aligned} & \varepsilon_{n\kappa}(z, \alpha(z), E_1(\mathbf{r}, \kappa), E_1(\mathbf{r}, 2\kappa), E_1(\mathbf{r}, 3\kappa)) \\ &= \varepsilon_{n\kappa}(z, \alpha(z), U(\kappa; z), U(2\kappa; z), U(3\kappa; z)) \\ &= \varepsilon^{(L)}(z) + \alpha(z) [ |U(\kappa; z)|^2 + |U(2\kappa; z)|^2 + |U(3\kappa; z)|^2 \\ & \quad + \delta_{n1} |U(\kappa; z)| |U(3\kappa; z)| \exp \{ i [-3\arg(U(\kappa; z)) + \arg(U(3\kappa; z))] \} \\ & \quad + \delta_{n2} |U(\kappa; z)| |U(3\kappa; z)| \exp \{ i [-2\arg(U(2\kappa; z)) + \arg(U(\kappa; z)) + \arg(U(3\kappa; z))] \} ], \\ & \quad n = 1, 2, 3. \end{aligned} \tag{19}$$

For the the components of the non-linear polarisation  $P_1^{(G)}(\mathbf{r}, n\kappa)$  (playing the role of the sources generating radiation in the right-hand sides of the system (16)) we have that

$$\begin{aligned} -4\pi\kappa^2 P_1^{(G)}(\mathbf{r}, \kappa) &= -\alpha(z)\kappa^2 U^2(2\kappa; z) \bar{U}(3\kappa; z) \exp(i\phi_\kappa y), \\ -4\pi(3\kappa)^2 P_1^{(G)}(\mathbf{r}, 3\kappa) &= -\alpha(z)(3\kappa)^2 \left\{ \frac{1}{3} U^3(\kappa; z) + U^2(2\kappa; z) \bar{U}(\kappa; z) \right\} \exp(i\phi_{3\kappa} y). \end{aligned}$$

A more detailed explanation of the condition (C2) can be found in (Angermann & Yatsyk, 2011, Sect. 3). In the considered case of spatially quasi-homogeneous (along the coordinate  $y$ ) electromagnetic fields (C1), the condition of the phase synchronism of waves (C2) reads as

$$\sin \varphi_{n\kappa} = \sin \varphi_\kappa, \quad n = 1, 2, 3.$$

Consequently, the given angle of incidence of a plane wave at the frequency  $\kappa$  coincides with the possible directions of the angles of incidence of plane waves at the multiple frequencies  $n\kappa$ . The angles of the wave scattered by the layer are equal to  $\varphi_{n\kappa}^{\text{scat}} = -\varphi_{n\kappa}$  in the zone of reflection  $z > 2\pi\delta$  and  $\varphi_{n\kappa}^{\text{scat}} = \pi + \varphi_{n\kappa}$  and in the zone of transmission of the non-linear layer  $z < -2\pi\delta$ , where all angles are measured counter-clockwise in the  $(y, z)$ -plane from the  $z$ -axis (cf. Fig. 1).

The conditions (C1), (C2) allow a further simplification of the system (16). Before we do so, we want to make a few comments on specific cases which have already been discussed in the literature. First we mention that the effect of a weak quasi-homogeneous electromagnetic field (C1) on the non-linear dielectric structure such that harmonics at multiple frequencies are not generated, i.e.  $E_1(\mathbf{r}, 2\kappa) = 0$  and  $E_1(\mathbf{r}, 3\kappa) = 0$ , reduces to find the electric field component  $E_1(\mathbf{r}, \kappa)$  determined by the first equation of the system (16). In this case, a diffraction problem



for a plane wave on a non-linear dielectric layer with a Kerr-type non-linearity  $\varepsilon_{n\kappa} = \varepsilon^{(L)}(z) + \alpha(z)|E_1(\mathbf{r}, \kappa)|^2$  and a vanishing right-hand side is to be solved, see Angermann & Yatsyk (2008); Kravchenko & Yatsyk (2007); Serov et al. (2004); Shestopalov & Yatsyk (2007); Smirnov et al. (2005); Yatsyk (2006; 2007). The generation process of a field at the triple frequency  $3\kappa$  by the non-linear dielectric structure is caused by a strong incident electromagnetic field at the frequency  $\kappa$  and can be described by the first and third equations of the system (16) only. Since the right-hand side of the second equation in (16) is equal to zero, we may set  $E_1(\mathbf{r}, 2\kappa) = 0$  corresponding to the homogeneous boundary condition w.r.t.  $E_1(\mathbf{r}, 2\kappa)$ . Therefore the second equation in (16) can be completely omitted, see Angermann & Yatsyk (2010).

A further interesting problem consists in the investigation of the influence of a packet of waves on the generation of the third harmonic, if a strong incident field at the basic frequency  $\kappa$  and, in addition, weak incident quasi-homogeneous electromagnetic fields at the double and triple frequencies  $2\kappa, 3\kappa$  (which alone do not generate harmonics at multiple frequencies) excite the non-linear structure. The system (16) allows to describe the corresponding process of the third harmonics generation. Namely, if such a wave packet consists of a strong field at the basic frequency  $\kappa$  and of a weak field at the triple frequency  $3\kappa$ , then we arrive, as in the situation described above, at the system (16) with  $E_1(\mathbf{r}, 2\kappa) = 0$ , i.e. it is sufficient to consider the first and third equations of (16) only. For wave packets consisting of a strong field at the basic frequency  $\kappa$  and of a weak field at the frequency  $2\kappa$ , (or of two weak fields at the frequencies  $2\kappa$  and  $3\kappa$ ) we have to take into account all three equations of system (16). This is caused by the inhomogeneity of the corresponding problem, where a weak incident field at the double frequency  $2\kappa$  (or two weak fields at the frequencies  $2\kappa$  and  $3\kappa$ ) excites (resp. excite) the dielectric medium.

So we consider the problem of scattering and generation of waves on a non-linear, layered, cubically polarisable structure, which is excited by a packet of plane waves consisting of a strong field at the frequency  $\kappa$  (which generates a field at the triple frequency  $3\kappa$ ) and of weak fields at the frequencies  $2\kappa$  and  $3\kappa$  (having an impact on the process of third harmonic generation due to the contribution of weak electromagnetic fields)

$$\left\{ E_1^{\text{inc}}(\mathbf{r}, n\kappa) := E_1^{\text{inc}}(n\kappa; y, z) := a_{n\kappa}^{\text{inc}} \exp \left( i(\phi_{n\kappa} y - \Gamma_{n\kappa}(z - 2\pi\delta)) \right) \right\}_{n=1}^3, \quad z > 2\pi\delta, \quad (20)$$

with amplitudes  $a_{n\kappa}^{\text{inc}}$  and angles of incidence  $\phi_{n\kappa}$ ,  $|\phi| < \pi/2$  (cf. Fig. 1), where  $\phi_{n\kappa} := n\kappa \sin \varphi_{n\kappa}$  are the longitudinal propagation constants (longitudinal wave-numbers) and  $\Gamma_{n\kappa} := \sqrt{(n\kappa)^2 - \phi_{n\kappa}^2}$  are the transverse propagation constants (transverse wave-numbers). In this setting, if a packet of plane waves excites a non-magnetic, isotropic, linearly polarised (i.e.

$$\mathbf{E}(\mathbf{r}, n\kappa) = (E_1(n\kappa; y, z), 0, 0)^\top, \quad \mathbf{H}(\mathbf{r}, n\kappa) = \left( 0, \frac{1}{i n \omega \mu_0} \frac{\partial E_1(n\kappa; y, z)}{\partial z}, -\frac{1}{i n \omega \mu_0} \frac{\partial E_1(n\kappa; y, z)}{\partial y} \right)^\top$$

(E-polarisation)), transversely inhomogeneous  $\varepsilon^{(L)} = \varepsilon^{(L)}(z) = 1 + 4\pi\chi_{11}^{(1)}(z)$  dielectric layer (see Fig. 1) with a cubic polarisability  $\mathbf{P}^{(NL)}(\mathbf{r}, n\kappa) = (P_1^{(NL)}(n\kappa; y, z), 0, 0)^\top$  of the medium, the complex amplitudes of the total fields

$$E_1(\mathbf{r}, n\kappa) =: E_1(n\kappa; y, z) := U(n\kappa; z) \exp(i\phi_{n\kappa} y) := E_1^{\text{inc}}(n\kappa; y, z) + E_1^{\text{scat}}(n\kappa; y, z)$$

satisfy the system of equations (cf. (16) – (18))

$$\begin{cases} \nabla^2 E_1(\mathbf{r}, \kappa) + \kappa^2 \varepsilon_\kappa(z, \alpha(z), E_1(\mathbf{r}, \kappa), E_1(\mathbf{r}, 2\kappa), E_1(\mathbf{r}, 3\kappa)) E_1(\mathbf{r}, \kappa) \\ \quad = -\alpha(z) \kappa^2 E_1^2(\mathbf{r}, 2\kappa) \bar{E}_1(\mathbf{r}, 3\kappa), \\ \nabla^2 E_1(\mathbf{r}, 2\kappa) + (2\kappa)^2 \varepsilon_{2\kappa}(z, \alpha(z), E_1(\mathbf{r}, \kappa), E_1(\mathbf{r}, 2\kappa), E_1(\mathbf{r}, 3\kappa)) E_1(\mathbf{r}, 2\kappa) = 0, \\ \nabla^2 E_1(\mathbf{r}, 3\kappa) + (3\kappa)^2 \varepsilon_{3\kappa}(z, \alpha(z), E_1(\mathbf{r}, \kappa), E_1(\mathbf{r}, 2\kappa), E_1(\mathbf{r}, 3\kappa)) E_1(\mathbf{r}, 3\kappa) \\ \quad = -\alpha(z) (3\kappa)^2 \left\{ \frac{1}{3} E_1^3(\mathbf{r}, \kappa) + E_1^2(\mathbf{r}, 2\kappa) \bar{E}_1(\mathbf{r}, \kappa) \right\} \end{cases} \quad (21)$$

together with the following conditions, where  $\mathbf{E}_{\text{tg}}(n\kappa; y, z)$  and  $\mathbf{H}_{\text{tg}}(n\kappa; y, z)$  denote the tangential components of the intensity vectors of the full electromagnetic field  $\{\mathbf{E}(n\kappa; y, z)\}_{n=1,2,3}$ ,  $\{\mathbf{H}(n\kappa; y, z)\}_{n=1,2,3}$ :

$$(C1) \quad E_1(n\kappa; y, z) = U(n\kappa; z) \exp(i\phi_{n\kappa} y), \quad n = 1, 2, 3$$

(the quasi-homogeneity condition w.r.t. the spatial variable  $y$  introduced above),

$$(C2) \quad \phi_{n\kappa} = n\phi_\kappa, \quad n = 1, 2, 3,$$

(the condition of phase synchronism of waves introduced above),

(C3)  $\mathbf{E}_{\text{tg}}(n\kappa; y, z)$  and  $\mathbf{H}_{\text{tg}}(n\kappa; y, z)$  (i.e.  $E_1(n\kappa; y, z)$  and  $H_2(n\kappa; y, z)$ ) are continuous at the boundary layers of the non-linear structure,

$$(C4) \quad E_1^{\text{scat}}(n\kappa; y, z) = \begin{Bmatrix} a_{n\kappa}^{\text{scat}} \\ b_{n\kappa}^{\text{scat}} \end{Bmatrix} \exp(i(\phi_{n\kappa} y \pm \Gamma_{n\kappa}(z \mp 2\pi\delta))), \quad z \gtrless \pm 2\pi\delta, \quad n = 1, 2, 3$$

(the radiation condition w.r.t. the scattered field).

The condition (C4) provides a physically consistent behaviour of the energy characteristics of scattering and guarantees the absence of waves coming from infinity (i.e.  $z = \pm\infty$ ), see Shestopalov & Sirenko (1989). We study the scattering properties of the non-linear layer, where in (C4) we always have

$$\Im \Gamma_{n\kappa} = 0, \quad \Re \Gamma_{n\kappa} > 0. \quad (22)$$

Note that (C4) is also applicable for the analysis of the wave-guide properties of the layer, where  $\Im \Gamma_{n\kappa} > 0$ ,  $\Re \Gamma_{n\kappa} = 0$ . The desired solution of the scattering and generation problem (21) under the conditions (C1) – (C4) can be represented as follows:

$$\begin{aligned} E_1(n\kappa; y, z) &= U(n\kappa; z) \exp(i\phi_{n\kappa} y) \\ &= \begin{cases} a_{n\kappa}^{\text{inc}} \exp(i(\phi_{n\kappa} y - \Gamma_{n\kappa}(z - 2\pi\delta))) + a_{n\kappa}^{\text{scat}} \exp(i(\phi_{n\kappa} y + \Gamma_{n\kappa}(z - 2\pi\delta))), & z > 2\pi\delta, \\ U(n\kappa; z) \exp(i\phi_{n\kappa} y), & |z| \leq 2\pi\delta, \\ b_{n\kappa}^{\text{scat}} \exp(i(\phi_{n\kappa} y - \Gamma_{n\kappa}(z + 2\pi\delta))), & z < -2\pi\delta, \end{cases} \quad (23) \\ & \quad n = 1, 2, 3. \end{aligned}$$

Substituting this representation into the system (21), the following system of non-linear ordinary differential equations results, where “’” denotes the differentiation w.r.t.  $z$ :

$$\begin{aligned} U''(n\kappa; z) + \{ \Gamma_{n\kappa}^2 - (n\kappa)^2 [1 - \varepsilon_{n\kappa}(z, \alpha(z), U(\kappa; z), U(2\kappa; z), U(3\kappa; z))] \} U(n\kappa; z) \\ = -(n\kappa)^2 \alpha(z) \left( \delta_{n1} U^2(2\kappa; z) \bar{U}(3\kappa; z) + \delta_{n3} \left\{ \frac{1}{3} U^3(\kappa; z) + U^2(2\kappa; z) \bar{U}(\kappa; z) \right\} \right), \quad (24) \\ |z| \leq 2\pi\delta, \quad n = 1, 2, 3. \end{aligned}$$

The boundary conditions follow from the continuity of the tangential components of the full fields of diffraction  $\{\mathbf{E}_{\text{tg}}(n\kappa; y, z)\}_{n=1,2,3}$   $\{\mathbf{H}_{\text{tg}}(n\kappa; y, z)\}_{n=1,2,3}$  at the boundary  $z = 2\pi\delta$  and  $z = -2\pi\delta$  of the non-linear layer (cf. (C3)). According to (C3) and the representation of the electrical components of the electromagnetic field (23), at the boundary of the non-linear layer we obtain:

$$\begin{aligned} U(n\kappa; 2\pi\delta) &= a_{n\kappa}^{\text{scat}} + a_{n\kappa}^{\text{inc}}, & U'(n\kappa; 2\pi\delta) &= i\Gamma_{n\kappa} (a_{n\kappa}^{\text{scat}} - a_{n\kappa}^{\text{inc}}), \\ U(n\kappa; -2\pi\delta) &= b_{n\kappa}^{\text{scat}}, & U'(n\kappa; -2\pi\delta) &= -i\Gamma_{n\kappa} b_{n\kappa}^{\text{scat}}, \quad n = 1, 2, 3. \end{aligned} \quad (25)$$

Eliminating in (25) the unknown values of the complex amplitudes  $\{a_{n\kappa}^{\text{scat}}\}_{n=1,2,3}$ ,  $\{b_{n\kappa}^{\text{scat}}\}_{n=1,2,3}$  of the scattered field and taking into consideration that  $a_{n\kappa}^{\text{inc}} = U^{\text{inc}}(n\kappa; 2\pi\delta)$ , we arrive at the desired boundary conditions for the problem (21), (C1) – (C4):

$$\begin{aligned} i\Gamma_{n\kappa} U(n\kappa; -2\pi\delta) + U'(n\kappa; -2\pi\delta) &= 0, \\ i\Gamma_{n\kappa} U(n\kappa; 2\pi\delta) - U'(n\kappa; 2\pi\delta) &= 2i\Gamma_{n\kappa} a_{n\kappa}^{\text{inc}}, \quad n = 1, 2, 3. \end{aligned} \quad (26)$$

The system of ordinary differential equations (24) and the boundary conditions (26) form a semi-linear boundary-value problem of Sturm-Liouville type, see also Angermann & Yatsyk (2010); Shestopalov & Yatsyk (2007; 2010); Yatsyk (2007).

#### 4. Existence and uniqueness of a weak solution of the non-linear boundary-value problem

Denote by  $\mathbf{u} = \mathbf{u}(z) := (u_1(z), u_2(z), u_3(z))^{\top} := (U(\kappa; z), U(2\kappa; z), U(3\kappa; z))^{\top}$  the (formal) solution of (24)&(26) and let, for  $\mathbf{w} = (w_1, w_2, w_3)^{\top} \in \mathbb{C}^3$ ,

$$\mathbf{F}(z, \mathbf{w}) := \begin{pmatrix} \{\Gamma_{\kappa}^2 - \kappa^2 [1 - \varepsilon_{\kappa}(z, \alpha(z), w_1, w_2, w_3)]\} w_1 + \alpha(z) \kappa^2 w_2^2 \bar{w}_3 \\ \{\Gamma_{2\kappa}^2 - (2\kappa)^2 [1 - \varepsilon_{2\kappa}(z, \alpha(z), w_1, w_2, w_3)]\} w_2 \\ \{\Gamma_{3\kappa}^2 - (3\kappa)^2 [1 - \varepsilon_{3\kappa}(z, \alpha(z), w_1, w_2, w_3)]\} w_3 + \alpha(z) (3\kappa)^2 \left\{ \frac{1}{3} w_1^3 + \bar{w}_1 w_1^2 \right\} \end{pmatrix}.$$

Then the system of differential equations (24) takes the form

$$-\mathbf{u}''(z) = \mathbf{F}(z, \mathbf{u}(z)), \quad z \in \mathcal{I} := (-2\pi\delta, 2\pi\delta). \quad (27)$$

The boundary conditions (26) can be written as

$$\mathbf{u}'(-2\pi\delta) + i\mathbf{G}\mathbf{u}(-2\pi\delta) = 0, \quad \mathbf{u}'(2\pi\delta) - i\mathbf{G}\mathbf{u}(2\pi\delta) = -2i\mathbf{G}\mathbf{a}^{\text{inc}}, \quad (28)$$

where  $\mathbf{G} := \text{diag}(\Gamma_{\kappa}, \Gamma_{2\kappa}, \Gamma_{3\kappa})$  and  $\mathbf{a}^{\text{inc}} := (a_{\kappa}^{\text{inc}}, a_{2\kappa}^{\text{inc}}, a_{3\kappa}^{\text{inc}})^{\top}$ . Taking an arbitrary complex-valued vector function  $\mathbf{v} : \mathcal{I}^{\text{cl}} := [-2\pi\delta, 2\pi\delta] \rightarrow \mathbb{C}^3$ ,  $\mathbf{v} = (v_1, v_2, v_3)^{\top}$ , multiplying the vector differential equation (27) by the complex conjugate  $\bar{\mathbf{v}}$  and integrating w.r.t.  $z$  over the interval  $\mathcal{I}$ , we arrive at the equation

$$-\int_{\mathcal{I}} \mathbf{u}'' \cdot \bar{\mathbf{v}} dz = \int_{\mathcal{I}} \mathbf{F}(z, \mathbf{u}) \cdot \bar{\mathbf{v}} dz.$$

Integrating formally by parts and using the boundary conditions (28), we obtain:

$$\begin{aligned} - \int_{\mathcal{I}} \mathbf{u}'' \cdot \bar{\mathbf{v}} dz &= \int_{\mathcal{I}} \mathbf{u}' \cdot \bar{\mathbf{v}} dz - (\mathbf{u}' \cdot \bar{\mathbf{v}}) (2\pi\delta) + (\mathbf{u}' \cdot \bar{\mathbf{v}}) (-2\pi\delta) \\ &= \int_{\mathcal{I}} \mathbf{u}' \cdot \bar{\mathbf{v}}' dz - i [((\mathbf{G}\mathbf{u}) \cdot \bar{\mathbf{v}}) (2\pi\delta) + ((\mathbf{G}\mathbf{u}) \cdot \bar{\mathbf{v}}) (-2\pi\delta)] + 2i(\mathbf{G}\mathbf{a}^{\text{inc}}) \cdot \bar{\mathbf{v}}(2\pi\delta). \end{aligned} \quad (29)$$

Now we take into consideration the complex Sobolev space  $H^1(\mathcal{I})$  consisting of functions with values in  $\mathbb{C}$ , which together with their weak derivatives belong to  $L_2(\mathcal{I})$ . According to (29) it is natural to introduce the following forms for  $\mathbf{w}, \mathbf{v} \in \mathbf{V} := [H^1(\mathcal{I})]^3$ :

$$\begin{aligned} a(\mathbf{w}, \mathbf{v}) &:= \int_{\mathcal{I}} \mathbf{w}' \cdot \bar{\mathbf{v}}' dz - i [((\mathbf{G}\mathbf{w}) \cdot \bar{\mathbf{v}}) (2\pi\delta) + ((\mathbf{G}\mathbf{w}) \cdot \bar{\mathbf{v}}) (-2\pi\delta)], \\ b(\mathbf{w}, \mathbf{v}) &:= \int_{\mathcal{I}} \mathbf{F}(z, \mathbf{w}) \cdot \bar{\mathbf{v}} dz - 2i(\mathbf{G}\mathbf{a}^{\text{inc}}) \cdot \bar{\mathbf{v}}(2\pi\delta). \end{aligned}$$

So we arrive at the following weak formulation of boundary-value problem (24):

$$\text{Find } \mathbf{u} \in \mathbf{V} \text{ such that } a(\mathbf{u}, \mathbf{v}) = b(\mathbf{u}, \mathbf{v}) \quad \forall \mathbf{v} \in \mathbf{V}. \quad (30)$$

The space  $\mathbf{V}$  is equipped with the usual norm and seminorm, resp.:

$$\|\mathbf{v}\|_{1,2,\mathcal{I}}^2 := \sum_{n=1}^3 [\|v_n\|_{0,2,\mathcal{I}}^2 + \|v_n'\|_{0,2,\mathcal{I}}^2], \quad |\mathbf{v}|_{1,2,\mathcal{I}}^2 := \sum_{n=1}^3 \|v_n'\|_{0,2,\mathcal{I}}^2,$$

where  $\|v\|_{0,2,\mathcal{I}}$ , for  $v \in L_2(\mathcal{I})$ , denotes the usual  $L_2(\mathcal{I})$ -norm. If  $\mathbf{v} \in [L_2(\mathcal{I})]^3$ , we will use the same notation, i.e.  $\|\mathbf{v}\|_{0,2,\mathcal{I}}^2 := \sum_{n=1}^3 \|v_n\|_{0,2,\mathcal{I}}^2$ . Then the above norm and seminorm in  $\mathbf{V}$  can be written in short as

$$\|\mathbf{v}\|_{1,2,\mathcal{I}}^2 := \|\mathbf{v}\|_{0,2,\mathcal{I}}^2 + \|\mathbf{v}'\|_{0,2,\mathcal{I}}^2, \quad |\mathbf{v}|_{1,2,\mathcal{I}} := \|\mathbf{v}'\|_{0,2,\mathcal{I}}. \quad (31)$$

Analogously, we will not make any notational difference between the absolute value  $|\cdot|$  of a (scalar) element of  $\mathbb{C}$  and the norm  $|\cdot|$  of a (vectorial) element of  $\mathbb{C}^3$ .

On  $\mathbf{V}$ , the following norm can be introduced:

$$\|\mathbf{v}\|_{\mathbf{V}}^2 := \sum_{n=1}^3 [|v_n(-2\pi\delta)|^2 + |v_n(2\pi\delta)|^2 + \|v_n'\|_{0,2,\mathcal{I}}^2] = |\mathbf{v}(-2\pi\delta)|^2 + |\mathbf{v}(2\pi\delta)|^2 + \|\mathbf{v}'\|_{0,2,\mathcal{I}}^2. \quad (32)$$

**Corollary 1.** *The norms defined in (31) and (32) are equivalent on  $\mathbf{V}$ , i.e.*

$$C_- \|\mathbf{v}\|_{1,2,\mathcal{I}} \leq \|\mathbf{v}\|_{\mathbf{V}} \leq C_+ \|\mathbf{v}\|_{1,2,\mathcal{I}} \quad \forall \mathbf{v} \in \mathbf{V}$$

with  $C_- := 1/\sqrt{16\pi^2\delta^2 + 1}$ ,  $C_+ := \sqrt{\max\left\{\frac{1}{2\pi\delta} + 1; 2\right\}}$ .

*Proof.* It is not difficult to verify the following inequality for any (scalar) element  $v \in H^1(\mathcal{I})$  (see, e.g., (Angermann & Yatsyk, 2008, Cor. 4)):

$$\|v\|_{0,2,\mathcal{I}}^2 \leq 4\pi\delta[|v(-2\pi\delta)|^2 + |v(2\pi\delta)|^2] + 16\pi^2\delta^2\|v'\|_{0,2,\mathcal{I}}^2. \quad (33)$$

Consequently, by (31),  $\|\mathbf{v}\|_{1,2,\mathcal{I}}^2 \leq 4\pi\delta[|\mathbf{v}(-2\pi\delta)|^2 + |\mathbf{v}(2\pi\delta)|^2] + (16\pi^2\delta^2 + 1)\|\mathbf{v}'\|_{0,2,\mathcal{I}}^2$ . Since  $4\pi\delta < 16\pi^2\delta^2 + 1$ , we immediately obtain the left-hand side of the desired estimate:

$$\|\mathbf{v}\|_{1,2,\mathcal{I}}^2 \leq (16\pi^2\delta^2 + 1)\|\mathbf{v}\|_{\mathbf{V}}^2.$$

On the other hand, a trace inequality (see, e.g., (Angermann & Yatsyk, 2008, Cor. 5)) says that we have the following estimate for any element  $v \in H^1(\mathcal{I})$ :

$$|v(-2\pi\delta)|^2 + |v(2\pi\delta)|^2 \leq \left(\frac{1}{2\pi\delta} + 1\right) \|v\|_{0,2,\mathcal{I}}^2 + \|v'\|_{0,2,\mathcal{I}}^2.$$

Thus  $\|\mathbf{v}\|_{\mathbf{V}}^2 \leq \left(\frac{1}{2\pi\delta} + 1\right) \|\mathbf{v}\|_{0,2,\mathcal{I}}^2 + 2\|\mathbf{v}'\|_{0,2,\mathcal{I}}^2$ , that is  $C_+^2 := \max\left\{\frac{1}{2\pi\delta} + 1; 2\right\}$ . ◀

**Lemma 1.** *If the matrix  $\mathbf{G}$  is positively definite, then the form  $a$  is coercive and bounded on  $\mathbf{V}$ , i.e.*

$$C_K \|\mathbf{v}\|_{1,2,\mathcal{I}}^2 \leq |a(\mathbf{v}, \mathbf{v})|, \quad |a(\mathbf{w}, \mathbf{v})| \leq C_b \|\mathbf{w}\|_{1,2,\mathcal{I}} \|\mathbf{v}\|_{1,2,\mathcal{I}}$$

for all  $\mathbf{w}, \mathbf{v} \in \mathbf{V}$  with  $C_K := \frac{\sqrt{2}}{2} \min\{1; \Gamma_\kappa; \Gamma_{2\kappa}; \Gamma_{3\kappa}\} C_-^2$ ,  $C_b := \max\{1; \Gamma_\kappa; \Gamma_{2\kappa}; \Gamma_{3\kappa}\} C_+^2$ .

**Remark 1.** *Due to (22), the assumption of the lemma is satisfied.*

**Proof** of the lemma: Obviously,

$$\begin{aligned} |a(\mathbf{v}, \mathbf{v})| &= \sqrt{|\Re a(\mathbf{v}, \mathbf{v})|^2 + |\Im a(\mathbf{v}, \mathbf{v})|^2} \geq \frac{\sqrt{2}}{2} [|\Re a(\mathbf{v}, \mathbf{v})| + |\Im a(\mathbf{v}, \mathbf{v})|] \\ &= \frac{\sqrt{2}}{2} \sum_{n=1}^3 \left[ \|v'_n\|_{0,2,\mathcal{I}}^2 + \Gamma_{n\kappa} |v_n(-2\pi\delta)|^2 + \Gamma_{n\kappa} |v_n(2\pi\delta)|^2 \right] \geq \frac{\sqrt{2}}{2} \min\{1; \Gamma_\kappa; \Gamma_{2\kappa}; \Gamma_{3\kappa}\} \|\mathbf{v}\|_{\mathbf{V}}^2, \end{aligned} \quad (34)$$

where we have used the convention  $\Gamma_{1\kappa} := \Gamma_\kappa$ . By Corollary 1, this estimate implies the coercivity of  $a$  on  $\mathbf{V}$ . The proof of the continuity runs in a similar way:

$$\begin{aligned} |a(\mathbf{w}, \mathbf{v})| &\leq \max\{1; \Gamma_\kappa; \Gamma_{2\kappa}; \Gamma_{3\kappa}\} \sum_{n=1}^3 [\|w'_n\|_{0,2,\mathcal{I}} \|v'_n\|_{0,2,\mathcal{I}} \\ &\quad + |w_n(-2\pi\delta)| |v_n(-2\pi\delta)| + |w_n(2\pi\delta)| |v_n(2\pi\delta)|] \\ &\leq \max\{1; \Gamma_\kappa; \Gamma_{2\kappa}; \Gamma_{3\kappa}\} \|\mathbf{w}\|_{\mathbf{V}} \|\mathbf{v}\|_{\mathbf{V}}, \end{aligned}$$

where the last estimate is a consequence of the Cauchy-Schwarz inequality for finite sums. From Corollary 1 we obtain the above expression for  $C_b$ . ◀

**Corollary 2.** *Under the assumption of Lemma 1, given an antilinear continuous functional  $\ell : \mathbf{V} \rightarrow \mathbb{C}$ , the problem to find an element  $\mathbf{u} \in \mathbf{V}$  such that*

$$a(\mathbf{u}, \mathbf{v}) = \ell(\mathbf{v}) \quad \forall \mathbf{v} \in \mathbf{V} \quad (35)$$

*is uniquely solvable and the following estimate holds:*

$$\|\mathbf{u}\|_{1,2,\mathcal{I}} \leq C_K^{-1} \|\ell\|_*, \quad \text{where} \quad \|\ell\|_* := \sup_{\mathbf{v} \in \mathbf{V}} \frac{|\ell(\mathbf{v})|}{\|\mathbf{v}\|_{1,2,\mathcal{I}}}.$$



*Proof.* This general result is well-known (see, e.g., (Showalter, 1994, Thm. 2.1)). ◀

**Corollary 3.** *If the antilinear continuous functional  $\ell : \mathbf{V} \rightarrow \mathbb{C}$  has the particular structure*

$$\ell(\mathbf{v}) := \int_{\mathcal{I}} \mathbf{f} \cdot \bar{\mathbf{v}} \, dz + \gamma_- \cdot \bar{\mathbf{v}}(-2\pi\delta) + \gamma_+ \cdot \bar{\mathbf{v}}(2\pi\delta),$$

where  $\mathbf{f} \in [L_2(\mathcal{I})]^3$  and  $\gamma_-, \gamma_+ \in \mathbb{C}^3$  are given, then

$$\|\ell\|_* \leq C_+ \sqrt{\max\{4\pi\delta + 1; 16\pi^2\delta^2\}} \left\{ \|\mathbf{f}\|_{0,2,\mathcal{I}}^2 + |\gamma_-|^2 + |\gamma_+|^2 \right\}^{1/2}.$$

*Proof.* By the Cauchy-Schwarz inequality for finite sums, we see that

$$\begin{aligned} |\ell(\mathbf{v})| &\leq \|\mathbf{f}\|_{0,2,\mathcal{I}} \|\mathbf{v}\|_{0,2,\mathcal{I}} + |\gamma_-| |\mathbf{v}(-2\pi\delta)| + |\gamma_+| |\mathbf{v}(2\pi\delta)| \\ &\leq \left\{ \|\mathbf{f}\|_{0,2,\mathcal{I}}^2 + |\gamma_-|^2 + |\gamma_+|^2 \right\}^{1/2} \left\{ \|\mathbf{v}\|_{0,2,\mathcal{I}}^2 + |\mathbf{v}(-2\pi\delta)|^2 + |\mathbf{v}(2\pi\delta)|^2 \right\}^{1/2}. \end{aligned}$$

Using the estimate (33), it follows

$$|\ell(\mathbf{v})| \leq \sqrt{\max\{4\pi\delta + 1; 16\pi^2\delta^2\}} \left\{ \|\mathbf{f}\|_{0,2,\mathcal{I}}^2 + |\gamma_-|^2 + |\gamma_+|^2 \right\}^{1/2} \|\mathbf{v}\|_{\mathbf{V}}. \quad (36)$$

It remains to apply Corollary 1. ◀

**Remark 2.** *Combining Corollary 2 and Corollary 3, we obtain the following estimate for the solution  $\mathbf{u}$  of (35):*

$$\|\mathbf{u}\|_{1,2,\mathcal{I}} \leq \frac{C_+ \sqrt{2 \max\{4\pi\delta + 1; 16\pi^2\delta^2\}}}{C_- \min\{1; \Gamma_\kappa; \Gamma_{2\kappa}; \Gamma_{3\kappa}\}} \left\{ \|\mathbf{f}\|_{0,2,\mathcal{I}}^2 + |\gamma_-|^2 + |\gamma_+|^2 \right\}^{1/2}.$$

The obtained constant suffers from the twice use of the norm equivalence in the proofs of Lemma 1 and Corollary 3, respectively. It can be improved if we start from the estimate (34). Namely, setting  $\mathbf{v} := \mathbf{u}$  in (35), we obtain from (34) and (36):

$$\begin{aligned} \frac{\sqrt{2}}{2} \min\{1; \Gamma_\kappa; \Gamma_{2\kappa}; \Gamma_{3\kappa}\} \|\mathbf{v}\|_{\mathbf{V}}^2 &\leq |a(\mathbf{u}, \mathbf{u})| = |\ell(\mathbf{u})| \\ &\leq \sqrt{\max\{4\pi\delta + 1; 16\pi^2\delta^2\}} \left\{ \|\mathbf{f}\|_{0,2,\mathcal{I}}^2 + |\gamma_-|^2 + |\gamma_+|^2 \right\}^{1/2} \|\mathbf{u}\|_{\mathbf{V}}. \end{aligned}$$

Therefore, by Corollary 1,

$$\|\mathbf{u}\|_{1,2,\mathcal{I}} \leq C_N \left\{ \|\mathbf{f}\|_{0,2,\mathcal{I}}^2 + |\gamma_-|^2 + |\gamma_+|^2 \right\}^{1/2} \text{ with } C_N := \frac{\sqrt{2 \max\{4\pi\delta + 1; 16\pi^2\delta^2\}}}{C_- \min\{1; \Gamma_\kappa; \Gamma_{2\kappa}; \Gamma_{3\kappa}\}}. \quad (37)$$

The identity

$$\mathcal{A}\mathbf{w}(\mathbf{v}) := a(\mathbf{w}, \mathbf{v}) \quad \forall \mathbf{w}, \mathbf{v} \in \mathbf{V}$$

defines a linear operator  $\mathcal{A} : \mathbf{V} \rightarrow \mathbf{V}^*$ , where  $\mathbf{V}^*$  is the dual space of  $\mathbf{V}$  consisting of all antilinear continuous functionals acting from  $\mathbf{V}$  to  $\mathbb{C}$ . By Lemma 1 and Corollary 2,  $\mathcal{A}$  is a bounded operator with a bounded inverse  $\mathcal{A}^{-1} : \mathbf{V}^* \rightarrow \mathbf{V}$ :

$$\|\mathbf{w}\|_{1,2,\mathcal{I}} \leq C_K^{-1} \|\mathcal{A}\mathbf{w}\|_* \quad \forall \mathbf{w} \in \mathbf{V}.$$

**Lemma 2.** If  $\varepsilon^{(L)}, \alpha \in L_\infty(\mathcal{I})$ , then the formal substitution  $\mathcal{N}(\mathbf{w})(z) := \mathbf{F}(z, \mathbf{w}(z))$  defines a Nemyckii operator  $\mathcal{N} : \mathbf{V} \rightarrow [L_2(\mathcal{I})]^3$ , and there is a constant  $C_S > 0$  such that

$$\|\mathcal{N}(\mathbf{w})\|_{0,2,\mathcal{I}} \leq \kappa^2 \left[ 9\|\varepsilon^{(L)} - \sin^2 \varphi_\kappa\|_{0,\infty,\mathcal{I}} + \sqrt{170} C_S^2 \|\alpha\|_{0,\infty,\mathcal{I}} \|\mathbf{w}\|_{1,2,\mathcal{I}}^2 \right] \|\mathbf{w}\|_{0,2,\mathcal{I}}.$$

*Proof.* It is sufficient to verify the estimate. According to the decomposition

$\mathbf{F}(z, \mathbf{w}) := \mathbf{F}^{(L)}(z, \mathbf{w}) + \mathbf{F}^{(NL)}(z, \mathbf{w})$  with

$$\mathbf{F}^{(L)}(z, \mathbf{w}) := \begin{pmatrix} \{\Gamma_\kappa^2 - \kappa^2 [1 - \varepsilon^{(L)}(z)]\} w_1 \\ \{\Gamma_{2\kappa}^2 - (2\kappa)^2 [1 - \varepsilon^{(L)}(z)]\} w_2 \\ \{\Gamma_{3\kappa}^2 - (3\kappa)^2 [1 - \varepsilon^{(L)}(z)]\} w_3 \end{pmatrix},$$

$$\mathbf{F}^{(NL)}(z, \mathbf{w}) := \begin{pmatrix} F_1^{(NL)}(z, \mathbf{w}) \\ F_2^{(NL)}(z, \mathbf{w}) \\ F_3^{(NL)}(z, \mathbf{w}) \end{pmatrix} := \alpha(z) \begin{pmatrix} \kappa^2 [|\mathbf{w}|^2 w_1 + \bar{w}_1^2 w_3 + w_2^2 \bar{w}_3] \\ (2\kappa)^2 [|\mathbf{w}|^2 w_2 + w_1 \bar{w}_2 w_3] \\ (3\kappa)^2 [|\mathbf{w}|^2 w_3 + \frac{1}{3} w_1^3 + \bar{w}_1 w_2^2] \end{pmatrix}$$

(cf. (19), (24)), it is convenient to split  $\mathcal{N}$  into a linear and a non-linear part as  $\mathcal{N}(\mathbf{w})(z) := \mathcal{N}^{(L)}(\mathbf{w})(z) + \mathcal{N}^{(NL)}(\mathbf{w})(z)$ , where  $\mathcal{N}^{(L)}(\mathbf{w})(z) := \mathbf{F}^{(L)}(z, \mathbf{w}(z))$  and  $\mathcal{N}^{(NL)}(\mathbf{w})(z) := \mathbf{F}^{(NL)}(z, \mathbf{w}(z))$ . Now, by the definition of the wave-numbers (see Section 3),

$$\Gamma_{n\kappa}^2 - (n\kappa)^2 [1 - \varepsilon^{(L)}(z)] = (n\kappa)^2 [\varepsilon^{(L)}(z) - \sin^2 \varphi_{n\kappa}] = (n\kappa)^2 [\varepsilon^{(L)}(z) - \sin^2 \varphi_\kappa], \quad n = 1, 2, 3,$$

where the last relation is a consequence of the condition (C2). Therefore,

$$\|\mathcal{N}^{(L)}(\mathbf{w})\|_{0,2,\mathcal{I}} \leq (3\kappa)^2 \|\varepsilon^{(L)} - \sin^2 \varphi_\kappa\|_{0,\infty,\mathcal{I}} \|\mathbf{w}\|_{0,2,\mathcal{I}}. \quad (38)$$

Next, since  $H^1(\mathcal{I})$  is continuously embedded into  $C(\mathcal{I}^1)$  by Sobolev's embedding theorem (see, e.g., (Adams, 1975, Thm. 5.4)), there exists a constant  $C_S > 0$  such that

$$\|\mathbf{w}\|_{0,\infty,\mathcal{I}} := \sup_{z \in \mathcal{I}} |\mathbf{w}(z)| = \sup_{z \in \mathcal{I}} \left\{ \sum_{n=1}^3 |w_n(z)|^2 \right\}^{1/2} \leq C_S \|\mathbf{w}\|_{1,2,\mathcal{I}}. \quad (39)$$

Using this fact we easily obtain the following triple of estimates:

$$\begin{aligned} \|F_1^{(NL)}(\cdot, \mathbf{w})\|_{0,2,\mathcal{I}} &\leq \kappa^2 \|\alpha\|_{0,\infty,\mathcal{I}} \left[ \| |\mathbf{w}|^2 w_1 \|_{0,2,\mathcal{I}} + \| \bar{w}_1^2 w_3 \|_{0,2,\mathcal{I}} + \| w_2^2 \bar{w}_3 \|_{0,2,\mathcal{I}} \right] \\ &\leq \kappa^2 \|\alpha\|_{0,\infty,\mathcal{I}} \left[ \|\mathbf{w}\|_{0,\infty,\mathcal{I}}^2 \|w_1\|_{0,2,\mathcal{I}} \right. \\ &\quad \left. + \|w_1\|_{0,\infty,\mathcal{I}}^2 \|w_3\|_{0,2,\mathcal{I}} + \|w_2\|_{0,\infty,\mathcal{I}} \|w_3\|_{0,\infty,\mathcal{I}} \|w_2\|_{0,2,\mathcal{I}} \right] \\ &\leq \kappa^2 \|\alpha\|_{0,\infty,\mathcal{I}} \|\mathbf{w}\|_{0,\infty,\mathcal{I}}^2 [\|w_1\|_{0,2,\mathcal{I}} + \|w_2\|_{0,2,\mathcal{I}} + \|w_3\|_{0,2,\mathcal{I}}] \\ &\leq \sqrt{3} \kappa^2 C_S^2 \|\alpha\|_{0,\infty,\mathcal{I}} \|\mathbf{w}\|_{1,2,\mathcal{I}}^2 \|\mathbf{w}\|_{0,2,\mathcal{I}}, \end{aligned}$$

$$\begin{aligned}
\|F_2^{(NL)}(\cdot, \mathbf{w})\|_{0,2,\mathcal{I}} &\leq (2\kappa)^2 \|\alpha\|_{0,\infty,\mathcal{I}} \left[ \|\mathbf{w}|^2 w_2\|_{0,2,\mathcal{I}} + \|w_1 \bar{w}_2 w_3\|_{0,2,\mathcal{I}} \right] \\
&\leq (2\kappa)^2 \|\alpha\|_{0,\infty,\mathcal{I}} \|\mathbf{w}\|_{0,\infty,\mathcal{I}}^2 [\|w_2\|_{0,2,\mathcal{I}} + \|w_3\|_{0,2,\mathcal{I}}] \\
&\leq \sqrt{2} (2\kappa)^2 C_S^2 \|\alpha\|_{0,\infty,\mathcal{I}} \|\mathbf{w}\|_{1,2,\mathcal{I}}^2 \|\mathbf{w}\|_{0,2,\mathcal{I}}, \\
\|F_3^{(NL)}(\cdot, \mathbf{w})\|_{0,2,\mathcal{I}} &\leq (3\kappa)^2 \|\alpha\|_{0,\infty,\mathcal{I}} \left[ \|\mathbf{w}|^2 w_3\|_{0,2,\mathcal{I}} + \frac{1}{3} \|w_1^3\|_{0,2,\mathcal{I}} + \|\bar{w}_1 w_2^2\|_{0,2,\mathcal{I}} \right] \\
&\leq (3\kappa)^2 \|\alpha\|_{0,\infty,\mathcal{I}} \|\mathbf{w}\|_{0,\infty,\mathcal{I}}^2 \left[ \frac{1}{3} \|w_1\|_{0,2,\mathcal{I}} + \|w_2\|_{0,2,\mathcal{I}} + \|w_3\|_{0,2,\mathcal{I}} \right] \\
&\leq \sqrt{\frac{5}{3}} (3\kappa)^2 C_S^2 \|\alpha\|_{0,\infty,\mathcal{I}} \|\mathbf{w}\|_{1,2,\mathcal{I}}^2 \|\mathbf{w}\|_{0,2,\mathcal{I}}.
\end{aligned}$$

These estimates immediately imply that

$$\|\mathcal{N}^{(NL)}(\mathbf{w})\|_{0,2,\mathcal{I}}^2 = \sum_{n=1}^3 \|F_n^{(NL)}(\cdot, \mathbf{w})\|_{0,2,\mathcal{I}}^2 \leq 170\kappa^4 C_S^4 \|\alpha\|_{0,\infty,\mathcal{I}}^2 \|\mathbf{w}\|_{1,2,\mathcal{I}}^4 \|\mathbf{w}\|_{0,2,\mathcal{I}}^2. \quad (40)$$

Putting the estimates (38) and (40) together, we obtain the desired estimate. ◀

As a consequence of Lemma 2, the following non-linear operator  $\mathcal{F} : \mathbf{V} \rightarrow \mathbf{V}^*$  can be introduced:

$$\mathcal{F}(\mathbf{w})(\mathbf{v}) := b(\mathbf{w}, \mathbf{v}) = \int_{\mathcal{I}} \mathcal{N}(\mathbf{w}) \cdot \bar{\mathbf{v}} dz - 2i(\mathbf{Ga}^{\text{inc}}) \cdot \bar{\mathbf{v}}(2\pi\delta) \quad \forall \mathbf{w}, \mathbf{v} \in \mathbf{V}.$$

Then the problem (30) is equivalent to the operator equation  $\mathcal{A}\mathbf{u} = \mathcal{F}(\mathbf{u})$  in  $\mathbf{V}^*$ . Furthermore, by Lemma 1, this equation is equivalent to the fixed-point problem

$$\mathbf{u} = \mathcal{A}^{-1} \mathcal{F}(\mathbf{u}) \quad \text{in } \mathbf{V}. \quad (41)$$

**Theorem 1.** Assume there is a number  $\varrho > 0$  such that

$$C_N \kappa^2 \left[ 9\|\varepsilon^{(L)} - \sin^2 \varphi_\kappa\|_{0,\infty,\mathcal{I}} + 3\sqrt{514} C_S^2 \|\alpha\|_{0,\infty,\mathcal{I}} \varrho^2 \right] \leq \frac{\sqrt{2}}{2} \quad \text{and} \quad C_N |\mathbf{Ga}^{\text{inc}}| \leq \frac{\sqrt{2}}{4} \varrho.$$

Then the problem (41) has a unique solution  $\mathbf{u} \in K_\varrho^{\text{cl}} := \{\mathbf{v} \in \mathbf{V} : \|\mathbf{v}\|_{1,2,\mathcal{I}} \leq \varrho\}$ .

*Proof.* Obviously,  $K_\varrho^{\text{cl}}$  is a closed nonempty subset of  $\mathbf{V}$ . We show that  $\mathcal{A}^{-1} \mathcal{F}(K_\varrho^{\text{cl}}) \subset K_\varrho^{\text{cl}}$ . By (37) with the particular choice  $\mathbf{f} := \mathcal{N}(\mathbf{w})$ ,  $\gamma_- := 0$ ,  $\gamma_+ := -2i\mathbf{Ga}^{\text{inc}}$ , for  $\mathbf{w} \in K_\varrho^{\text{cl}}$  we have that

$$\begin{aligned}
\|\mathcal{A}^{-1} \mathcal{F}(\mathbf{w})\|_{1,2,\mathcal{I}} &\leq C_N \left\{ \|\mathcal{N}(\mathbf{w})\|_{0,2,\mathcal{I}}^2 + 4|\mathbf{Ga}^{\text{inc}}|^2 \right\}^{1/2} \\
&\leq C_N \left\{ \kappa^4 \left[ 9\|\varepsilon^{(L)} - \sin^2 \varphi_\kappa\|_{0,\infty,\mathcal{I}} + \sqrt{170} C_S^2 \|\alpha\|_{0,\infty,\mathcal{I}} \|\mathbf{w}\|_{1,2,\mathcal{I}}^2 \right]^2 \|\mathbf{w}\|_{0,2,\mathcal{I}}^2 + 4|\mathbf{Ga}^{\text{inc}}|^2 \right\}^{1/2} \\
&\leq C_N \left\{ \kappa^4 \left[ 9\|\varepsilon^{(L)} - \sin^2 \varphi_\kappa\|_{0,\infty,\mathcal{I}} + \sqrt{170} C_S^2 \|\alpha\|_{0,\infty,\mathcal{I}} \varrho^2 \right]^2 \varrho^2 + 4|\mathbf{Ga}^{\text{inc}}|^2 \right\}^{1/2} \leq \varrho.
\end{aligned}$$

Next, from (37) with the choice  $\mathbf{f} := \mathcal{N}(\mathbf{w}) - \mathcal{N}(\mathbf{v})$ ,  $\gamma_- := \gamma_+ := 0$  we conclude that

$$\begin{aligned} \|\mathcal{A}^{-1}\mathcal{F}(\mathbf{w}) - \mathcal{A}^{-1}\mathcal{F}(\mathbf{v})\|_{1,2,\mathcal{I}} &\leq C_N \|\mathcal{N}(\mathbf{w}) - \mathcal{N}(\mathbf{v})\|_{0,2,\mathcal{I}} \\ &\leq C_N \left\{ \|\mathcal{N}^{(L)}(\mathbf{w}) - \mathcal{N}^{(L)}(\mathbf{v})\|_{0,2,\mathcal{I}} + \|\mathcal{N}^{(NL)}(\mathbf{w}) - \mathcal{N}^{(NL)}(\mathbf{v})\|_{0,2,\mathcal{I}} \right\}. \end{aligned}$$

The linear term can be estimated as in the proof of Lemma 2 (cf. (38)):

$$\begin{aligned} \|\mathcal{N}^{(L)}(\mathbf{w}) - \mathcal{N}^{(L)}(\mathbf{v})\|_{0,2,\mathcal{I}} &= \|\mathcal{N}^{(L)}(\mathbf{w} - \mathbf{v})\|_{0,2,\mathcal{I}} \\ &\leq (3\kappa)^2 \|\varepsilon^{(L)} - \sin^2 \varphi_\kappa\|_{0,\infty,\mathcal{I}} \|\mathbf{w} - \mathbf{v}\|_{0,2,\mathcal{I}}. \end{aligned}$$

To treat the non-linear term, we start with the following estimates:

$$\begin{aligned} &\|F_1^{(NL)}(\cdot, \mathbf{w}) - F_1^{(NL)}(\cdot, \mathbf{v})\|_{0,2,\mathcal{I}} \\ &\leq \kappa^2 \|\alpha\|_{0,\infty,\mathcal{I}} \left[ \|\mathbf{w}|^2 w_1 - |\mathbf{v}|^2 v_1\|_{0,2,\mathcal{I}} + \|\bar{w}_1^2 w_3 - \bar{v}_1^2 v_3\|_{0,2,\mathcal{I}} + \|w_2^2 \bar{w}_3 - v_2^2 \bar{v}_3\|_{0,2,\mathcal{I}} \right], \\ &\|F_2^{(NL)}(\cdot, \mathbf{w}) - F_2^{(NL)}(\cdot, \mathbf{v})\|_{0,2,\mathcal{I}} \\ &\leq (2\kappa)^2 \|\alpha\|_{0,\infty,\mathcal{I}} \left[ \|\mathbf{w}|^2 w_2 - |\mathbf{v}|^2 v_2\|_{0,2,\mathcal{I}} + \|w_1 \bar{w}_2 w_3 - v_1 \bar{v}_2 v_3\|_{0,2,\mathcal{I}} \right], \\ &\|F_3^{(NL)}(\cdot, \mathbf{w}) - F_3^{(NL)}(\cdot, \mathbf{v})\|_{0,2,\mathcal{I}} \\ &\leq (3\kappa)^2 \|\alpha\|_{0,\infty,\mathcal{I}} \left[ \|\mathbf{w}|^2 w_3 - |\mathbf{v}|^2 v_3\|_{0,2,\mathcal{I}} + \frac{1}{3} \|w_1^3 - v_1^3\|_{0,2,\mathcal{I}} + \|\bar{w}_1 w_2^2 - \bar{v}_1 v_2^2\|_{0,2,\mathcal{I}} \right]. \end{aligned}$$

The subsequent collection of simple estimates shows that the absolute value of all terms appearing in the  $L_2(\mathcal{I})$ -terms of the right-hand sides above can be bounded by one and the same upper bound. Namely, since

$$\begin{aligned} |\mathbf{w}|^2 w_n - |\mathbf{v}|^2 v_n &= |\mathbf{w}|^2 (w_n - v_n) + v_n (|\mathbf{w}|^2 - |\mathbf{v}|^2) \\ &= |\mathbf{w}|^2 (w_n - v_n) + v_n (|\mathbf{w}| + |\mathbf{v}|)(|\mathbf{w}| - |\mathbf{v}|) \end{aligned}$$

and

$$||\mathbf{w}| - |\mathbf{v}|| \leq |\mathbf{w} - \mathbf{v}|,$$

we obtain

$$||\mathbf{w}|^2 w_n - |\mathbf{v}|^2 v_n| \leq [|\mathbf{w}|^2 + |\mathbf{w}||\mathbf{v}| + |\mathbf{v}|^2] |\mathbf{w} - \mathbf{v}|, \quad n = 1, 2, 3.$$

Similarly,

$$\begin{aligned} |\bar{w}_1^2 w_3 - \bar{v}_1^2 v_3| &\leq [|\mathbf{w}|^2 + |\mathbf{w}||\mathbf{v}| + |\mathbf{v}|^2] |\mathbf{w} - \mathbf{v}|, \\ |w_1 \bar{w}_2 w_3 - v_1 \bar{v}_2 v_3| &\leq [|\mathbf{w}|^2 + |\mathbf{w}||\mathbf{v}| + |\mathbf{v}|^2] |\mathbf{w} - \mathbf{v}|, \\ |w_1^3 - v_1^3| &\leq [|\mathbf{w}|^2 + |\mathbf{w}||\mathbf{v}| + |\mathbf{v}|^2] |\mathbf{w} - \mathbf{v}|. \end{aligned}$$

Therefore

$$\begin{aligned}
& \|F_1^{(NL)}(\cdot, \mathbf{w}) - F_1^{(NL)}(\cdot, \mathbf{v})\|_{0,2,\mathcal{I}} \\
& \leq 3\kappa^2 \|\alpha\|_{0,\infty,\mathcal{I}} \left[ \|\mathbf{w}\|_{0,\infty,\mathcal{I}}^2 + \|\mathbf{w}\|_{0,\infty,\mathcal{I}} \|\mathbf{v}\|_{0,\infty,\mathcal{I}} + \|\mathbf{v}\|_{0,\infty,\mathcal{I}}^2 \right] \|\mathbf{w} - \mathbf{v}\|_{0,2,\mathcal{I}} \\
& \leq 3\kappa^2 \|\alpha\|_{0,\infty,\mathcal{I}} C_S^2 \left[ \|\mathbf{w}\|_{1,2,\mathcal{I}}^2 + \|\mathbf{w}\|_{1,2,\mathcal{I}} \|\mathbf{v}\|_{1,2,\mathcal{I}} + \|\mathbf{v}\|_{1,2,\mathcal{I}}^2 \right] \|\mathbf{w} - \mathbf{v}\|_{0,2,\mathcal{I}}, \\
& \|F_2^{(NL)}(\cdot, \mathbf{w}) - F_2^{(NL)}(\cdot, \mathbf{v})\|_{0,2,\mathcal{I}} \\
& \leq 2(2\kappa)^2 \|\alpha\|_{0,\infty,\mathcal{I}} C_S^2 \left[ \|\mathbf{w}\|_{1,2,\mathcal{I}}^2 + \|\mathbf{w}\|_{1,2,\mathcal{I}} \|\mathbf{v}\|_{1,2,\mathcal{I}} + \|\mathbf{v}\|_{1,2,\mathcal{I}}^2 \right] \|\mathbf{w} - \mathbf{v}\|_{0,2,\mathcal{I}} \\
& \|F_3^{(NL)}(\cdot, \mathbf{w}) - F_3^{(NL)}(\cdot, \mathbf{v})\|_{0,2,\mathcal{I}} \\
& \leq \frac{7}{3} (3\kappa)^2 \|\alpha\|_{0,\infty,\mathcal{I}} C_S^2 \left[ \|\mathbf{w}\|_{1,2,\mathcal{I}}^2 + \|\mathbf{w}\|_{1,2,\mathcal{I}} \|\mathbf{v}\|_{1,2,\mathcal{I}} + \|\mathbf{v}\|_{1,2,\mathcal{I}}^2 \right] \|\mathbf{w} - \mathbf{v}\|_{0,2,\mathcal{I}}.
\end{aligned}$$

It follows that

$$\begin{aligned}
& \|\mathcal{N}^{(NL)}(\mathbf{w}) - \mathcal{N}^{(NL)}(\mathbf{v})\|_{0,2,\mathcal{I}}^2 = \sum_{n=1}^3 \|F_n^{(NL)}(\cdot, \mathbf{w}) - F_n^{(NL)}(\cdot, \mathbf{v})\|_{0,2,\mathcal{I}}^2 \\
& \leq 514\kappa^4 \|\alpha\|_{0,\infty,\mathcal{I}}^2 C_S^4 \left[ \|\mathbf{w}\|_{1,2,\mathcal{I}}^2 + \|\mathbf{w}\|_{1,2,\mathcal{I}} \|\mathbf{v}\|_{1,2,\mathcal{I}} + \|\mathbf{v}\|_{1,2,\mathcal{I}}^2 \right]^2 \|\mathbf{w} - \mathbf{v}\|_{0,2,\mathcal{I}}^2.
\end{aligned}$$

Hence, for  $\mathbf{w}, \mathbf{v} \in K_\varrho^{\text{cl}}$ :  $\|\mathcal{N}^{(NL)}(\mathbf{w}) - \mathcal{N}^{(NL)}(\mathbf{v})\|_{0,2,\mathcal{I}} \leq 3\sqrt{514}\kappa^2 C_S^2 \|\alpha\|_{0,\infty,\mathcal{I}} \varrho^2 \|\mathbf{w} - \mathbf{v}\|_{0,2,\mathcal{I}}$ .  
In summary, by assumption we arrive at the estimate

$$\begin{aligned}
& \|\mathcal{A}^{-1}\mathcal{F}(\mathbf{w}) - \mathcal{A}^{-1}\mathcal{F}(\mathbf{v})\|_{1,2,\mathcal{I}} \\
& \leq C_N \kappa^2 \left[ 9\|\varepsilon^{(L)} - \sin^2 \varphi_\kappa\|_{0,\infty,\mathcal{I}} + 3\sqrt{514} C_S^2 \|\alpha\|_{0,\infty,\mathcal{I}} \varrho^2 \right] \|\mathbf{w} - \mathbf{v}\|_{0,2,\mathcal{I}} \leq \frac{\sqrt{2}}{2} \|\mathbf{w} - \mathbf{v}\|_{1,2,\mathcal{I}}.
\end{aligned}$$

By Banach's fixed-point theorem, the problem (41) has a unique solution  $\mathbf{u} \in K_\varrho^{\text{cl}}$ . ◀

## 5. The non-linear problem and the equivalent system of non-linear integral equations

The problem (21), (C1) – (C4) can be reduced to finding solutions of one-dimensional non-linear integral equations w.r.t. the components  $U(n\kappa; z)$ ,  $n = 1, 2, 3$ ,  $z \in [-2\pi\delta, 2\pi\delta]$ , of the fields scattered and generated in the non-linear layer. Similar to the results of the papers Angermann & Yatsyk (2011), Angermann & Yatsyk (2010), Shestopalov & Yatsyk (2010), Yatsyk (2007), Shestopalov & Yatsyk (2007), Kravchenko & Yatsyk (2007), Shestopalov & Sirenko (1989), we give the derivation of these equations for the case of excitation of the non-linear structure by a plane-wave packet (20).

Taking into account the representation (23), the solution of (21), (C1) – (C4) in the whole space  $Q := \{q = (y, z) : |y| < \infty, |z| < \infty\}$  is obtained using the properties of the canonical Green's function of the problem (21), (C1) – (C4) (for the special case  $\varepsilon_{n\kappa} \equiv 1$ ) which is defined, for



$Y > 0$ , in the strip  $Q_{\{Y,\infty\}} := \{q = (y, z) : |y| < Y, |z| < \infty\} \subset Q$  by

$$\begin{aligned} G_0(n\kappa; q, q_0) &:= \frac{i}{4Y} \exp \{i [\phi_{n\kappa} (y - y_0) + \Gamma_{n\kappa} |z - z_0|]\} / \Gamma_{n\kappa} \\ &= \exp (\pm i \phi_{n\kappa} y) \frac{i\pi}{4Y} \int_{-\infty}^{\infty} H_0^{(1)} \left( n\kappa \sqrt{(\check{y} - y_0)^2 + (z - z_0)^2} \right) \exp (\mp i \phi_{n\kappa} \check{y}) d\check{y}, \quad n = 1, 2, 3, \end{aligned} \quad (42)$$

where  $H_0^{(1)}$  as usual denotes the Hankel function of the first kind of order zero (cf. Shestopalov & Sirenko (1989); Sirenko et al. (1985)).

The system of non-linear integral equations is obtained by means of an iterative approach Angermann & Yatsyk (2011), Yatsyk (2007), Shestopalov & Yatsyk (2007), Shestopalov & Sirenko (1989), Titchmarsh (1961). Denote both the scattered and the generated full fields of diffraction at each frequency  $n\kappa$ ,  $n = 1, 2, 3$ , i.e. the solution of the problem (21), (C1) – (C4), by  $E_1(n\kappa; q|_{q=(y,z)}) = U(n\kappa; z) \exp(i\phi_{n\kappa} y)$  (cf. (23)), and write the system (21) in the form

$$\begin{aligned} (\nabla^2 + (n\kappa)^2) E_1(n\kappa; q) &= [1 - \varepsilon_{n\kappa}(q, \alpha(q), E_1(\kappa; q), E_1(2\kappa; q), E_1(3\kappa; q))] (n\kappa)^2 E_1(n\kappa; q) \\ &\quad - \delta_{n1} \alpha(q) (n\kappa)^2 E_1^2(2\kappa; q) \bar{E}_1(3\kappa; q) \\ &\quad - \delta_{n3} \alpha(q) (n\kappa)^2 \left\{ \frac{1}{3} E_1^3(\kappa; q) + E_1^2(2\kappa; q) \bar{E}_1(\kappa; q) \right\}, \quad n = 1, 2, 3. \end{aligned} \quad (43)$$

At the right-hand side of the system (43), the first term outside the layer vanishes, since, by assumption, the permittivity of the medium in which the non-linear layer is situated is equal to one, i.e.  $1 - \varepsilon_{n\kappa}(q, \alpha(q), E_1(\kappa; q), E_1(2\kappa; q), E_1(3\kappa; q)) \equiv 0$  for  $|z| > 2\pi\delta$ .

The excitation field of the non-linear structure can be represented in the form of a packet of incident plane waves  $\{E_1^{\text{inc}}(n\kappa; q)\}_{n=1,2,3}$  satisfying the condition of phase synchronism (C2), where

$$E_1^{\text{inc}}(n\kappa; q) = a_{n\kappa}^{\text{inc}} \exp \{i [\phi_{n\kappa} y - \Gamma_{n\kappa} (z - 2\pi\delta)]\}, \quad n = 1, 2, 3. \quad (44)$$

Furthermore, in the present situation described by the system (43), we assume that the excitation field  $E_1^{\text{inc}}(\kappa; q)$  of the non-linear structure at the frequency  $\kappa$  is sufficiently strong (i.e. the amplitude  $a_{\kappa}^{\text{inc}}$  is sufficiently large such that the third harmonic generation is possible), whereas the amplitudes  $a_{2\kappa}^{\text{inc}}, a_{3\kappa}^{\text{inc}}$  corresponding to excitation fields  $E_1^{\text{inc}}(2\kappa; q), E_1^{\text{inc}}(3\kappa; q)$  at the frequencies  $2\kappa, 3\kappa$ , respectively, are selected sufficiently weak such that no generation of multiple harmonics occurs.

In the whole space  $Q$ , for each frequency  $n\kappa$ ,  $n = 1, 2, 3$ , the fields  $\{E_1^{\text{inc}}(n\kappa; q)\}_{n=1,2,3}$  of incident plane waves satisfy a system of homogeneous Helmholtz equations:

$$(\nabla^2 + (n\kappa)^2) E_1^{\text{inc}}(n\kappa; q) = 0, \quad q \in Q, \quad n = 1, 2, 3. \quad (45)$$

For  $z > 2\pi\delta$ , the incident fields  $\{E_1^{\text{inc}}(n\kappa; q)\}_{n=1,2,3}$  are fields of plane waves approaching the layer, while, for  $z < 2\pi\delta$ , they move away from the layer and satisfy the radiation condition (since, in the representation of the fields  $E_1^{\text{inc}}(n\kappa; q)$ ,  $n = 1, 2, 3$ , the transverse propagation constants  $\Gamma_{n\kappa} > 0$ ,  $n = 1, 2, 3$  are positive).

Following Angermann & Yatsyk (2011), we construct a sequence  $\{E_{1,s}(n\kappa; q)\}_{s=0}^{\infty}$ ,  $n = 1, 2, 3$ , of functions in the region  $Q$  (where each function, starting with the index  $p = 1$ , satisfies the conditions (C1) – (C4)) such that the limit functions  $E_1(n\kappa; q) = \lim_{s \rightarrow \infty} E_{1,s}(n\kappa; q)$  at the

frequencies  $n\kappa$ ,  $n = 1, 2, 3$ , satisfy (21), (C1) – (C4), i.e.

$$\begin{aligned}
 (\nabla^2 + (n\kappa)^2) E_{1,0}(n\kappa; q) &= 0, \\
 (\nabla^2 + (n\kappa)^2) E_{1,1}(n\kappa; q) &= [1 - \varepsilon_{n\kappa}(q, \alpha(q), E_{1,0}(\kappa; q), E_{1,0}(2\kappa; q), E_{1,0}(3\kappa; q))] \\
 &\quad \times (n\kappa)^2 E_{1,0}(n\kappa; q) - \delta_{n1} \alpha(q) (n\kappa)^2 E_{1,0}^2(2\kappa; q) \bar{E}_{1,0}(3\kappa; q) \\
 &\quad - \delta_{n3} \alpha(q) (n\kappa)^2 \left\{ \frac{1}{3} E_{1,0}^3(\kappa; q) + E_{1,0}^2(2\kappa; q) \bar{E}_{1,0}(\kappa; q) \right\}, \dots, \\
 (\nabla^2 + (n\kappa)^2) E_{1,s+1}(n\kappa; q) &= [1 - \varepsilon_{n\kappa}(q, \alpha(q), E_{1,s}(\kappa; q), E_{1,s}(2\kappa; q), E_{1,s}(3\kappa; q))] \\
 &\quad \times (n\kappa)^2 E_{1,s}(n\kappa; q) - \delta_{n1} \alpha(q) (n\kappa)^2 E_{1,s}^2(2\kappa; q) \bar{E}_{1,s}(3\kappa; q) \\
 &\quad - \delta_{n3} \alpha(q) (n\kappa)^2 \left\{ \frac{1}{3} E_{1,s}^3(\kappa; q) + E_{1,s}^2(2\kappa; q) \bar{E}_{1,s}(\kappa; q) \right\}, \dots, \\
 &\quad n = 1, 2, 3.
 \end{aligned} \tag{46}$$

The system of equations (46) is formally equivalent to the following one:

$$\begin{aligned}
 E_{1,0}(n\kappa; q) &:= E_1^{\text{inc}}(n\kappa; q), \\
 E_{1,1}(n\kappa; q) &= -(n\kappa)^2 \iint_{Q_\delta} G_0(n\kappa; q, q_0) \times \\
 &\quad \times [1 - \varepsilon_{n\kappa}(q_0, \alpha(q_0), E_{1,0}(\kappa; q_0), E_{1,0}(2\kappa; q_0), E_{1,0}(3\kappa; q_0))] E_{1,0}(n\kappa; q_0) dq_0 \\
 &\quad + \delta_{n1} (n\kappa)^2 \iint_{Q_\delta} G_0(n\kappa; q, q_0) \alpha(q_0) E_{1,0}^2(2\kappa; q_0) \bar{E}_{1,0}(3\kappa; q_0) dq_0 \\
 &\quad + \delta_{n3} (n\kappa)^2 \iint_{Q_\delta} G_0(n\kappa; q, q_0) \alpha(q_0) \left\{ \frac{1}{3} E_{1,0}^3(\kappa; q_0) + E_{1,0}^2(2\kappa; q_0) \bar{E}_{1,0}(\kappa; q_0) \right\} dq_0 \\
 &\quad + E_{1,0}(n\kappa; q), \dots, \\
 E_{1,s+1}(n\kappa; q) &= -(n\kappa)^2 \iint_{Q_\delta} G_0(n\kappa; q, q_0) \times \\
 &\quad \times [1 - \varepsilon_{n\kappa}(q_0, \alpha(q_0), E_{1,s}(\kappa; q_0), E_{1,s}(2\kappa; q_0), E_{1,s}(3\kappa; q_0))] E_{1,s}(n\kappa; q_0) dq_0 \\
 &\quad + \delta_{n1} (n\kappa)^2 \iint_{Q_\delta} G_0(n\kappa; q, q_0) \alpha(q_0) E_{1,s}^2(2\kappa; q_0) \bar{E}_{1,s}(3\kappa; q_0) dq_0 \\
 &\quad + \delta_{n3} (n\kappa)^2 \iint_{Q_\delta} G_0(n\kappa; q, q_0) \alpha(q_0) \left\{ \frac{1}{3} E_{1,s}^3(\kappa; q_0) + E_{1,s}^2(2\kappa; q_0) \bar{E}_{1,s}(\kappa; q_0) \right\} dq_0 \\
 &\quad + E_{1,0}(n\kappa; q), \dots, \quad q \in Q, \quad n = 1, 2, 3.
 \end{aligned} \tag{47}$$

Here  $Q_\delta := \{q = (y, z) : |y| < \infty, |z| \leq 2\pi\delta\}$  denotes the strip filled by the non-linear dielectric layer. The extension of the permitted values  $q \in Q_{\{Y, \infty\}} \subset Q$  from the strip  $Q_{\{Y, \infty\}}$  (where the Green's function (42) is defined) to the whole space  $Q$  is realised by passing to the limit  $Y \rightarrow \infty$  (where this procedure is admissible because of the free choice of the parameter  $Y$  and the asymptotic behaviour of the integrands as  $\mathcal{O}(Y^{-1})$ , see (42)). Letting  $s$  tend to infinity in (47), we obtain the integral representations of the unknown diffraction fields in the region  $Q$ :

$$\begin{aligned}
 E_1(n\kappa; q) &= -(n\kappa)^2 \iint_{Q_\delta} G_0(n\kappa; q, q_0) \times \\
 &\quad \times [1 - \varepsilon_{n\kappa}(q_0, \alpha(q_0), E_1(\kappa; q_0), E_1(2\kappa; q_0), E_1(3\kappa; q_0))] E_1(n\kappa; q_0) dq_0 \\
 &\quad + \delta_{n1} (n\kappa)^2 \iint_{Q_\delta} G_0(n\kappa; q, q_0) \alpha(q_0) E_1^2(2\kappa; q_0) \bar{E}_1(3\kappa; q_0) dq_0 \\
 &\quad + \delta_{n3} (n\kappa)^2 \iint_{Q_\delta} G_0(n\kappa; q, q_0) \alpha(q_0) \left\{ \frac{1}{3} E_1^3(\kappa; q_0) + E_1^2(2\kappa; q_0) \bar{E}_1(\kappa; q_0) \right\} dq_0 \\
 &\quad + E_1^{\text{inc}}(n\kappa; q), \quad q \in Q, \quad n = 1, 2, 3.
 \end{aligned} \tag{48}$$

Now, substituting the representation (42) for the canonical Green's function  $G_0$  into the system (48) and taking into consideration the expressions for the permittivity

$$\varepsilon_{n\kappa}(q_0, \alpha(q_0), E_1(\kappa; q_0), E_1(2\kappa; q_0), E_1(3\kappa; q_0)) = \varepsilon_{n\kappa}(z_0, \alpha(z_0), U(\kappa; z_0), U(2\kappa; z_0), U(3\kappa; z_0)),$$

we get the following system w.r.t. the unknown quasi-homogeneous fields

$$E_1(n\kappa; q|_{q \equiv (y,z)}) = U(n\kappa; z) \exp(i\phi_{n\kappa} y), \quad n = 1, 2, 3, \quad |z| \leq 2\pi\delta:$$

$$\begin{aligned} & U(n\kappa; z) \exp(i\phi_{n\kappa} y) \\ &= - \lim_{Y \rightarrow \infty} \left( \frac{i(n\kappa)^2}{4Y\Gamma_{n\kappa}} \exp(i\phi_{n\kappa} y) \int_{-2\pi\delta}^{2\pi\delta} \int_{-Y}^Y \exp(i\Gamma_{n\kappa}|z - z_0|) \times \right. \\ & \quad \times [1 - \varepsilon_{n\kappa}(z_0, \alpha(z_0), U(\kappa; z_0), U(2\kappa; z_0), U(3\kappa; z_0))] U(n\kappa; z_0) dy_0 dz_0 \\ &+ \lim_{Y \rightarrow \infty} \left( \delta_{n1} \frac{i(n\kappa)^2}{4Y\Gamma_{n\kappa}} \exp(i\phi_{n\kappa} y) \times \right. \\ & \quad \times \int_{-2\pi\delta}^{2\pi\delta} \int_{-Y}^Y \exp(i\Gamma_{n\kappa}|z - z_0|) \alpha(z_0) U^2(2\kappa; z_0) \bar{U}(3\kappa; z_0) dy_0 dz_0 \\ &+ \lim_{Y \rightarrow \infty} \left( \delta_{n3} \frac{i(n\kappa)^2}{4Y\Gamma_{n\kappa}} \exp(i\phi_{n\kappa} y) \times \right. \\ & \quad \times \int_{-2\pi\delta}^{2\pi\delta} \int_{-Y}^Y \exp(i\Gamma_{n\kappa}|z - z_0|) \alpha(z_0) \left\{ \frac{1}{3} U^3(\kappa; z_0) + U^2(2\kappa; z_0) \bar{U}(\kappa; z_0) \right\} dy_0 dz_0 \\ &+ U^{\text{inc}}(n\kappa; z) \exp(i\phi_{n\kappa} y), \quad |z| \leq 2\pi\delta, \quad n = 1, 2, 3. \end{aligned}$$

Integrating in the region  $Q_\delta$  w.r.t. the variable  $y_0$ , we arrive at a system of non-linear Fredholm integral equations of the second kind w.r.t. the unknown functions  $U(n\kappa; \cdot) \in L_2(-2\pi\delta, 2\pi\delta)$ :

$$\begin{aligned} & U(n\kappa; z) + \frac{i(n\kappa)^2}{2\Gamma_{n\kappa}} \int_{-2\pi\delta}^{2\pi\delta} \exp(i\Gamma_{n\kappa}|z - z_0|) \times \\ & \quad \times [1 - \varepsilon_{n\kappa}(z_0, \alpha(z_0), U(\kappa; z_0), U(2\kappa; z_0), U(3\kappa; z_0))] U(n\kappa; z_0) dz_0 \\ &= \delta_{n1} \frac{i(n\kappa)^2}{2\Gamma_{n\kappa}} \int_{-2\pi\delta}^{2\pi\delta} \exp(i\Gamma_{n\kappa}|z - z_0|) \alpha(z_0) U^2(2\kappa; z_0) \bar{U}(3\kappa; z_0) dz_0 \\ &+ \delta_{n3} \frac{i(n\kappa)^2}{2\Gamma_{n\kappa}} \int_{-2\pi\delta}^{2\pi\delta} \exp(i\Gamma_{n\kappa}|z - z_0|) \alpha(z_0) \left\{ \frac{1}{3} U^3(\kappa; z_0) + U^2(2\kappa; z_0) \bar{U}(\kappa; z_0) \right\} dz_0 \\ &+ U^{\text{inc}}(n\kappa; z), \quad |z| \leq 2\pi\delta, \quad n = 1, 2, 3. \end{aligned} \tag{49}$$

Here  $U^{\text{inc}}(n\kappa; z) = a_{n\kappa}^{\text{inc}} \exp[-i\Gamma_{n\kappa}(z - 2\pi\delta)]$ ,  $n = 1, 2, 3$ .

The solution of the original problem (21), (C1) – (C4), represented as (23), can be obtained from (49) using the formulas

$$U(n\kappa; 2\pi\delta) = a_{n\kappa}^{\text{inc}} + a_{n\kappa}^{\text{scat}}, \quad U(n\kappa; -2\pi\delta) = b_{n\kappa}^{\text{scat}}, \quad n = 1, 2, 3, \tag{50}$$

(cf. (C3)). The derivation of the system of non-linear integral equations (49) shows that (49) can be regarded as an integral representation of the desired solution of (21), (C1) – (C4) (i.e. solutions of the form  $E_1(n\kappa; y, z) = U(n\kappa; z) \exp(i\phi_{n\kappa} y)$ ,  $n = 1, 2, 3$ , see (23)) for points located outside the non-linear layer:  $\{(y, z) : |y| < \infty, |z| > 2\pi\delta\}$ . Indeed, given the solution of non-linear integral equations (49) in the region  $|z| \leq 2\pi\delta$ , the substitution into the integrals of (49) leads to explicit expressions of the desired solutions  $U(n\kappa; z)$  for points  $|z| > 2\pi\delta$  outside the non-linear layer at each frequency  $n\kappa$ ,  $n = 1, 2, 3$ .

## 6. A sufficient condition for the existence of solutions of the system of non-linear equations

In the case of a linear system (49), i.e. if  $\alpha \equiv 0$ , the problem of existence and uniqueness of solutions has been investigated in Sirenko et al. (1985), Shestopalov & Sirenko (1989). In the general situation, the system of non-linear integral equations can have a unique solution, no solution or several solutions, depending on the properties of the kernel and the right-hand side.

We start with the derivation of sufficient conditions for the existence of solutions of the system (49) (cf. Shestopalov & Yatsyk (2010), Shestopalov & Yatsyk (2007), Kravchenko & Yatsyk (2007)). To do so, in the region  $|z| \leq 2\pi\delta$  we consider two sequences of solutions  $\{U_s(n\kappa; z), n = 1, 2, 3\}_{s=0}^\infty$  and  $\{\Psi_s(n\kappa; z), n = 1, 2, 3\}_{s=0}^\infty$  of the following systems of integral equations:

$$\begin{aligned}
 & U_{s+1}(n\kappa; z) + \frac{i(n\kappa)^2}{2\Gamma_{n\kappa}} \int_{-2\pi\delta}^{2\pi\delta} \exp(i\Gamma_{n\kappa}|z - z_0|) \\
 & \quad \times [1 - \varepsilon_{n\kappa}(z_0, \alpha(z_0), U_s(\kappa; z_0), U_s(2\kappa; z_0), U_s(3\kappa; z_0))] U_s(n\kappa; z_0) dz_0 \\
 & = \delta_{n1} \frac{i(n\kappa)^2}{2\Gamma_{n\kappa}} \int_{-2\pi\delta}^{2\pi\delta} \exp(i\Gamma_{n\kappa}|z - z_0|) \alpha(z_0) U_s^2(2\kappa; z_0) \bar{U}_s(3\kappa; z_0) dz_0 \\
 & \quad + \delta_{n3} \frac{i(n\kappa)^2}{2\Gamma_{n\kappa}} \int_{-2\pi\delta}^{2\pi\delta} \exp(i\Gamma_{n\kappa}|z - z_0|) \\
 & \quad \times \alpha(z_0) \left\{ \frac{1}{3} U_s^3(\kappa; z_0) + U_s^2(2\kappa; z_0) \bar{U}_s(\kappa; z_0) \right\} dz_0 + U^{\text{inc}}(n\kappa; z), \quad |z| \leq 2\pi\delta, \quad n = 1, 2, 3, \\
 & \Psi_s(n\kappa; z) + \frac{i(n\kappa)^2}{2\Gamma_{n\kappa}} \int_{-2\pi\delta}^{2\pi\delta} \exp(i\Gamma_{n\kappa}|z - z_0|) \\
 & \quad \times [1 - \varepsilon_{n\kappa}(z_0, \alpha(z_0), U_s(\kappa; z_0), U_s(2\kappa; z_0), U_s(3\kappa; z_0))] \Psi_s(n\kappa; z_0) dz_0 \\
 & = \delta_{n1} \frac{i(n\kappa)^2}{2\Gamma_{n\kappa}} \int_{-2\pi\delta}^{2\pi\delta} \exp(i\Gamma_{n\kappa}|z - z_0|) \alpha(z_0) U_s^2(2\kappa; z_0) \bar{U}_s(3\kappa; z_0) dz_0 \\
 & \quad + \delta_{n3} \frac{i(n\kappa)^2}{2\Gamma_{n\kappa}} \int_{-2\pi\delta}^{2\pi\delta} \exp(i\Gamma_{n\kappa}|z - z_0|) \\
 & \quad \times \alpha(z_0) \left\{ \frac{1}{3} U_s^3(\kappa; z_0) + U_s^2(2\kappa; z_0) \bar{U}_s(\kappa; z_0) \right\} dz_0 + U^{\text{inc}}(n\kappa; z), \quad |z| \leq 2\pi\delta, \quad n = 1, 2, 3.
 \end{aligned} \tag{51}$$

The first system of equations (51) coincides with the iterative scheme (47) for the solution of the non-linear system (49). The second system w.r.t.  $\Psi_s(n\kappa; z)$ ,  $n = 1, 2, 3$ , is nothing else than the linearisation of the non-linear system (49) around  $U_s(n\kappa; z)$ ,  $n = 1, 2, 3$ .

In the case that the functions  $\Psi_s(n\kappa; z)$ ,  $n = 1, 2, 3$ , are not eigen-functions of the linearised problem under consideration with the induced permittivity of the layer (cf. 19))

$$\begin{aligned}
 & \varepsilon_{n\kappa}(z, \alpha(z), U_s(\kappa; z), U_s(2\kappa; z), U_s(3\kappa; z)) \\
 & = \varepsilon^{(L)}(z) + \varepsilon_{n\kappa}^{(NL)}(\alpha(z), U_s(\kappa; z), U_s(2\kappa; z), U_s(3\kappa; z)) \\
 & = \varepsilon^{(L)}(z) + \alpha(z) \{ |U_s(\kappa; z)|^2 + |U_s(2\kappa; z)|^2 + |U_s(3\kappa; z)|^2 \\
 & \quad + \delta_{n1} |U_s(\kappa; z)| |U_s(3\kappa; z)| \exp[i\{-3\arg U_s(\kappa; z) + \arg U_s(3\kappa; z)\}] \\
 & \quad + \delta_{n2} |U_s(\kappa; z)| |U_s(3\kappa; z)| \exp[i\{-2\arg U_s(2\kappa; z) + \arg U_s(\kappa; z) + \arg U_s(3\kappa; z)\}] \}, \\
 & \quad |z| \leq 2\pi\delta, \quad n = 1, 2, 3,
 \end{aligned} \tag{52}$$

a solution of the second system in (51) exists uniquely (Sirenko et al. (1985), Shestopalov & Sirenko (1989)) and can be represented as

$$\Psi_s(n\kappa; z) = \Psi(n\kappa; z, \alpha(z), U_s(\kappa; z), U_s(2\kappa; z), U_s(3\kappa; z)), \quad n = 1, 2, 3. \quad (53)$$

Moreover, at each iteration step (i.e. for any iteration parameter  $s \in \{0, 1, 2, \dots\}$ ) the solution (53) which is caused by the exciting wave packet  $\{|U^{\text{inc}}(n\kappa; z)| = a_{n\kappa}^{\text{inc}}\}_{n=1}^3$ , satisfies the estimate

$$|\Psi_s(n\kappa; z)|^2 \leq \sum_{m=1}^3 (a_{m\kappa}^{\text{inc}})^2, \quad \forall s \in \{0, 1, 2, \dots\}, \quad n = 1, 2, 3 \quad (54)$$

due to energy relations. In particular,

$$\begin{aligned} & |\varepsilon_{n\kappa}(z, \alpha(z), U_s(\kappa; z), U_s(2\kappa; z), U_s(3\kappa; z))| \\ & \leq |\varepsilon^{(L)}(z)| + |\alpha(z)|(3 + \delta_{n1} + \delta_{n2}) \sum_{m=1}^3 (a_{m\kappa}^{\text{inc}})^2, \quad \forall s \in \{0, 1, 2, \dots\}, \quad n = 1, 2, 3. \end{aligned} \quad (55)$$

The analysis of appropriate convergence criteria for the sequences  $\{U_s(n\kappa; z), n = 1, 2, 3\}_{s=0}^\infty$  and  $\{\Psi_s(n\kappa; z), n = 1, 2, 3\}_{s=0}^\infty$  given by (51) provides a sufficient condition for the existence and uniqueness of solutions of the non-linear integral equations (49). Since the kernels of the integral equations (51) are identical, it is easy to estimate the distance between the elements  $U_{s+1}(n\kappa; z)$  and  $\Psi_s(n\kappa; z)$ :

$$\begin{aligned} \varrho(U_{s+1}(n\kappa; z), \Psi_s(n\kappa; z)) &= \left[ \int_{-2\pi\delta}^{2\pi\delta} |U_{s+1}(n\kappa; z) - \Psi_s(n\kappa; z)|^2 dz \right]^{1/2} \\ &= \left| \frac{i(n\kappa)^2}{2\Gamma_{n\kappa}} \left[ \int_{-2\pi\delta}^{2\pi\delta} \left| \int_{-2\pi\delta}^{2\pi\delta} \exp(i\Gamma_{n\kappa}|z - z_0|) \right. \right. \right. \\ &\quad \times [1 - \varepsilon_{n\kappa}(z_0, \alpha(z_0), U_s(\kappa; z_0), U_s(2\kappa; z_0), U_s(3\kappa; z_0))] (U_s(n\kappa; z_0) - \Psi_s(n\kappa; z_0)) dz_0 \Big|^2 dz \Big]^{1/2} \\ &= \frac{(n\kappa)^2}{2\Gamma_{n\kappa}} \left[ \int_{-2\pi\delta}^{2\pi\delta} \left| \int_{-2\pi\delta}^{2\pi\delta} [1 - \varepsilon_{n\kappa}(z_0, \alpha(z_0), U_s(\kappa; z_0), U_s(2\kappa; z_0), U_s(3\kappa; z_0))] \right. \right. \\ &\quad \times (U_s(n\kappa; z_0) - \Psi_s(n\kappa; z_0)) dz_0 \Big|^2 dz \Big]^{1/2} \\ &\leq \frac{(n\kappa)^2}{2\Gamma_{n\kappa}} \left[ \int_{-2\pi\delta}^{2\pi\delta} \int_{-2\pi\delta}^{2\pi\delta} |1 - \varepsilon_{n\kappa}(z_0, \alpha(z_0), U_s(\kappa; z_0), U_s(2\kappa; z_0), U_s(3\kappa; z_0))|^2 dz_0 dz \right]^{1/2} \\ &\quad \times \left[ \int_{-2\pi\delta}^{2\pi\delta} |U_s(n\kappa; z_0) - \Psi_s(n\kappa; z_0)|^2 dz_0 \right]^{1/2} \\ &\leq \frac{(n\kappa)^2}{2\Gamma_{n\kappa}} 4\pi\delta \max_{z \in [-2\pi\delta, 2\pi\delta]} \left( |1 - \varepsilon^{(L)}(z)| + |\varepsilon_{n\kappa}(z, \alpha(z), U_s(\kappa; z), U_s(2\kappa; z), U_s(3\kappa; z))| \right) \\ &\quad \times \varrho(U_s(n\kappa; z), \Psi_s(n\kappa; z)) \\ &\leq \frac{(n\kappa)^2}{2\Gamma_{n\kappa}} 4\pi\delta \max_{z \in [-2\pi\delta, 2\pi\delta]} \left( |1 - \varepsilon^{(L)}(z)| + 4|\alpha(z)| \sum_{m=1}^3 (a_{m\kappa}^{\text{inc}})^2 \right) \varrho(U_s(n\kappa; z), \Psi_s(n\kappa; z)), \quad (56) \\ &\quad n = 1, 2, 3. \end{aligned}$$



The last inequality in (56) is a consequence of (55). The estimate (56) shows that the iterative process defined by the first system of equations (51) converges to a unique solution determined by the second system of equations (51) if in (56) the factor in front of  $\varrho(U_s(n\kappa; z), \Psi_s(n\kappa; z))$  satisfies the condition

$$\frac{(n\kappa)^2}{2\Gamma_{n\kappa}} 4\pi\delta \max_{z \in [-2\pi\delta, 2\pi\delta]} \left( |1 - \varepsilon^{(L)}(z)| + 4|\alpha(z)| \sum_{m=1}^3 (a_{m\kappa}^{\text{inc}})^2 \right) < 1, \quad n = 1, 2, 3.$$

Taking into account the expressions for the transverse propagation constants  $\Gamma_{n\kappa} = ((n\kappa)^2 - \phi_{n\kappa}^2)^{1/2} = ((n\kappa)^2 - (n\kappa \sin \varphi_{n\kappa})^2)^{1/2} = n\kappa \cos \varphi_{n\kappa}$ ,  $n = 1, 2, 3$ , and the condition of phase synchronism (C2)  $\varphi_\kappa = \varphi_{n\kappa}$ ,  $n = 1, 2, 3$ , these inequalities can be represented as

$$n\kappa 2\pi\delta \max_{z \in [-2\pi\delta, 2\pi\delta]} \left( |1 - \varepsilon^{(L)}(z)| + 4|\alpha(z)| \sum_{m=1}^3 (a_{m\kappa}^{\text{inc}})^2 \right) < \cos \varphi_\kappa, \quad n = 1, 2, 3. \quad (57)$$

In summary, we have proved the following result.

**Theorem 2.** *The condition (57) is a sufficient condition for the existence of solutions of the non-linear integral equations (49). Such a solution can be obtained by using the iterative process given the first system of equations in (51), or by using the equivalent iterative process that can be built on the basis of the second system of equations in (51). The solution  $\Psi_s(n\kappa; z)$ ,  $n = 1, 2, 3$ , should be regarded as an  $(s + 1)$ st approximation  $U_{s+1}(n\kappa; z) := \Psi_s(n\kappa; z)$  to the desired solution  $U(n\kappa; z)$ ,  $n = 1, 2, 3$ :*

$$\begin{aligned} & U_{s+1}(n\kappa; z) + \frac{i(n\kappa)^2}{2\Gamma_{n\kappa}} \int_{-2\pi\delta}^{2\pi\delta} \exp(i\Gamma_{n\kappa}|z - z_0|) \\ & \quad \times [1 - \varepsilon_{n\kappa}(z_0, \alpha(z_0), U_s(\kappa; z_0), U_s(2\kappa; z_0), U_s(3\kappa; z_0))] U_{s+1}(n\kappa; z_0) dz_0 \\ & = \delta_{n1} \frac{i(n\kappa)^2}{2\Gamma_{n\kappa}} \int_{-2\pi\delta}^{2\pi\delta} \exp(i\Gamma_{n\kappa}|z - z_0|) \alpha(z_0) U_s^2(2\kappa; z_0) \bar{U}_s(3\kappa; z_0) dz_0 \\ & \quad + \delta_{n3} \frac{i(n\kappa)^2}{2\Gamma_{n\kappa}} \int_{-2\pi\delta}^{2\pi\delta} \exp(i\Gamma_{n\kappa}|z - z_0|) \\ & \quad \times \alpha(z_0) \left\{ \frac{1}{3} U_s^3(\kappa; z_0) + U_s^2(2\kappa; z_0) \bar{U}_s(\kappa; z_0) \right\} dz_0 + U^{\text{inc}}(n\kappa; z), \quad |z| \leq 2\pi\delta, \quad n = 1, 2, 3. \end{aligned} \quad (58)$$

Moreover, if the elements  $\Psi_s(n\kappa; z) \equiv U_{s+1}(n\kappa; z)$ ,  $n = 1, 2, 3$ , are not eigen-functions of the linearised problem (49) with the induced permittivity of the layer (52) (i.e. solutions of the homogeneous system (58)), then this solution is unique.

## 7. A self-consistent approach to the numerical analysis of the non-linear integral equations

According to Angermann & Yatsyk (2011), Angermann & Yatsyk (2010), the application of suitable quadrature rules to the system of non-linear integral equations (49) leads to a system of complex-valued non-linear algebraic equations of the second kind:

$$\begin{cases} (\mathbf{I} - \mathbf{B}_\kappa(\mathbf{U}_\kappa, \mathbf{U}_{2\kappa}, \mathbf{U}_{3\kappa})) \mathbf{U}_\kappa = \mathbf{C}_\kappa(\mathbf{U}_{2\kappa}, \mathbf{U}_{3\kappa}) + \mathbf{U}_\kappa^{\text{inc}}, \\ (\mathbf{I} - \mathbf{B}_{2\kappa}(\mathbf{U}_\kappa, \mathbf{U}_{2\kappa}, \mathbf{U}_{3\kappa})) \mathbf{U}_{2\kappa} = \mathbf{U}_{2\kappa}^{\text{inc}}, \\ (\mathbf{I} - \mathbf{B}_{3\kappa}(\mathbf{U}_\kappa, \mathbf{U}_{2\kappa}, \mathbf{U}_{3\kappa})) \mathbf{U}_{3\kappa} = \mathbf{C}_{3\kappa}(\mathbf{U}_\kappa, \mathbf{U}_{2\kappa}) + \mathbf{U}_{3\kappa}^{\text{inc}}, \end{cases} \quad (59)$$

where  $\{z_l\}_{l=1}^N$  is a discrete set of nodes such that  $-2\pi\delta =: z_1 < z_2 < \dots < z_l < \dots < z_N =: 2\pi\delta$ .

$\mathbf{U}_{n\kappa} := \{U_l(n\kappa)\}_{l=1}^N \approx \{U(n\kappa; z_l)\}_{l=1}^N$  denotes the vector of the unknown approximate solution values corresponding to the frequencies  $n\kappa$ ,  $n = 1, 2, 3$ . The matrices are of the form

$$\mathbf{B}_{n\kappa}(\mathbf{U}_\kappa, \mathbf{U}_{2\kappa}, \mathbf{U}_{3\kappa}) = \{A_m K_{lm}(n\kappa, \mathbf{U}_\kappa, \mathbf{U}_{2\kappa}, \mathbf{U}_{3\kappa})\}_{l,m=1}^N$$

with entries

$$\begin{aligned} K_{lm}(n\kappa, \mathbf{U}_\kappa, \mathbf{U}_{2\kappa}, \mathbf{U}_{3\kappa}) := & -\frac{i(n\kappa)^2}{2\Gamma_{n\kappa}} \exp(i\Gamma_{n\kappa}|z_l - z_m|) \left[ 1 - \left\{ \varepsilon^{(L)}(z_m) \right. \right. \\ & + \alpha(z_m) \left( |U_m(\kappa)|^2 + |U_m(2\kappa)|^2 + |U_m(3\kappa)|^2 \right. \\ & + \delta_{n1} |U_m(\kappa)| |U_m(3\kappa)| \exp\{i[-3\arg U_m(\kappa) + \arg U_m(3\kappa)]\} \\ & \left. \left. + \delta_{n2} |U_m(\kappa)| |U_m(3\kappa)| \exp\{i[-2\arg U_m(2\kappa) + \arg U_m(\kappa) + \arg U_m(3\kappa)]\} \right) \right\} \right]. \end{aligned} \quad (60)$$

The numbers  $A_m$  are the coefficients determined by the quadrature rule,  $\mathbf{I} := \{\delta_{lm}\}_{l,m=1}^N$  is the identity matrix, and  $\delta_{lm}$  is Kronecker's symbol.

The right-hand side of (59) is defined by

$$\mathbf{U}_{n\kappa}^{\text{inc}} := \{a_{n\kappa}^{\text{inc}} \exp[-i\Gamma_{n\kappa}(z_l - 2\pi\delta)]\}_{l=1}^N,$$

$$\mathbf{C}_\kappa(\mathbf{U}_{2\kappa}, \mathbf{U}_{3\kappa}) := \left\{ \frac{i\kappa^2}{2\Gamma_\kappa} \sum_{m=1}^N A_m \exp(i\Gamma_\kappa|z_l - z_m|) \alpha(z_m) U_m^2(2\kappa) \overline{U}_m(3\kappa) \right\}_{l=1}^N,$$

$$\mathbf{C}_{3\kappa}(\mathbf{U}_\kappa, \mathbf{U}_{2\kappa}) := \left\{ \frac{i(3\kappa)^2}{2\Gamma_{3\kappa}} \sum_{m=1}^N A_m \exp(i\Gamma_{3\kappa}|z_l - z_m|) \alpha(z_m) \left[ \frac{1}{3} U_m^3(\kappa) + U_m^2(2\kappa) \overline{U}_m(\kappa) \right] \right\}_{l=1}^N.$$

The solution of (59) is approximated by means of the following iterative method:

$$\left\{ \begin{aligned} & \left\{ \left[ \mathbf{I} - \mathbf{B}_\kappa \left( \mathbf{U}_\kappa^{(s-1)}, \mathbf{U}_{2\kappa}^{(S_2(q))}, \mathbf{U}_{3\kappa}^{(S_3(q))} \right) \right] \mathbf{U}_\kappa^{(s)} \right. \\ & \quad \left. = \mathbf{C}_\kappa \left( \mathbf{U}_{2\kappa}^{(S_2(q))}, \mathbf{U}_{3\kappa}^{(S_3(q))} \right) + \mathbf{U}_\kappa^{\text{inc}} \right\}_{s=1}^{S_1(q): \|\mathbf{U}_\kappa^{(S_1(q))} - \mathbf{U}_\kappa^{(S_1(q)-1)}\| / \|\mathbf{U}_\kappa^{(S_1(q))}\| < \xi} \\ & \left\{ \left[ \mathbf{I} - \mathbf{B}_{2\kappa} \left( \mathbf{U}_\kappa^{(S_1(q))}, \mathbf{U}_{2\kappa}^{(s-1)}, \mathbf{U}_{3\kappa}^{(S_3(q))} \right) \right] \mathbf{U}_{2\kappa}^{(s)} \right. \\ & \quad \left. = \mathbf{U}_{2\kappa}^{\text{inc}} \right\}_{s=1}^{S_2(q): \|\mathbf{U}_{2\kappa}^{(S_2(q))} - \mathbf{U}_{2\kappa}^{(S_2(q)-1)}\| / \|\mathbf{U}_{2\kappa}^{(S_2(q))}\| < \xi} \\ & \left\{ \left[ \mathbf{I} - \mathbf{B}_{3\kappa} \left( \mathbf{U}_\kappa^{(S_1(q))}, \mathbf{U}_{2\kappa}^{(S_2(q))}, \mathbf{U}_{3\kappa}^{(s-1)} \right) \right] \mathbf{U}_{3\kappa}^{(s)} \right. \\ & \quad \left. = \mathbf{C}_{3\kappa} \left( \mathbf{U}_\kappa^{(S_1(q))}, \mathbf{U}_{2\kappa}^{(S_2(q))} \right) + \mathbf{U}_{3\kappa}^{\text{inc}} \right\}_{s=1}^{S_3(q): \|\mathbf{U}_{3\kappa}^{(S_3(q))} - \mathbf{U}_{3\kappa}^{(S_3(q)-1)}\| / \|\mathbf{U}_{3\kappa}^{(S_3(q))}\| < \xi} \end{aligned} \right\}_{q=1}^Q, \quad (61)$$

where, for a given relative error tolerance  $\xi > 0$ , the terminating index  $Q \in \mathbb{N}$  is defined by the requirement

$$\max \left\{ \|\mathbf{U}_\kappa^{(Q)} - \mathbf{U}_\kappa^{(Q-1)}\| / \|\mathbf{U}_\kappa^{(Q)}\|, \|\mathbf{U}_{2\kappa}^{(Q)} - \mathbf{U}_{2\kappa}^{(Q-1)}\| / \|\mathbf{U}_{2\kappa}^{(Q)}\|, \|\mathbf{U}_{3\kappa}^{(Q)} - \mathbf{U}_{3\kappa}^{(Q-1)}\| / \|\mathbf{U}_{3\kappa}^{(Q)}\| \right\} < \xi.$$

## 8. Eigen-modes of the linearised problems of scattering and generation of waves on the cubically polarisable layer

The solution of the system of non-linear equations (49) is approximated by the solution of the linearised system of non-linear equations (58), for given values of the induced dielectric permittivity and of the source functions at the right-hand side of the system. The solution can be found by the help of algorithm (61), where at each step a system of linearised non-linear complex-valued algebraic equations of the second kind is solved iteratively. The analytic continuation of the linearised non-linear problems into the region of complex values of the frequency parameter allows us to switch to the analysis of spectral problems. That is, the eigen-frequencies and the corresponding eigen-fields of the homogeneous linear problems with an induced non-linear permittivity are to be determined. The results of the development of a spectral theory of linear problems for structures with non-compact boundaries can be found in Yatsyk (2000), Shestopalov & Yatsyk (1997), Sirenko et al. (1985), Shestopalov & Sirenko (1989), Sirenko et al. (2007), Sirenko & Ström (2010).

As mentioned above, the classical formulation of the problem of scattering and generation of waves, described by the *system* of boundary value problems (21), (C1) – (C4), can be reformulated as a *set* of independent spectral problems in the following way:

Find the eigen-frequencies  $\kappa_n$  and the corresponding eigen-functions  $E_1(\mathbf{r}, \kappa_n)$  (i.e.  $\{\kappa_n \in \Omega_{n\kappa} \subset H_{n\kappa}, E_1(\mathbf{r}, \kappa_n)\}_{n=1}^3$ , where  $\Omega_{n\kappa}$  are the sets of eigen-frequencies lying on the two-sheeted Riemann surfaces  $H_{n\kappa}$ , see Fig. 2 and the more detailed explanations below) satisfying the equations

$$\nabla^2 E_1(\mathbf{r}, \kappa_n) + \kappa_n^2 \varepsilon_{n\kappa}(z, \alpha(z), E_1(r, \kappa), E_1(\mathbf{r}, 2\kappa), E_1(\mathbf{r}, 3\kappa)) E_1(\mathbf{r}, \kappa_n) = 0, \quad n = 1, 2, 3, \quad (62)$$

together with the following conditions:

$$(CS1) \quad E_1(\kappa_n; y, z) = U(\kappa_n; z) \exp(i\phi_{n\kappa} y), \quad n = 1, 2, 3$$

(the quasi-homogeneity condition w.r.t. the spatial variable  $y$ ),

$$(CS2) \quad \phi_{n\kappa} = n\phi_\kappa, \quad n = 1, 2, 3 \quad (\text{the condition of phase synchronism of waves}),$$

$$(CS3) \quad \mathbf{E}_{tg}(\kappa_n; y, z) \text{ and } \mathbf{H}_{tg}(\kappa_n; y, z) \text{ (i.e. } E_1(\kappa_n; y, z) \text{ and } H_2(\kappa_n; y, z)) \text{ are continuous at the boundary layers of the structure with the induced permittivity } \varepsilon_{n\kappa} \text{ for } \kappa := \kappa^{inc}, \quad n = 1, 2, 3,$$

$$(CS4) \quad E_1(\kappa_n; y, z) = \begin{cases} a_{\kappa_n} \\ b_{\kappa_n} \end{cases} \exp(i(\phi_{n\kappa} y \pm \Gamma_{\kappa_n}(\kappa_n, \phi_{n\kappa})(z \mp 2\pi\delta))), \quad z \gtrless \pm 2\pi\delta, \quad n = 1, 2, 3$$

(the radiation condition w.r.t. the eigen-field).

For real values of the parameters  $\kappa_n$  and  $\phi_{n\kappa}$ , the condition (CS4) meets the physically reasonable requirement of the absence of radiation fields of waves coming from infinity  $z = \pm\infty$ :

$$\Im \Gamma_{\kappa_n}(\kappa_n, \phi_{n\kappa}) \geq 0, \quad \Re \Gamma_{\kappa_n}(\kappa_n, \phi_{n\kappa}) \Re \kappa_n \geq 0 \quad \text{for} \quad \Im \phi_{n\kappa} = 0, \quad \Im \kappa_n = 0, \quad n = 1, 2, 3. \quad (63)$$

The non-trivial solutions (eigen-fields) of problem (62), (CS1) – (CS4) can be represented as

$$E_1(\kappa_n; y, z) = U(\kappa_n; z) \exp(i\phi_{n\kappa} y) = \begin{cases} a_{\kappa_n} \exp(i(\phi_{n\kappa} y + \Gamma_{\kappa_n}(\kappa_n, \phi_{n\kappa})(z - 2\pi\delta))), & z > 2\pi\delta, \\ U(\kappa_n; z) \exp(i\phi_{n\kappa} y), & |z| \leq 2\pi\delta, \\ b_{\kappa_n} \exp(i(\phi_{n\kappa} y - \Gamma_{\kappa_n}(\kappa_n, \phi_{n\kappa})(z + 2\pi\delta))), & z < -2\pi\delta, \end{cases} \quad \kappa_n \in \Omega_{n\kappa} \subset H_{n\kappa}, \quad n = 1, 2, 3, \quad (64)$$

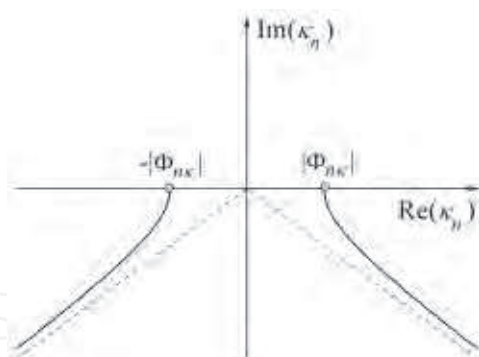


Fig. 2. The geometry of the two-sheeted Riemann surfaces  $H_{n\kappa}$

where  $\kappa := \kappa^{\text{inc}}$  is a given constant equal to the value of the excitation frequency of the non-linear structure,  $\Gamma_{\kappa_n}(\kappa_n, \phi_{n\kappa}) := (\kappa_n^2 - \phi_{n\kappa}^2)^{1/2}$  are the transverse propagation functions depending on the complex frequency spectral variables  $\kappa_n$ ,  $\phi_{n\kappa} := n\kappa \sin(\varphi_{n\kappa})$  denote the given real values of the longitudinal propagation constants,

$\varepsilon_{n\kappa} = \varepsilon_{n\kappa}(z, \alpha(z), E_1(\mathbf{r}, \kappa), E_1(\mathbf{r}, 2\kappa), E_1(\mathbf{r}, 3\kappa))$  are the induced dielectric permittivities at the frequencies  $n\kappa$  corresponding to the parameter  $\kappa := \kappa^{\text{inc}}$ ,  $\Omega_{n\kappa}$  are the sets of eigen-frequencies and  $H_{n\kappa}$  are two-sheeted Riemann surfaces (cf. Fig. 2),  $n = 1, 2, 3$ . The range of the spectral parameters  $\kappa_n \in \Omega_{n\kappa}$  is completely determined by the boundaries of those regions in which the analytic continuation (consistent with the condition (63)) of the canonical Green's functions

$$G_0(\kappa_n; q, q_0) = \frac{i}{4Y} \exp \{i [\phi_{n\kappa} (y - y_0) + \Gamma_{\kappa_n}(\kappa_n, \phi_{n\kappa}) |z - z_0|]\} / \Gamma_{\kappa_n}(\kappa_n, \phi_{n\kappa}), \quad n = 1, 2, 3,$$

(cf. (42)) into the complex space of the spectral parameters  $\kappa_n$  of the unperturbed problems (62), (CS1) – (CS4) (i.e. for the special case  $\varepsilon_{n\kappa} \equiv 1$ ,  $n = 1, 2, 3$ ) is possible. These complex spaces are two-sheeted Riemann surfaces  $H_{n\kappa}$  (see Fig. 2) with real algebraic branch points of second order  $\kappa_n^\pm : \Gamma_{\kappa_n}(\kappa_n^\pm, \phi_{n\kappa}) = 0$  (i.e.  $\kappa_n^\pm = \pm |\phi_{n\kappa}|$ ,  $n = 1, 2, 3$ ) and with cuts starting at these points and extending along the lines

$$(\Re \kappa_n)^2 - (\Im \kappa_n)^2 - \phi_{n\kappa}^2 = 0, \quad \Im \kappa_n \leq 0, \quad n = 1, 2, 3. \quad (65)$$

The first, “physical” sheets (i.e. the pair of values  $\{\kappa_n, \Gamma_{\kappa_n}(\kappa_n, \phi_{n\kappa})\}$ ) on each of the surfaces  $H_{n\kappa}$ ,  $n = 1, 2, 3$ , are completely determined by the condition (63) and the cuts (65). At the first sheets of  $H_{n\kappa}$  the signs of the pairs  $\{\kappa_n, \Re \Gamma_{\kappa_n}\}$  and  $\{\kappa_n, \Im \Gamma_{\kappa_n}\}$  are distributed as follows:  $\Im \Gamma_{\kappa_n} > 0$  for  $0 < \arg \kappa_n < \pi$ ,  $\Re \Gamma_{\kappa_n} \geq 0$  for  $0 < \arg \kappa_n < \pi/2$  and  $\Re \Gamma_{\kappa_n} \leq 0$  for  $\pi/2 \leq \arg \kappa_n < \pi$ . For points  $\kappa_n$  with  $3\pi/2 \leq \arg \kappa_n \leq 2\pi$ , the function values (where  $(\Re \kappa_n)^2 - (\Im \kappa_n)^2 - \phi_{n\kappa}^2 > 0$ ) are determined by the condition  $\Im \Gamma_{\kappa_n} < 0$ ,  $\Re \Gamma_{\kappa_n} > 0$ , for the remaining points  $\kappa_n$  the function  $\Gamma_{\kappa_n}(\kappa_n, \phi_{n\kappa})$  is determined by the condition  $\Im \Gamma_{\kappa_n} > 0$ ,  $\Re \Gamma_{\kappa_n} \leq 0$ . In the region  $\pi < \arg \kappa_n < 3\pi/2$  the situation is similar to the previous one up to the change of the sign of  $\Re \Gamma_{\kappa_n}$ . The second, “unphysical” sheets of the surfaces  $H_{n\kappa}$ ,  $n = 1, 2, 3$  are different from the “physical” ones in that, for each  $\kappa_n$ , the signs of both  $\Re \Gamma_{\kappa_n}$  and  $\Im \Gamma_{\kappa_n}$  are reversed.

The qualitative analysis of the eigen-modes of the linearised problems (62), (CS1) – (CS4) is carried out using the equivalent formulation of spectral problems for the linearised non-linear integral equations (49). It is based on the analytic continuation of (49) (see also (58)) into the space of spectral values  $\kappa_n \in \Omega_{n\kappa} \subset H_{n\kappa}$ ,  $n = 1, 2, 3$ .

The spectral problem reduces to finding non-trivial solutions  $U(\kappa_n; z)$  of a set of homogeneous (i.e. with vanishing right-hand sides), linear (i.e. linearised equations (49)) integral equations with the induced dielectric permittivity at the frequencies  $n\kappa$  of excitation and generation:

$$U(\kappa_n; z) + \frac{i\kappa_n^2}{2\Gamma_{\kappa_n}(\kappa_n, \phi_{n\kappa})} \int_{-2\pi\delta}^{2\pi\delta} \exp(i\Gamma_{\kappa_n}(\kappa_n, \phi_{n\kappa})|z - z_0|) \times [1 - \varepsilon_{n\kappa}(z_0, \alpha(z_0), U(\kappa; z_0), U(2\kappa; z_0), U(3\kappa; z_0))] U(\kappa_n; z_0) dz_0 = 0; \quad (66)$$

$$|z| \leq 2\pi\delta, \quad \kappa := \kappa^{\text{inc}}, \quad \kappa_n \in \Omega_{n\kappa} \subset H_{n\kappa}, \quad n = 1, 2, 3.$$

The solution of the problem (62), (CS1) – (CS4) can be obtained from the solution of the equivalent problem (66), where – according to (CS3) – in the representation of the eigen-fields (64) the following formulas are used:

$$U(\kappa_n; 2\pi\delta) = a_{\kappa_n}, \quad U(\kappa_n; -2\pi\delta) = b_{\kappa_n}, \quad n = 1, 2, 3. \quad (67)$$

The analyticity w.r.t. the argument  $\kappa_n \in H_{n\kappa}$ ,  $n = 1, 2, 3$ , and the compactness of the operator functions (cf. (66))  $B_{n\kappa}(\kappa_n) [U(\kappa_n; \cdot)] : L_2(-2\pi\delta, 2\pi\delta) \rightarrow L_2(-2\pi\delta, 2\pi\delta)$ ,  $n = 1, 2, 3$ , where

$$B_{n\kappa}(\kappa_n) [U(\kappa_n; z)] = -\frac{i\kappa_n^2}{2\Gamma_{\kappa_n}(\kappa_n, \phi_{n\kappa})} \int_{-2\pi\delta}^{2\pi\delta} \exp(i\Gamma_{\kappa_n}(\kappa_n, \phi_{n\kappa})|z - z_0|) \times [1 - \varepsilon_{n\kappa}(z_0, \alpha(z_0), U(\kappa; z_0), U(2\kappa; z_0), U(3\kappa; z_0))] U(\kappa_n; z_0) dz_0, \quad \kappa := \kappa^{\text{inc}}, \quad n = 1, 2, 3, \quad (68)$$

are necessary conditions in the analytic Fredholm theorem (see (Reed & Simon, 1980, Thm. VI.14)). Taking into account that the resolvent set of (66) is non-empty in  $H_{n\kappa}$ , the theorem implies that the resolvent operator  $(I - B_{n\kappa}(\kappa_n))^{-1}$  (where  $I$  is the identity operator) exists and is a holomorphic operator function of the parameters  $\kappa_n \in H_{n\kappa}$ , with the exception of not more than countable sets of isolated points  $\Omega_{n\kappa}$ ,  $n = 1, 2, 3$  (i.e. sets that have no accumulation points in the finite part of each of the surfaces  $H_{n\kappa}$ ,  $n = 1, 2, 3$ ). In this case  $(I - B_{n\kappa}(\kappa_n))^{-1}$  is meromorphic in  $H_{n\kappa}$ , the residues at the poles are operators of finite rank and, if  $\kappa_n \in \Omega_{n\kappa}$ , then the equation (66)  $B_{n\kappa}(\kappa_n)U = U$  has a non-trivial solution in  $H_{n\kappa}$ ,  $n = 1, 2, 3$ . Summarizing the above discussion, we obtain the following result.

**Theorem 3.** *The spectra  $\Omega_{n\kappa}$  of the problem (62), (CS1) – (CS4), and also of the equivalent problem (66) for the dielectric layer with the induced piecewise continuous permittivity at the frequencies  $n\kappa$  of excitation and generation, consist of not more than countable sets of isolated points, without accumulation points in the finite part of each of the surfaces  $H_{n\kappa}$ ,  $n = 1, 2, 3$ . The resolvents of the spectral problems at these points are poles of finite order.*

## 9. Algorithm for the numerical analysis of the eigen-modes of the linearised problems

The qualitative analysis of the spectral characteristics allows to develop algorithms for solving the spectral problems (62), (CS1) – (CS4) by reducing them to the equivalent spectral problem of finding non-trivial solutions of the integral equations (66), see Shestopalov & Yatsyk (1997), Yatsyk (2000). The solvability of (66) follows from an analysis of the basic qualitative characteristics of the spectra. Applying to the integral equations (66) appropriate quadrature formulas, we obtain a set of independent systems of linear algebraic equations of second kind depending non-linearly on the spectral parameter:  $(\mathbf{I} - \mathbf{B}_{n\kappa}(\kappa_n))\mathbf{U}_{\kappa_n} = \mathbf{0}$ , where  $\kappa_n \in H_{n\kappa}$ ,  $\kappa := \kappa^{\text{inc}}$ ,  $n = 1, 2, 3$ . Consequently, the spectral problem of finding the eigen-frequencies



$\kappa_n \in \Omega_{n\kappa} \subset H_{n\kappa}$  and the corresponding eigen-fields (i.e. the non-trivial solutions of the integral equations (66)) reduces to the following algorithm:

$$\begin{cases} f_{n\kappa}(\kappa_n) := \det(\mathbf{I} - \mathbf{B}_{n\kappa}(\kappa_n)) = 0, \\ (\mathbf{I} - \mathbf{B}_{n\kappa}(\kappa_n))\mathbf{U}_{\kappa_n} = \mathbf{0}, \\ \kappa := \kappa^{\text{inc}}, \kappa_n \in \Omega_{n\kappa} \subset H_{n\kappa}, \quad n = 1, 2, 3. \end{cases} \quad (69)$$

Here we use a similar notation to that in Section 7.  $\kappa_n$  are the desired eigen-frequencies, and  $\mathbf{U}_{\kappa_n} = \{U(\kappa_n; z_l)\}_{l=1}^N := \{U_l(\kappa_n)\}_{l=1}^N$  are the vectors of the unknown approximate solution values corresponding to the frequencies  $\kappa_n$ . The matrices are of the form

$$\mathbf{B}_{n\kappa}(\kappa_n) := \mathbf{B}_{n\kappa}(\kappa_n; \mathbf{U}_\kappa, \mathbf{U}_{2\kappa}, \mathbf{U}_{3\kappa}) = \{A_m K_{lm}(\kappa_n, \mathbf{U}_\kappa, \mathbf{U}_{2\kappa}, \mathbf{U}_{3\kappa})\}_{l,m=1}^N \quad (70)$$

with given values of the vectors of the scattered and generated fields  $\mathbf{U}_{n\kappa} = \{U(n\kappa; z_l)\}_{l=1}^N := \{U_l(n\kappa)\}_{l=1}^N$ ,  $n = 1, 2, 3$ . The numbers  $A_m$  are the coefficients determined by the quadrature rule, and the entries  $K_{lm}(\kappa_n, \mathbf{U}_\kappa, \mathbf{U}_{2\kappa}, \mathbf{U}_{3\kappa})$  are calculated by means of (60), where the first argument  $n\kappa$  is replaced by  $\kappa_n$ . The eigen-frequencies  $\kappa_n \in \Omega_{n\kappa} \subset H_{n\kappa}$ ,  $n = 1, 2, 3$ , i.e. the characteristic numbers of the dispersion equations of the problem (69), are obtained by solving the corresponding dispersion equations  $f_{n\kappa}(\kappa_n) := \det(\mathbf{I} - \mathbf{B}_{n\kappa}(\kappa_n)) = 0$  by the help of Newton's method or its modifications. The non-trivial solutions  $\mathbf{U}_{\kappa_n}$  of the homogeneous systems of linear algebraic equations (69) corresponding to these characteristic numbers are the eigen-fields (64) of the linearised non-linear layered structures with an induced dielectric constant (52). Since the solutions  $\mathbf{U}_{\kappa_n}$  are unique up to multiplication by an arbitrary constant, we require  $U(\kappa_n; 2\pi\delta) = a_{\kappa_n} := 1$  (cf. (64)). According to (70), the matrix entries in (69) depend on the dielectric permittivities. The latter are defined by the scattered and generated fields  $\mathbf{U}_\kappa, \mathbf{U}_{2\kappa}, \mathbf{U}_{3\kappa}$  of the problem (49) by means of the algorithm (61). This defines the basic design of the implemented numerical algorithm. The investigation of the eigen-modes of the linearised non-linear structures (69) should always precede the solution of the non-linear scattering and generation problem in the self-consistent formulation (61). Note that, in the analysis of the linear structures, the problem of excitation (scattering) and the spectral problem can be solved independently.

In physical applications, a very useful theorem (see (Sánchez-Palencia, 1980, Thm. 7.2)) asserts the continuous dependence of the operator (68) (or (70)) of the spectral problem on some non-spectral parameter  $\tau$  of the problem under consideration, i.e.  $B_{n\kappa}(\kappa_n, \tau)$  (or  $\mathbf{B}_{n\kappa}(\kappa_n, \tau)$ ). In particular, this theorem implies that the characteristic numbers  $\kappa_n(\tau)$ , i.e. the poles of  $(I - B_{n\kappa}(\kappa_n, \tau))^{-1}$  (or  $(\mathbf{I} - \mathbf{B}_{n\kappa}(\kappa_n, \tau))^{-1}$ ) continuously depend on  $\tau$  and, therefore, they may appear or disappear only at the boundary of any given open, connected region  $D \subset H_{n\kappa}$ ,  $n = 1, 2, 3$ . Further, we interpret  $\kappa_n(\tau) \in \Omega_{n\kappa}(\tau) \subset H_{n\kappa}$  as a branch of the dispersion curves in the eigen-fields  $U(\kappa_n(\tau), z)$  of the problem under investigation. Finally we mention that the classification of scattered, generated or eigen-fields of the dielectric layer by the  $H_{m,l,p}$ -type adopted in our paper is identical to that given in Shestopalov & Sirenko (1989), Shestopalov & Yatsyk (1997), Yatsyk (2000). In the case of E-polarisation, see (12),  $H_{m,l,p}$  (or  $TE_{m,l,p}$ ) denotes the type of polarisation of the wave field under investigation. The subscripts indicate the number of local maxima of  $|E_1|$  (or  $|U|$ , as  $|E_1| = |U|$ , see (23), (64)) along the coordinate axes  $x$ ,  $y$  and  $z$  (see Fig. 1). Since the considered waves are homogeneous along the  $x$ -axis and quasi-homogeneous along the  $y$ -axis, we study actually fields of the type  $H_{0,0,p}$  (or  $TE_{0,0,p}$ ),

where the subscript  $p$  is equal to the number of local maxima of the function  $|U|$  of the argument  $z \in [-2\pi\delta, 2\pi\delta]$ .

### 10. Numerical analysis. Third-harmonic generation by resonant scattering of a wave on a layer with negative and positive values of the cubic susceptibility

Consider the excitation of the non-linear structure by a strong electromagnetic field at the basic frequency only (see (20)), i.e.

$$\{E_1^{\text{inc}}(\kappa; q) \neq 0, E_1^{\text{inc}}(2\kappa; q) = 0, E_1^{\text{inc}}(3\kappa; q) = 0\}, \quad \text{where} \quad \{a_\kappa^{\text{inc}} \neq 0, a_{2\kappa}^{\text{inc}} = a_{3\kappa}^{\text{inc}} = 0\}. \quad (71)$$

In this case, the number of equations in the systems can be reduced. The second equations in all the systems (21), (24) and (49), corresponding to a problem at the double frequency  $2\kappa$  with a trivial right-hand side, can be eliminated by setting  $E_1(\mathbf{r}, 2\kappa) := 0$  (cf. Angermann & Yatsyk (2010), Angermann & Yatsyk (2011)). The dielectric permittivity of the non-linear layer (cf. (19)) in the case (71) simplifies to

$$\begin{aligned} \varepsilon_{n\kappa}(z, \alpha(z), E_1(\mathbf{r}, \kappa), 0, E_1(\mathbf{r}, 3\kappa)) &= \varepsilon_{n\kappa}(z, \alpha(z), U(\kappa; z), U(3\kappa; z)) \\ &=: \varepsilon^{(L)}(z) + \varepsilon_{n\kappa}^{\text{NL}}(\alpha(z), U(\kappa; z), U(3\kappa; z)) \\ &= \varepsilon^{(L)}(z) + \alpha(z) [|U(\kappa; z)|^2 + |U(3\kappa; z)|^2] \\ &\quad + \delta_{n,1} \alpha(z) |U(\kappa; z)| |U(3\kappa; z)| \exp[i\{-3\arg U(\kappa; z) + \arg U(3\kappa; z)\}], \quad n = 1, 3. \end{aligned} \quad (72)$$

The desired solution of the scattering and generation problem (21), (C1) – (C4) (or of the equivalent problems (24) and (49)) can be represented as follows (cf. (23)):

$$\begin{aligned} E_1(n\kappa; y, z) &= U(n\kappa; z) \exp(i\phi_{n\kappa} y) \\ &= \begin{cases} \delta_{n1} a_{n\kappa}^{\text{inc}} \exp(i(\phi_{n\kappa} y - \Gamma_{n\kappa}(z - 2\pi\delta))) + a_{n\kappa}^{\text{scat}} \exp(i(\phi_{n\kappa} y + \Gamma_{n\kappa}(z - 2\pi\delta))), & z > 2\pi\delta, \\ U(n\kappa; z) \exp(i\phi_{n\kappa} y), & |z| \leq 2\pi\delta, \\ b_{n\kappa}^{\text{scat}} \exp(i(\phi_{n\kappa} y - \Gamma_{n\kappa}(z + 2\pi\delta))), & z < -2\pi\delta, \end{cases} \\ &\quad n = 1, 3, \end{aligned} \quad (73)$$

where  $U(\kappa; z)$ ,  $U(3\kappa; z)$ ,  $|z| \leq 2\pi\delta$ , are the solutions of the reduced systems (24) or (49). According to (25) we determine the values of complex amplitudes  $\{a_{n\kappa}^{\text{scat}}, b_{n\kappa}^{\text{scat}} : n = 1, 3\}$  in (73) for the scattered and generated fields by means of the formulas

$$U(n\kappa; 2\pi\delta) = \delta_{n1} a_{n\kappa}^{\text{inc}} + a_{n\kappa}^{\text{scat}}, \quad U(n\kappa; -2\pi\delta) = b_{n\kappa}^{\text{scat}}, \quad n = 1, 3. \quad (74)$$

According to the results of Section 7, the solution of (21), (C1) – (C4) reduces in the case of (71) to the following system (cf. (59)):

$$\begin{cases} (\mathbf{I} - \mathbf{B}_\kappa(\mathbf{U}_\kappa, \mathbf{U}_{3\kappa})) \mathbf{U}_\kappa = \mathbf{U}_\kappa^{\text{inc}}, \\ (\mathbf{I} - \mathbf{B}_{3\kappa}(\mathbf{U}_\kappa, \mathbf{U}_{3\kappa})) \mathbf{U}_{3\kappa} = \mathbf{C}_{3\kappa}(\mathbf{U}_\kappa). \end{cases} \quad (75)$$

The system (75) is written taking into account (71), i.e.  $\mathbf{U}_{2\kappa}^{\text{inc}} = \mathbf{0}$ ,  $\mathbf{U}_{3\kappa}^{\text{inc}} = \mathbf{0}$ ,  $\mathbf{U}_{2\kappa} = \mathbf{0}$ . Here (cf. (59))  $\mathbf{B}_{n\kappa}(\mathbf{U}_\kappa, \mathbf{U}_{3\kappa}) = \mathbf{B}_{n\kappa}(\mathbf{U}_\kappa, \mathbf{0}, \mathbf{U}_{3\kappa})$ ,  $n = 1, 3$ , denote the matrices of the complex-valued non-linear algebraic equations, and  $\mathbf{U}_\kappa^{\text{inc}}$ ,  $\mathbf{C}_{3\kappa}(\mathbf{U}_\kappa) = \mathbf{C}_{3\kappa}(\mathbf{U}_\kappa, \mathbf{0})$ ,  $\mathbf{C}_\kappa(\mathbf{0}, \mathbf{U}_\kappa) = \mathbf{0}$  are the right-hand side vectors. The solution of (75) is obtained by means of successive approximations using the self-consistent approach based on the iterative algorithm (61).

In order to describe the scattering and generation properties of the non-linear structure in the zones of reflection  $z > 2\pi\delta$  and transmission  $z < -2\pi\delta$ , we introduce the following notation:

$$R_{n\kappa} := |a_{n\kappa}^{\text{scat}}|^2 / |a_{n\kappa}^{\text{inc}}|^2 \quad \text{and} \quad T_{n\kappa} := |b_{n\kappa}^{\text{scat}}|^2 / |a_{n\kappa}^{\text{inc}}|^2.$$

The quantities  $R_{n\kappa}$ ,  $T_{n\kappa}$  are called *reflection*, *transmission* or *generation coefficients* of the waves w.r.t. the intensity of the excitation field.

We note that in the considered case of the excitation  $\{a_{n\kappa}^{\text{inc}} \neq 0, a_{2\kappa}^{\text{inc}} = 0, a_{3\kappa}^{\text{inc}} = 0\}$  and for non-absorbing media with  $\Im[\varepsilon^{(L)}(z)] = 0$ , the energy balance equation  $R_{n\kappa} + T_{n\kappa} + R_{3\kappa} + T_{3\kappa} = 1$  is satisfied. This equation represents the law of conservation of energy (Shestopalov & Sirenko (1989), Vainstein (1988)). The quantity  $W_{3\kappa}/W_{n\kappa}$ , which characterises the portion of energy generated in the third harmonic in comparison to the energy scattered in the non-linear layer, is of particular interest. Here by  $W_{n\kappa} = |a_{n\kappa}^{\text{scat}}|^2 + |b_{n\kappa}^{\text{scat}}|^2$  we denote the total energy of the scattered and generated fields at the frequencies  $n\kappa$ ,  $n = 1, 3$ .

The spectral characteristics of the linearised non-linear problems (62), (CS1) – (CS4) with the induced dielectric permittivity (72) at the frequency  $\kappa$  of excitation and the frequency  $3\kappa$  of generation were calculated by means of the algorithm (69). In the graphical illustration of the eigen-fields  $U_{\kappa_n}$  in the representation (64) we have set  $a_{\kappa_n} := 1$  for  $\kappa_n \in \Omega_{n\kappa} \subset H_{n\kappa}$ ,  $n = 1, 3$ .

In what follows we want to discuss some results of the numerical analysis of scattering and generation properties of cubic non-linear polarisable layers with both negative and positive values of the cubic susceptibility of the medium. We consider non-linear dielectric layers (see Fig. 1) with a dielectric permittivity  $\varepsilon_{n\kappa}(z, \alpha(z), U(\kappa; z), U(3\kappa; z)) = \varepsilon^{(L)}(z) + \varepsilon_{n\kappa}^{(NL)}$  of the form (72), where

$$\{\varepsilon^{(L)}(z), \alpha(z)\} = \{\varepsilon^{(L)} = 16, \alpha = \mp 0.01, z \in [-2\pi\delta, 2\pi\delta]\}$$

with the parameter  $\delta := 0.5$ , the excitation frequency  $\kappa^{\text{inc}} := \kappa := 0.375$ , the generation frequency of the third harmonic field  $\kappa^{\text{gen}} := 3\kappa := 1.125$ , and the angle of incidence of the plane wave  $\varphi_{\kappa} \in [0^\circ, 90^\circ]$ .

### 10.1 A non-linear layer with a negative value of the cubic susceptibility of the medium

The results of the numerical analysis of scattering and generation properties as well as the eigen-modes of the dielectric layer with a negative value of the cubic susceptibility of the medium ( $\alpha = -0.01$ ) are presented in Fig. 3 – Fig. 9.

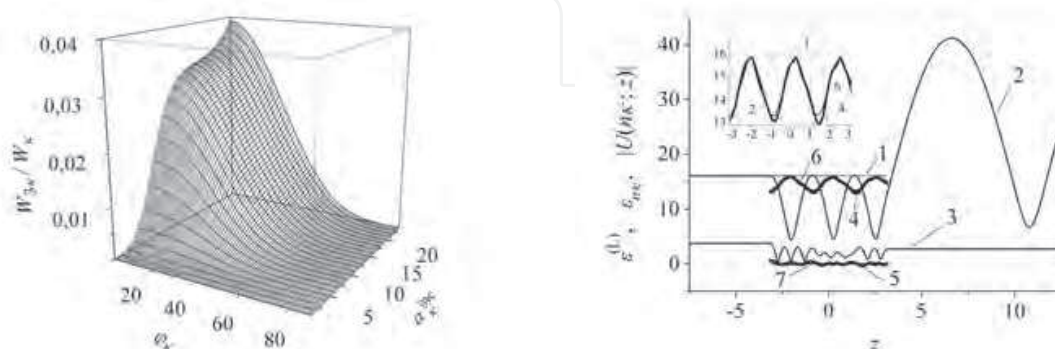


Fig. 3. The portion of energy generated in the third harmonic (left) and some graphs describing the properties of the non-linear layer at  $a_{\kappa}^{\text{inc}} = 24$  and  $\varphi_{\kappa} = 0^\circ$  (right): #1 ...  $\varepsilon^{(L)}$ , #2 ...  $|U(\kappa; z)|$ , #3 ...  $|U(3\kappa; z)|$ , #4 ...  $\Re(\varepsilon_{\kappa})$ , #5 ...  $\Im(\varepsilon_{\kappa})$ , #6 ...  $\Re(\varepsilon_{3\kappa})$ , #7 ...  $\Im(\varepsilon_{3\kappa}) \equiv 0$

Fig. 3 (left) shows the dependence of  $W_{3\kappa}/W_\kappa$  on the angle of incidence  $\varphi_\kappa$  and on the amplitude  $a_\kappa^{\text{inc}}$  of the incident field. It describes the portion of energy generated in the third harmonic by the non-linear layer when a plane wave at the excitation frequency  $\kappa$  and with the amplitude  $a_\kappa^{\text{inc}}$  is passing the layer under the angle of incidence  $\varphi_\kappa$ . In particular,  $W_{3\kappa}/W_\kappa = 0.039$  at  $a_\kappa^{\text{inc}} = 24$  and  $\varphi_\kappa = 0^\circ$ , i.e.  $W_{3\kappa}$  amounts to 3.9% of the total energy  $W_\kappa$  scattered at the frequency of excitation  $\kappa$ . Fig. 3 (right) displays some graphs characterising the scattering and generation properties of the non-linear structure. Graphs #4 and #5 show the real and imaginary parts of the permittivity at the frequency of excitation, while graphs #6 and #7 display the corresponding values at the generation frequency. The figure also shows the absolute values  $|U(\kappa; z)|$  of the amplitudes of the full scattered field  $H_{0,0,4}$  at the frequency of excitation  $\kappa$  (graph #2) and  $|U(3\kappa; z)|$  of the generated field of the  $H_{0,0,9}$ -type at the frequency  $3\kappa$  (graph #3). The values  $|U(\kappa; z)|$  and  $|U(3\kappa; z)|$  are given in the non-linear layered structure ( $|z| \leq 2\pi\delta$ ) and outside it (i.e. in the zones of reflection  $z > 2\pi\delta$  and transmission  $z < -2\pi\delta$ ).

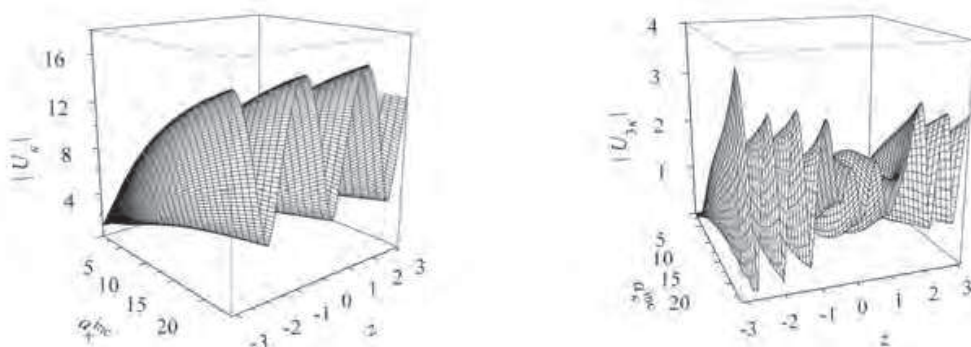


Fig. 4. Graphs of the scattered and generated fields in the non-linear layered structure for  $\varphi_\kappa = 0^\circ$ :  $|U_\kappa[a_\kappa^{\text{inc}}, z]|$  (left),  $|U_{3\kappa}[a_\kappa^{\text{inc}}, z]|$  (right)

Figs. 4 and 5 show the numerical results obtained for the scattered and the generated fields in the non-linear structure and for the non-linear dielectric permittivity of the layered structure in dependence on the amplitude  $a_\kappa^{\text{inc}}$  at normal incidence  $\varphi_\kappa = 0^\circ$  of the plane wave.

Fig. 4 shows the graphs of  $|U_\kappa[a_\kappa^{\text{inc}}, z]|$  and  $|U_{3\kappa}[a_\kappa^{\text{inc}}, z]|$  demonstrating the dynamic behaviour of the scattered and the generated fields  $|U(\kappa; z)|$  and  $|U(3\kappa; z)|$  in the non-linear layered structure in dependence on an increasing amplitude  $a_\kappa^{\text{inc}}$  at normal incidence  $\varphi_\kappa = 0^\circ$  of the plane wave of the frequency  $\kappa$ . We mention that, in the range of amplitudes  $a_\kappa^{\text{inc}} \in (0, 24]$  under consideration, the scattered field is of the type  $H_{0,0,4}$ , see Fig. 4 (left). The generation of the third harmonic field can be observed within the range  $a_\kappa^{\text{inc}} \in [4, 24]$ , see Fig. 4 (right). The generated field has the type  $H_{0,0,10}$  for  $a_\kappa^{\text{inc}} \in [4, 23)$ , and  $H_{0,0,9}$  for  $a_\kappa^{\text{inc}} \in [23, 24]$ . The change of type of the generated field from  $H_{0,0,10}$  to  $H_{0,0,9}$  for an increasing amplitude  $a_\kappa^{\text{inc}}$  is due to the loss of one local maximum of the function  $|U(3\kappa; z)|$ ,  $z \in [-2\pi\delta, 2\pi\delta]$ , at  $a_\kappa^{\text{inc}} = 23$  (see the point with coordinates  $(a_\kappa^{\text{inc}} = 23, z = 1.15, |U_{3\kappa}| = 1.61)$  in Fig. 4 (right)).

The non-linear parts  $\varepsilon_{n\kappa}^{(NL)}$  of the dielectric permittivity at each frequency  $\kappa$  and  $3\kappa$  depend on the values  $U_\kappa := U(\kappa; z)$  and  $U_{3\kappa} := U(3\kappa; z)$  of the fields, see (72). The variation of the non-linear parts  $\varepsilon_{n\kappa}^{(NL)}$  of the dielectric permittivity for an increasing amplitude  $a_\kappa^{\text{inc}}$  of the incident field are illustrated by the behaviour of  $\Re(\varepsilon_\kappa[a_\kappa^{\text{inc}}, z])$  (Fig. 5 (top left)) and  $\Im(\varepsilon_\kappa[a_\kappa^{\text{inc}}, z])$  (Fig. 5 (top right)) at the frequency  $\kappa$ , and by  $\varepsilon_{3\kappa}[a_\kappa^{\text{inc}}, z]$  at the triple frequency  $3\kappa$  (Fig. 5 (bottom left)). In Fig. 5 (top right) the graph of  $\Im(\varepsilon_\kappa[a_\kappa^{\text{inc}}, z])$  for a given amplitude  $a_\kappa^{\text{inc}}$  characterises the loss of energy in the non-linear medium (at the frequency of excitation  $\kappa$ )



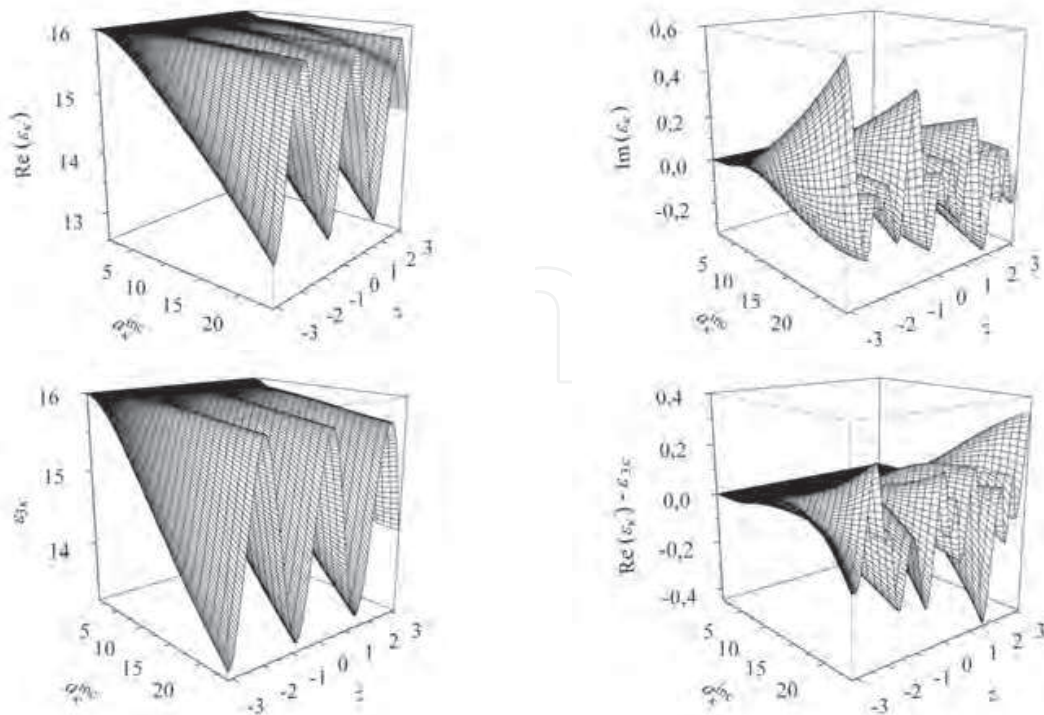


Fig. 5. Graphs characterising the non-linear dielectric permittivity at normal incidence of the plane wave  $\varphi_K = 0^\circ$ :  $\Re(\varepsilon_K [a_K^{\text{inc}}, z])$  (top left),  $\Im(\varepsilon_K [a_K^{\text{inc}}, z])$  (top right),  $\varepsilon_{3K} [a_K^{\text{inc}}, z]$  (bottom left),  $\Re(\varepsilon_K [a_K^{\text{inc}}, z]) - \varepsilon_{3K} [a_K^{\text{inc}}, z]$  (bottom right)

caused by the generation of the electromagnetic field of the third harmonic (at the frequency  $3\kappa$ ). In our case  $\Im[\varepsilon^{(L)}(z)] = 0$  and  $\Im[\alpha(z)] = 0$ , therefore, according to (72),

$$\Im(\varepsilon_K) = \alpha(z)|U(\kappa; z)||U(3\kappa; z)|\Im(\exp[i\{-3\arg U(\kappa; z) + \arg U(3\kappa; z)\}]). \quad (76)$$

From Fig. 5 (top right) we see that a small value of  $a_K^{\text{inc}}$  induces a small amplitude of the function  $\Im(\varepsilon_K)$ , i.e.  $|\Im(\varepsilon_K)| \approx 0$ . The increase of  $a_K^{\text{inc}}$  corresponds to a strong field excitation and leads to the generation of a third harmonic field  $U(3\kappa; z)$ . Fig. 5 (top right) shows the dynamic behaviour of  $\Im(\varepsilon_K)$ . It can be seen that the values of  $\Im(\varepsilon_K)$  may be *positive or negative* along the height of the non-linear layer, i.e. in the interval  $z \in [-2\pi\delta, 2\pi\delta]$ . The zero values of  $\Im(\varepsilon_K)$  are determined by the phase relation between the scattered and the generated fields  $U(\kappa; z)$ ,  $U(3\kappa; z)$  in the non-linear layer, see (76),  $-3\arg U(\kappa; z) + \arg U(3\kappa; z) = p\pi$ ,  $p = 0, \pm 1, \dots$ . We mention that the behaviour of both the quantities  $\Im(\varepsilon_K)$  and

$$\Re(\varepsilon_K) - \varepsilon_{3K} = \alpha(z)|U(\kappa; z)||U(3\kappa; z)|\Re(\exp[i\{-3\arg U(\kappa; z) + \arg U(3\kappa; z)\}])$$

plays an essential role in the process of third harmonic generation because of the presence of the last term in (72). Fig. 5 (bottom right) shows the graph describing the behaviour of  $\Re(\varepsilon_K [a_K^{\text{inc}}, z]) - \varepsilon_{3K} [a_K^{\text{inc}}, z]$ .

The scattering and generation properties of the non-linear structure in the range  $\varphi_K \in [0^\circ, 90^\circ]$ ,  $a_K^{\text{inc}} \in [1, 24]$  of the parameters of the excitation field are presented in Figs. 6 – 7. The graphs show the dynamics of the scattering ( $R_K [\varphi_K, a_K^{\text{inc}}]$ ,  $T_K [\varphi_K, a_K^{\text{inc}}]$ , see Fig. 6 (top)) and generation ( $R_{3K} [\varphi_K, a_K^{\text{inc}}]$ ,  $T_{3K} [\varphi_K, a_K^{\text{inc}}]$ , see Fig. 6 (bottom)) properties of the structure. Fig. 7

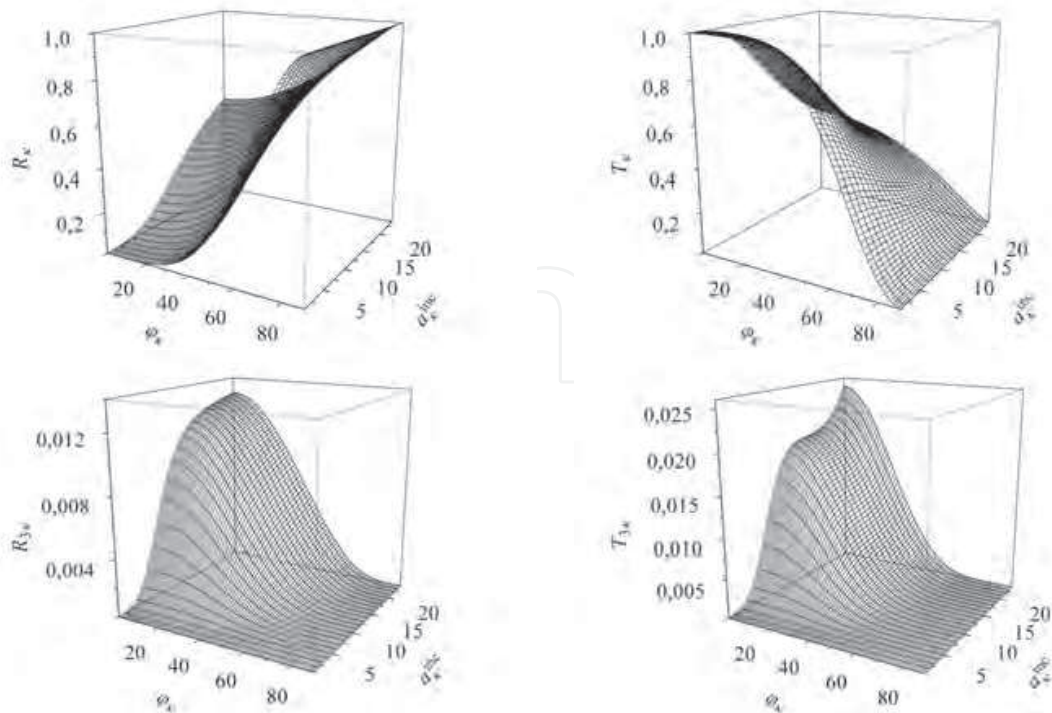


Fig. 6. The scattering and generation properties of the non-linear structure:  $R_{\kappa} [\varphi_{\kappa}, a_{\kappa}^{\text{inc}}]$  (top left),  $T_{\kappa} [\varphi_{\kappa}, a_{\kappa}^{\text{inc}}]$  (top right),  $R_{3\kappa} [\varphi_{\kappa}, a_{\kappa}^{\text{inc}}]$  (bottom left),  $T_{3\kappa} [\varphi_{\kappa}, a_{\kappa}^{\text{inc}}]$  (bottom right)

shows cross sections of the graphs depicted in Figs. 6 and 3 by the planes  $\varphi_{\kappa} = 0^{\circ}$  and  $a_{\kappa}^{\text{inc}} = 20$ .

In the resonant range of wave scattering and generation frequencies, i.e.  $\kappa^{\text{scat}} := \kappa^{\text{inc}} = \kappa$  and  $\kappa^{\text{gen}} = 3\kappa$ , resp., the dynamic behaviour of the characteristic quantities depicted in Figs. 6 – 7 has the following causes. The scattering and generation frequencies are close to the corresponding eigen-frequencies of the linear ( $\alpha = 0$ ) and linearised non-linear ( $\alpha \neq 0$ ) spectral problems (62), (CS1) – (CS4). Furthermore, the distance between the corresponding eigen-frequencies of the spectral problems with  $\alpha = 0$  and  $\alpha \neq 0$  is small. Thus, the graphs in Fig. 7 can be compared with the dynamic behaviour of the branches of the eigen-frequencies of the spectral problems presented in Fig. 8. The graphs of the eigen-fields corresponding to the branches of the considered eigen-frequencies are shown in Fig. 9.

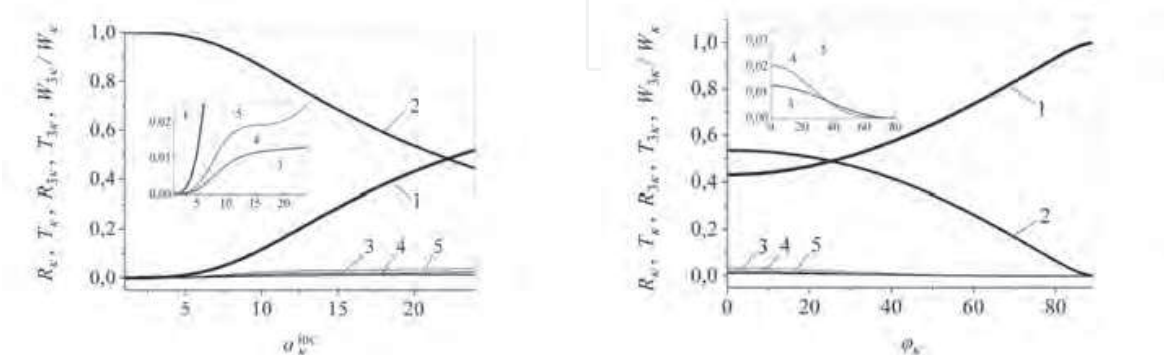


Fig. 7. The curves  $R_{\kappa}$  (#1),  $T_{\kappa}$  (#2),  $R_{3\kappa}$  (#3),  $T_{3\kappa}$  (#4),  $W_{3\kappa}/W_{\kappa}$  (#5) for  $\varphi_{\kappa} = 0^{\circ}$  (left) and  $a_{\kappa}^{\text{inc}} = 20$  (right)



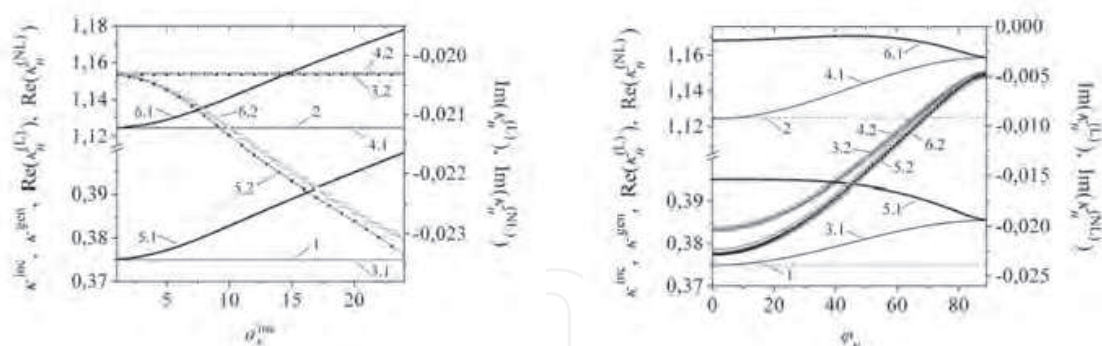


Fig. 8. The curves  $\kappa := \kappa^{\text{inc}} := 0.375$  (#1),  $3\kappa = \kappa^{\text{gen}} = 3\kappa^{\text{inc}} = 1.125$  (#2), the complex eigen-frequencies  $\Re(\kappa_1^{(L)})$  (#3.1),  $\Im(\kappa_1^{(L)})$  (#3.2),  $\Re(\kappa_3^{(L)})$  (#4.1),  $\Im(\kappa_3^{(L)})$  (#4.2) of the linear problem ( $\alpha = 0$ ) and  $\Re(\kappa_1^{(NL)})$  (#5.1),  $\Im(\kappa_1^{(NL)})$  (#5.2),  $\Re(\kappa_3^{(NL)})$  (#6.1),  $\Im(\kappa_3^{(NL)})$  (#6.2) of the linearised non-linear problem ( $\alpha = -0.01$ ) for  $\varphi_\kappa = 0^\circ$  (left) and  $a_\kappa^{\text{inc}} = 20$  (right)

Fig. 8 illustrates the dispersion characteristics of the linear ( $\alpha = 0$ ) and the linearised non-linear ( $\alpha = -0.01$ ) layer  $\varepsilon_{n\kappa} = \varepsilon^{(L)} + \varepsilon_{n\kappa}^{(NL)}$ ,  $n = 1, 3$ , see (72). The non-linear components of the permittivity at the scattering (excitation) frequencies  $\kappa^{\text{scat}} := \kappa^{\text{inc}} = \kappa$  and the generation frequencies  $\kappa^{\text{gen}} := \kappa$  depend on the amplitude  $a_\kappa^{\text{inc}}$  and the angle of incidence  $\varphi_\kappa$  of the incident field. This is reflected in the dynamics of the behaviour of the complex-valued eigen-frequencies of the linear and the linearised non-linear layer. Comparing the results shown in Fig. 8 and Fig. 7, we note the following. The dynamics of the change of the scattering properties  $R_\kappa$ ,  $T_\kappa$  of the non-linear layer (compare the behaviour of curves #1 and #2 in Fig. 7) depends on the magnitude of the distance between the curves #3.1 and #5.1 in Fig. 8. Decanalising properties of the layer occur when  $\alpha < 0$ . A previously transparent (Fig. 7 (left)) or reflective (Fig. 7 (right)) structure loses its properties. It becomes transparent and the reflection and transmission coefficients become comparable. The greater the distance between the curves #4.1 and #6.1 (see Fig. 8), the greater the values of  $R_{3\kappa}$ ,  $T_{3\kappa}$ ,  $W_{3\kappa}/W_\kappa$ , characterising the generating properties of the non-linear layer, see Fig. 7. The magnitudes of the absolute

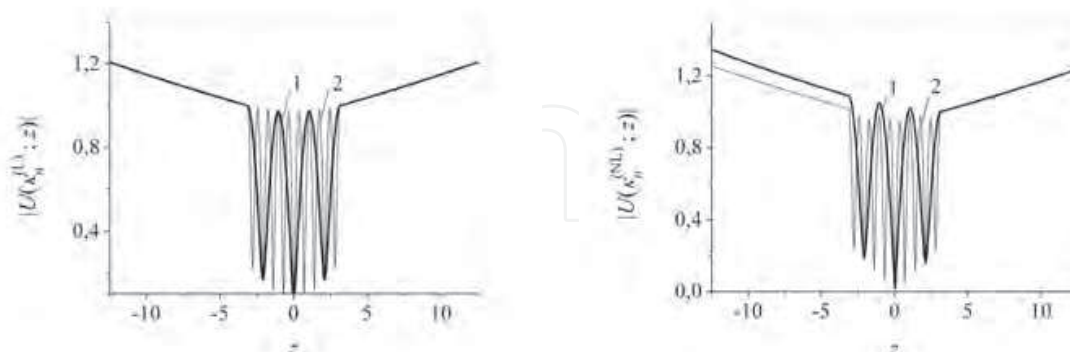


Fig. 9. The graphs of the eigen-fields of the layer for  $\varphi_\kappa = 0^\circ$ ,  $a_\kappa^{\text{inc}} = 20$ . The linear problem ( $\alpha = 0$ , left figure):  $|U(\kappa_1^{(L)}; z)|$  with  $\kappa_1^{(L)} = 0.3749822 - i 0.02032115$  (#1),  $|U(\kappa_3^{(L)}; z)|$  with  $\kappa_3^{(L)} = 1.124512 - i 0.02028934$  (#2), the linearised non-linear problem ( $\alpha = -0.01$ , right figure):  $|U(\kappa_1^{(NL)}; z)|$  with  $\kappa_1^{(NL)} = 0.3949147 - i 0.02278218$  (#1),  $|U(\kappa_3^{(NL)}; z)|$  with  $\kappa_3^{(NL)} = 1.168264 - i 0.02262382$  (#2)

values of the eigen-fields shown in Fig. 9 correspond to the branches of the eigen-frequencies of the linear and the linearised non-linear spectral problems, see Fig. 8. The curves in Fig. 9 are labeled by #1 for an eigen-field of type  $H_{0,0,4}$  and by #2 for an eigen-field of type  $H_{0,0,10}$ . The loss of symmetry in the eigen-fields with respect to the  $z$ -axis in Fig. 9 (right) is due to the violation of the symmetry (w.r.t. the axis  $z = 0$ ) in the induced dielectric permittivity at both the scattering (excitation) and the oscillation frequencies, see Fig. 5.

## 10.2 A non-linear layer with a positive value of the cubic susceptibility of the medium

The results of the numerical analysis of scattering and generation properties as well as the eigen-modes of the dielectric layer with a positive value of the cubic susceptibility of the medium ( $\alpha = +0.01$ ) are presented in Fig. 10 – Fig. 16.

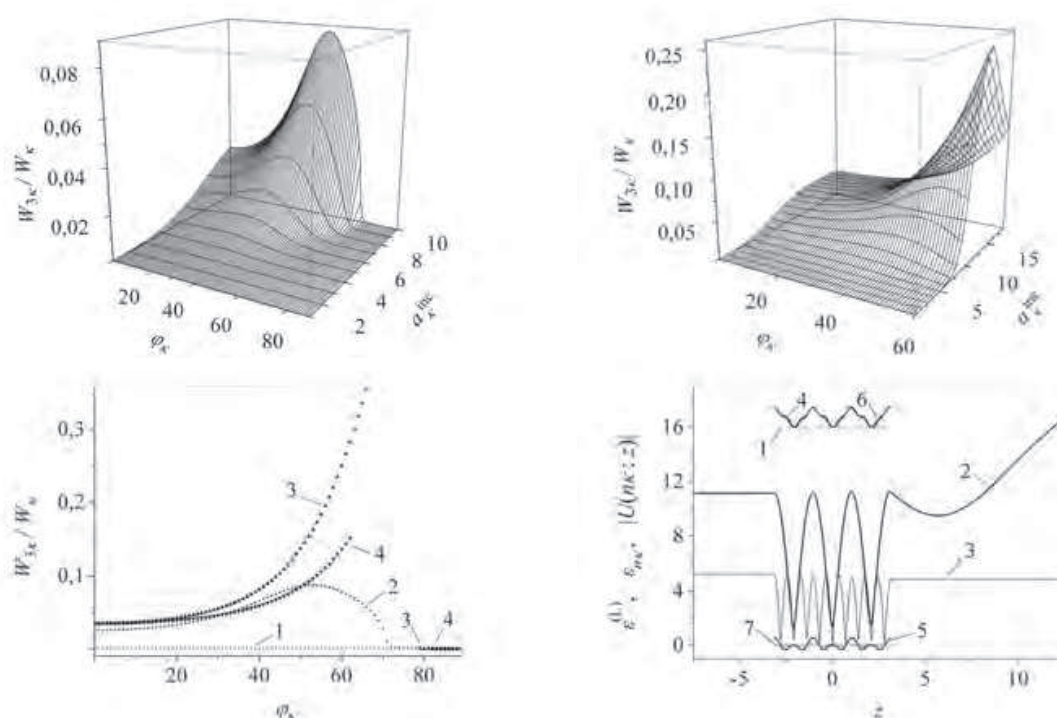


Fig. 10. The portion of energy generated in the third harmonic (top left/right and bottom left): #1 ...  $a_{\kappa}^{\text{inc}} = 1$ , #2 ...  $a_{\kappa}^{\text{inc}} = 9.93$ , #3 ...  $a_{\kappa}^{\text{inc}} = 14$ , #4 ...  $a_{\kappa}^{\text{inc}} = 19$ , and some graphs describing the properties of the non-linear layer for  $a_{\kappa}^{\text{inc}} = 14$  and  $\varphi_{\kappa} = 66^\circ$  (bottom right): #1 ...  $\varepsilon^{(L)}$ , #2 ...  $|U(\kappa; z)|$ , #3 ...  $|U(3\kappa; z)|$ , #4 ...  $\Re(\varepsilon_{\kappa})$ , #5 ...  $\Im(\varepsilon_{\kappa})$ , #6 ...  $\Re(\varepsilon_{3\kappa})$ , #7 ...  $\Im(\varepsilon_{3\kappa}) \equiv 0$

The results shown in Fig. 10 (top left/right and bottom left) allow us to track the dynamic behaviour of the quantity  $W_{3\kappa}/W_{\kappa}$  characterising the ratio of the generated and scattered energies. In particular, the value  $W_{3\kappa}/W_{\kappa} = 0.3558$  for  $a_{\kappa}^{\text{inc}} = 14$  and  $\varphi_{\kappa} = 66^\circ$  (see the graph #3 in Fig. 10 (bottom left)) indicates that  $W_{3\kappa}$  is 35.58% of  $W_{\kappa}$ . This is the maximal value of  $W_{3\kappa}/W_{\kappa}$  that has been achieved. The numerical analysis of the processes displayed by the curves #3 in the range of angles  $\varphi_{\kappa} \in (66^\circ, 79^\circ)$  and #4 in the range of angles  $\varphi_{\kappa} \in (62^\circ, 82^\circ)$  did not lead to the convergence of the computational algorithm. Among the results shown in Fig. 10 (bottom right) we mention that the curve #2 describes the scattered field of type  $H_{0,0,4}$ , and the curve #3 the generated field of type  $H_{0,0,10}$ .

The results of Fig. 11 (left) show that, in the range  $a_K^{\text{inc}} \in (0, 22]$  of the amplitude of the incident field and for an incident angle  $\varphi_K = 60^\circ$  of the plane wave, the scattered field has the type  $H_{0,0,4}$ . The generated field, observed in the range  $a_K^{\text{inc}} \in [5, 22]$ , is of the type  $H_{0,0,10}$ , see Fig. 11 (right). The surfaces presented in Fig. 12 characterise the non-linear dielectric permittivity of the layer (72) induced by the scattered and generated fields shown in Fig. 11. Here, as in Subsection 10.1, the quantity  $\Im(\varepsilon_K)$  takes both positive and negative values along the height of the non-linear layer (i.e. in the interval  $z \in [-2\pi\delta, 2\pi\delta]$ ), see Fig. 12 (top right). For a given amplitude  $a_K^{\text{inc}}$ , the graph of  $\Im(\varepsilon_K[a_K^{\text{inc}}, z])$  characterises the *loss of energy* in the non-linear layer at the excitation frequency caused by the *generation* of the electromagnetic field of the third harmonic.

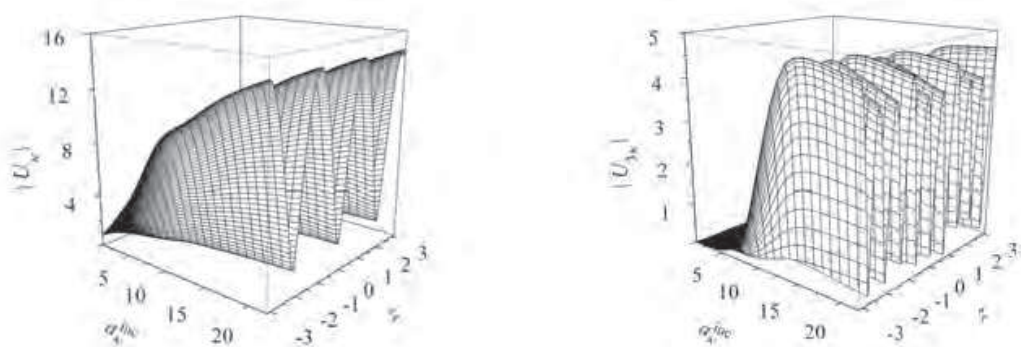


Fig. 11. Graphs of the scattered and generated fields in the non-linear layered structure for  $\varphi_K = 60^\circ$ :  $|U_K[a_K^{\text{inc}}, z]|$  (left),  $|U_{3K}[a_K^{\text{inc}}, z]|$  (right)

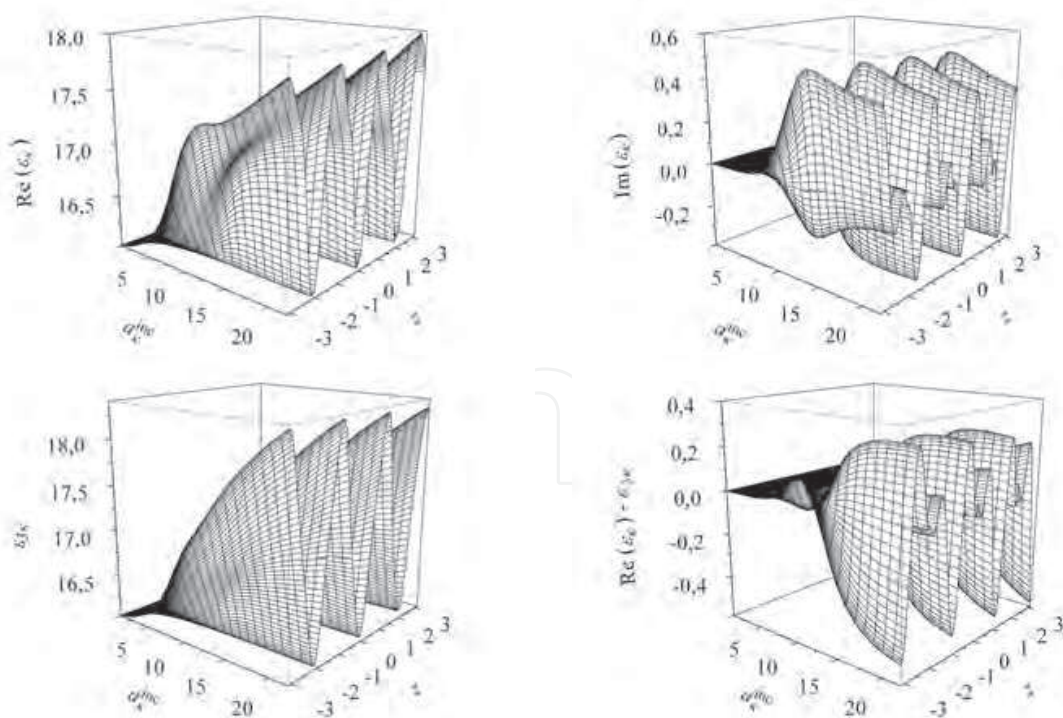


Fig. 12. Graphs characterising the non-linear dielectric permittivity for  $\varphi_K = 60^\circ$ :  $\Re(\varepsilon_K[a_K^{\text{inc}}, z])$  (top left),  $\Im(\varepsilon_K[a_K^{\text{inc}}, z])$  (top right),  $\varepsilon_{3K}[a_K^{\text{inc}}, z]$  (bottom left),  $\Re(\varepsilon_K[a_K^{\text{inc}}, z]) - \varepsilon_{3K}[a_K^{\text{inc}}, z]$  (bottom right)



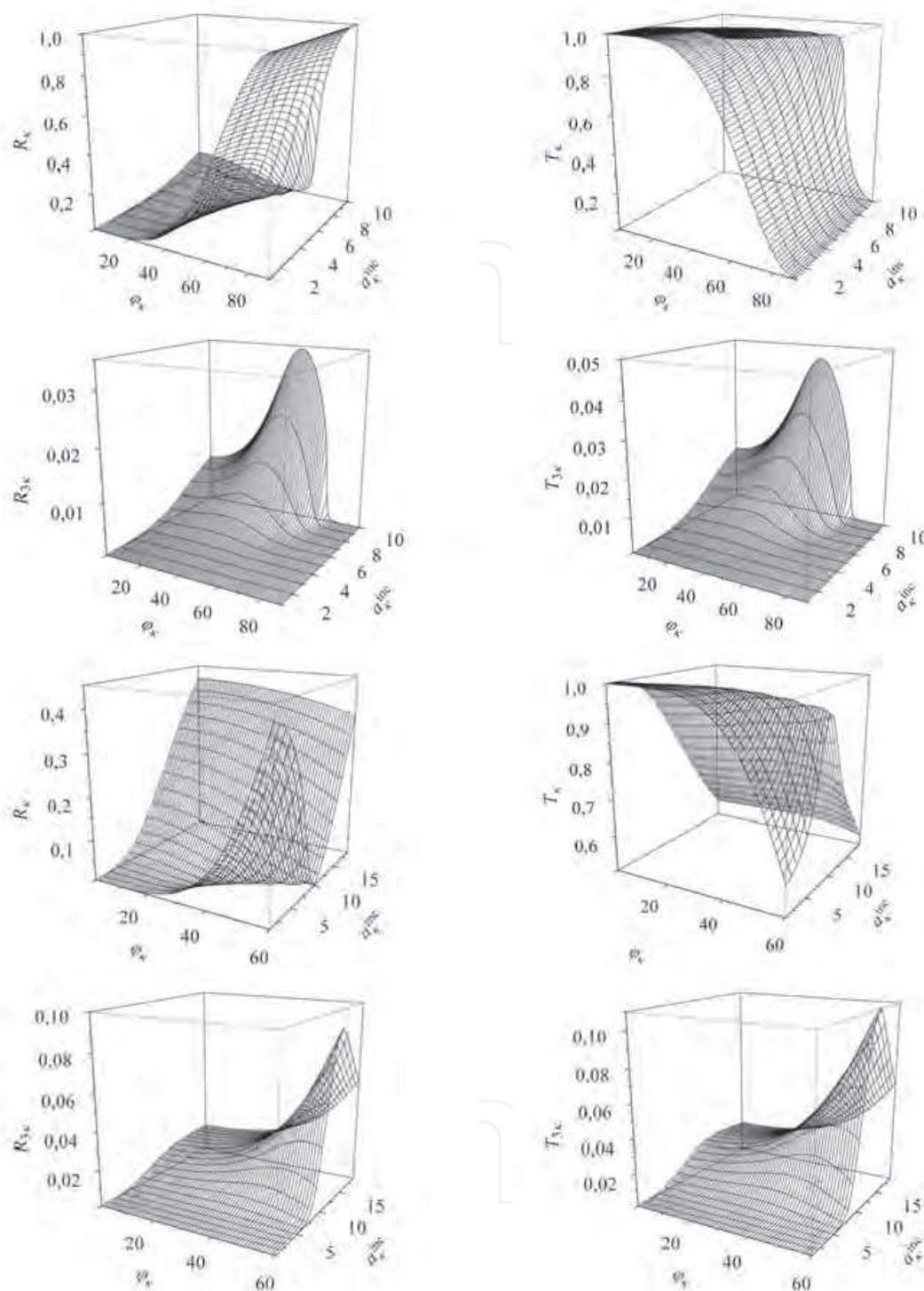


Fig. 13. The scattering and generation properties of the non-linear structure:  $R_K [\varphi_K, a_K^{\text{inc}}]$  (top left, second to the last left),  $T_K [\varphi_K, a_K^{\text{inc}}]$  (top right, second to the last right),  $R_{3K} [\varphi_K, a_K^{\text{inc}}]$  (second from top left, bottom left),  $T_{3K} [\varphi_K, a_K^{\text{inc}}]$  (second from top right, bottom right)

The scattering and generation properties of the non-linear structure in the ranges  $\varphi_K \in [0^\circ, 90^\circ)$ ,  $a_K^{\text{inc}} \in [1, 9.93]$  and  $\varphi_K \in [0^\circ, 60^\circ]$ ,  $a_K^{\text{inc}} \in [1, 19]$  of the parameters of the excitation field are presented in Fig. 13 (top 4) and (last 4), respectively. Fig. 14 shows cross sections of the surfaces depicted in Fig. 13 and of the graph of  $W_{3K}/W_K [\varphi_K, a_K^{\text{inc}}]$  (see Fig. 10 (top)) by

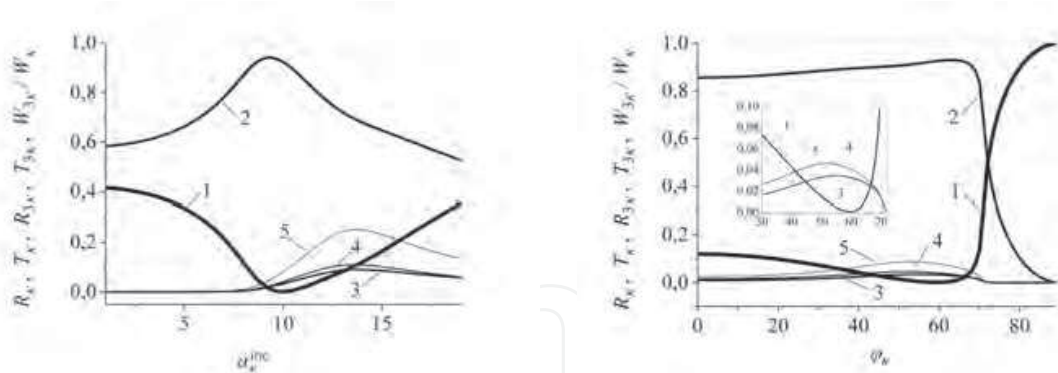


Fig. 14. The curves  $R_\kappa$  (#1),  $T_\kappa$  (#2),  $R_{3\kappa}$  (#3),  $T_{3\kappa}$  (#4),  $W_{3\kappa}/W_\kappa$  (#5) for  $\varphi_\kappa = 60^\circ$  (left) and  $a_\kappa^{\text{inc}} = 9.93$  (right)

the planes  $\varphi_\kappa = 60^\circ$  and  $a_\kappa^{\text{inc}} = 9.93$ . The dynamic behaviour of the characteristic quantities depicted in Figs. 13 and 14 is caused by the fact that the corresponding eigen-frequencies of the problems (62), (CS1) – (CS4) with  $\alpha = 0$  and with  $\alpha \neq 0$  are close together. They also depend on the proximity of the corresponding eigen-frequencies to the scattering (excitation) and generation frequencies  $\kappa^{\text{scat}} := \kappa^{\text{inc}} = \kappa$  and  $\kappa^{\text{gen}} := 3\kappa$  of the waves.

We start the analysis of the results of our calculations with the comparison of the dispersion relations given by the branches of the eigen-frequencies (curves #3.1, #3.2 and #5.1, #5.2) near the scattering frequency (curve #1, corresponding to the excitation frequency) and (curves #4.1, #4.2, #6.1, #6.2) near the oscillation frequency (line #2) in the situations presented in Fig. 8 (where  $\alpha < 0$ ) and Fig. 15 (where  $\alpha > 0$ ). We point out that the situations shown in Fig. 8 and Fig. 15 are fundamentally different. In the case of Fig. 8 ( $\alpha < 0$ ), the graph #5.1 lies above the graph #3.1 and the graph #6.1 above the graph #4.1 in the vicinity of the lines #1 and #2, respectively. This is the typical for the case of decanalisation, see Subsection 10.1.

In the situation of Fig. 15 ( $\alpha > 0$ ) we observe a different behaviour. Here, near the lines #1 and #2, respectively, the graph #5.1 lies below the graph #3.1 and the graph #6.1 below the graph #4.1. That is, canalising properties (properties of transparency) of the non-linear layer occur if  $\alpha > 0$ . This case is characterised by the increase of the angle of transparency of the non-linear structure at the excitation frequency with an increasing amplitude of the incident field (see

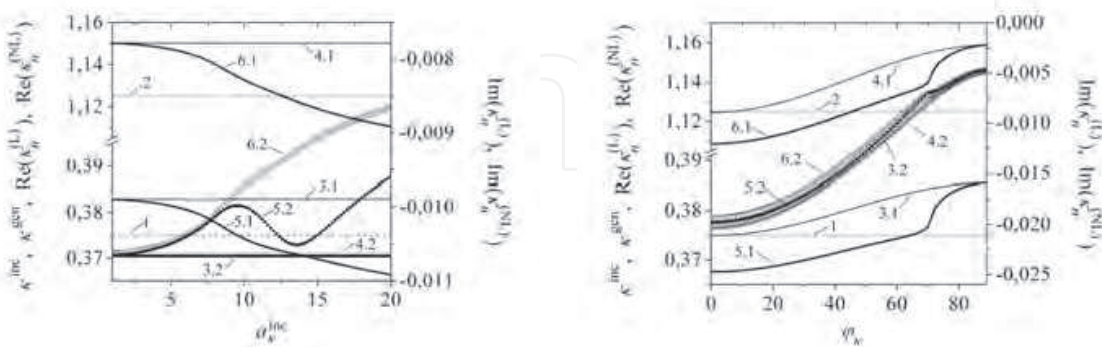


Fig. 15. The curves  $\kappa := \kappa^{\text{inc}} := 0.375$  (#1),  $3\kappa = \kappa^{\text{gen}} = 3\kappa^{\text{inc}} = 1.125$  (#2), the complex eigen-frequencies  $\Re(\kappa_1^{(L)})$  (#3.1),  $\Im(\kappa_1^{(L)})$  (#3.2),  $\Re(\kappa_3^{(L)})$  (#4.1),  $\Im(\kappa_3^{(L)})$  (#4.2) of the linear problem ( $\alpha = 0$ ) and  $\Re(\kappa_1^{(NL)})$  (#5.1),  $\Im(\kappa_1^{(NL)})$  (#5.2),  $\Re(\kappa_3^{(NL)})$  (#6.1),  $\Im(\kappa_3^{(NL)})$  (#6.2) of the linearised non-linear problem ( $\alpha = +0.01$ ) for  $\varphi_\kappa = 60^\circ$  (left) and  $a_\kappa^{\text{inc}} = 9.93$  (right)

Fig. 13 (top left), (second to the last left), there where the reflection coefficient is close to zero). The analysis of the eigen-modes of Fig. 15 ( $\alpha > 0$ ) allows us to explain the mechanisms of the canalisation phenomena (transparency) (see Fig. 13 (top left), (second to the last left), Fig. 14) and wave generation (see Fig. 13 (second from top), (bottom), Fig. 14).

Comparing the results shown in Fig. 14 and Fig. 15 we note the following. The intersection of the curves #1 and #5.1 in Fig. 15 defines certain parameters, in the neighborhood of which the canalisation effect (transparency) of the non-linear structure can be observed in Fig. 14. For example, in Fig. 15 (left) the curves #1 and #5.1 intersect at  $a_k^{\text{inc}} = 9.5$ , also here the curve #5.2 achieves a local maximum. Near this value, we see the phenomenon of canalisation (transparency) of the layer in Fig. 14 (left). If we compare the Figs. 14 (right) and 15 (right), we detect a similar situation. The intersection of the curves #1 and #5.1 defines the parameter  $\varphi_k = 64^\circ$ , near which we observe the canalisation effect in Fig. 15 (right). The same is true – to some extent – for the description of the wave generation processes. For example, for similar values of the imaginary parts of the branches of the eigen-frequencies #5.2 and #6.2 in Fig. 15 (right), the intersection of the curves #2 and #6.1 defines the parameter  $\varphi_k = 45^\circ$ . Near this value, stronger generation properties of the layer can be observed, see Fig. 14 and Fig. 13 (second from top), at  $\varphi_k = 45^\circ$ . Let us also consider the situation in Fig. 15 (left). Here, at the point of intersection of the curves #2 and #6.1, the graph #5.2 starts to decrease monotonically in some interval. The intersection of the curves #2 and #6.1 defines the parameter  $a_k^{\text{inc}} = 12.6$ , which falls into the range  $[9.5, 13.6]$  of values of the amplitudes at which the curve #5.2 is monotonically decreasing. This leads to a shift in the imaginary part of the eigen-frequency of the scattering structure (graph #5.2) with respect to the eigen-frequency of the generating structure (graph #6.2). The magnitude of the shift depends on the distance between the curves of #6.2 and #5.2 at the given value  $a_k^{\text{inc}}$ . The maximal distance between the graphs #6.2 and #5.2 is achieved at the local minimum of the graph #5.2 at  $a_k^{\text{inc}} = 13.6$ . Right from this point, i.e. with an increasing amplitude  $a_k^{\text{inc}}$ , the distance between the graphs #6.2 and #5.2 shows no significant change. The maximum value of the generation is achieved at an amplitude close to the intersection of curves #2 and #6.1, but shifted to the point of the local minimum of the curve #5.2, see  $R_{3k}$ ,  $T_{3k}$ ,  $W_{3k}/W_k$  in Fig. 14 (left), Fig. 13 (bottom) and Fig. 10 (top right).

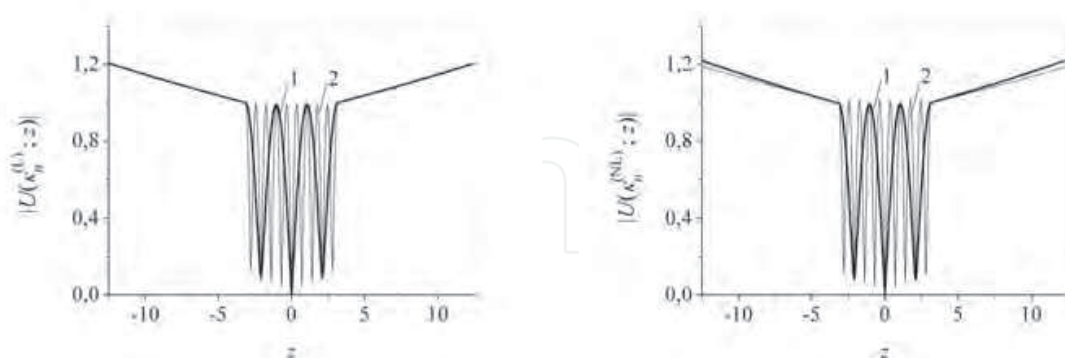


Fig. 16. The graphs of the eigen-fields of the layer for  $\varphi_k = 60^\circ$ ,  $a_k^{\text{inc}} = 14$ . The linear problem ( $\alpha = 0$ , left figure):  $|U(\kappa_1^{(L)}; z)|$  with  $\kappa_1^{(L)} = 0.3829155 - i 0.01066148$  (#1),  $|U(\kappa_3^{(L)}; z)|$  with  $\kappa_3^{(L)} = 1.150293 - i 0.01062912$  (#2), the linearised non-linear problem ( $\alpha = +0.01$ , right figure):  $|U(\kappa_1^{(NL)}; z)|$  with  $\kappa_1^{(NL)} = 0.3705110 - i 0.01049613$  (#1),  $|U(\kappa_3^{(NL)}; z)|$  with  $\kappa_3^{(NL)} = 1.121473 - i 0.009194824$  (#2)



Fig. 16 presents the characteristic distribution of the eigen-fields corresponding to the branches of the eigen-frequencies under consideration. The graphs of the eigen-fields of type  $H_{0,0,4}$  are labeled by #1, the graphs of the eigen-fields of type  $H_{0,0,10}$  by #2.

The numerical results presented in this paper were obtained using an approach based on the description of the wave scattering and generation processes in a non-linear, cubically polarisable layer by a system of non-linear integral equations (49), and of the corresponding spectral problems by the non-trivial solutions of the integral equations (66). We have considered an excitation of the non-linear layer defined by the condition (71). For this case we passed from (49) to (75) and from (66) to (69) by the help of Simpson's quadrature rule. The numerical solution of (75) was obtained using the self-consistent iterative algorithm (61). The problem (69) was solved by means of Newton's method. In the investigated range of parameters, the dimension of the resulting systems of algebraic equations was  $N = 301$ , and the relative error of calculations did not exceed  $\xi = 10^{-7}$ .

## 11. Conclusion

We have investigated the problem of scattering and generation of waves on a non-linear, layered, cubically polarisable structure, which is excited by a packet of waves, in the range of resonant frequencies. The theoretical and numerical results complement the previously presented investigations from Angermann & Yatsyk (2011), Angermann & Yatsyk (2010), Shestopalov & Yatsyk (2010). The mathematical description of the wave scattering and generation processes on a non-linear, layered, cubically polarisable structure reduces to a system of non-linear boundary-value problems. This classical formulation of the problem is equivalent to a system of boundary-value problems of Sturm-Liouville type and to a system of one-dimensional non-linear Fredholm integral equations of the second kind. In this paper, for each of these problems we have obtained sufficient conditions for existence and uniqueness of the solution and we have developed self-consistent algorithms for the numerical analysis. Within the framework of the self-consistent approach we could show that the variation of the imaginary part of the permittivity of the layer at the excitation frequency can take both positive and negative values along the height of the non-linear layer. This effect is caused by the energy consumption in the non-linear medium at the frequency of the incident field which is spent for the generation of the electromagnetic field of the third harmonic. It was shown that layers with negative and positive values of the coefficient of cubic susceptibility of the non-linear medium have fundamentally different scattering and generation properties in the range of resonance. So, for the considered here layer with a negative value of the susceptibility, the maximal portion of the total energy generated in the third harmonic was observed in the direction normal to the structure and amounted to 3.9% of the total dissipated energy. For a layer with a positive value of the susceptibility it was possible to reach such intensities of the excitation field under which the maximum of the relative portion of the total energy was 36% and was observed near the angle of transparency which increasingly deviates from the direction normal to the layer with increasing intensity of the incident field.

The approximate solution of the non-linear problems was obtained by means of solutions of linear problems with an induced non-linear dielectric permeability. The analytical continuation of these linear problems into the region of complex values of the frequency parameter allowed us to switch to the analysis of spectral problems. In the frequency domain, the resonant scattering and generation properties of non-linear structures are determined by the proximity of the excitation frequencies of the non-linear structures to the complex

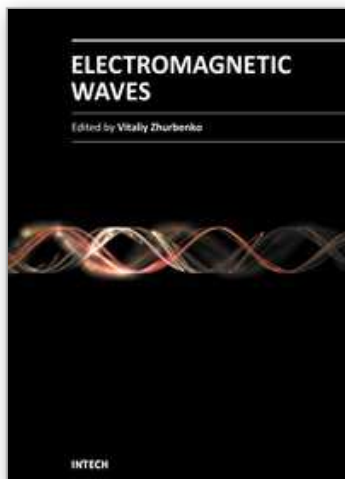
eigen-frequencies of the corresponding homogeneous linear spectral problems with the induced non-linear dielectric permeability of the medium.

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