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Generation and Resonance Scattering of Waves on Cubically Polarisable Layered Structures

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1. Introduction

In this paper, mathematical models for the analysis of processes of generation and resonance scattering of wave packets on a transversely inhomogeneous, isotropic, cubically polarisable, non-magnetic, linearly polarised (*E* polarisation) medium with a non-linear, layered dielectric structure, and methods of their numerical simulation are considered. In general, electromagnetic waves in a non-linear medium with a cubic polarisability can be described by an infinite system of non-linear differential equations. In the study of particular non-linear effects it proves to be possible to restrict the examination to a finite number of equations, and also to leave certain terms in the representation of the polarisation coefficients, which characterise the physical problem under investigation.

Here we investigate the situation where the incident field consists of a packet of three waves oscillating with single, double and triple frequency. An intense field at the basic frequency leads to the generation of the third harmonic, i.e. of a field at the triple frequency. In this case it is possible to reduce the mathematical model to a system of two equations, where only the non-trivial terms in the expansion of the polarisation coefficients are taken into account (see Angermann & Yatsyk (2010)). The consideration of a weak field at the double frequency or at both the double and triple frequencies allows to analyse its influence on the generation process of the third harmonic. In this situation, the mathematical model consists of three differential equations.

The rigorous formulation finally leads to a system of boundary-value problems of Sturm-Liouville type, which can be equivalently transformed into a system of one-dimensional non-linear integral equations (defined along the height of the structure) with respect to the complex Fourier amplitudes of the scattered fields in the non-linear layer at the basic and multiple frequencies. In the paper both the variational approach to the approximate solution of the system of non-linear boundary-value problems of Sturm-Liouville type (based on the application of a finite element method) and an iterative scheme of the solution of the system of non-linear integral equations (based on the application of a quadrature rule to each of the non-linear integral equations) are considered.

The numerical simulation of the generation of the third harmonic and the resonance scattering problem by excitation by a plane wave packet passing a non-linear three-layered structure is described. Results of the numerical experiments for the values of the non-linear dielectric constants depending on the given amplitudes and angles of the incident fields are presented. Also the obtained diffraction characteristics of the scattered and generated fields are discussed. The dependence characterising the portion of generated energy in the third harmonic on the values of the amplitudes of the excitation fields of the non-linear structure and on the angles of incidence is given. Within the framework of the closed system under consideration it is shown that the imaginary part of the dielectric constant, determined by the value of the non-linear part of the polarisation at a frequency of the incident field, characterises the loss of energy in the non-linear medium which is spent for the generation of the third harmonic, where the contributions caused be the influence of the weak electromagnetic fields of diffraction are taken into account.

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

Electrodynamical and optical wave phenomena in charge- and current-free media can be described by the Maxwell equations

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

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 ∇ 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 $^\top$ denotes the transposition. In addition, the system (1) is completed by the material equations

$$\mathbf{D} = \mathbf{E} + 4\pi\mathbf{P}, \qquad \mathbf{B} = \mathbf{H} + 4\pi\mathbf{M}, \tag{2}$$

where $\mathbf{P}$ and $\mathbf{M}$ are the vectors of the polarisation and magnetic moment, respectively. In general, the polarisation vector $\mathbf{P}$ is non-linear with respect to the intensity and non-local both in time and space.

In the present paper, the non-linear medium under consideration is located in the region Ω^{cl}, where Ω^{cl} denotes the closure of the set Ω defined by

$$\Omega := \{\mathbf{r} = (x,y,z)^\top \in \mathbb{R}^3 : |z| < 2\pi\delta\}$$

for some $\delta > 0$ being fixed. That is, the non-linear medium represents an infinite plate of thickness $4\pi\delta$.

As in the book Akhmediev & Ankevich (2003), the investigations will be restricted to non-linear media having a spatially non-local response function, i.e. the spatial dispersion is ignored (cf. Agranovich & Ginzburg (1966)). In this case, the polarisation vector can be expanded in terms of the electric field intensity as follows:

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

where $\boldsymbol{\chi}^{(1)}$, $\boldsymbol{\chi}^{(2)}$, $\boldsymbol{\chi}^{(3)}$ 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

$$\mathbf{P} = \mathbf{P}^{(L)} + \mathbf{P}^{(NL)},$$

where $\mathbf{P}^{(L)} := \boldsymbol{\chi}^{(1)}\mathbf{E}$. Similarly, with $\boldsymbol{\varepsilon} := \mathbf{I} + 4\pi\boldsymbol{\chi}^{(1)}$ and $\mathbf{D}^{(L)} := \boldsymbol{\varepsilon}\mathbf{E}$, where $\mathbf{I}$ denotes the identity in $\mathbb{C}^3$, the displacement field in (2) can be decomposed as

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

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

$$\mathbf{M} = 0, \tag{5}$$

so that

$$\mathbf{B} = \mathbf{H} \tag{6}$$

by (2). Resolving the equations (1), (4) and (6) with respect to $\mathbf{H}$, a single vector-valued equation results:

$$\nabla^2\mathbf{E} - \nabla(\nabla \cdot \mathbf{E}) - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\mathbf{D}^{(L)} - \frac{4\pi}{c^2}\frac{\partial^2}{\partial t^2}\mathbf{P}^{(NL)} = 0. \tag{7}$$

Equation (7) is of rather general character and is used, together with the material equations (4), in electrodynamics and optics. In each particular case, specific assumptions are made that allow to simplify its form. For example, the second term in (7) may be ignored in a number of cases. One such case is the study of isotropic media considered here, where

$$\boldsymbol{\varepsilon} = \varepsilon^{(L)}\mathbf{I}$$

with a scalar, possibly complex-valued function $\varepsilon^{(L)}$. Then

$$\nabla \cdot (\boldsymbol{\varepsilon}\mathbf{E}) = \nabla\varepsilon^{(L)} \cdot \mathbf{E} + \varepsilon^{(L)}\nabla \cdot \mathbf{E}. \tag{8}$$

From (1), (4) and (8) we see that

$$0 = \nabla \cdot \mathbf{D} = \nabla \cdot (\boldsymbol{\varepsilon}\mathbf{E}) + 4\pi\nabla \cdot \mathbf{P}^{(NL)} = \nabla\varepsilon^{(L)} \cdot \mathbf{E} + \varepsilon^{(L)}\nabla \cdot \mathbf{E} + 4\pi\nabla \cdot \mathbf{P}^{(NL)},$$

hence

$$\nabla \cdot \mathbf{E} = -\frac{1}{\varepsilon^{(L)}}\nabla\varepsilon^{(L)} \cdot \mathbf{E} - \frac{4\pi}{\varepsilon^{(L)}}\nabla \cdot \mathbf{P}^{(NL)}. \tag{9}$$

In addition, if the media under consideration are transversely inhomogeneous w.r.t. z, i.e. $\varepsilon^{(L)} = \varepsilon^{(L)}(z)$, 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.

$$\mathbf{E}(\mathbf{r}, t) = (E_1(t; y, z), 0, 0)^\top, \tag{10}$$

then the first term of the r.h.s in (9) vanishes.

For linear media, in particular in $\mathbb{R}^3 \setminus \Omega^{cl}$, the second term of the r.h.s in (9) is not present. In the layer medium the expansion (3) together with (10) implies that the vector $\mathbf{P}^{(NL)}$ has only one non-trivial component which is homogeneous w.r.t. x, i.e. $\mathbf{P}^{(NL)}(\mathbf{r}, t) = (P_1(t; y, z), 0, 0)^\top$.

Then the second term of the r.h.s in (9) vanishes in Ω^{cl}, too. Consequently, the second term in equation (7) disappears completely, and we arrive at

$$\nabla^2 \mathbf{E} - \frac{\varepsilon^{(L)}}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{E} - \frac{4\pi}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{P}^{(NL)} = 0, \tag{11}$$

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

In this paper we consider resonance effects caused by the irradiation of a non-linear dielectric layer by an intense electromagnetic field of the frequency ω, where we also take into consideration the higher-order harmonics of the electromagnetic field. A mathematical model for the case of a weakly non-linear Kerr-type dielectric layer can be found in Yatsyk (2007); Shestopalov & Yatsyk (2007); Kravchenko & Yatsyk (2007).
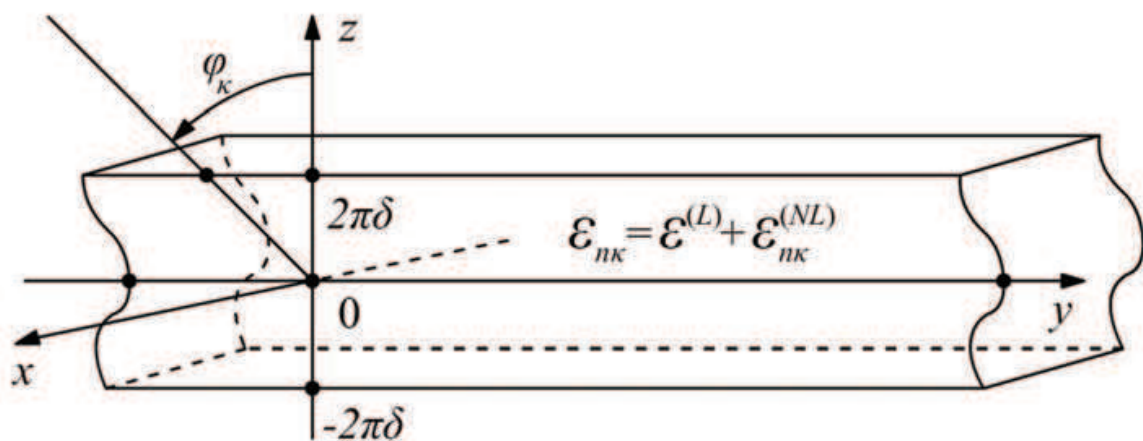

Fig. 1. The non-linear dielectric layered structure

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 direct and inverse Fourier transforms:

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

where $\mathbf{F}$ is one of the vector fields $\mathbf{E}$ or $\mathbf{P}^{(NL)}$.

Applying formally the Fourier transform to equation (11), we obtain the following representation in the frequency domain:

$$\nabla^2 \hat{\mathbf{E}}(\mathbf{r},\hat{\omega}) + \frac{\varepsilon^{(L)}\hat{\omega}^2}{c^2} \hat{\mathbf{E}}(\mathbf{r},\hat{\omega}) + \frac{4\pi\hat{\omega}^2}{c^2} \hat{\mathbf{P}}^{(NL)}(\mathbf{r},\hat{\omega}) = 0. \tag{12}$$

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 Agranovich & Ginzburg (1966), Vinogradova et al. (1990)). Therefore, the quantities describing the

electromagnetic field in the time domain subject to equation (11) can be represented as Fourier series

$$\mathbf{F}(\mathbf{r},t) = \frac{1}{2}\sum_{n\in\mathbb{Z}}\mathbf{F}(\mathbf{r},n\omega)e^{-in\omega t}, \qquad \mathbf{F} \in \{\mathbf{E},\mathbf{P}^{(NL)}\}. \tag{13}$$

Applying to (13) the Fourier transform, we obtain

$$\hat{\mathbf{F}}(\mathbf{r},\hat{\omega}) = \frac{1}{2}\int_{\mathbb{R}}\sum_{n\in\mathbb{Z}}\mathbf{F}(\mathbf{r},n\omega)e^{-in\omega t}e^{i\hat{\omega}t}dt = \frac{\sqrt{2\pi}}{2}\mathbf{F}(\mathbf{r},n\omega)\delta(\hat{\omega},n\omega), \qquad \mathbf{F} \in \{\mathbf{E},\mathbf{P}^{(NL)}\}, \tag{14}$$

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 (14) into (12), we obtain an infinite system of equations with respect to the Fourier amplitudes of the electric field intensities of the non-linear structure in the frequency domain:

$$\nabla^2\mathbf{E}(\mathbf{r},s\omega) + \frac{\varepsilon^{(L)}(s\omega)^2}{c^2}\mathbf{E}(\mathbf{r},s\omega) + \frac{4\pi(s\omega)^2}{c^2}\mathbf{P}^{(NL)}(\mathbf{r},s\omega) = 0, \quad s\in\mathbb{Z}. \tag{15}$$

For linear electrodynamic objects, the equations in system (15) are independent. In a non-linear structure, the presence of the functions $\mathbf{P}^{(NL)}(\mathbf{r},s\omega)$ makes them coupled since every harmonic depends on a series of $\mathbf{E}(\mathbf{r},s\omega)$. Indeed, consider a three-component E-polarised electromagnetic field $\mathbf{E}(\mathbf{r},s\omega) = (E_1(s\omega;y,z),0,0)^\top$, $\mathbf{H}(\mathbf{r},s\omega) = (0;H_2(s\omega;y,z),H_3(s\omega;y,z))^\top$. Since the field $\mathbf{E}$ has only one non-trivial component, the system (15) reduces to a system of scalar equations with respect to E_1:

$$\nabla^2 E_1(\mathbf{r},s\omega) + \frac{\varepsilon^{(L)}(s\omega)^2}{c^2}E_1(\mathbf{r},s\omega) + \frac{4\pi(s\omega)^2}{c^2}P_1^{(NL)}(\mathbf{r},s\omega) = 0, \quad s\in\mathbb{N}. \tag{16}$$

In writing equation (16), the property $E_1(\mathbf{r};j\omega) = E_1^*(\mathbf{r};-j\omega)$ 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)). 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 $\chi^{(3)}$, that is characteristic for a non-linear isotropic medium with cubic polarisability. In the time domain, this component can be represented in the form (cf. (3) and (13)):

$$\begin{aligned}
P_1^{(NL)}(\mathbf{r},t) &= \frac{1}{2}\sum_{s\in\mathbb{Z}\setminus\{0\}}P_1^{(NL)}(\mathbf{r},s\omega)e^{-is\omega t} \doteq \chi_{1111}^{(3)}E_1(\mathbf{r},t)E_1(\mathbf{r},t)E_1(\mathbf{r},t) \\
&\doteq \frac{1}{8}\sum_{\substack{n,m,p,s\in\mathbb{Z}\setminus\{0\} \\ n+m+p=s}}\chi_{1111}^{(3)}(s\omega;n\omega,m\omega,p\omega)E_1(\mathbf{r},n\omega)E_1(\mathbf{r},m\omega)E_1(\mathbf{r},p\omega)e^{-is\omega t},
\end{aligned}$$

$$(17)$$

where the symbol $\doteq$ means that higher-order terms are neglected. Applying to (17) the Fourier transform with respect to time (14) we obtain an expansion in the frequency domain:

$$
\begin{aligned}
P_1^{(NL)}(\mathbf{r}, s\omega) \quad = \quad & \frac{1}{4} \sum_{\substack{n,m,p\in\mathbb{Z}\setminus\{0\} \\ n+m+p=s}} \chi_{1111}^{(3)}(s\omega; n\omega, m\omega, p\omega) E_1(\mathbf{r}, n\omega) E_1(\mathbf{r}, m\omega) E_1(\mathbf{r}, p\omega) \\
= \quad & \frac{1}{4} \sum_{j\in\mathbb{N}} 3\chi_{1111}^{(3)}(s\omega; j\omega, -j\omega, s\omega) |E_1(\mathbf{r}, j\omega)|^2 E_1(\mathbf{r}, s\omega) \\
& + \frac{1}{4} \sum_{\substack{n,m,p\in\mathbb{Z}\setminus\{0\} \\ n\neq-m,\, p=s \\ m\neq-p,\, n=s \\ n\neq-p,\, m=s \\ n+m+p=s}} \chi_{1111}^{(3)}(s\omega; n\omega, m\omega, p\omega) E_1(\mathbf{r}, n\omega) E_1(\mathbf{r}, m\omega) E_1(\mathbf{r}, p\omega).
\end{aligned}
\tag{18}
$$

The addends in the first sum of the last representation of $P_1^{(NL)}(\mathbf{r}, s\omega)$ in (18) are usually called *phase self-modulation (PSM) terms* (cf. Akhmediev & Ankevich (2003)). We denote them by $P_1^{(FSM)}(\mathbf{r}, s\omega)$. Since the terms in formula (18) contain the factor $E_1(\mathbf{r}, s\omega)$, they are responsible for the variation of the dielectric permittivity of the non-linear medium influenced by a variation of the amplitude of the field of excitation. We obtained them taking into account the property of the Fourier coefficients $E_1(\mathbf{r}; j\omega) = E_1^*(\mathbf{r}; -j\omega)$, where the factor 3 appears as a result of permutations $\{j\omega, -j\omega, s\omega\}$ of the three last parameters in the terms

$$
\chi_{1111}^{(3)}(s\omega; j\omega, -j\omega, s\omega).
$$

The addends in the second sum of the last representation of $P_1^{(NL)}(\mathbf{r}, s\omega)$ in (18) are responsible for the generation of the multiple harmonics. Some of them generate radiation at multiple frequencies, others describe the mutual influence of the generated fields at multiple frequencies on the electromagnetic field being investigated. Moreover, those of them which clearly depend at the multiple frequency $s\omega$ on the unknown field of diffraction induce a complex contribution to the dielectric permittivity of the non-linear medium. They are denoted by $P_1^{(GC)}(\mathbf{r}, s\omega)$. The remaining terms of the second sum are denoted by $P_1^{(G)}(\mathbf{r}, s\omega)$. They play the role of the sources generating radiation. In summary, we have the representation

$$
P_1^{(NL)}(\mathbf{r}, s\omega) = P_1^{(FSM)}(\mathbf{r}, s\omega) + P_1^{(GC)}(\mathbf{r}, s\omega) + P_1^{(G)}(\mathbf{r}, s\omega).
\tag{19}
$$

Thus, under the above assumption, the electromagnetic waves in a non-linear medium with a cubic polarisability are described by an infinite system (16)&(18) of 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 $\kappa = \frac{\omega}{c}$.

In the study of particular non-linear effects it proves to be possible to restrict the examination of the system (16)&(18) to a finite number of equations, and also to leave particular terms in the representation of the polarisation coefficients, which characterise the physical problem under investigation. For example, in the analysis of the non-linear effects caused by the generation of harmonics only at three combined frequencies (i.e., neglecting the influence of

higher harmonics), it is possible to restrict the investigation to a system of three equations. Taking into account only the non-trivial terms in the expansion of the polarisation coefficients, we arrive at the following system:

$$
\begin{cases}
\nabla^2 E_1(\mathbf{r},\kappa) + \varepsilon^{(L)}\kappa^2 E_1(\mathbf{r},\kappa) + 4\pi\kappa^2 P_1^{(NL)}(\mathbf{r},\kappa) &= 0, \\
\nabla^2 E_1(\mathbf{r},2\kappa) + \varepsilon^{(L)}(2\kappa)^2 E_1(\mathbf{r},2\kappa) + 4\pi(2\kappa)^2 P_1^{(NL)}(\mathbf{r},2\kappa) &= 0, \\
\nabla^2 E_1(\mathbf{r},3\kappa) + \varepsilon^{(L)}(3\kappa)^2 E_1(\mathbf{r},3\kappa) + 4\pi(3\kappa)^2 P_1^{(NL)}(\mathbf{r},3\kappa) &= 0,
\end{cases}
$$

$$
\begin{aligned}
P_1^{(NL)}(\mathbf{r},n\kappa) =\ & \frac{3}{4}\Big(\chi_{1111}^{(3)}(n\kappa;\kappa,-\kappa,n\kappa)|E_1(\mathbf{r},\kappa)|^2 + \chi_{1111}^{(3)}(n\kappa;2\kappa,-2\kappa,n\kappa)|E_1(\mathbf{r},2\kappa)|^2 \\
& +\chi_{1111}^{(3)}(n\kappa;3\kappa,-3\kappa,n\kappa)|E_1(\mathbf{r},3\kappa)|^2\Big)E_1(\mathbf{r},n\kappa) \\
& +\delta_{n1}\frac{3}{4}\Big\{\chi_{1111}^{(3)}(\kappa;-\kappa,-\kappa,3\kappa)\left[E_1^*(\mathbf{r},\kappa)\right]^2 E_1(\mathbf{r},3\kappa) \\
& \qquad + \chi_{1111}^{(3)}(\kappa;2\kappa,2\kappa,-3\kappa)E_1^2(\mathbf{r},2\kappa)E_1^*(\mathbf{r},3\kappa)\Big\} \\
& +\delta_{n2}\frac{3}{4}\chi_{1111}^{(3)}(2\kappa;-2\kappa,\kappa,3\kappa)E_1^*(\mathbf{r},2\kappa)E_1(\mathbf{r},\kappa)E_1(\mathbf{r},3\kappa) \\
& +\delta_{n3}\Big\{\frac{1}{4}\chi_{1111}^{(3)}(3\kappa;\kappa,\kappa,\kappa)E_1^3(\mathbf{r},\kappa) + \frac{3}{4}\chi_{1111}^{(3)}(3\kappa;2\kappa,2\kappa,-\kappa)E_1^2(\mathbf{r},2\kappa)E_1^*(\mathbf{r},\kappa)\Big\}, \\
& \hspace{8cm} n = 1,2,3,
\end{aligned}
\tag{20}
$$

where δ_{nm} denotes Kronecker's symbol. Using (19), we obtain

$$
\begin{cases}
\nabla^2 E_1(\mathbf{r},\kappa) + \varepsilon^{(L)}\kappa^2 E_1(\mathbf{r},\kappa) + 4\pi\kappa^2\left(P_1^{(FSM)}(\mathbf{r},\kappa) + P_1^{(GC)}(\mathbf{r},\kappa)\right) \\
\hspace{8cm} = -4\pi\kappa^2 P_1^{(G)}(\mathbf{r},\kappa), \\
\nabla^2 E_1(\mathbf{r},2\kappa) + \varepsilon^{(L)}(2\kappa)^2 E_1(\mathbf{r},2\kappa) + 4\pi(2\kappa)^2\left(P_1^{(FSM)}(\mathbf{r},2\kappa) + P_1^{(GC)}(\mathbf{r},2\kappa)\right) = 0, \\
\nabla^2 E_1(\mathbf{r},3\kappa) + \varepsilon^{(L)}(3\kappa)^2 E_1 r(\mathbf{r},3\kappa) + 4\pi(3\kappa)^2 P_1^{(FSM)}(\mathbf{r},3\kappa) \\
\hspace{8cm} = -4\pi(3\kappa)^2 P_1^{(G)}(\mathbf{r},3\kappa),
\end{cases}
$$

$$
\begin{aligned}
P_1^{(FSM)}(\mathbf{r},n\kappa) =\ & \frac{3}{4}(\chi_{1111}^{(3)}(n\kappa;\kappa,-\kappa,n\kappa)|E_1(\mathbf{r},\kappa)|^2 + \chi_{1111}^{(3)}(n\kappa;2\kappa,-2\kappa,n\kappa)|E_1(\mathbf{r},2\kappa)|^2 \\
& +\chi_{1111}^{(3)}(n\kappa;3\kappa,-3\kappa,n\kappa)|E_1(\mathbf{r},3\kappa)|^2)E_1(\mathbf{r},n\kappa), \quad n = 1,2,3, \\
P_1^{(GC)}(\mathbf{r},\kappa) =\ & \frac{3}{4}\chi_{1111}^{(3)}(\kappa;-\kappa,-\kappa,3\kappa)\left[E_1^*(\mathbf{r},\kappa)\right]^2 E_1(\mathbf{r},3\kappa) \\
=\ & \frac{3}{4}\chi_{1111}^{(3)}(\kappa;-\kappa,-\kappa,3\kappa)\frac{\left[E_1^*(\mathbf{r},\kappa)\right]^2}{E_1(\mathbf{r},\kappa)}E_1(\mathbf{r},3\kappa)E_1(\mathbf{r},\kappa), \\
P_1^{(G)}(\mathbf{r},\kappa) =\ & \frac{3}{4}\chi_{1111}^{(3)}(\kappa;2\kappa,2\kappa,-3\kappa)E_1^2(\mathbf{r},2\kappa)E_1^*(\mathbf{r},3\kappa), \\
P_1^{(GC)}(\mathbf{r},2\kappa) =\ & \frac{3}{4}\chi_{1111}^{(3)}(2\kappa;-2\kappa,\kappa,3\kappa)E_1^*(\mathbf{r},2\kappa)E_1(\mathbf{r},\kappa)E_1(\mathbf{r},3\kappa) \\
=\ & \frac{3}{4}\chi_{1111}^{(3)}(2\kappa;-2\kappa,\kappa,3\kappa)\frac{E_1^*(\mathbf{r},2\kappa)}{E_1(\mathbf{r},2\kappa)}E_1(\mathbf{r},\kappa)E_1(\mathbf{r},3\kappa)E_1(\mathbf{r},2\kappa), \\
P_1^{(G)}(\mathbf{r},3\kappa) =\ & \frac{3}{4}\Big\{\frac{1}{3}\chi_{1111}^{(3)}(3\kappa;\kappa,\kappa,\kappa)E_1^3(\mathbf{r},\kappa) + \chi_{1111}^{(3)}(3\kappa;2\kappa,2\kappa,-\kappa)E_1^2(\mathbf{r},2\kappa)E_1^*(\mathbf{r},\kappa)\Big\}.
\end{aligned}
\tag{21}
$$

The analysis of the problem can be significantly simplified by reducing the number of parameters, i.e. the coefficients of the cubic susceptibility of the non-linear medium. Thus,

by Kleinman's rule (Kleinman (1962), Miloslavski (2008)),

$$
\begin{aligned}
\chi^{(3)}_{1111}(n\kappa;\kappa,-\kappa,n\kappa) &= \chi^{(3)}_{1111}(n\kappa;2\kappa,-2\kappa,n\kappa) &= \chi^{(3)}_{1111}(n\kappa;3\kappa,-3\kappa,n\kappa) \\
= \chi^{(3)}_{1111}(\kappa;-\kappa,-\kappa,3\kappa) &= \chi^{(3)}_{1111}(\kappa;2\kappa,2\kappa,-3\kappa) &= \chi^{(3)}_{1111}(2\kappa;-2\kappa,\kappa,3\kappa) \\
= \chi^{(3)}_{1111}(3\kappa;\kappa,\kappa,\kappa) &= \chi^{(3)}_{1111}(3\kappa;2\kappa,2\kappa,-\kappa) &=: \chi^{(3)}_{1111}, \quad n=1,2,3.
\end{aligned}
$$

Therefore, the system (21) can be written in the form

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

$$
\begin{aligned}
P_1^{(FSM)}(\mathbf{r},n\kappa) &= \frac{3}{4}\chi^{(3)}_{1111}\left(|E_1(\mathbf{r},\kappa)|^2 + |E_1(\mathbf{r},2\kappa)|^2 + |E_1(\mathbf{r},3\kappa)|^2\right)E_1(\mathbf{r},n\kappa), \quad n=1,2,3, \\
P_1^{(GC)}(\mathbf{r},\kappa) &= \frac{3}{4}\chi^{(3)}_{1111}\frac{\left[E_1^*(\mathbf{r},\kappa)\right]^2}{E_1(\mathbf{r},\kappa)}E_1(\mathbf{r},3\kappa)E_1(\mathbf{r},\kappa), \\
P_1^{(G)}(\mathbf{r},\kappa) &= \frac{3}{4}\chi^{(3)}_{1111}E_1^2(\mathbf{r},2\kappa)E_1^*(\mathbf{r},3\kappa), \\
P_1^{(GC)}(\mathbf{r},2\kappa) &= \frac{3}{4}\chi^{(3)}_{1111}\frac{E_1^*(\mathbf{r},2\kappa)}{E_1(\mathbf{r},2\kappa)}E_1(\mathbf{r},\kappa)E_1(\mathbf{r},3\kappa)E_1(\mathbf{r},2\kappa), \quad P_1^{(G)}(\mathbf{r},2\kappa) := 0, \\
P_1^{(G)}(\mathbf{r},3\kappa), &= \frac{3}{4}\chi^{(3)}_{1111}\left\{\frac{1}{3}E_1^3(\mathbf{r},\kappa) + E_1^2(\mathbf{r},2\kappa)E_1^*(\mathbf{r},\kappa)\right\}, \quad P_1^{(GC)}(\mathbf{r},3\kappa) := 0.
\end{aligned}
$$

$$(22)$$

The permittivity of the non-linear medium filling a layer (see Fig. 1) can be represented as

$$
\varepsilon_{n\kappa} = \varepsilon^{(L)} + \varepsilon^{(NL)}_{n\kappa} \quad \text{for} \quad |z| \le 2\pi\delta. \tag{23}
$$

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

$$
\varepsilon^{(L)} = \frac{D_1^{(L)}(\mathbf{r},n\kappa)}{E_1(\mathbf{r},n\kappa)} = 1 + 4\pi\chi^{(1)}_{11}, \tag{24}
$$

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 $P_1^{(L)}(\mathbf{r},n\kappa) = \chi^{(1)}_{11} E_1(\mathbf{r},n\kappa)$ are taken into account. Similarly, the third term of each equation of the system makes it possible to write the non-linear component of the permittivity in the form

$$
\begin{aligned}
\varepsilon^{(NL)}_{n\kappa} &= 4\pi\frac{P_1^{(FSM)}(\mathbf{r},n\kappa) + P_1^{(GC)}(\mathbf{r},n\kappa)}{E_1(\mathbf{r},n\kappa)} \\
&= \alpha(z)\Big[|E_1(\mathbf{r},\kappa)|^2 + |E_1(\mathbf{r},2\kappa)|^2 + |E_1(\mathbf{r},3\kappa)|^2 \\
&\quad + \delta_{n1}\frac{\left[E_1^*(\mathbf{r},\kappa)\right]^2}{E_1(\mathbf{r},\kappa)}E_1(\mathbf{r},3\kappa) + \delta_{n2}\frac{E_1^*(\mathbf{r},2\kappa)}{E_1(\mathbf{r},2\kappa)}E_1(\mathbf{r},\kappa)E_1(\mathbf{r},3\kappa)\Big],
\end{aligned} \tag{25}
$$

where $\alpha(z) := 3\pi\chi_{1111}^{(3)}(z)$ is the so-called function of the cubic susceptibility of the non-linear medium.

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 (cf. (24)) is described by a piecewise smooth or a piecewise constant function. Similarly, the function of the cubic susceptibility $\alpha = \alpha(z)$ is also a piecewise smooth or 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.

3. The condition of phase synchronism. Quasi-homogeneous electromagnetic fields in a transversely inhomogeneous non-linear dielectric layered structure.

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

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).

The dielectric permittivities of the layered structure at the multiple frequencies $n\kappa$ are determined by the values of the transverse components of the Fourier amplitudes of the scattered and generated fields, i.e. by the redistribution of energy of the electric fields at multiple frequencies, where the angles of incidence are given and the non-linear structure under consideration is transversely inhomogeneous. The condition of the longitudinal homogeneity (along the coordinate y) of the non-linear dielectric constant of the layered structure can be written as

$$\varepsilon_{n\kappa}^{(NL)}(z, \alpha(z), E_1(\mathbf{r}, \kappa), E_1(\mathbf{r}, 2\kappa), E_1(\mathbf{r}, 3\kappa)) = \varepsilon_{n\kappa}^{(NL)}(z, \alpha(z), U(\kappa; z), U(2\kappa; z), U(3\kappa; z)). \quad (26)$$

Using the representation (25) and the conditions (C1), (26), we obtain the following physically consistent requirement, which we call *the condition of the phase synchronism of waves:*

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

Indeed, from (25) and (C1) it follows that

$$
\begin{aligned}
\varepsilon_{n\kappa}^{(NL)} &= \alpha(z)\Big[|E_1(\mathbf{r}, \kappa)|^2 + |E_1(\mathbf{r}, 2\kappa)|^2 + |E_1(\mathbf{r}, 3\kappa)|^2 \\
&\quad + \delta_{n1}\frac{[E_1^*(\mathbf{r}, \kappa)]^2}{E_1(\mathbf{r}, \kappa)}E_1(\mathbf{r}, 3\kappa) + \delta_{n2}\frac{E_1^*(\mathbf{r}, 2\kappa)}{E_1(\mathbf{r}, 2\kappa)}E_1(\mathbf{r}, \kappa)E_1(\mathbf{r}, 3\kappa)\Big], \\
&= \alpha(z)\Big[|U(\kappa; z)|^2 + |U(2\kappa; z)|^2 + |U(3\kappa; z)|^2 \\
&\quad + \delta_{n1}\frac{[U^*(\mathbf{r}, \kappa)]^2}{U(\mathbf{r}, \kappa)}U(3\kappa; z)\exp\{i[-3\phi_\kappa + \phi_{3\kappa}]y\} \\
&\quad + \delta_{n2}\frac{U^*(\mathbf{r}, 2\kappa)}{U(\mathbf{r}, 2\kappa)}U(\kappa; z)U(3\kappa; z)\exp\{i[-2\phi_{2\kappa} + \phi_\kappa + \phi_{3\kappa}]y\}\Big], \quad n = 1, 2, 3.
\end{aligned}
\quad (27)
$$

Therefore the condition (26) is satisfied if

$$
\begin{cases}
-3\phi_\kappa + \phi_{3\kappa} &= 0, \\
-2\phi_{2\kappa} + \phi_\kappa + \phi_{3\kappa} &= 0.
\end{cases}
\quad (28)
$$

From this system we obtain the condition (C2).

According to (23), (24), (27) and (C2), the permittivity of the non-linear layer can be expressed as

$$
\begin{aligned}
&\varepsilon_{n\kappa}(z,\alpha(z),E_1(\mathbf{r},\kappa),E_1(\mathbf{r},2\kappa),E_1(\mathbf{r},3\kappa))\\
={}&\varepsilon_{n\kappa}(z,\alpha(z),U(\kappa;z),U(2\kappa;z),U(3\kappa;z))\\
={}&\varepsilon^{(L)}(z)+\alpha(z)\big[|U(\kappa;z)|^2+|U(2\kappa;z)|^2+|U(3\kappa;z)|^2\\
&+\delta_{n1}U^*(\kappa;z)\exp\{-2i\arg(U(\kappa;z))\}\,U(3\kappa;z)\\
&+\delta_{n2}\exp\{-2i\arg(U(2\kappa;z))\}\,U(\kappa,z)U(3\kappa;z)\big]\\
={}&\varepsilon^{(L)}(z)+\alpha(z)\big[|U(\kappa;z)|^2+|U(2\kappa;z)|^2+|U(3\kappa;z)|^2\\
&+\delta_{n1}|U(\kappa;z)||U(3\kappa;z)|\exp\{i[-3\arg(U(\kappa;z))-3\phi_\kappa y+\arg(U(3\kappa;z))+\phi_{3\kappa}y]\}\\
&+\delta_{n2}|U(\kappa;z)||U(3\kappa;z)|\exp\{i[-2\arg(U(2\kappa;z))-2\phi_{2\kappa}y+\arg(U(\kappa;z))+\phi_\kappa y\\
&\qquad\qquad\qquad\qquad+\arg(U(3\kappa;z))+\phi_{3\kappa}y]\}\big]\\
={}&\varepsilon^{(L)}(z)+\alpha(z)\big[|U(\kappa;z)|^2+|U(2\kappa;z)|^2+|U(3\kappa;z)|^2\\
&+\delta_{n1}|U(\kappa;z)||U(3\kappa;z)|\exp\{i[-3\arg(U(\kappa;z))+\arg(U(3\kappa;z))]\}\\
&+\delta_{n2}|U(\kappa;z)||U(3\kappa;z)|\exp\{i[-2\arg(U(2\kappa;z))+\arg(U(\kappa;z))+\arg(U(3\kappa;z))]\}\big],\\
&\hspace{9cm} n=1,2,3.
\end{aligned}
\tag{29}
$$

The investigation of the quasi-homogeneous fields $E_1(n\kappa;y,z)$ (cf. condition (C1)) in a transversely inhomogeneous non-linear dielectric layer shows that, if the condition of the phase synchronism (C2) is satisfied, 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 (22)) satisfy the quasi-homogeneity condition, too. Indeed, using (25) and (C1), the right-hand sides of the first and third equations of (22) can be rewritten as

$$
\begin{aligned}
-4\pi\kappa^2 P_1^{(G)}(\mathbf{r},\kappa) &= -\alpha(z)\kappa^2 E_1^2(\mathbf{r},2\kappa)E_1^*(\mathbf{r},3\kappa)\\
&= -\alpha(z)\kappa^2 U^2(2\kappa;z)U^*(3\kappa;z)\exp\{i[2\phi_{2\kappa}-\phi_{3\kappa}]y\}\\
&= -\alpha(z)\kappa^2 U^2(2\kappa;z)U^*(3\kappa;z)\exp(i\phi_\kappa y)
\end{aligned}
$$

and

$$
\begin{aligned}
-4\pi(3\kappa)^2 P_1^{(G)}(\mathbf{r},3\kappa) &= -\alpha(z)(3\kappa)^2\left\{\frac{1}{3}E_1^3(\mathbf{r},\kappa)+E_1^2(\mathbf{r},2\kappa)E_1^*(\mathbf{r},\kappa)\right\}\\
&= -\alpha(z)(3\kappa)^2\left\{\frac{1}{3}U^3(\kappa;z)\exp(3i\phi_\kappa y)\right.\\
&\qquad\qquad\qquad\left.+U^2(2\kappa;z)U^*(\kappa;z)\exp\{i[2\phi_{2\kappa}-\phi_\kappa]y\}\right\}\\
&= -\alpha(z)(3\kappa)^2\left\{\frac{1}{3}U^3(\kappa;z)+U^2(2\kappa;z)U^*(\kappa;z)\right\}\exp(i\phi_{3\kappa}y),
\end{aligned}
$$

respectively. This shows that the quasi-homogeneity condition for the components of the non-linear polarisation $P_1^{(G)}(\mathbf{r},n\kappa)$ is satisfied.

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 κ 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).

4. The diffraction of a packet of plane waves on a non-linear layered dielectric structure. The third harmonics generation

As a first observation 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 (22). 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 Yatsyk (2007); Shestopalov & Yatsyk (2007); Kravchenko & Yatsyk (2007); Angermann & Yatsyk (2008); Yatsyk (2006); Smirnov et al. (2005); Serov et al. (2004).

The generation process of a field at the triple frequency 3κ by the non-linear dielectric structure is caused by a strong incident electromagnetic field at the frequency κ and can be described by the first and third equations of the system (22) only. Since the right-hand side of the second equation in (22) 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 (22) can be completely omitted.

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 κ and, in addition, weak incident quasi-homogeneous electromagnetic fields at the double and triple frequencies 2κ, 3κ (which alone do not generate harmonics at multiple frequencies) excite the non-linear structure. The system (22) 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 κ and of a weak field at the triple frequency 3κ, then we arrive, as in the situation described above, at the system (22) with $E_1(\mathbf{r}, 2\kappa) = 0$, i.e. it is sufficient to consider the first and third equations of (22) only. For wave packets consisting of a strong field at the basic frequency κ and of a weak field at the frequency 2κ, (or of two weak fields at the frequencies 2κ and 3κ) we have to take into account all three equations of system (22). This is caused by the inhomogeneity of the corresponding diffraction problem, where a weak incident field at the double frequency 2κ (or two weak fields at the frequencies 2κ and 3κ) excites (resp. excite) the dielectric medium.

So we consider the problem of diffraction of a packet of plane waves consisting of a strong field at the frequency κ (which generates a field at the triple frequency 3κ) and of weak fields at the frequencies 2κ and 3κ (having an impact on the process of third harmonic generation due to the contribution of weak electromagnetic fields of diffraction)

$$\left\{ E_1^{\text{inc}}(\mathbf{r}, \kappa) := E_1^{\text{inc}}(\kappa; y, z) := a_{n\kappa}^{\text{inc}} \exp\left(i\left(\phi_{n\kappa} y - \Gamma_{n\kappa}(z - 2\pi\delta)\right)\right) \right\}_{n=1}^{3}, \quad z > 2\pi\delta, \quad (30)$$

with amplitudes $a_{n\kappa}^{\text{inc}}$ and angles of incidence $\varphi_{n\kappa}$, $|\varphi| < \pi/2$ (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, the complex amplitudes of the total fields of diffraction

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

of a plane wave (30) in a non-magnetic, isotropic, linearly polarised

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

(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 (see (20)) satisfies the system of equations (cf. (22) – (25))

$$
\begin{cases}
\nabla^2 E_1(\mathbf{r}, \kappa) + \kappa^2 \varepsilon_\kappa(z, \alpha(z), E_1(\mathbf{r}, \kappa), E_1(\mathbf{r}, 2\kappa), E_1(\mathbf{r}, 3\kappa)) E_1(\mathbf{r}, \kappa) \\
\qquad\qquad = -\alpha(z)\kappa^2 E_1^2(\mathbf{r}, 2\kappa) E_1^*(\mathbf{r}, 3\kappa), \\
\nabla^2 E_1(\mathbf{r}, 2\kappa) + (2\kappa)^2 \varepsilon_{2\kappa}(z, \alpha(z), E_1(\mathbf{r}, \kappa), E_1(\mathbf{r}, 2\kappa), E_1(\mathbf{r}, 3\kappa)) E_1(\mathbf{r}, 2\kappa) = 0, \\
\nabla^2 E_1(\mathbf{r}, 3\kappa) + (3\kappa)^2 \varepsilon_{3\kappa}(z, \alpha(z), E_1(\mathbf{r}, \kappa), E_1(\mathbf{r}, 2\kappa), E_1(\mathbf{r}, 3\kappa)) E_1(\mathbf{r}, 3\kappa) \\
\qquad\qquad = -\alpha(z)(3\kappa)^2 \left\{ \frac{1}{3} E_1^3(\mathbf{r}, \kappa) + E_1^2(\mathbf{r}, 2\kappa) E_1^*(\mathbf{r}, \kappa) \right\}
\end{cases}
\tag{31}
$$

together with the following conditions, where $\mathbf{E}_{\mathrm{tg}}(n\kappa; y, z)$ and $\mathbf{H}_{\mathrm{tg}}(n\kappa; y, z)$ 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) $E_1(n\kappa; y, z) = U(n\kappa; z) \exp(i\phi_{n\kappa} y)$, $n = 1, 2, 3$

   (the quasi-homogeneity condition w.r.t. the spatial variable y introduced in Section 3),

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

   (the condition of phase synchronism of waves introduced in Section 3),

– (C3) $\mathbf{E}_{\mathrm{tg}}(n\kappa; y, z)$ and $\mathbf{H}_{\mathrm{tg}}(n\kappa; y, z)$ (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) $E_1^{\mathrm{scat}}(n\kappa; y, z) = \begin{Bmatrix} a_{n\kappa}^{\mathrm{scat}} \\ b_{n\kappa}^{\mathrm{scat}} \end{Bmatrix} \exp\left(i \left(\phi_{n\kappa} y \pm \Gamma_{n\kappa}(z \mp 2\pi\delta) \right) \right),$ $z \gtrless \pm 2\pi\delta$, $n = 1, 2, 3$

   (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 $\mathfrak{Im}\,\Gamma_{n\kappa} = 0$, $\mathfrak{Re}\,\Gamma_{n\kappa} > 0$. Note that (C4) is also applicable for the analysis of the wave-guide properties of the layer, where $\mathfrak{Im}\,\Gamma_{n\kappa} > 0$, $\mathfrak{Re}\,\Gamma_{n\kappa} = 0$.

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 $\exp(-in\omega t)$, where $\omega := \kappa c$ is the dimensionless circular frequency and κ 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 λ, 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 ($\mathfrak{Im}\,c = 0$). ε_0 and μ_0 are the material parameters of the medium. The absolute values of the true variables $\mathbf{r}', t', \omega'$ are given by the formulas $\mathbf{r}' = h\mathbf{r}/4\pi\delta$, $t' = th/4\pi\delta$, $\omega' = \omega 4\pi\delta/h$.

The desired solution of the diffraction problem (31), (C1) – (C4) can be represented as follows:

$$E_1(n\kappa;y,z) = U(n\kappa;z)\exp(i\phi_{n\kappa}y)$$
$$= \begin{cases} a_{n\kappa}^{\text{inc}}\exp(i(\phi_{n\kappa}y - \Gamma_{n\kappa}(z - 2\pi\delta))) + a_{n\kappa}^{\text{scat}}\exp(i(\phi_{n\kappa}y + \Gamma_{n\kappa}(z - 2\pi\delta))), & z > 2\pi\delta, \\ U(n\kappa;z)\exp(i\phi_{n\kappa}y), & |z| \le 2\pi\delta, \\ b_{n\kappa}^{\text{scat}}\exp(i(\phi_{n\kappa}y - \Gamma_{n\kappa}(z + 2\pi\delta))), & z < -2\pi\delta, \end{cases}$$
$$n = 1,2,3.$$
(32)

Note that depending on the magnitudes of the amplitudes $\{a_\kappa^{\text{inc}}, a_{2\kappa}^{\text{inc}}, a_{3\kappa}^{\text{inc}}\}$ of the packet of incident plane waves, the amplitudes $\{a_{n\kappa}^{\text{scat}}, b_{n\kappa}^{\text{scat}}\}_{n=1}^3$ of the scattered fields can be considered as the amplitudes of the diffraction field, of the generation field or of the sum of the diffraction and generation fields. If the components $\{a_\kappa^{\text{inc}} = a_\kappa^{\text{inc(w)}}, a_{2\kappa}^{\text{inc}} = a_{2\kappa}^{\text{inc(w)}}, a_{3\kappa}^{\text{inc}} = a_{3\kappa}^{\text{inc(w)}}\}$ of the packet consist of the amplitudes of weak fields, then $\{a_{n\kappa}^{\text{scat}} = a_{n\kappa}^{\text{dif}}, b_{n\kappa}^{\text{scat}} = b_{n\kappa}^{\text{dif}}\}_{n=1}^3$.
The presence of an amplitude of a strong field at the basic frequency κ in the packet $\{a_\kappa^{\text{inc}} = a_\kappa^{\text{inc(s)}}, a_{2\kappa}^{\text{inc}} = a_{2\kappa}^{\text{inc(w)}}, a_{3\kappa}^{\text{inc}} = a_{3\kappa}^{\text{inc(w)}}\}$ leads to non-trivial right-hand sides in the problem (31), (C1) – (C4). In this case the analysis of the following situations is of interest (see (32)):

$$\left.\begin{cases} a_\kappa^{\text{inc}} = a_\kappa^{\text{inc(s)}} \ne 0, \\ a_{2\kappa}^{\text{inc}} = a_{2\kappa}^{\text{inc(w)}} := 0, \\ a_{3\kappa}^{\text{inc}} = a_{3\kappa}^{\text{inc(w)}} := 0 \end{cases}\right\} \Rightarrow \begin{cases} a_\kappa^{\text{scat}} = a_\kappa^{\text{dif}}, & a_{2\kappa}^{\text{scat}} = 0, & a_{3\kappa}^{\text{scat}} = a_{3\kappa}^{\text{gen}} \\ b_\kappa^{\text{scat}} = b_\kappa^{\text{dif}}, & b_{2\kappa}^{\text{scat}} = 0, & b_{3\kappa}^{\text{scat}} = b_{3\kappa}^{\text{gen}} \end{cases}\right\},$$

$$\left.\begin{cases} a_\kappa^{\text{inc}} = a_\kappa^{\text{inc(s)}} \ne 0, \\ a_{2\kappa}^{\text{inc}} = a_{2\kappa}^{\text{inc(w)}} := 0, \\ a_{3\kappa}^{\text{inc}} = a_{3\kappa}^{\text{inc(w)}} \ne 0 \end{cases}\right\} \Rightarrow \begin{cases} a_\kappa^{\text{scat}} = a_\kappa^{\text{dif}}, & a_{2\kappa}^{\text{scat}} = 0, & a_{3\kappa}^{\text{scat}} = a_{3\kappa}^{\text{dif}} + a_{3\kappa}^{\text{gen}} \\ b_\kappa^{\text{scat}} = b_\kappa^{\text{dif}}, & b_{2\kappa}^{\text{scat}} = 0, & b_{3\kappa}^{\text{scat}} = b_{3\kappa}^{\text{dif}} + b_{3\kappa}^{\text{gen}} \end{cases}\right\},$$

$$\left.\begin{cases} a_\kappa^{\text{inc}} = a_\kappa^{\text{inc(s)}} \ne 0, \\ a_{2\kappa}^{\text{inc}} = a_{2\kappa}^{\text{inc(w)}} \ne 0, \\ a_{3\kappa}^{\text{inc}} = a_{3\kappa}^{\text{inc(w)}} := 0 \end{cases}\right\} \Rightarrow \begin{cases} a_\kappa^{\text{scat}} = a_\kappa^{\text{dif}} + a_\kappa^{\text{gen}}, & a_{2\kappa}^{\text{scat}} = a_{2\kappa}^{\text{dif}}, & a_{3\kappa}^{\text{scat}} = a_{3\kappa}^{\text{gen}} \\ b_\kappa^{\text{scat}} = b_\kappa^{\text{dif}} + b_\kappa^{\text{gen}}, & b_{2\kappa}^{\text{scat}} = b_{2\kappa}^{\text{dif}}, & b_{3\kappa}^{\text{scat}} = b_{3\kappa}^{\text{gen}} \end{cases}\right\},$$

$$\left.\begin{cases} a_\kappa^{\text{inc}} = a_\kappa^{\text{inc(s)}} \ne 0, \\ a_{2\kappa}^{\text{inc}} = a_{2\kappa}^{\text{inc(w)}} \ne 0, \\ a_{3\kappa}^{\text{inc}} = a_{3\kappa}^{\text{inc(w)}} \ne 0 \end{cases}\right\} \Rightarrow \begin{cases} a_\kappa^{\text{scat}} = a_\kappa^{\text{dif}} + a_\kappa^{\text{gen}}, & a_{2\kappa}^{\text{scat}} = a_{2\kappa}^{\text{dif}}, & a_{3\kappa}^{\text{scat}} = a_{3\kappa}^{\text{dif}} + a_{3\kappa}^{\text{gen}} \\ b_\kappa^{\text{scat}} = b_\kappa^{\text{dif}} + b_\kappa^{\text{gen}}, & b_{2\kappa}^{\text{scat}} = b_{2\kappa}^{\text{dif}}, & b_{3\kappa}^{\text{scat}} = b_{3\kappa}^{\text{dif}} + b_{3\kappa}^{\text{gen}} \end{cases}\right\}.$$

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 presentation of the electrical components of the electromagnetic field (32), at the boundary of the non-linear layer we obtain:

$$\begin{aligned} U(n\kappa;2\pi\delta) &= a_{n\kappa}^{\text{scat}} + a_{n\kappa}^{\text{inc}}, & U'(n\kappa;2\pi\delta) &= i\Gamma_{n\kappa}(a_{n\kappa}^{\text{scat}} - a_{n\kappa}^{\text{inc}}), \\ U(n\kappa;-2\pi\delta) &= b_{n\kappa}^{\text{scat}}, & U'(n\kappa;-2\pi\delta) &= -i\Gamma_{n\kappa}b_{n\kappa}^{\text{scat}}, \quad n = 1,2,3, \end{aligned}$$
(33)

where $''''$ denotes the differentiation w.r.t. z. Eliminating in (33) 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 (31), (C1) – (C4):

$$\begin{aligned} i\Gamma_{n\kappa}U(n\kappa;-2\pi\delta) &+ U'(n\kappa;-2\pi\delta) &= 0, \\ i\Gamma_{n\kappa}U(n\kappa;2\pi\delta) &- U'(n\kappa;2\pi\delta) &= 2i\Gamma_{n\kappa}a_{n\kappa}^{\text{inc}}, \quad n = 1,2,3. \end{aligned}$$
(34)

Substituting the representation (32) for the desired solution into the system (31), the resulting system of non-linear ordinary differential equations together with the boundary conditions (34) forms a semi-linear boundary-value problem of Sturm-Liouville type, see also Shestopalov & Yatsyk (2010); Yatsyk (2007); Shestopalov & Yatsyk (2007); Angermann & Yatsyk (2010).

5. The system of non-linear integral equations

Similarly to the results given in Yatsyk (2007); Shestopalov & Yatsyk (2007); Kravchenko & Yatsyk (2007); Angermann & Yatsyk (2010); Shestopalov & Sirenko (1989), the problem (31), (C1) – (C4) reduces to finding solutions of one-dimensional non-linear integral equations (along the height $z \in (-2\pi\delta, 2\pi\delta)$ of the structure) w.r.t. the components $U(n\kappa; z)$, $n = 1, 2, 3$, of the fields scattered and generated in the non-linear layer. We give the derivation of this system of equations in the case of excitation of the non-linear structure by a plane wave packet (30). The solution of (31), (C1) – (C4) in the whole space $Q := \{q = (y,z) \colon |y| < \infty, |z| < \infty\}$ is obtained using the properties of the canonical Green's function of the problem (31), (C1) – (C4) (for the special case $\varepsilon_{n\kappa} \equiv 1$) which is defined, for $Y > 0$, in the strip $Q_{\{Y,\infty\}} := \{q = (y,z) \colon |y| < Y, |z| < \infty\} \subset Q$ by

$$
\begin{aligned}
G_0(n\kappa; q, q_0) \\
:= \quad & \frac{i}{4Y} \exp\left\{i\left[\phi_{n\kappa}(y - y_0) + \Gamma_{n\kappa}|z - z_0|\right]\right\} / \Gamma_{n\kappa} \\
= \quad & \exp\left(\pm i\phi_{n\kappa}y\right) \frac{i\pi}{4Y} \int_{-\infty}^{\infty} H_0^{(1)}\left(n\kappa\sqrt{(\breve{y} - y_0)^2 + (z - z_0)^2}\right) \exp\left(\mp i\phi_{n\kappa}\breve{y}\right) d\breve{y}, \\
& \hspace{9cm} n = 1, 2, 3
\end{aligned}
\tag{35}
$$

(cf. Shestopalov & Sirenko (1989); Sirenko et al. (1985)).

We derive the system of non-linear integral equations by the same classical approach as described in Smirnov (1981) (see also Shestopalov & Yatsyk (2007)). 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 (31), (C1) – (C4), by $E_1\left(n\kappa; q|_{q=(y,z)}\right) = U(n\kappa; z) \exp\left(i\phi_{n\kappa}y\right)$ (cf. (32)), and write the system of equations (31) in the form

$$
\begin{cases}
\left(\nabla^2 + \kappa^2\right) E_1(\kappa; q) &= \left[1 - \varepsilon_\kappa\left(q, \alpha(q), E_1(\kappa; q), E_1(2\kappa; q), E_1(3\kappa; q)\right)\right] \kappa^2 E_1(\kappa; q) \\
& \quad - \alpha(q)\kappa^2 E_1^2(2\kappa; q) E_1^*(3\kappa; q), \\[2mm]
\left(\nabla^2 + (2\kappa)^2\right) E_1(2\kappa; q) &= \left[1 - \varepsilon_{2\kappa}\left(q, \alpha(q), E_1(\kappa; q), E_1(2\kappa; q), E_1(3\kappa; q)\right)\right](2\kappa)^2 E_1(2\kappa; q), \\[2mm]
\left(\nabla^2 + (3\kappa)^2\right) E_1(3\kappa; q) &= \left[1 - \varepsilon_{3\kappa}\left(q, \alpha(q), E_1(\kappa; q), E_1(2\kappa; q), E_1(3\kappa; q)\right)\right](3\kappa)^2 E_1(3\kappa; q) \\
& \quad - \alpha(q)(3\kappa)^2 \left\{\frac{1}{3} E_1^3(\kappa; q) + E_1^2(2\kappa; q) E_1^*(\kappa; q)\right\},
\end{cases}
$$

or, shorter,

$$
\begin{aligned}
\left(\nabla^2 + (n\kappa)^2\right) E_1(n\kappa; q) &= \left[1 - \varepsilon_{n\kappa}\left(q, \alpha(q), E_1(\kappa; q), E_1(2\kappa; q), E_1(3\kappa; q)\right)\right](n\kappa)^2 E_1(n\kappa; q) \\
& \quad - \delta_{n1}\alpha(q)(n\kappa)^2 E_1^2(2\kappa; q) E_1^*(3\kappa; q) \\
& \quad - \delta_{n3}\alpha(q)(n\kappa)^2 \left\{\frac{1}{3} E_1^3(\kappa; q) + E_1^2(2\kappa; q) E_1^*(\kappa; q)\right\}, \quad n = 1, 2, 3.
\end{aligned}
\tag{36}
$$

At the right-hand side of the system of equations (36), 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 $\left\{E_1^{\mathrm{inc}}(n\kappa;q)\right\}_{n=1,2,3}$ satisfying the condition of phase synchronism, where

$$E_1^{\mathrm{inc}}(n\kappa;q) = a_{n\kappa}^{\mathrm{inc}} \exp\left\{i\left[\phi_{n\kappa}y - \Gamma_{n\kappa}(z - 2\pi\delta)\right]\right\}, \quad n = 1,2,3. \tag{37}$$

Furthermore, in the present situation described by the system of equations (36), we assume that the excitation field $E_1^{\mathrm{inc}}(\kappa;q)$ of the non-linear structure at the frequency κ is sufficiently strong (i.e. the amplitude a_κ^{inc} is sufficiently large such that the third harmonic generation is possible), whereas the amplitudes $a_{2\kappa}^{\mathrm{inc}}$, $a_{3\kappa}^{\mathrm{inc}}$ corresponding to excitation fields $E_1^{\mathrm{inc}}(2\kappa;q)$, $E_1^{\mathrm{inc}}(3\kappa;q)$ at the frequencies 2κ, 3κ, respectively, are selected sufficiently weak such that no generation of multiple harmonics occurs.

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

$$\left(\nabla^2 + (n\kappa)^2\right) E_1^{\mathrm{inc}}(n\kappa;q) = 0, \quad q \in Q, \quad n = 1,2,3. \tag{38}$$

For $z > 2\pi\delta$, the incident fields $\left\{E_1^{\mathrm{inc}}(n\kappa;q)\right\}_{n=1,2,3}$ 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 $E_1^{\mathrm{inc}}(n\kappa;q)$, $n = 1,2,3$, the transverse propagation constants $\Gamma_{n\kappa} > 0$, $n = 1,2,3$ are positive).

Subtracting the incident fields $E_1^{\mathrm{inc}}(n\kappa;q)$, from the corresponding total fields $E_1(n\kappa;q)$, cf. (32), we obtain the following equations w.r.t. the scattered fields $E_1(n\kappa;q) - E_1^{\mathrm{inc}}(n\kappa;q) =: E_1^{\mathrm{scat}}(n\kappa;q)$ in the zone of reflection $z > 2\pi\delta$, the fields $E_1(n\kappa;q)$, $|z| \leq 2\pi\delta$, scattered in the layer and the fields $E_1(n\kappa;q) =: E_1^{\mathrm{scat}}(n\kappa;q)$, $z < 2\pi\delta$, passing through the layer:

$$
\begin{aligned}
\left(\nabla^2 + (n\kappa)^2\right)\left[E_1(n\kappa;q)\right. &- & \left. E_1^{\mathrm{inc}}(n\kappa;q)\right] &= 0, \quad z > 2\pi\delta, \\
\left(\nabla^2 + (n\kappa)^2\right) E_1(n\kappa;q) &= & \left[1 - \varepsilon_{n\kappa}\left(q, \alpha(q), E_1(\kappa;q), E_1(2\kappa;q), E_1(3\kappa;q)\right)\right](n\kappa)^2 E_1(n\kappa;q) & \\
& & - \delta_{n1}\alpha(q)(n\kappa)^2 E_1^2(2\kappa;q) E_1^*(3\kappa;q) & \\
& & - \delta_{n3}\alpha(q)(n\kappa)^2 \left\{\tfrac{1}{3}E_1^3(\kappa;q) + E_1^2(2\kappa;q) E_1^*(\kappa;q)\right\}, & |z| \leq 2\pi\delta, \\
\left(\nabla^2 + (n\kappa)^2\right) E_1(n\kappa;q) &= & 0, \quad z < -2\pi\delta, \quad n = 1,2,3. &
\end{aligned}
\tag{39}
$$

Since the canonical Green's functions satisfy the equations

$$\left(\nabla^2 + (n\kappa)^2\right) G_0(n\kappa;q,q_0) = -\delta(q,q_0), \quad n = 1,2,3, \tag{40}$$

where $\delta(q,q_0)$ denotes the Dirac delta-function, it is easy to obtain from the above equations (39), with q replaced by q_0, the following system:

$$
\begin{aligned}
&\left[E_1(n\kappa;q_0) - E_1^{\text{inc}}(n\kappa;q_0)\right]\nabla^2 G_0(n\kappa;q,q_0) - G_0(n\kappa;q,q_0)\nabla^2\left[E_1(n\kappa;q_0) - E_1^{\text{inc}}(n\kappa;q_0)\right] \\
={}& -\left[E_1(n\kappa;q_0) - E_1^{\text{inc}}(n\kappa;q_0)\right]\delta(q,q_0), \quad z > 2\pi\delta, \\[4pt]
&E_1(n\kappa;q_0)\nabla^2 G_0(n\kappa;q,q_0) - G_0(n\kappa;q,q_0)\nabla^2 E_1(n\kappa;q_0) \\
={}& -E_1(n\kappa;q_0)\delta(q,q_0) \\
&- G_0(n\kappa;q,q_0)\left[1 - \varepsilon_{n\kappa}\left(q_0,\alpha(q_0),E_1(\kappa;q_0),E_1(2\kappa;q_0),E_1(3\kappa;q_0)\right)\right](n\kappa)^2 E_1(n\kappa;q_0) \\
&+ \delta_{n1}G_0(n\kappa;q,q_0)\alpha(q)(n\kappa)^2 E_1^2(2\kappa;q)E_1^*(3\kappa;q) \\
&+ \delta_{n3}G_0(n\kappa;q,q_0)\alpha(q)(n\kappa)^2\left\{\tfrac{1}{3}E_1^3(\kappa;q) + E_1^2(2\kappa;q)E_1^*(\kappa;q)\right\}, \quad |z|\leq 2\pi\delta, \\[4pt]
&E_1(n\kappa;q_0)\nabla^2 G_0(n\kappa;q,q_0) - G_0(n\kappa;q,q_0)\nabla^2 E_1(n\kappa;q_0) \\
={}& -E_1(n\kappa;q_0)\delta(q,q_0), \quad z < -2\pi\delta, \quad n = 1,2,3.
\end{aligned}
$$
$$(41)$$

Given $Y > 0$, $Z > 2\pi\delta$, now we consider in the space Q the rectangular domain

$$
Q_{\{Y,Z\}} := \{q = (y,z) : |y| < Y, \ |z| < Z\},
$$

and the subsets

$$
\begin{aligned}
Q_{\{Y,Z\},\,z>2\pi\delta} &:= \{q = (y,z) : |y| < Y, \ 2\pi\delta < z \leq Z\}, \\
Q_{\{Y,Z\},\,|z|\leq 2\pi\delta} &:= \{q = (y,z) : |y| < Y, \ |z| \leq 2\pi\delta\}, \\
Q_{\{Y,Z\},\,z<-2\pi\delta} &:= \{q = (y,z) : |y| < Y, \ -Z \leq z < -2\pi\delta\},
\end{aligned}
$$

and make use of Green's formula.

We also mention that in the case of a non-linear layered structure consisting of a finite number of layers the applicability of Green's formula in the region $Q_{\{Y,Z\},\,|z|\leq 2\pi\delta}$ occupied by the dielectric follows from the continuity condition (C3) w.r.t. $\mathbf{E}_{\text{tg}}(n\kappa;q)$, $\mathbf{H}_{\text{tg}}(n\kappa;q)$ at the boundaries. Indeed, consider a covering of $Q_{\{Y,Z\}}$ by a finite number of disjoint rectangles such that the restrictions of $\varepsilon_{n\kappa}\left(q_0,\alpha(q_0),E_1(\kappa;q_0),E_1(2\kappa;q_0),E_1(3\kappa;q_0)\right)$ to each of these rectangles are smooth functions. At the common interfaces of these regions (i.e. at the boundaries of the separate layers of the structure) due to the continuity of the components $\mathbf{E}_{\text{tg}}(n\kappa;q)$ and $\mathbf{H}_{\text{tg}}(n\kappa;q)$ of the electromagnetic field (cf. (C3)), $E_1(n\kappa;q)$ and $\partial E_1(n\kappa;q)/\partial\mathbf{n}$ are continuous (where $\mathbf{n}$ denotes the outward unit normal w.r.t. each of the regions). Now, by Green's formula and condition (C3) it is easy to obtain the system of non-linear integral equations w.r.t. the unknown solutions $E_1(n\kappa;q)$, $n = 1,2,3$, in the region $Q_{\{Y,Z\},\,|z|\leq 2\pi\delta}$. This system forms an integral representation of the solution in the exterior $Q_{\{Y,Z\}} \setminus Q_{\{Y,Z\},\,|z|\leq 2\pi\delta}$ of the region occupied by the dielectric layer. Consequently, the desired functions $\{E_1(n\kappa;q)\}_{n=1,2,3}$, which are twice continuously differentiable both within (i.e. $Q_{\{Y,Z\},\,|z|\leq 2\pi\delta}$) and outside (i.e. $Q_{\{Y,Z\},\,|z|>2\pi\delta}$) of the region occupied by the dielectric layer, are continuous and have continuous derivatives throughout the whole region $Q_{\{Y,Z\}}$ up to and including the boundary $\partial Q_{\{Y,Z\}}$, i.e. $E_1(n\kappa;q) \in C^2\left(Q_{\{Y,Z\}}\right) \cap C^1\left(\overline{Q_{\{Y,Z\}}}\right)$, $n = 1,2,3$. The system of non-linear integral equations and the corresponding integral representations of the desired solution are obtained by applying, in each of the rectangles $Q_{\{Y,Z\},\,z>2\pi\delta}$, $Q_{\{Y,Z\},\,|z|\leq 2\pi\delta}$, $Q_{\{Y,Z\},\,z<-2\pi\delta}$, Green's formula to the functions $E_1(n\kappa;q_0) - E_1^{\text{inc}}(n\kappa;q_0) =: E_1^{\text{scat}}(n\kappa;q_0)$ for $q_0 \in Q_{\{Y,Z\},\,z>2\pi\delta}$, $E_1(n\kappa;q_0) =: E_1^{\text{scat}}(n\kappa;q_0)$ for $q_0 \in Q_{\{Y,Z\},\,|z|\leq 2\pi\delta}$, $E_1(n\kappa;q_0) =: E_1^{\text{scat}}(n\kappa;q_0)$ for $q_0 \in Q_{\{Y,Z\}}$, $z < -2\pi\delta$, and $G_0(n\kappa;q,q_0)$ for $q,q_0 \in Q_{\{Y,Z\}}$:

$$\iint_{Q_{\{Y,Z\},z>2\pi\delta}} \left(\left[E_1 - E_1^{\text{inc}} \right] \nabla^2 G_0 - G_0 \nabla^2 \left[E_1 - E_1^{\text{inc}} \right] \right) dq_0$$

$$= \int_{Q_{\{Y,Z\},z>2\pi\delta}} \left(\left[E_1 - E_1^{\text{inc}} \right] \frac{\partial G_0}{\partial \mathbf{n}} - G_0 \frac{\partial \left[E_1 - E_1^{\text{inc}} \right]}{\partial \mathbf{n}} \right) dq_0,$$

$$\iint_{Q_{\{Y,Z\},|z|\le 2\pi\delta}} \left(E_1 \nabla^2 G_0 - G_0 \nabla^2 E_1 \right) dq_0 = \int_{Q_{\{Y,Z\},|z|\le 2\pi\delta}} \left(E_1 \frac{\partial G_0}{\partial \mathbf{n}} - G_0 \frac{\partial E_1}{\partial \mathbf{n}} \right) dq_0,$$

$$\iint_{Q_{\{Y,Z\},z<-2\pi\delta}} \left(E_1 \nabla^2 G_0 - G_0 \nabla^2 E_1 \right) dq_0 = \int_{Q_{\{Y,Z\},z<-2\pi\delta}} \left(E_1 \frac{\partial G_0}{\partial \mathbf{n}} - G_0 \frac{\partial E_1}{\partial \mathbf{n}} \right) dq_0, \quad n = 1,2,3.$$

$$(42)$$

Taking into account the relations (41), we get

$$\left\{ \begin{array}{ll} E_1(n\kappa;q) - E_1^{\text{inc}}(n\kappa;q), & q \in Q_{\{Y,Z\},z>2\pi\delta} \\ 0, & q \in Q_{\{Y,Z\}} \setminus \partial Q_{\{Y,Z\},z>2\pi\delta} \end{array} \right\}$$

$$= -\int_{\partial Q_{\{Y,Z\},z>2\pi\delta}} \left(\left[E_1(n\kappa;q_0) - E_1^{\text{inc}}(n\kappa;q_0) \right] \frac{\partial G_0(n\kappa;q,q_0)}{\partial \mathbf{n}} \right.$$
$$\left. - G_0(n\kappa;q,q_0) \frac{\partial \left[E_1(n\kappa;q_0) - E_1^{\text{inc}}(n\kappa;q_0) \right]}{\partial \mathbf{n}} \right) dq_0,$$

$$\left\{ \begin{array}{ll} E_1(n\kappa;q), & q \in Q_{\{Y,Z\},|z|\le 2\pi\delta} \\ 0, & q \in Q_{\{Y,Z\}} \setminus Q_{\{Y,Z\},|z|\le 2\pi\delta} \end{array} \right\}$$

$$= -(n\kappa)^2 \iint_{Q_{\{Y,Z\},|z|\le 2\pi\delta}} G_0(n\kappa;q,q_0) \times$$
$$\times \left[1 - \varepsilon_{n\kappa} \left(q_0, \alpha(q_0), E_1(\kappa;q_0), E_1(2\kappa;q_0), E_1(3\kappa;q_0) \right) \right] E_1(n\kappa;q_0) dq_0$$
$$+ \delta_{n1}(n\kappa)^2 \iint_{Q_{\{Y,Z\},|z|\le 2\pi\delta}} G_0(n\kappa;q,q_0) \alpha(q_0) E_1^2(2\kappa;q_0) E_1^*(3\kappa;q_0) dq_0$$
$$+ \delta_{n3}(n\kappa)^2 \iint_{Q_{\{Y,Z\},|z|\le 2\pi\delta}} G_0(n\kappa;q,q_0) \alpha(q_0) \left\{ \frac{1}{3} E_1^3(\kappa;q_0) + E_1^2(2\kappa;q_0) E_1^*(\kappa;q_0) \right\} dq_0$$
$$- \int_{\partial Q_{\{Y,Z\},|z|\le 2\pi\delta}} \left(E_1(n\kappa;q_0) \frac{\partial G_0(n\kappa;q,q_0)}{\partial \mathbf{n}} - G_0(n\kappa;q,q_0) \frac{\partial E_1(n\kappa;q_0)}{\partial \mathbf{n}} \right) dq_0,$$

$$\left\{ \begin{array}{ll} E_1(n\kappa;q), & q \in Q_{\{Y,Z\},z<-2\pi\delta} \\ 0, & q \in Q_{\{Y,Z\}} Q_{\{Y,Z\},z<-2\pi\delta} \end{array} \right\}$$

$$= -\int_{\partial Q_{\{Y,Z\},z<-2\pi\delta}} \left(E_1(n\kappa;q_0) \frac{\partial G_0(n\kappa;q,q_0)}{\partial \mathbf{n}} - G_0(n\kappa;q,q_0) \frac{\partial E_1(n\kappa;q_0)}{\partial \mathbf{n}} \right) dq_0, \quad n = 1,2,3.$$

$$(43)$$

Suppose $q \in Q_{\{Y,Z\},|z|\le 2\pi\delta}$, i.e. it lies in a rectangle containing the non-linear structure. Then the equations of (43) take the form

$$
\begin{aligned}
0 &= -\int_{\partial Q_{\{Y,Z\},\,z>2\pi\delta}} \left(\left[E_1(n\kappa;q_0) - E_1^{\mathrm{inc}}(n\kappa;q_0) \right] \frac{\partial G_0(n\kappa;q,q_0)}{\partial \mathbf{n}} \right.\\
&\qquad\qquad\qquad \left. - G_0(n\kappa;q,q_0) \frac{\partial \left[E_1(n\kappa;q_0) - E_1^{\mathrm{inc}}(n\kappa;q_0) \right]}{\partial \mathbf{n}} \right) dq_0,\\[6pt]
E_1(n\kappa;q) &= -(n\kappa)^2 \iint_{Q_{\{Y,Z\},\,|z|\le 2\pi\delta}} G_0(n\kappa;q,q_0) \times\\
&\qquad \times \left[1 - \varepsilon_{n\kappa}\left(q_0,\alpha(q_0),E_1(\kappa;q_0),E_1(2\kappa;q_0),E_1(3\kappa;q_0)\right) \right] E_1(n\kappa;q_0)dq_0\\[4pt]
&\quad + \delta_{n1}(n\kappa)^2 \iint_{Q_{\{Y,Z\},\,|z|\le 2\pi\delta}} G_0(n\kappa;q,q_0)\alpha(q_0)E_1^2(2\kappa;q_0)E_1^*(3\kappa;q_0)dq_0\\[4pt]
&\quad + \delta_{n3}(n\kappa)^2 \iint_{Q_{\{Y,Z\},\,|z|\le 2\pi\delta}} G_0(n\kappa;q,q_0)\alpha(q_0) \times\\
&\qquad\qquad \times \left\{ \frac{1}{3}E_1^3(\kappa;q_0) + E_1^2(2\kappa;q_0)E_1^*(\kappa;q_0) \right\} dq_0\\[4pt]
&\quad - \int_{\partial Q_{\{Y,Z\},\,|z|\le 2\pi\delta}} \left(E_1(n\kappa;q_0) \frac{\partial G_0(n\kappa;q,q_0)}{\partial \mathbf{n}} - G_0(n\kappa;q,q_0)\frac{\partial E_1(n\kappa;q_0)}{\partial \mathbf{n}} \right) dq_0,\\[6pt]
0 &= -\int_{\partial Q_{\{Y,Z\},\,z<-2\pi\delta}} \left(E_1(n\kappa;q_0) \frac{\partial G_0(n\kappa;q,q_0)}{\partial \mathbf{n}} - G_0(n\kappa;q,q_0)\frac{\partial E_1(n\kappa;q_0)}{\partial \mathbf{n}} \right) dq_0,
\end{aligned}
$$

$$ n = 1,2,3. \tag{44} $$

If the parameter Z increases to infinity, $Z \to \infty$, the line integrals appearing in the first and third equations of (44) along the lower $[(-Z,-Y),(-Z,Y)]$ and upper $[(Z,Y),(Z,-Y)]$ parts of the boundary $\partial Q_{\{Y,Z\}}$ tend to zero for all $n = 1,2,3$. This is a consequence of the fact that, for all frequencies $n\kappa$, $n = 1,2,3$, the reflected field $E_1(n\kappa;q) - E_1^{\mathrm{inc}}(n\kappa;q) =: E_1^{\mathrm{scat}}(n\kappa;q)$, given by the first equation of (44), and the field $E_1(n\kappa;q) =: E_1^{\mathrm{scat}}(n\kappa;q)$, passing through the layer and described by the third equation of (44), satisfy the radiation condition (C4), and of the asymptotic properties of the canonical Green's function (35). The line integrals along the left $[(-Z,Y),(Z,Y)]$ and right $[(Z,-Y),(-Z,-Y)]$ sides of the boundary $\partial Q_{\{Y,Z\}}$ cancel out each other in all equations of the system (44).

Next we consider the components of the total fields $E_1(n\kappa;q)$ (i.e. $\mathbf{E}_{\mathrm{tg}}(n\kappa;q)$ and $\frac{\partial E_1(n\kappa;q)}{\partial \mathbf{n}}$) (i.e. $\mathbf{H}_{\mathrm{tg}}(n\kappa;q)$) at the common boundaries of neighbouring rectangles. At the upper $z = 2\pi\delta$ and lower $z = -2\pi\delta$ boundaries of the non-linear medium, they are continuous, cf. the interface condition (C3). The orientations of the outer normals in the line integrals of the system (44) (for the first and second equations, and for the second and third equations, for each $n = 1,2,3$) at these common boundaries are opposite. Adding all equations of the system (44), we obtain

$$
\begin{aligned}
& E_1(n\kappa;q) \\
&= -(n\kappa)^2 \iint_{Q_{\{Y,Z\}, |z|\leq 2\pi\delta}} G_0(n\kappa;q,q_0) \times \\
& \qquad \times [1 - \varepsilon_{n\kappa}(q_0, \alpha(q_0), E_1(\kappa;q_0), E_1(2\kappa;q_0), E_1(3\kappa;q_0))] E_1(n\kappa;q_0) dq_0 \\
& + \delta_{n1}(n\kappa)^2 \iint_{Q_{\{Y,Z\}, |z|\leq 2\pi\delta}} G_0(n\kappa;q,q_0)\alpha(q_0)E_1^2(2\kappa;q_0)E_1^*(3\kappa;q_0) dq_0 \\
& + \delta_{n3}(n\kappa)^2 \iint_{Q_{\{Y,Z\}, |z|\leq 2\pi\delta}} G_0(n\kappa;q,q_0)\alpha(q_0)\left\{\frac{1}{3}E_1^3(\kappa;q_0) + E_1^2(2\kappa;q_0)E_1^*(\kappa;q_0)\right\} dq_0 \\
& + \int_{\underline{\partial Q_{\{Y,Z=\infty\}, z>2\pi\delta}}} \left(E_1(n\kappa;q_0)\frac{\partial G_0(n\kappa;q,q_0)}{\partial\mathbf{n}} - G_0(n\kappa;q,q_0)\frac{\partial E_1(n\kappa;q_0)}{\partial\mathbf{n}}\right) dq_0, \\
& \hspace{6cm} q \in Q_{\{Y,Z\}, |z|\leq 2\pi\delta}, \quad n = 1,2,3.
\end{aligned}
\tag{45}
$$

In the line integrals of equation (45), at each of the frequencies $n\kappa$, $n = 1,2,3$, the integration runs along the lower boundary $\underline{\partial Q_{\{Y,Z=\infty\}, z>2\pi\delta}}$ of the half-space $Q_{\{Y,Z=\infty\}, z>2\pi\delta}$, where the normal vector $\mathbf{n}$ points into the non-linear layer. Changing the orientation of the normal vector (which is equivalent to changing the sign of the integral) and considering the line integrals as integrals along the upper boundary $\overline{\partial Q_{\{Y,Z\}, z\leq 2\pi\delta}}$ of the region $Q_{\{Y,Z\}, z\leq 2\pi\delta}$, we get

$$
\begin{aligned}
& E_1(n\kappa;q) \\
&= -(n\kappa)^2 \iint_{Q_{\{Y,Z\}, |z|\leq 2\pi\delta}} G_0(n\kappa;q,q_0) \times \\
& \qquad \times [1 - \varepsilon_{n\kappa}(q_0, \alpha(q_0), E_1(\kappa;q_0), E_1(2\kappa;q_0), E_1(3\kappa;q_0))] E_1(n\kappa;q_0) dq_0 \\
& + \delta_{n1}(n\kappa)^2 \iint_{Q_{\{Y,Z\}, |z|\leq 2\pi\delta}} G_0(n\kappa;q,q_0)\alpha(q_0)E_1^2(2\kappa;q_0)E_1^*(3\kappa;q_0) dq_0 \\
& + \delta_{n3}(n\kappa)^2 \iint_{Q_{\{Y,Z\}, |z|\leq 2\pi\delta}} G_0(n\kappa;q,q_0)\alpha(q_0)\left\{\frac{1}{3}E_1^3(\kappa;q_0) + E_1^2(2\kappa;q_0)E_1^*(\kappa;q_0)\right\} dq_0 \\
& - \int_{\overline{Q_{\{Y,Z\}, |z|\leq 2\pi\delta}}} \left(E_1(n\kappa;q_0)\frac{\partial G_0(n\kappa;q,q_0)}{\partial\mathbf{n}} - G_0(n\kappa;q,q_0)\frac{\partial E_1(n\kappa;q_0)}{\partial\mathbf{n}}\right) dq_0,
\end{aligned}
\tag{46}
$$

$$
q \in Q_{\{Y,Z\}, |z|\leq 2\pi\delta}, \quad n = 1,2,3.
$$

The line integrals in (46) represent the values of the incident fields at the frequencies $n\kappa$, $n = 1,2,3$, in the points $q \in Q_{\{Y,Z\}, |z|\leq 2\pi\delta}$:

$$
E_1^{\text{inc}}(n\kappa;q) = -\int_{\overline{Q_{\{Y,Z\}, |z|\leq 2\pi\delta}}} \left(E_1(n\kappa;q_0)\frac{\partial G_0(n\kappa;q,q_0)}{\partial\mathbf{n}} - G_0(n\kappa;q,q_0)\frac{\partial E_1(n\kappa;q_0)}{\partial\mathbf{n}}\right) dq_0,
$$

$$
q \in Q_{\{Y,Z\}, |z|\leq 2\pi\delta}, \quad n = 1,2,3.
\tag{47}
$$

Indeed, applying Green's formula to the functions $G(n\kappa;q,q_0)$ and $E_1^{\text{inc}}(n\kappa;q)$ in the region $Q_{\{Y,Z\}, |z|\leq 2\pi\delta} \cup Q_{\{Y,Z\}, z<-2\pi\delta}$ (where $q \in Q_{\{Y,Z\}, |z|\leq 2\pi\delta} \cup Q_{\{Y,Z\}, z<-2\pi\delta}$) and letting $\partial Q_{\{Y,Z\}, z<-2\pi\delta} \to -\infty$, we arrive at (47). Substituting (47) into (46), we obtain the following system of non-linear integral equations w.r.t. the unknown total diffraction field:

$$
\begin{aligned}
&E_1(n\kappa;q) \\
&= -(n\kappa)^2 \iint_{Q_{\{Y,Z\}, |z|\le 2\pi\delta}} G_0(n\kappa;q,q_0) \times \\
&\qquad \times [1 - \varepsilon_{n\kappa}(q_0, \alpha(q_0), E_1(\kappa;q_0), E_1(2\kappa;q_0), E_1(3\kappa;q_0))] E_1(n\kappa;q_0) dq_0 \\
&\quad + \delta_{n1}(n\kappa)^2 \iint_{Q_{\{Y,Z\}, |z|\le 2\pi\delta}} G_0(n\kappa;q,q_0)\alpha(q_0) E_1^2(2\kappa;q_0) E_1^*(3\kappa;q_0) dq_0 \\
&\quad + \delta_{n3}(n\kappa)^2 \iint_{Q_{\{Y,Z\}, |z|\le 2\pi\delta}} G_0(n\kappa;q,q_0)\alpha(q_0) \left\{ \frac{1}{3}E_1^3(\kappa;q_0) + E_1^2(2\kappa;q_0) E_1^*(\kappa;q_0) \right\} dq_0 \\
&\quad + E_1^{\mathrm{inc}}(n\kappa;q), \quad q \in Q_{\{Y,Z\}, |z|\le 2\pi\delta}, \quad n = 1,2,3.
\end{aligned}
$$

Passing in the above equations to the limit $Y \to \infty$ (where this procedure is admissible because of the free choice of the parameter Y and the asymptotic behaviour of the integrands as $\mathcal{O}\left(Y^{-1}\right)$, see (C1) and (35)) we arrive at a system of non-linear integral equations w.r.t. the total diffraction fields in the strip $Q_\delta := Q_{\{Y=\infty,Z\}, |z|\le 2\pi\delta} = \{q = (y,z): |y| < \infty, |z| \le 2\pi\delta\}$ filled by the non-linear dielectric layer:

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

The integral representations of the total diffraction fields $E_1(n\kappa;q)$, $n = 1,2,3$, in the points $q \notin Q_\delta$ located outside the layer can be derived similarly to the approach described above (see (35) – (48)). For this situation it is sufficient to consider in (43) the points lying above ($q \in Q_{\{Y=\infty,Z=\infty\}, z>2\pi\delta}$) and below ($q \in Q_{\{Y=\infty,Z=\infty\}, z<-2\pi\delta}$) the layer. As a result, we get that the integral representations (48) are valid for all points in the region $q \in Q := Q_{\{Y=\infty,Z=\infty\}, z>2\pi\delta} \cup Q_\delta \cup Q_{\{Y=\infty,Z=\infty\}, z<-2\pi\delta}$, that is

$$
\begin{aligned}
&E_1(n\kappa;q) \\
&= -(n\kappa)^2 \iint_{Q_\delta} G_0(n\kappa;q,q_0) \times \\
&\qquad \times [1 - \varepsilon_{n\kappa}(q_0, \alpha(q_0), E_1(\kappa;q_0), E_1(2\kappa;q_0), E_1(3\kappa;q_0))] E_1(n\kappa;q_0) dq_0 \\
&\quad + \delta_{n1}(n\kappa)^2 \iint_{Q_\delta} G_0(n\kappa;q,q_0)\alpha(q_0) E_1^2(2\kappa;q_0) E_1^*(3\kappa;q_0) dq_0 \\
&\quad + \delta_{n3}(n\kappa)^2 \iint_{Q_\delta} G_0(n\kappa;q,q_0)\alpha(q_0) \left\{ \frac{1}{3}E_1^3(\kappa;q_0) + E_1^2(2\kappa;q_0) E_1^*(\kappa;q_0) \right\} dq_0 \\
&\quad + E_1^{\mathrm{inc}}(n\kappa;q), \quad q \in Q, \quad n = 1,2,3.
\end{aligned}
\tag{49}
$$

The expressions in (49) form a system of non-linear integral equations in the points $q \in Q_\delta$. Provided that a solution of this system exists, it can be substituted into the right-hand side of (49). In this way we also obtain an integral representation of the total diffraction field at points located outside the layer, i.e. $q \in Q_{\{Y=\infty,Z=\infty\}, z>2\pi\delta}$ or $q \in Q_{\{Y=\infty,Z=\infty\}, z<-2\pi\delta}$.

Alternatively, the system (49) can be derived by means of an iterative approach developed in Shestopalov & Sirenko (1989). Schematically it can be represented as follows (see also Yatsyk

(2007)). In the region Q we construct a sequence $\left\{E_{1,p}(n\kappa;q)\right\}_{p=0}^{\infty}$, $n=1,2,3$, of functions (where each function, starting with the index $p=1$, satisfies the conditions (C1) – (C4)) such that the limit functions $E_1(n\kappa;q) = \lim\limits_{p\to\infty} E_{1,p}(n\kappa;q)$ at the frequencies $n\kappa$, $n=1,2,3$, satisfy (31), (C1) – (C4), i.e.

$$
\begin{aligned}
&\left(\nabla^2 + (n\kappa)^2\right) E_{1,0}(n\kappa;q) = 0, \\
&\left(\nabla^2 + (n\kappa)^2\right) E_{1,1}(n\kappa;q) \\
={}& \left[1 - \varepsilon_{n\kappa}\left(q,\alpha(q),E_{1,0}(\kappa;q),E_{1,0}(2\kappa;q),E_{1,0}(3\kappa;q)\right)\right](n\kappa)^2 E_{1,0}(n\kappa;q) \\
&- \delta_{n1}\alpha(q)(n\kappa)^2 E_{1,0}^2(2\kappa;q)E_{1,0}^*(3\kappa;q) \\
&- \delta_{n3}\alpha(q)(n\kappa)^2\left\{\tfrac{1}{3}E_{1,0}^3(\kappa;q) + E_{1,0}^2(2\kappa;q)E_{1,0}^*(\kappa;q)\right\},\dots, \\
&\left(\nabla^2 + (n\kappa)^2\right) E_{1,p+1}(n\kappa;q) \\
={}& \left[1 - \varepsilon_{n\kappa}\left(q,\alpha(q),E_{1,p}(\kappa;q),E_{1,p}(2\kappa;q),E_{1,p}(3\kappa;q)\right)\right](n\kappa)^2 E_{1,p}(n\kappa;q) \\
&- \delta_{n1}\alpha(q)(n\kappa)^2 E_{1,p}^2(2\kappa;q)E_{1,p}^*(3\kappa;q) \\
&- \delta_{n3}\alpha(q)(n\kappa)^2\left\{\tfrac{1}{3}E_{1,p}^3(\kappa;q) + E_{1,p}^2(2\kappa;q)E_{1,p}^*(\kappa;q)\right\},\dots, \\
&\hspace{9cm} n=1,2,3.
\end{aligned}
\tag{50}
$$

The system of equations (50) is formally equivalent to the following:

$$
\begin{aligned}
&E_{1,0}(n\kappa;q) := E_1^{\mathrm{inc}}(n\kappa;q), \\
&E_{1,1}(n\kappa;q) \\
={}& -(n\kappa)^2 \iint_{Q_\delta} G_0(n\kappa;q,q_0) \times \\
&\quad\times \left[1 - \varepsilon_{n\kappa}\left(q_0,\alpha(q_0),E_{1,0}(\kappa;q_0),E_{1,0}(2\kappa;q_0),E_{1,0}(3\kappa;q_0)\right)\right] E_{1,0}(n\kappa;q_0)dq_0 \\
&+ \delta_{n1}(n\kappa)^2 \iint_{Q_\delta} G_0(n\kappa;q,q_0)\alpha(q_0)E_{1,0}^2(2\kappa;q_0)E_{1,0}^*(3\kappa;q_0)dq_0 \\
&+ \delta_{n3}(n\kappa)^2 \iint_{Q_\delta} G_0(n\kappa;q,q_0)\alpha(q_0)\left\{\tfrac{1}{3}E_{1,0}^3(\kappa;q_0) + E_{1,0}^2(2\kappa;q_0)E_{1,0}^*(\kappa;q_0)\right\}dq_0 \\
&+ E_{1,0}(n\kappa;q),\dots, \\
&E_{1,p+1}(n\kappa;q) \\
={}& -(n\kappa)^2 \iint_{Q_\delta} G_0(n\kappa;q,q_0) \times \\
&\quad\times \left[1 - \varepsilon_{n\kappa}\left(q_0,\alpha(q_0),E_{1,p}(\kappa;q_0),E_{1,p}(2\kappa;q_0),E_{1,p}(3\kappa;q_0)\right)\right] E_{1,p}(n\kappa;q_0)dq_0 \\
&+ \delta_{n1}(n\kappa)^2 \iint_{Q_\delta} G_0(n\kappa;q,q_0)\alpha(q_0)E_{1,p}^2(2\kappa;q_0)E_{1,p}^*(3\kappa;q_0)dq_0 \\
&+ \delta_{n3}(n\kappa)^2 \iint_{Q_\delta} G_0(n\kappa;q,q_0)\alpha(q_0)\left\{\tfrac{1}{3}E_{1,p}^3(\kappa;q_0) + E_{1,p}^2(2\kappa;q_0)E_{1,p}^*(\kappa;q_0)\right\}dq_0 \\
&+ E_{1,0}(n\kappa;q),\dots, \\
&\hspace{7cm} q \in Q, \quad n=1,2,3.
\end{aligned}
\tag{51}
$$

Letting in (51) p tend to infinity, we obtain (49) – the integral representations of the unknown diffraction fields in the region Q.

We consider now the variation of the parameter q in the strip occupied by the dielectric layer, i.e. $q \in Q_\delta$. Then the representation (49) can be converted into a system of non-linear integral equations w.r.t. the unknown fields $E_1(n\kappa;q)$, $n=1,2,3$, $q \in Q_\delta$, scattered in the non-linear structure, see (32). Namely, substituting the representations for the canonical Green's functions (35) into (49) and taking into consideration the expressions for the permittivity

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

we get the following system w.r.t. the unknown quasi-homogeneous fields
$E_1\left(n\kappa;q|_{q\equiv(y,z)}\right)=U(n\kappa;z)\exp\left(i\phi_{n\kappa}y\right)$, $n=1,2,3$, $|z|\leq2\pi\delta$:

$$
\begin{aligned}
&U(n\kappa;z)\exp\left(i\phi_{n\kappa}y\right)\\
=&-\lim_{Y\to\infty}\left(\frac{i(n\kappa)^2}{4Y\Gamma_{n\kappa}}\exp(i\phi_{n\kappa}y)\int_{-2\pi\delta}^{2\pi\delta}\int_{-Y}^{Y}\exp(i\Gamma_{n\kappa}|z-z_0|)\times\right.\\
&\left.\times\left[1-\varepsilon_{n\kappa}\left(z_0,\alpha(z_0),U(\kappa;z_0),U(2\kappa;z_0),U(3\kappa;z_0)\right)\right]U(n\kappa;z_0)\,dy_0dz_0\right)\\
&+\lim_{Y\to\infty}\left(\delta_{n1}\frac{i(n\kappa)^2}{4Y\Gamma_{n\kappa}}\exp(i\phi_{n\kappa}y)\times\right.\\
&\left.\times\int_{-2\pi\delta}^{2\pi\delta}\int_{-Y}^{Y}\exp(i\Gamma_{n\kappa}|z-z_0|)\alpha(z_0)U^2(2\kappa;z_0)U^*(3\kappa;z_0)\,dy_0dz_0\right)\\
&+\lim_{Y\to\infty}\left(\delta_{n3}\frac{i(n\kappa)^2}{4Y\Gamma_{n\kappa}}\exp(i\phi_{n\kappa}y)\times\right.\\
&\left.\times\int_{-2\pi\delta}^{2\pi\delta}\int_{-Y}^{Y}\exp(i\Gamma_{n\kappa}|z-z_0|)\alpha(z_0)\left\{\frac{1}{3}U^3(\kappa;z_0)+U^2(2\kappa;z_0)U^*(\kappa;z_0)\right\}dy_0dz_0\right)\\
&+U^{\text{inc}}(n\kappa;z)\exp(i\phi_{n\kappa}y),\quad|z|\leq2\pi\delta,\quad n=1,2,3.
\end{aligned}
$$

Integrating in the region Q_δ 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 $U(n\kappa;z)\in L_2(-2\pi\delta,2\pi\delta)$:

$$
\begin{aligned}
&U(n\kappa;z)+\frac{i(n\kappa)^2}{2\Gamma_{n\kappa}}\int_{-2\pi\delta}^{2\pi\delta}\exp(i\Gamma_{n\kappa}|z-z_0|)\times\\
&\qquad\times\left[1-\varepsilon_{n\kappa}\left(z_0,\alpha(z_0),U(\kappa;z_0),U(2\kappa;z_0),U(3\kappa;z_0)\right)\right]U(n\kappa;z_0)dz_0\\
=&\;\delta_{n1}\frac{i(n\kappa)^2}{2\Gamma_{n\kappa}}\int_{-2\pi\delta}^{2\pi\delta}\exp(i\Gamma_{n\kappa}|z-z_0|)\alpha(z_0)U^2(2\kappa;z_0)U^*(3\kappa;z_0)dz_0\\
&+\delta_{n3}\frac{i(n\kappa)^2}{2\Gamma_{n\kappa}}\int_{-2\pi\delta}^{2\pi\delta}\exp(i\Gamma_{n\kappa}|z-z_0|)\alpha(z_0)\left\{\frac{1}{3}U^3(\kappa;z_0)+U^2(2\kappa;z_0)U^*(\kappa;z_0)\right\}dz_0\\
&+U^{\text{inc}}(n\kappa;z),\quad|z|\leq2\pi\delta,\quad n=1,2,3.
\end{aligned}
$$

$$(52)$$

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

The solution of the original problem (31), (C1) – (C4), represented as (32), can be obtained from (52) using the formulas

$$U(n\kappa;2\pi\delta)=a_{n\kappa}^{\text{inc}}+a_{n\kappa}^{\text{scat}},\quad U(n\kappa;-2\pi\delta)=b_{n\kappa}^{\text{scat}},\quad n=1,2,3,\qquad(53)$$

(cf. (C3)).

The derivation of the system of non-linear integral equations (52) shows that (52) can be regarded as an integral representation of the desired solution of (31), (C1) – (C4) (i.e. solutions of the form $E_1\left(n\kappa;y,z\right)=U(n\kappa;z)\exp\left(i\phi_{n\kappa}y\right)$, $n=1,2,3$, see (32)) 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 (52) in the region $|z|\leq2\pi\delta$, the substitution into the integrals of (52) 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. The system of non-linear Sturm-Liouville boundary value problems

The system of non-linear integral equations (52), as well as the problem (31), (C1) – (C4) reduce to a system of non-linear Sturm-Liouville problems.

Indeed, applying the approach described in Yatsyk (2007), Shestopalov & Yatsyk (2007), Kravchenko & Yatsyk (2007), Angermann & Yatsyk (2008), we write the system (52) for arguments z lying in the non-linear layer, i.e. for $|z| \leq 2\pi\delta$, in the form

$$
U(n\kappa;z) + \frac{i(n\kappa)^2}{2\Gamma_{n\kappa}}\left[F_{+,n\kappa}(z) + F_{-,n\kappa}(z)\right] = (\delta_{n1} + \delta_{n3})\frac{i(n\kappa)^2}{2\Gamma_{n\kappa}}\left[P_{+,n\kappa}(z) + P_{-,n\kappa}(z)\right] \\ + U^{\mathrm{inc}}(n\kappa;z), \quad |z| \leq 2\pi\delta, \quad n = 1,2,3,
\tag{54}
$$

where

$$
\begin{aligned}
F_{+,n\kappa}(z) &:= \int_{-2\pi\delta}^{z} \exp(i\Gamma_{n\kappa}(z - z_0)) \times \\
&\quad \times [1 - \varepsilon_{n\kappa}(z_0, \alpha(z_0), U(\kappa;z_0), U(2\kappa;z_0), U(3\kappa;z_0))] U(n\kappa;z_0)\, dz_0, \\
F_{-,n\kappa}(z) &:= \int_{z}^{2\pi\delta} \exp(-i\Gamma_{n\kappa}(z - z_0)) \times \\
&\quad \times [1 - \varepsilon_{n\kappa}(z_0, \alpha(z_0), U(\kappa;z_0), U(2\kappa;z_0), U(3\kappa;z_0))] U(n\kappa;z_0)\, dz_0, \\
&\qquad\qquad n = 1,2,3,
\end{aligned}
$$

and

$$
\begin{aligned}
P_{+,\kappa}(z) &:= \int_{-2\pi\delta}^{z} \exp(i\Gamma_\kappa(z - z_0))\alpha(z_0)U^2(2\kappa;z_0)U^*(3\kappa;z_0)dz_0, \\
P_{-,\kappa}(z) &:= \int_{z}^{2\pi\delta} \exp(-i\Gamma_\kappa(z - z_0))\alpha(z_0)U^2(2\kappa;z_0)U^*(3\kappa;z_0)dz_0, \\
P_{+,3\kappa}(z) &:= \int_{-2\pi\delta}^{z} \exp(i\Gamma_{3\kappa}(z - z_0))\alpha(z_0)\left\{\frac{1}{3}U^3(\kappa;z_0) + U^2(2\kappa;z_0)U^*(\kappa;z_0)\right\}dz_0, \\
P_{-,3\kappa}(z) &:= \int_{z}^{2\pi\delta} \exp(-i\Gamma_{3\kappa}(z - z_0))\alpha(z_0)\left\{\frac{1}{3}U^3(\kappa;z_0) + U^2(2\kappa;z_0)U^*(\kappa;z_0)\right\}dz_0.
\end{aligned}
$$

The integrands and their partial derivatives w.r.t. z are continuous on the set $-2\pi\delta \leq z \leq 2\pi\delta$, $-2\pi\delta \leq z_0 \leq 2\pi\delta$. Therefore we may differentiate w.r.t. the argument z by means of the Leibniz rule. Differentiating (54) twice w.r.t. z, we obtain the following system of integro-differential equations:

$$
\begin{aligned}
&\frac{d^2}{dz^2}U(n\kappa;z) + \frac{i(n\kappa)^2}{2\Gamma_{n\kappa}}\left[F''_{+,n\kappa}(z) + F''_{-,n\kappa}(z)\right] \\
&= (\delta_{n1} + \delta_{n3})\frac{i(n\kappa)^2}{2\Gamma_{n\kappa}}\left[P''_{+,n\kappa}(z) + P''_{-,n\kappa}(z)\right] - \Gamma_{n\kappa}^2 U^{\mathrm{inc}}(n\kappa;z), \quad |z| \leq 2\pi\delta, \quad n = 1,2,3.
\end{aligned}
\tag{55}
$$

Because of

$$
\begin{aligned}
F''_{+,n\kappa}(z) + F''_{-,n\kappa}(z) &= i\Gamma_{n\kappa}\left[F'_{+,n\kappa}(z) - F'_{-,n\kappa}(z)\right], \quad n = 1,2,3, \\
P''_{+,n\kappa}(z) + P''_{-,n\kappa}(z) &= i\Gamma_{n\kappa}\left[P'_{+,n\kappa}(z) - P'_{-,n\kappa}(z)\right], \quad n = 1,3,
\end{aligned}
$$

where

$$
\begin{aligned}
F'_{+,n\kappa}(z) &= i\Gamma_{n\kappa}F_{+,n\kappa}(z) + [1 - \varepsilon_{n\kappa}(z,\alpha(z),U(\kappa;z),U(2\kappa;z),U(3\kappa;z))]\,U(n\kappa;z), \\
F'_{-,n\kappa}(z) &= -i\Gamma_{n\kappa}F_{-,n\kappa}(z) - [1 - \varepsilon_{n\kappa}(z,\alpha(z),U(\kappa;z),U(2\kappa;z),U(3\kappa;z))]\,U(n\kappa;z), \\
& \qquad n = 1,2,3, \\
P'_{+,\kappa}(z) &= i\Gamma_{\kappa}P_{+,\kappa}(z) + \alpha(z)U^2(2\kappa;z)U^*(3\kappa;z), \\
P'_{-,\kappa}(z) &= -i\Gamma_{\kappa}P_{-,\kappa}(z) - \alpha(z)U^2(2\kappa;z)U^*(3\kappa;z), \\
P'_{+,3\kappa}(z) &= i\Gamma_{3\kappa}P_{+,3\kappa}(z) + \alpha(z)\left\{\frac{1}{3}U^3(\kappa;z) + U^2(2\kappa;z)U^*(\kappa;z)\right\}, \\
P'_{-,3\kappa}(z) &= -i\Gamma_{3\kappa}P_{-,3\kappa}(z) - \alpha(z)\left\{\frac{1}{3}U^3(\kappa;z) + U^2(2\kappa;z)U^*(\kappa;z)\right\},
\end{aligned}
\tag{56}
$$

we see that

$$
\begin{aligned}
F'_{+,n\kappa}(z) - F'_{-,n\kappa}(z) &= i\Gamma_{n\kappa}[F_{+,n\kappa}(z) + F_{-,n\kappa}(z)] \\
& \quad + 2[1 - \varepsilon_{n\kappa}(z,\alpha(z),U(\kappa;z),U(2\kappa;z),U(3\kappa;z))]\,U(n\kappa;z), \\
& \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad n = 1,2,3, \\
P'_{+,\kappa}(z) - P'_{-,\kappa}(z) &= i\Gamma_{\kappa}[P_{+,\kappa}(z) + P_{-,\kappa}(z)] + 2\alpha(z)U^2(2\kappa;z)U^*(3\kappa;z), \\
P'_{+,3\kappa}(z) - P'_{-,3\kappa}(z) &= i\Gamma_{3\kappa}[P_{+,3\kappa}(z) + P_{-,3\kappa}(z)] + 2\alpha(z)\left\{\frac{1}{3}U^3(\kappa;z) + U^2(2\kappa;z)U^*(\kappa;z)\right\}.
\end{aligned}
$$

Consequently, the system (55) takes the form

$$
\left\{
\begin{aligned}
& \frac{d^2}{dz^2}U(n\kappa;z) - \Gamma_{n\kappa}\frac{i(n\kappa)^2}{2}[F_{+,n\kappa}(z) + F_{-,n\kappa}(z)] \\
& - (n\kappa)^2[1 - \varepsilon_{n\kappa}(z,\alpha(z),U(\kappa;z),U(2\kappa;z),U(3\kappa;z))]\,U(n\kappa;z) \\
=\ & -(\delta_{n1} + \delta_{n3})\frac{i(n\kappa)^2}{2}\Gamma_{n\kappa}[P_{+,n\kappa}(z) + P_{-,n\kappa}(z)] \\
& - (n\kappa)^2\alpha(z)\left(\delta_{n1}U^2(2\kappa;z)U^*(3\kappa;z) + \delta_{n3}\left\{\frac{1}{3}U^3(\kappa;z) + U^2(2\kappa;z)U^*(\kappa;z)\right\}\right) \\
& - \Gamma_{n\kappa}^2 U^{\mathrm{inc}}(n\kappa;z), \quad |z| \le 2\pi\delta, \quad n = 1,2,3.
\end{aligned}
\right.
$$

Making use of the integral representations of the desired solution $\{U(n\kappa;z)\}_{n=1,2,3}$ given by (54), the elimination of the integral terms results in the following system of non-linear second-order ordinary differential equations of Sturm-Liouville type:

$$
\begin{aligned}
& \frac{d^2}{dz^2}U(n\kappa;z) + \left\{\Gamma_{n\kappa}^2 - (n\kappa)^2[1 - \varepsilon_{n\kappa}(z,\alpha(z),U(\kappa;z),U(2\kappa;z),U(3\kappa;z))]\right\}U(n\kappa;z) \\
=\ & -(n\kappa)^2\alpha(z)\left(\delta_{n1}U^2(2\kappa;z)U^*(3\kappa;z) + \delta_{n3}\left\{\frac{1}{3}U^3(\kappa;z) + U^2(2\kappa;z)U^*(\kappa;z)\right\}\right), \\
& \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad |z| \le 2\pi\delta, \quad n = 1,2,3.
\end{aligned}
\tag{57}
$$

The boundary conditions at $z = \pm 2\pi\delta$ for each of the equations from system (57) are derived from those first-order integro-differential equations, which are obtained by differentiating the integral equations (54) w.r.t. the argument z, i.e.

$$
\begin{aligned}
& \frac{d}{dz}U(n\kappa;z) + \frac{i(n\kappa)^2}{2\Gamma_{n\kappa}}[F'_{+,n\kappa}(z) + F'_{-,n\kappa}(z)] \\
=\ & (\delta_{n1} + \delta_{n3})\frac{i(n\kappa)^2}{2\Gamma_{n\kappa}}[P'_{+,n\kappa}(z) + P'_{-,n\kappa}(z)] - i\Gamma_{n\kappa}U^{\mathrm{inc}}(n\kappa;z), \quad |z| \le 2\pi\delta, \quad n = 1,2,3.
\end{aligned}
$$

Because of

$$
\begin{aligned}
F'_{+,n\kappa}(z) + F'_{-,n\kappa}(z) &= i\Gamma_{n\kappa}\left[F_{+,n\kappa}(z) - F_{-,n\kappa}(z)\right], \quad n = 1,2,3, \\
P'_{+,n\kappa}(z) + P'_{-,n\kappa}(z) &= i\Gamma_{n\kappa}\left[P_{+,n\kappa}(z) - P_{-,n\kappa}(z)\right], \quad n = 1,3,
\end{aligned}
$$

(cf. (56)) we get

$$
\begin{aligned}
&\frac{d}{dz}U(n\kappa;z) + \frac{i(n\kappa)^2}{2\Gamma_{n\kappa}}i\Gamma_{n\kappa}\left[F_{+,n\kappa}(z) - F_{-,n\kappa}(z)\right] \\
&= (\delta_{n1} + \delta_{n3})\frac{i(n\kappa)^2}{2\Gamma_{n\kappa}}i\Gamma_{n\kappa}\left[P_{+,n\kappa}(z) - P_{-,n\kappa}(z)\right] - i\Gamma_{n\kappa}U^{\text{inc}}(n\kappa;z), \quad |z| \leq 2\pi\delta, \quad n = 1,2,3.
\end{aligned}
$$

(58)

Accordingly, at the boundary $z = \pm 2\pi\delta$ the system of integro-differential and integral equations (58), (54) can be represented as

$$
\begin{aligned}
&\frac{d}{dz}U\left(n\kappa; \left\{\begin{array}{c} 2\pi\delta \\ -2\pi\delta \end{array}\right\}\right) + \frac{i(n\kappa)^2}{2\Gamma_{n\kappa}}i\Gamma_{n\kappa}\left[\left\{\begin{array}{c} F_{+,n\kappa}(2\pi\delta) \\ 0 \end{array}\right\} - \left\{\begin{array}{c} 0 \\ F_{-,n\kappa}(-2\pi\delta) \end{array}\right\}\right] \\
&= (\delta_{n1} + \delta_{n3})\frac{i(n\kappa)^2}{2\Gamma_{n\kappa}}i\Gamma_{n\kappa}\left[\left\{\begin{array}{c} P_{+,n\kappa}(2\pi\delta) \\ 0 \end{array}\right\} - \left\{\begin{array}{c} 0 \\ P_{-,n\kappa}(-2\pi\delta) \end{array}\right\}\right] - i\Gamma_{n\kappa}U^{\text{inc}}\left(n\kappa; \left\{\begin{array}{c} 2\pi\delta \\ -2\pi\delta \end{array}\right\}\right), \\
&\hspace{10cm} n = 1,2,3,
\end{aligned}
$$

and

$$
\begin{aligned}
&U\left(n\kappa; \left\{\begin{array}{c} 2\pi\delta \\ -2\pi\delta \end{array}\right\}\right) + \frac{i(n\kappa)^2}{2\Gamma_{n\kappa}}\left[\left\{\begin{array}{c} F_{+,n\kappa}(2\pi\delta) \\ 0 \end{array}\right\} - \left\{\begin{array}{c} 0 \\ F_{-,n\kappa}(-2\pi\delta) \end{array}\right\}\right] \\
&= (\delta_{n1} + \delta_{n3})\frac{i(n\kappa)^2}{2\Gamma_{n\kappa}}\left[\left\{\begin{array}{c} P_{+,n\kappa}(2\pi\delta) \\ 0 \end{array}\right\} - \left\{\begin{array}{c} 0 \\ P_{-,n\kappa}(-2\pi\delta) \end{array}\right\}\right] + U^{\text{inc}}\left(n\kappa; \left\{\begin{array}{c} 2\pi\delta \\ -2\pi\delta \end{array}\right\}\right), \\
&\hspace{10cm} n = 1,2,3.
\end{aligned}
$$

Eliminating from both equations the terms containing the integrals, we obtain the boundary conditions of third kind:

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

(59)

Therefore, the system of non-linear integral equations (54) (or (52)) according to (57) and (59) is reduced to an equivalent system of non-linear Sturm-Liouville boundary value problems:

$$
\begin{aligned}
&\frac{d^2}{dz^2}U(n\kappa;z) + \left\{\Gamma_{n\kappa}^2 - (n\kappa)^2\left[1 - \varepsilon_{n\kappa}(z,\alpha(z),U(\kappa;z),U(2\kappa;z),U(3\kappa;z))\right]\right\}U(n\kappa;z) \\
&= -(n\kappa)^2\alpha(z)\left(\delta_{n1}U^2(2\kappa;z)U^*(3\kappa;z) + \delta_{n3}\left\{\frac{1}{3}U^3(\kappa;z) + U^2(2\kappa;z)U^*(\kappa;z)\right\}\right), \\
&\hspace{9cm} |z| \leq 2\pi\delta, \quad (60) \\
&i\Gamma_{n\kappa}U(n\kappa;-2\pi\delta) + \frac{d}{dz}U(n\kappa;-2\pi\delta) = 0, \\
&i\Gamma_{n\kappa}U(n\kappa;2\pi\delta) - \frac{d}{dz}U(n\kappa;2\pi\delta) = 2i\Gamma_{n\kappa}U^{\text{inc}}(n\kappa;2\pi\delta), \\
&\hspace{10cm} n = 1,2,3.
\end{aligned}
$$

We recall that the boundary problem (60) on the interval $|z| \leq 2\pi\delta$ can also be obtained by starting from the original problem (31), (C1) – (C4) and the representation of the

desired diffraction field (32), as shown at the end of Section 4. The system of non-linear ordinary differential equations of Sturm-Liouville type follows directly from substituting the representations (32) for the desired solutions, i.e. $\{E_1(n\kappa;y,z) = U(n\kappa;z)\exp(i\phi_{n\kappa}y)\}_{n=1,2,3}$ for $|z| \leq 2\pi\delta$, into the system of equations (31), using the relations $\Gamma_{n\kappa}^2 = (n\kappa)^2 - \phi_{n\kappa}^2$, $n = 1,2,3$, for the longitudinal and transverse propagation constants. The boundary conditions follow from the continuity condition (C3) of the tangential components of the full field of diffraction $\{\mathbf{E}_{\mathrm{tg}}(n\kappa;y,z)\}_{n=1,3}$ $\{\mathbf{H}_{\mathrm{tg}}(n\kappa;y,z)\}_{n=1,3}$ at the boundary $z = \pm 2\pi\delta$ of the non-linear layer:

$$
\begin{array}{rclcrcl}
U(n\kappa;2\pi\delta) & = & a_{n\kappa}^{\mathrm{scat}} + a_{n\kappa}^{\mathrm{inc}}, & & \dfrac{d}{dz}U(n\kappa;2\pi\delta) & = & i\Gamma_{n\kappa}\left(a_{n\kappa}^{\mathrm{scat}} - a_{n\kappa}^{\mathrm{inc}}\right), \\[2mm]
U(n\kappa;-2\pi\delta) & = & b_{n\kappa}^{\mathrm{scat}}, & & \dfrac{d}{dz}U(n\kappa;-2\pi\delta) & = & -i\Gamma_{n\kappa}b_{n\kappa}^{\mathrm{scat}}, \quad n = 1,2,3.
\end{array}
\tag{61}
$$

Eliminating in (61) the unknown values of the complex amplitudes $\{a_{n\kappa}^{\mathrm{scat}}\}_{n=1,2,3}$, $\{b_{n\kappa}^{\mathrm{scat}}\}_{n=1,2,3}$ of the scattered field at the boundary $z = \pm 2\pi\delta$ and taking into consideration that $a_{n\kappa}^{\mathrm{inc}} = U^{\mathrm{inc}}(n\kappa;2\pi\delta)$, we arrive at the same boundary conditions as in problem (60).

Thus we have established the equivalence of the non-linear problem (31), (C1) – (C4), of the system of non-linear integral equations (52) and of the system of non-linear boundary-value problems of Sturm-Liouville type (60) (cf. Angermann & Yatsyk (2010), Shestopalov & Yatsyk (2007)).

7. Numerical solution of the non-linear boundary value problem by the finite element method

Using the results given in Angermann & Yatsyk (2008), Angermann & Yatsyk (2010), we can apply the finite element method (FEM) to obtain an approximate solution of the non-linear boundary value problem (60). Let

$$
\mathbf{U}(z) := \begin{pmatrix} U(\kappa;z) \\ U(2\kappa;z) \\ U(3\kappa;z) \end{pmatrix},
$$

$$
\mathbf{F}(z,\mathbf{U}) := \begin{pmatrix}
\left\{\Gamma_{\kappa}^2 - \kappa^2\left[1 - \varepsilon_{\kappa}(z,\alpha(z),U(\kappa;z),U(2\kappa;z),U(3\kappa;z))\right]\right\}U(\kappa;z) \\
\qquad\qquad\qquad + \alpha(z)\kappa^2 U^2(2\kappa;z)U^*(3\kappa;z) \\[1mm]
\left\{\Gamma_{2\kappa}^2 - (2\kappa)^2\left[1 - \varepsilon_{2\kappa}(z,\alpha(z),U(\kappa;z),U(2\kappa;z),U(3\kappa;z))\right]\right\}U(2\kappa;z) \\[1mm]
\left\{\Gamma_{3\kappa}^2 - (3\kappa)^2\left[1 - \varepsilon_{3\kappa}(z,\alpha(z),U(\kappa;z),U(2\kappa;z),U(3\kappa;z))\right]\right\}U(3\kappa;z) \\
\qquad\qquad + \alpha(z)(3\kappa)^2\left\{\frac{1}{3}U^3(\kappa;z) + U^2(2\kappa;z)U^*(\kappa;z)\right\}
\end{pmatrix}.
$$

Then the system of differential equations in (60) takes the form

$$
-\mathbf{U}''(z) = \mathbf{F}(z,\mathbf{U}(z)), \quad z \in \mathcal{I} := (-2\pi\delta, 2\pi\delta).
\tag{62}
$$

The boundary conditions in (60) can be written as

$$
\begin{array}{rcl}
\mathbf{U}'(-2\pi\delta) & = & -i\mathbf{G}\mathbf{U}(-2\pi\delta), \\
\mathbf{U}'(2\pi\delta) & = & i\mathbf{G}\mathbf{U}(2\pi\delta) - 2i\mathbf{G}\mathbf{a}^{\mathrm{inc}},
\end{array}
\tag{63}
$$

where

$$
\mathbf{G} := \begin{pmatrix} \Gamma_{\kappa} & 0 & 0 \\ 0 & \Gamma_{2\kappa} & 0 \\ 0 & 0 & \Gamma_{3\kappa} \end{pmatrix} \quad \text{and} \quad \mathbf{a}^{\mathrm{inc}} := \begin{pmatrix} a_{\kappa}^{\mathrm{inc}} \\ a_{2\kappa}^{\mathrm{inc}} \\ a_{3\kappa}^{\mathrm{inc}} \end{pmatrix}.
$$

Taking an arbitrary complex-valued vector function $\mathbf{v} : [-2\pi\delta, 2\pi\delta] \to \mathbb{C}^3$, $\mathbf{v} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$, multiplying the vector differential equation (62) by the complex conjugate $\mathbf{v}^*$ and integrating w.r.t. z over the interval $\mathcal{I}$, we arrive at the equation

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

Integrating the left-hand side of this equation by parts and using the boundary conditions (63), we obtain:

$$\begin{aligned}
-\int_{\mathcal{I}} \mathbf{U}'' \cdot \mathbf{v}^* \, dz &= \int_{\mathcal{I}} \mathbf{U}' \cdot \mathbf{v}^* \, dz - (\mathbf{U}' \cdot \mathbf{v}^*)(2\pi\delta) + (\mathbf{U}' \cdot \mathbf{v}^*)(-2\pi\delta) \\
&= \int_{\mathcal{I}} \mathbf{U}' \cdot \mathbf{v}^{*\prime} \, dz - i\left[((\mathbf{GU}) \cdot \mathbf{v}^*)(2\pi\delta) + ((\mathbf{GU}) \cdot \mathbf{v}^*)(-2\pi\delta)\right] \\
&\quad + 2i(\mathbf{Ga}^{\text{inc}}) \cdot \mathbf{v}^*(2\pi\delta).
\end{aligned}$$

Now we consider the complex Sobolev space $H^1(\mathcal{I})$ consisting of functions with values in $\mathbb{C}$, which, together with their weak derivatives belong to $L_2(\mathcal{I})$. For $\mathbf{w}, \mathbf{v} \in \left[H^1(\mathcal{I})\right]^3$, we introduce the following forms:

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

So we arrive at the following weak formulation of boundary value problem (60):

Find $\mathbf{U} \in \left[H^1(\mathcal{I})\right]^3$ such that

$$a(\mathbf{U}, \mathbf{v}) = b(\mathbf{U}, \mathbf{v}) \quad \forall \mathbf{v} \in \left[H^1(\mathcal{I})\right]^3. \tag{64}$$

Based on the variational equation (64), we obtain the numerical method. We consider N nodes $\{z_i\}_{i=1}^N$ such that $-2\pi\delta =: z_1 < z_2 < \ldots < z_{N-1} < z_N := 2\pi\delta$, and define the intervals $\mathcal{I}_i := (z_i, z_{i+1})$ with the lengths $h_i := z_{i+1} - z_i$ and the parameter $h := \max_{i \in \{1, \ldots, N-1\}} h_i$. Then, for $i \in \{1, \ldots, N\}$ we introduce the basis functions $\psi_i : [-2\pi\delta, 2\pi\delta] \to \mathbb{R}$ by the formula

$$\psi_i(z) := \begin{cases} (z - z_{i-1})/h_{i-1}, & z \in \mathcal{I}_{i-1} \text{ and } i \geq 2, \\ (z_{i+1} - z)/h_i, & z \in \mathcal{I}_i \text{ and } i \leq N-1, \\ 0, & \text{otherwise} \end{cases}$$

and the corresponding space $V_h := \left\{ v_h = \sum_{i=1}^N \lambda_i \psi_i : \lambda_i \in \mathbb{C} \right\}$ (defined by a set of all linear combinations of the basis functions). It is well-known that $V_h \subset H^1(\mathcal{I})$ (cf. Samarskij & Gulin (2003)). Therefore the following discrete finite element formulation of the problem (64) is well-defined (see Angermann & Yatsyk (2008), Samarskij & Gulin (2003)):

Find $\mathbf{U}_h \subset V_h^3$ such that

$$a(\mathbf{U}_h, \mathbf{v}_h) = b_h(\mathbf{U}_h, \mathbf{v}_h) \quad \forall \mathbf{v}_h := \begin{pmatrix} v_{h1} \\ v_{h2} \\ v_{h3} \end{pmatrix} \in V_h^3. \tag{65}$$

The non-linear discrete form b_h is a slight modification of the right-hand side b of the problem (64) defined as follows:

$$b_h(\mathbf{w}_h, \mathbf{v}_h) := \int_{\mathcal{I}} \left[\mathbf{F}_h^{(L)}(z, \mathbf{w}_h) + \mathbf{F}_h^{(NL)}(z, \mathbf{w}_h)\right] \cdot \mathbf{v}_h^* \, dz - 2i(\mathbf{Ga}^{\text{inc}}) \cdot \mathbf{v}_h^*(2\pi\delta),$$

where

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

$$\mathbf{F}_h^{(NL)}(z, \mathbf{w}_h) \quad := \quad \begin{pmatrix} \kappa^2 \sum_{i=1}^N \left[\varepsilon_\kappa^{(NL)}\left(z_i, \alpha(z_i), w_{1i}, w_{2i}, w_{3i}\right) w_{1i} \right. \\ \left. + \; \alpha(z_i) w_{2i}^2 w_{3i}^* \right] \psi_i \\ (2\kappa)^2 \sum_{i=1}^N \varepsilon_{2\kappa}^{(NL)}\left(z_i, \alpha(z_i), w_{1i}, w_{2i}, w_{3i}\right) w_{2i}\, \psi_i \\ (3\kappa)^2 \sum_{i=1}^N \left[\varepsilon_{3\kappa}^{(NL)}\left(z_i, \alpha(z_i), w_{1i}, w_{2i}, w_{3i}\right) w_{3i} \right. \\ \left. + \; \alpha(z_i) \left\{ \tfrac{1}{3} w_{1i}^3 + w_{2i}^2 w_{1i}^* \right\} \right] \psi_i \end{pmatrix}.$$

In fact, the problem (65) reduces to solving a non-linear system of algebraic equations w.r.t. $3N$ complex scalars.

As in Angermann & Yatsyk (2008) the weak formulation (64) and the discrete formulation (65) can be used to prove, under certain assumptions, the existence and uniqueness of the solutions $\mathbf{U} \in \left[H^1(\mathcal{I})\right]^3$ and $\mathbf{U}_h \in V_h^3$, respectively. Furthermore, the convergence of the finite element solution to the weak solution can be established.

8. Third harmonic generation and resonant scattering of a strong electromagnetic field by the non-linear structure. A numerical algorithm for solving systems of non-linear integral equations

Consider the excitation of the non-linear structure by a strong electromagnetic field at the basic frequency κ only (see (30)), i.e.

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

In this case, the number of equations in the system of non-linear boundary-value problems (31), (C1) – (C4) and in the equivalent system of Sturm-Liouville problems (60), and the number of non-linear integral equations in the system (52) can be reduced (cf. Angermann & Yatsyk (2010)). As noted above, the second equation in each of the systems (31), (60) and (52), corresponding to a problem at the double frequency 2κ with a trivial right-hand side, can be eliminated by setting $E_1(\mathbf{r}, 2\kappa) := 0$. The dielectric permittivity of the non-linear layer depends on the component $U(\kappa; z)$ of the scattered field and on the component $U(3\kappa; z)$ of the generated field, i.e. the expression (29) simplifies to

$$
\begin{aligned}
& \varepsilon_{n\kappa}\left(z, \alpha(z), E_1(\mathbf{r}, \kappa), 0, E_1(\mathbf{r}, 3\kappa)\right) = \varepsilon_{n\kappa}\left(z, \alpha(z), U(\kappa; z), U(3\kappa; z)\right) \\
=: \;\; & \varepsilon^{(L)}(z) + \varepsilon_{n\kappa}^{(NL)}\left(\alpha(z), U(\kappa; z), U(3\kappa; z)\right) \\
= \;\; & \varepsilon^{(L)}(z) + \alpha(z)\left[|U(\kappa; z)|^2 + |U(3\kappa; z)|^2\right] \\
& + \delta_{n,1}\alpha(z)|U(\kappa; z)||U(3\kappa; z)| \exp\left[i\left\{-3\arg U(\kappa; z) + \arg U(3\kappa; z)\right\}\right], \quad n = 1, 3.
\end{aligned}
\tag{66}
$$

Now we discuss the numerical realisation of the approach based on the non-linear integral equations (52). In the case under consideration, the problem is reduced to finding solutions to one-dimensional non-linear integral equations (along the height $z \in [-2\pi\delta, 2\pi\delta]$ of the structure) w.r.t. the components $U(n\kappa; z)$, $U(3n\kappa; z)$:

$$
\begin{cases}
U(\kappa;z) + \dfrac{i\kappa^2}{2\Gamma_\kappa} \displaystyle\int_{-2\pi\delta}^{2\pi\delta} \exp(i\Gamma_\kappa|z-z_0|)\left[1 - \varepsilon_\kappa\left(z_0, \alpha(z_0), U(\kappa;z_0), U(3\kappa;z_0)\right)\right] U(\kappa;z_0)dz_0 \\
\qquad = U^{\mathrm{inc}}(\kappa;z), & |z| \le 2\pi\delta, \\[4pt]
U(3\kappa;z) + \dfrac{i(3\kappa)^2}{2\Gamma_{3\kappa}} \displaystyle\int_{-2\pi\delta}^{2\pi\delta} \exp(i\Gamma_{3\kappa}|z-z_0|)\left[1 - \varepsilon_{3\kappa}(z_0, \alpha(z_0), U(\kappa;z_0), U(3\kappa;z_0))\right] U(3\kappa;z_0)dz_0 \\
\qquad = \dfrac{i(3\kappa)^2}{6\Gamma_{3\kappa}} \displaystyle\int_{-2\pi\delta}^{2\pi\delta} \exp(i\Gamma_{3\kappa}|z-z_0|)\alpha(z_0)U^3(\kappa;z_0)dz_0, & |z| \le 2\pi\delta,
\end{cases}
\tag{67}
$$

where $U^{\mathrm{inc}}(\kappa;z) = a_\kappa^{\mathrm{inc}} \exp\left[-i\Gamma_\kappa(z - 2\pi\delta)\right]$.

The desired solution of the diffraction problem (31), (C1) – (C4) can be represented as follows (cf. (32)):

$$
\begin{aligned}
E_1(n\kappa;y,z) &= U(n\kappa;z)\exp(i\phi_{n\kappa}y) \\
&= \begin{cases}
\delta_{n1}a_{n\kappa}^{\mathrm{inc}}\exp(i(\phi_{n\kappa}y - \Gamma_{n\kappa}(z - 2\pi\delta))) + a_{n\kappa}^{\mathrm{scat}}\exp(i(\phi_{n\kappa}y + \Gamma_{n\kappa}(z - 2\pi\delta))), & z > 2\pi\delta, \\
U(n\kappa;z)\exp(i\phi_{n\kappa}y), & |z| \le 2\pi\delta, \\
b_{n\kappa}^{\mathrm{scat}}\exp(i(\phi_{n\kappa}y - \Gamma_{n\kappa}(z + 2\pi\delta))), & z < -2\pi\delta, \\
\end{cases} \\
& n = 1,3,
\end{aligned}
\tag{68}
$$

where $U(\kappa;z)$, $U(3\kappa;z)$, $|z| \le 2\pi\delta$, are the solutions of the system (67). According to (53) we determine the values of complex amplitudes $\left\{a_{n\kappa}^{\mathrm{scat}}, b_{n\kappa}^{\mathrm{scat}} : n = 1,3\right\}$ in (68) for the scattered and generated fields by means of the formulas

$$
U(n\kappa;2\pi\delta) = \delta_{n1}a_{n\kappa}^{\mathrm{inc}} + a_{n\kappa}^{\mathrm{scat}}, \quad U(n\kappa;-2\pi\delta) = b_{n\kappa}^{\mathrm{scat}}, \quad n = 1,3.
\tag{69}
$$

The solution of the system of non-linear integral equations (67) can be approximated numerically by the help of an iterative method. The proposed algorithm is based on the application of a quadrature rule to each of the non-linear integral equations of the system (67). The resulting system of complex non-linear inhomogeneous algebraic equations is solved by a block-iterative method, cf. Yatsyk (September 21-24, 2009), Yatsyk (June 21-26, 2010).

Thus, using Simpson's quadrature rule, the system of non-linear integral equations (67) reduces to a system of non-linear algebraic equations of the second kind:

$$
\begin{cases}
(\mathbf{I} - \mathbf{B}_\kappa(\mathbf{U}_\kappa, \mathbf{U}_{3\kappa}))\mathbf{U}_\kappa &= \mathbf{U}_\kappa^{\mathrm{inc}}, \\
(\mathbf{I} - \mathbf{B}_{3\kappa}(\mathbf{U}_\kappa, \mathbf{U}_{3\kappa}))\mathbf{U}_{3\kappa} &= \mathbf{C}_{3\kappa}(\mathbf{U}_\kappa),
\end{cases}
\tag{70}
$$

where, as in Section 7, $\{z_i\}_{i=1}^N$ is a discrete set of nodes $-2\pi\delta =: z_1 < z_2 < ... < z_n < ... < z_N =: 2\pi\delta$.

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

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

with entries

$$
\begin{aligned}
K_{nm}(p\kappa, \mathbf{U}_\kappa, \mathbf{U}_{3\kappa}) \quad := \quad & -\dfrac{i(p\kappa)^2}{2\Gamma_{p\kappa}}\exp\left(i\Gamma_{p\kappa}|z_n - z_m|\right)\Big[1 - \Big\{\varepsilon^{(L)}(z_m) \\
& + \alpha(z_m)\left(|U_m(\kappa)|^2 + |U_m(3\kappa)|^2\right. \\
& + \left.\delta_{p1}|U_m(\kappa)||U_m(3\kappa)|\exp\left\{i\left[-3\arg U_m(\kappa) + \arg U_m(3\kappa)\right]\right\}\right)\Big\}\Big].
\end{aligned}
$$

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

The right-hand side of (70) is defined by

$$
\begin{aligned}
\mathbf{U}_\kappa^{\text{inc}} &:= \left\{ a_\kappa^{\text{inc}} \exp\left[-i\Gamma_\kappa(z_n - 2\pi\delta)\right]\right\}_{n=1}^N, \\
\mathbf{C}_{3\kappa}(\mathbf{U}_\kappa) &:= \left\{ \frac{i(3\kappa)^2}{6\,\Gamma_{3\kappa}} \sum_{m=1}^N A_m \exp\left(i\Gamma_{3\kappa}|z_n - z_m|\right) \alpha(z_m) U_m^3(\kappa) \right\}_{n=1}^N .
\end{aligned}
$$

Given a relative error tolerance $\xi > 0$, the approximate solution of (70) is obtained by means of the following iterative method:

$$
\left\{
\begin{aligned}
&\left\{\left[\mathbf{I} - \mathbf{B}_\kappa\left(\mathbf{U}_\kappa^{(s-1)}, \mathbf{U}_{3\kappa}^{(S_{3q})}\right)\right]\mathbf{U}_\kappa^{(s)} = \mathbf{U}_\kappa^{\text{inc}}\right\}_{s=1}^{S_q: \|\mathbf{U}_\kappa^{(S_q)} - \mathbf{U}_\kappa^{(S_q-1)}\|/\|\mathbf{U}_\kappa^{(S_q)}\| < \xi} \\
&\left\{\left[\mathbf{I} - \mathbf{B}_{3\kappa}\left(\mathbf{U}_\kappa^{(S_q)}, \mathbf{U}_{3\kappa}^{(s-1)}\right)\right]\mathbf{U}_{3\kappa}^{(s)} = \mathbf{C}_{3\kappa}\left(\mathbf{U}_\kappa^{(S_q)}\right)\right\}_{s=1}^{S_{3q}: \|\mathbf{U}_{3\kappa}^{(S_{3q})} - \mathbf{U}_{3\kappa}^{(S_{3q}-1)}\|/\|\mathbf{U}_{3\kappa}^{(S_{3q})}\| < \xi}
\end{aligned}
\right\}_{q=1}^Q , \quad (71)
$$

where the terminating index $Q \in \mathbb{N}$ is defined by the requirement

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

We mention that, as in Yatsyk (2006), Shestopalov & Yatsyk (2007), a sufficient condition for convergence of the iterative process (71) can be derived. Similarly, under appropriate assumptions, a condition for existence and uniqueness of the solution of the problem can be obtained.

9. Numerical analysis. Resonant scattering of waves and the generation of the third harmonic

We consider a non-linear dielectric layered structure (see Fig. 1), the dielectric permittivity

$$
\varepsilon_{n\kappa}(z, \alpha(z), U(\kappa;z), U(3\kappa;z)) = \varepsilon^{(L)} + \varepsilon_{n\kappa}^{(NL)}
$$

of which is given by (29), where

$$
\left\{\varepsilon^{(L)}(z), \alpha(z)\right\} = \left\{
\begin{aligned}
&\left\{\varepsilon^{(L)} = 16,\ \alpha = \alpha_1\right\}, &&z \in [-2\pi\delta, z_1 = -2\pi\delta/3) \\
&\left\{\varepsilon^{(L)} = 64,\ \alpha = \alpha_2\right\}, &&z \in [z_1 = -2\pi\delta/3,\ z_2 = 2\pi\delta/3] \\
&\left\{\varepsilon^{(L)} = 16,\ \alpha = \alpha_3\right\}, &&z \in (z_2 = 2\pi\delta/3,\ 2\pi\delta]
\end{aligned}
\right\},
$$

$\alpha_1 = \alpha_3 = 0.01$, $\alpha_2 = -0.01$, $\delta = 0.5$. The excitation frequency is given by $\kappa = 0.25$, and the angle of incidence of the plane wave at the basic frequency κ is $\varphi_\kappa \in [0°, 90°)$.

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 $n\kappa$, $n = 1, 3$. Thus W_κ is the total energy scattered at the frequency κ of excitation, and $W_{3\kappa}$ is the total energy generated at the frequency 3κ. Fig. 2 (left) shows the dependence of $W_{3\kappa}/W_\kappa$ on the angle of incidence φ_κ and on the amplitude a_κ^{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 with angle of incidence φ_κ and amplitude a_κ^{inc} is passing the layer.
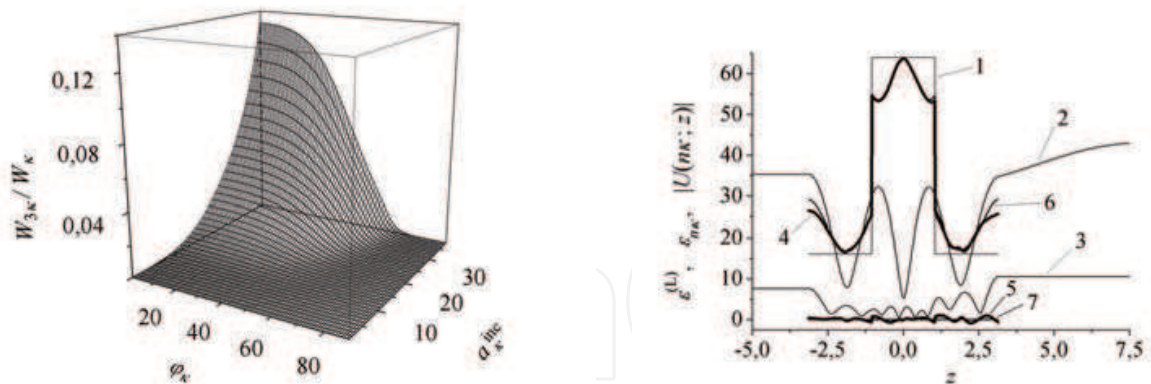
Fig. 2. The portion of energy generated in the third harmonic (left) and some graphs describing the properties of the structure at $a_\kappa^{\mathrm{inc}} = 38$ and $\varphi_\kappa = 0°$ (right): #1 ... $\varepsilon^{(L)}$, #2 ... $|U(\kappa;z)|$, #3 ... $|U(3\kappa;z)|$, #4 ... $\Re(\varepsilon_\kappa)$, #5 ... $\Im(\varepsilon_\kappa)$, #6 ... $\Re(\varepsilon_{3\kappa})$, #7 ... $\Im(\varepsilon_{3\kappa}) \equiv 0$

In particular, $W_{3\kappa}/W_\kappa = 0.132$ at $a_\kappa^{\mathrm{inc}} = 38$, i.e. $W_{3\kappa}$ amounts to 13.2% of the total energy W_κ scattered at the frequency of excitation κ.

Fig. 2 (right) shows the absolute values of the amplitudes of the full scattered field (total diffraction field) $|U(\kappa;z)|$ at the frequency of excitation κ (graph #2) and of the generated field $|U(3\kappa;z)|$ at the frequency 3κ (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. 2 (right) also displays some graphs characterising the scattering and generation properties of the non-linear structure. Graph #1 illustrates the value of the linear part $\varepsilon^{(L)}$ of the permittivity of the non-linear layered structure. Graphs #4 and #5 show the real and imaginary part of the permittivity at the frequency of excitation, while graphs #6 and #7 display the corresponding values at the generation frequency.

Figs. 3, 4 and 5 show the numerical results obtained for the scattered and the generated fields and for the non-linear dielectric permittivity in dependence on the amplitude a_κ^{inc} at normal incidence $\varphi_\kappa = 0°$ of the plane wave.

Fig. 3 shows the graphs of $|U_\kappa[a_\kappa^{\mathrm{inc}},z]|$ and $|U_{3\kappa}[a_\kappa^{\mathrm{inc}},z]|$ demonstrating the behaviour of the scattered and the generated fields, $|U(\kappa;z)|$ and $|U(3\kappa;z)|$, in the non-linear layered
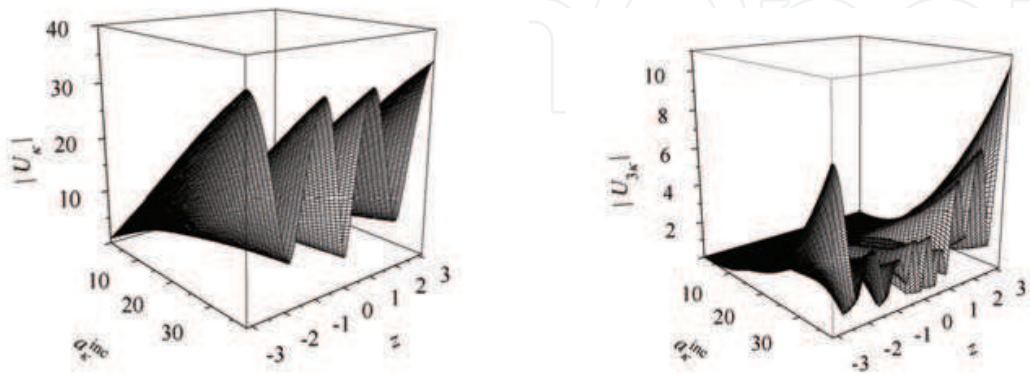

Fig. 3. Graphs of the scattered and generated fields in the non-linear layered structure for $\varphi_\kappa = 0°$: $|U_\kappa[a_\kappa^{\mathrm{inc}},z]|$ at $\kappa = 0.25$ (left), $|U_{3\kappa}[a_\kappa^{\mathrm{inc}},z]|$ at $3\kappa = 0.75$ (right)
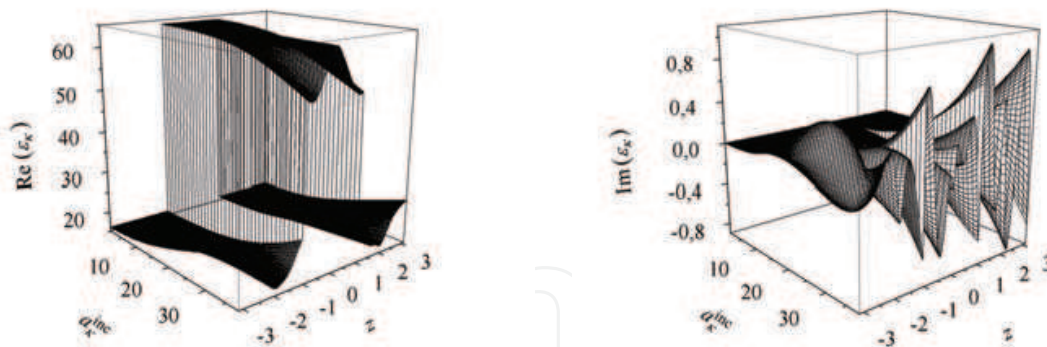
Fig. 4. Graphs of the permittivity at the frequency of excitation $\kappa = 0.25$ at normal incidence of the plane wave $\varphi_\kappa = 0°$: $\mathfrak{Re}\left(\varepsilon_\kappa\left[a_\kappa^{\mathrm{inc}},z\right]\right)$ (left), $\mathfrak{Im}\left(\varepsilon_\kappa\left[a_\kappa^{\mathrm{inc}},z\right]\right)$ (right)

structure in dependence on an increasing amplitude a_κ^{inc} at normal incidence $\varphi_\kappa = 0°$ of the plane wave of the frequency $\kappa = 0.25$. According to (66), the non-linear parts $\varepsilon_{n\kappa}^{(NL)}$ of the dielectric permittivity at each frequency κ and 3κ depend on the values $U_\kappa := U(\kappa;z)$ and $U_{3\kappa} := U(3\kappa;z)$ of the fields. The variation of the non-linear parts $\varepsilon_{n\kappa}^{(NL)}$ of the dielectric permittivity for an increasing amplitude a_κ^{inc} of the incident field are illustrated by the behaviour of $\mathfrak{Re}\left(\varepsilon_\kappa\left[a_\kappa^{\mathrm{inc}},z\right]\right)$ (Fig. 4 (left)) and $\mathfrak{Im}\left(\varepsilon_\kappa\left[a_\kappa^{\mathrm{inc}},z\right]\right)$ (Fig. 4 (right)) at the frequency κ, and by $\varepsilon_{3\kappa}\left[a_\kappa^{\mathrm{inc}},z\right]$ at the triple frequency 3κ (Fig. 5 (left)).

In Fig. 4 (right) the graph of $\mathfrak{Im}(\varepsilon_\kappa)$ for a given amplitude a_κ^{inc} (denoted by $\mathfrak{Im}\left(\varepsilon_\kappa\left[a_\kappa^{\mathrm{inc}},z\right]\right)$) characterises the loss of energy in the non-linear medium (at the frequency of excitation κ) caused by the generation of the electromagnetic field of the third harmonic (at the frequency 3κ). In our case $\mathfrak{Im}\left[\varepsilon^{(L)}(z)\right] = 0$ and $\mathfrak{Im}\left[\alpha(z)\right] = 0$, therefore, according to (66),

$$\mathfrak{Im}(\varepsilon_\kappa) = \alpha(z)|U(\kappa;z)||U(3\kappa;z)|\mathfrak{Im}\left(\exp\left[i\left\{-3\mathrm{arg}U(\kappa;z) + \mathrm{arg}U(3\kappa;z)\right\}\right]\right). \qquad (72)$$

Fig. 4 (right) shows that the third harmonic generation is insignificant, i.e. $U(3\kappa;z) \approx 0$, if the non-linear structure is excited by a weak field (cf. also Figs. 4 (left), 5 and 3). In this case, for a small value of $|a_\kappa^{\mathrm{inc}}|$ in Fig. 4 (right) we observe a small amplitude of the function $\mathfrak{Im}(\varepsilon_\kappa)$, i.e. $|\mathfrak{Im}(\varepsilon_\kappa)| \approx 0$. The increase of $|a_\kappa^{\mathrm{inc}}|$ corresponds to a strong field excitation and leads to the generation of a third harmonic field $U(3\kappa;z)$. In this case, the variation of the absolute
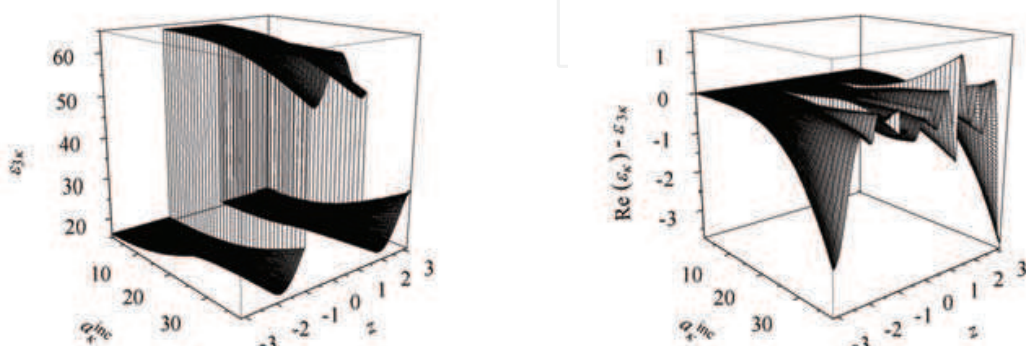

Fig. 5. Graph of the dielectric permittivity $\varepsilon_{3\kappa}\left[a_\kappa^{\mathrm{inc}},z\right]$ at the triple frequency $3\kappa = 0.75$ for $\varphi_\kappa = 0°$ (left), behaviour of $\mathfrak{Re}\left(\varepsilon_\kappa\left[a_\kappa^{\mathrm{inc}},z\right]\right) - \varepsilon_{3\kappa}\left[a_\kappa^{\mathrm{inc}},z\right]$ (right)

values $|U(\kappa;z)|$, $|U(3\kappa;z)|$ of the scattered and generated fields increase, see Fig. 3. Fig. 4 (right) shows that the values of $\Im\mathrm{m}(\varepsilon_\kappa)$ 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 $\Im\mathrm{m}(\varepsilon_\kappa)$ 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 (72),

$$-3\mathrm{arg}U(\kappa;z) + \mathrm{arg}U(3\kappa;z) = p\pi, \quad p = 0, \pm 1, \ldots$$

We mention that the behaviour of both the quantities $\Im\mathrm{m}(\varepsilon_\kappa)$ and

$$\Re\mathfrak{e}(\varepsilon_\kappa) - \varepsilon_{3\kappa} = \alpha(z)|U(\kappa;z)||U(3\kappa;z)|\Re\mathfrak{e}\left(\exp\left[i\left\{-3\mathrm{arg}U(\kappa;z) + \mathrm{arg}U(3\kappa;z)\right\}\right]\right)$$

plays a role in the process of third harmonic generation because of the presence of the last term in (66). Fig. 5 (right) shows the graph describing the behaviour of $\Re\mathfrak{e}\left(\varepsilon_\kappa\left[a_\kappa^{\mathrm{inc}},z\right]\right) - \varepsilon_{3\kappa}\left[a_\kappa^{\mathrm{inc}},z\right]$.

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:

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

The quantities $R_{n\kappa}$, $T_{n\kappa}$ represent the portions of energy of the reflected and the transmitted waves (at the excitation frequency κ), or the portions of energy of the generated waves in the zones of reflection and transmission (at the frequency 3κ), with respect to the energy of the incident field (at the frequency κ). We call them *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 $\{a_\kappa^{\mathrm{inc}} \neq 0, a_{2\kappa}^{\mathrm{inc}} = 0, a_{3\kappa}^{\mathrm{inc}} = 0\}$ and for non-absorbing media with $\Im\mathrm{m}\left[\varepsilon^{(L)}(z)\right] = 0$, the energy balance equation

$$R_\kappa + T_\kappa + R_{3\kappa} + T_{3\kappa} = 1$$

is satisfied. This equation represents the law of conservation of energy (Shestopalov & Sirenko (1989), Vainstein (1988)). It can be obtained by writing the energy conservation law for each frequency κ and 3κ, adding the resulting equations and taking into consideration the fact that the loss of energy at the frequency κ (spent for the generation of the third harmonic) is equal to the amount of energy generated at the frequency 3κ.

The scattering and generation properties of the non-linear structure are presented in Figs. 6 – 8. We consider the following range of parameters of the excitation field: the angle $\varphi_\kappa \in [0°, 90°)$, the amplitude of the incident plane wave $a_\kappa^{\mathrm{inc}} \in [1, 38]$ at the frequency $\kappa = 0.25$. The graphs show the dynamics of the scattering ($R_\kappa\left[\varphi_\kappa, a_\kappa^{\mathrm{inc}}\right]$, $T_\kappa\left[\varphi_\kappa, a_\kappa^{\mathrm{inc}}\right]$, see Fig. 6) and generation ($R_{3\kappa}\left[\varphi_\kappa, a_\kappa^{\mathrm{inc}}\right]$, $T_{3\kappa}\left[\varphi_\kappa, a_\kappa^{\mathrm{inc}}\right]$, see Fig. 7) properties of the structure.

Fig. 8 shows cross sections of the graphs depicted in Figs. 6 – 7 by the planes $\varphi_\kappa = 0°$ and $a_\kappa^{\mathrm{inc}} = 38$. We see that increasing the amplitude of the excitation field of the non-linear layer leads to the third harmonic generation (Fig. 8 (left)). In the range $29 < a_\kappa^{\mathrm{inc}} \leq 38$ (i.e. right from the intersection of the graphs #1 and #3 in Fig. 8 (left)) we see that $R_{3\kappa} > R_\kappa$. In this case, $0.053 < W_{3\kappa}/W_\kappa \leq 0.132$, cf. Fig. 2. If $34 < a_\kappa^{\mathrm{inc}} \leq 38$ (i.e. right from the intersection of the graphs #1 and #4 in Fig. 8 (left)) the field generated at the triple frequency in the zones of reflection and transmission is stronger than the reflected field at the excitation frequency κ: $R_{3\kappa} > T_{3\kappa} > R_\kappa$. Here, $0.088 < W_{3\kappa}/W_\kappa \leq 0.132$, cf. Fig. 2.

Fig. 8 (right) shows the dependence of the coefficients of the scattered and generated waves on the angle of incidence $\varphi_\kappa \in [0°, 90°)$ of a plane wave with a constant amplitude $a_\kappa^{\mathrm{inc}} = 38$
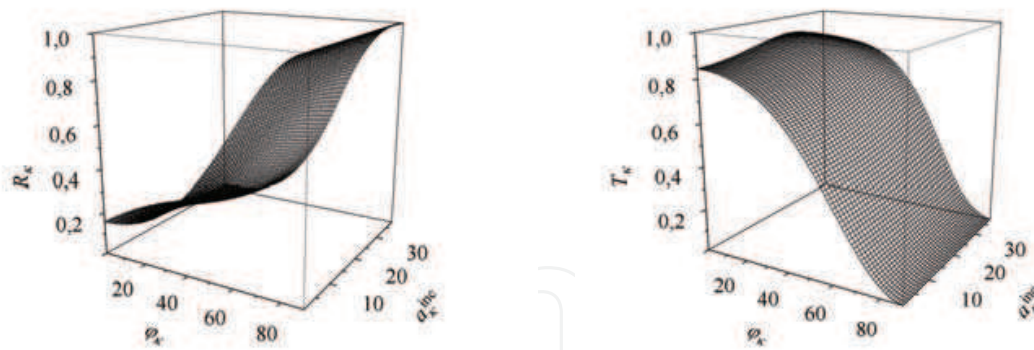
Fig. 6. The scattering properties of the non-linear structure at the excitation frequency
$\kappa = 0.25$: $R_\kappa \left[\varphi_\kappa, a_\kappa^{\text{inc}} \right]$ (left), $T_\kappa \left[\varphi_\kappa, a_\kappa^{\text{inc}} \right]$ (right)

of the incident field. It is seen that an increasing angle φ_κ leads to a weakening of the third harmonic generation. In the range of angles $0° \leq \varphi_\kappa < 21°$ (i.e. left from the intersection of the graphs #1 and #4 in Fig. 8 (right)) we see that $T_{3\kappa} > R_\kappa$. In this case, $0.125 < W_{3\kappa}/W_\kappa \leq 0.132$, cf. Fig. 2. The value of the coefficient of the third harmonic generation in the zone of reflection exceeds the value of the reflection coefficient at the excitation frequency, i.e. $R_{3\kappa} > R_\kappa$, in the range of angles $0° \leq \varphi_\kappa < 27°$ (i.e. left from the intersection of the graphs #1 and #3 in Fig. 8 (right)). Here, according to Fig. 2, $0.117 < W_{3\kappa}/W_\kappa \leq 0.132$. We mention that, at the normal incidence $\varphi_\kappa = 0°$ of a plane wave with amplitude $a_\kappa^{\text{inc}} = 38$, the coefficients of generation in the zones of reflection $R_{3\kappa} \left[\varphi_\kappa = 0°, a_\kappa^{\text{inc}} = 38 \right] = 0.076$ and transmission $T_{3\kappa} \left[\varphi_\kappa = 0°, a_\kappa^{\text{inc}} = 38 \right] = 0.040$ reach their maximum values, see Fig.s 7 and 8. In this case, the coefficients describing the portion of reflected and transmitted waves at the frequency of excitation $\kappa = 0.25$ of the structure take the following values: $R_\kappa \left[\varphi_\kappa = 0°, a_\kappa^{\text{inc}} = 38 \right] = 0.017$, $T_\kappa \left[\varphi_\kappa = 0°, a_\kappa^{\text{inc}} = 38 \right] = 0.866$.

The results shown in Figs. 2 - 8 are obtained by means of the iterative scheme (71). We point out some features of the numerical realisation of the algorithm (71). Figs. 9 and 10 display the number Q of iterations of the algorithm (71) that were necessary to obtain the results (analysis of scattering and generation properties of the non-linear structure) shown in Fig. 8. In Fig. 9 (left) we can see the number of iterations of the algorithm (71) for $\varphi_\kappa = 0°$, the range of amplitudes $a_\kappa^{\text{inc}} \in [0, 38]$ and the range of increments $\Delta a_\kappa^{\text{inc}} = 1$. Similarly, in Fig. 9 (right), we have the following parameters: $a_\kappa^{\text{inc}} = 38$, $\varphi_\kappa \in [0°, 90°)$ and $\Delta \varphi_\kappa = 1°$. The results
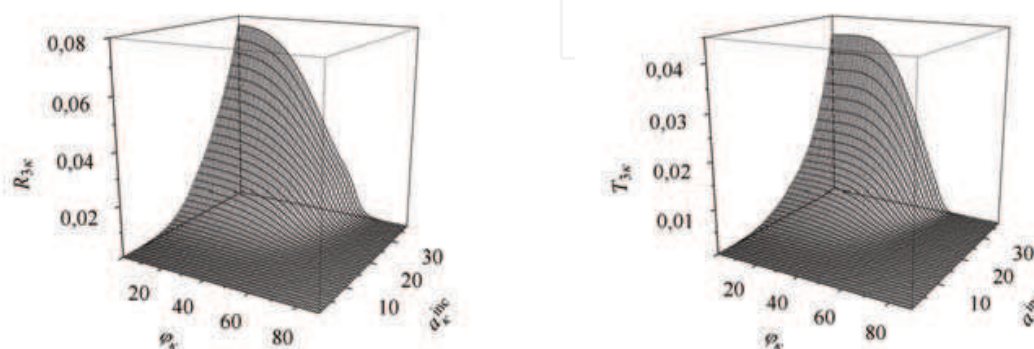

Fig. 7. Generation properties of the non-linear structure at the frequency of the third harmonic $3\kappa = 0.75$: $R_{3\kappa} \left[\varphi_\kappa, a_\kappa^{\text{inc}} \right]$ (left), $T_{3\kappa} \left[\varphi_\kappa, a_\kappa^{\text{inc}} \right]$ (right)
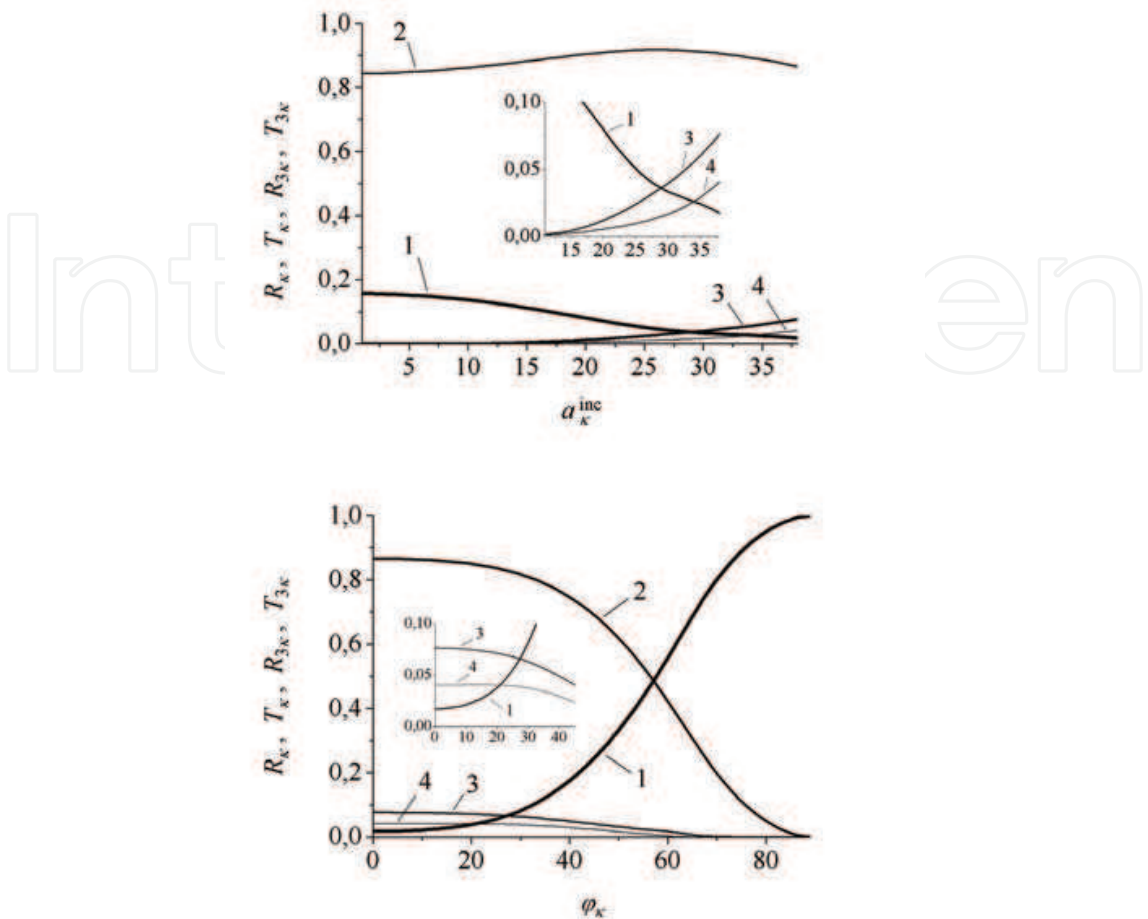
Fig. 8. Scattering and generation properties of the non-linear structure, $\kappa = 0.25$, $3\kappa = 0.75$, for $\varphi_\kappa = 0°$ (left) and $a_\kappa^{\mathrm{inc}} = 38$ (right): #1 … R_κ, #2 … T_κ, #3 … $R_{3\kappa}$, #4 … $T_{3\kappa}$

shown in Fig. 9 are also reflected in Fig. 10. Here the dependencies on the portion of the total energy generated in the third harmonic $W_{3\kappa}/W_\kappa$ are presented that characterise the iterative processes. We see that the number of iterations essentially depends on the energy generated
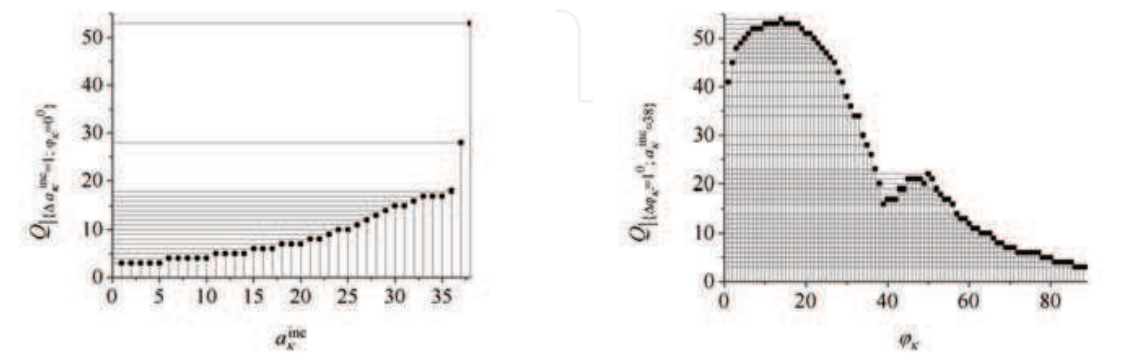
Fig. 9. The number of iterations of the algorithm in the analysis of the generating and scattering properties of the non-linear structure ($\kappa = 0.25$, $3\kappa = 0.75$): $Q|_{\{\Delta a_\kappa^{\mathrm{inc}}=1,\ \varphi_\kappa=0°\}}$ for $\Delta a_\kappa^{\mathrm{inc}} = 1$ and $\varphi_\kappa = 0°$ (left), $Q|_{\{\Delta\varphi_\kappa=1°,\ a_\kappa^{\mathrm{inc}}=38\}}$ for $\Delta\varphi_\kappa = 1°$ and $a_\kappa^{\mathrm{inc}} = 38$ (right)
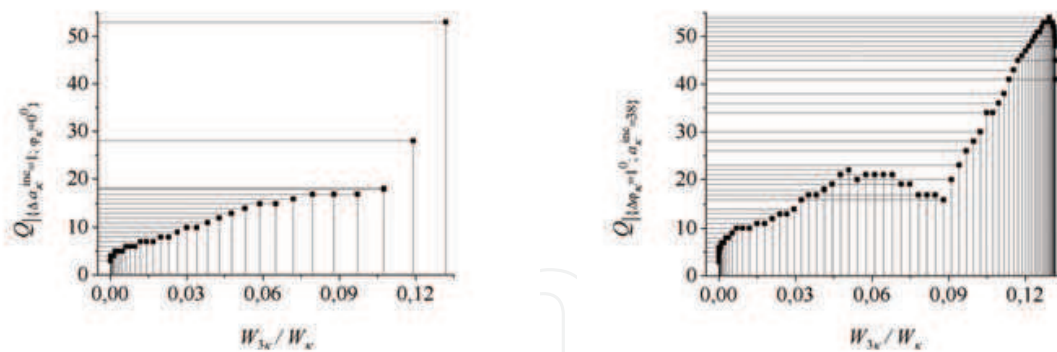
Fig. 10. The number of iterations of the algorithm in the analysis of the generating and scattering properties of the non-linear structure ($\kappa = 0.25$, $3\kappa = 0.75$) in dependence on the value $W_{3\kappa}/W_\kappa$: $Q|_{\{\Delta a_\kappa^{\mathrm{inc}}=1,\ \varphi_\kappa=0°\}}$ for $\Delta a_\kappa^{\mathrm{inc}} = 1$ and $\varphi_\kappa = 0°$ (left), $Q|_{\{\Delta \varphi_\kappa=1°,\ a_\kappa^{\mathrm{inc}}=38\}}$ for $\Delta \varphi_\kappa = 1°$ and $a_\kappa^{\mathrm{inc}} = 38$ (right)

in the third harmonic of the field by the non-linear structure.

The numerical results presented above were obtained by the iterative scheme (71) based on Simpson's quadrature rule, see Angermann & Yatsyk (2010). In the investigated range of parameters of the non-linear problem, the dimension of the resulting system of algebraic equations was $N = 501$, the relative error of calculations did not exceed $\xi = 10^{-7}$. Finally, it should be mentioned that the analysis of the problem (31), (C1) – (C4) can be carried out by solving the system of non-linear integral equations (52) and (55) as well as by solving the non-linear boundary value problems of Sturm-Liouville type (60). The numerical investigation of the non-linear boundary value problems (60) is based on the application of the finite element method Angermann & Yatsyk (2008), Angermann & Yatsyk (2010) Samarskij & Gulin (2003).

10. Conclusion

We presented a mathematical model and numerical simulations for the problem of resonance scattering and generation of harmonics by the diffraction of an incident wave packet by a non-linear layered cubically polarised structure. This model essentially extends the model proposed earlier in Yatsyk (September 21-24, 2009), Angermann & Yatsyk (2010), where only the case of normal incidence of the wave packet has been investigated. The involvment of the condition of phase synchronism into the boundary conditions of the problem allowed us to eliminate this restriction. The incident wave packet may fall onto the non-linear layered structure under an arbitrary angle. The wave packets under consideration consist of a strong field leading to the generation of waves and of weak fields which do not lead to the generation of harmonics but have a certain influence on the process of scattering and wave generation by the non-linear structure. The research was focused on the construction of algorithms for the analysis of resonant scattering and wave generation by a cubically non-linear layered structure. Results of calculations of the scattering field of a plane wave including the effect of the third harmonic generation by the structure were given. In particular, within the framework of the closed system of boundary value problems under consideration it could be shown that the imaginary part of the dielectric permittivity, which depends on the value of the non-linear part of the polarisation at the excitation frequency, characterises the loss of energy in the non-linear medium (at the frequency of the incident field) caused by to

the generation of the electromagnetic field of the third harmonic (at the triple frequency). For a sufficiently strong excitation field, the magnitude of the total energy generated by the non-linear structure at the triple frequency reaches 13.2 % of the total energy dissipated at the frequency of excitation. In addition, the paper presented the results describing the scattering and generation properties of the non-linear layered structure.

11. References

Agranovich, V. & Ginzburg, V. (1966). *Spatial Dispersion in Crystal Optics and the Theory of Excitons*, Interscience, Innsbruck.

Akhmediev, N. & Ankevich, A. (2003). *Solitons*, Fizmatlit, Moscow.

Angermann, L. & Yatsyk, V. (2008). Numerical simulation of the diffraction of weak electromagnetic waves by a Kerr-type nonlinear dielectric layer, *Int. J. Electromagnetic Waves and Electronic Systems* 13(12): 15–30.

Angermann, L. & Yatsyk, V. (2010). Mathematical models of the analysis of processes of resonance scattering and generation of the third harmonic by the diffraction of a plane wave through a layered, cubically polarisable structure, *Int. J. Electromagnetic Waves and Electronic Systems* 15(1): 36–49. In Russian.

Butcher, P. (1965). Nonlinear optical phenomena, *Bulletin 200*, Ohio State University, Columbus.

Kleinman, D. (1962). Nonlinear dielectric polarization in optical media, *Phys. Rev.* 126(6): 1977–1979.

Kravchenko, V. & Yatsyk, V. (2007). Effects of resonant scattering of waves by layered dielectric structure with Kerr-type nonlinearity, *Int. J. Electromagnetic Waves and Electronic Systems* 12(12): 17–40.

Miloslavski, V. (2008). *Nonlinear Optics*, V.N. Karazin Kharkov National University, Kharkov.

Samarskij, A. & Gulin, A. (2003). *Chislennye metody matematicheskoi fiziki (Numerical Methods of Mathematical Physics)*, Nauchnyi Mir, Moscow. In Russian.

Schürmann, H. W., Serov, V. & Shestopalov, Y. (2001). Reflection and transmission of a TE-plane wave at a lossless nonlinear dielectric film, *Physica D* 158: 197–215.

Serov, V., Schürmann, H. & Svetogorova, E. (2004). Integral equation approach to reflection and transmission of a plane te-wave at a (linear/nonlinear) dielectric film with spatially varying permittivities, *J. Phys. A: Math. Gen.* 37: 3489–3500.

Shestopalov, V. & Sirenko, Y. (1989). *Dynamical Theory of Gratings*, Naukova, Dumka, Kiev.

Shestopalov, Y. & Yatsyk, V. (2007). Resonance scattering of electromagnetic waves by a Kerr nonlinear dielectric layer, *Radiotekhnika i Elektronika (J. of Communications Technology and Electronics)* 52(11): 1285–1300.

Shestopalov, Y. & Yatsyk, V. (2010). Diffraction of electromagnetic waves by a layer filled with a Kerr-type nonlinear medium, *J. of Nonlinear Math. Physics* . 17(3): 311-335.

Sirenko, Y., Shestopalov, V. & Yatsyk, V. (1985). Elements of the spectral theory of gratings, *Preprint 266*, IRE NAS Ukraine, Kharkov.

Smirnov, V. (1981). *Course of Higher Mathematics, Vol. 4, Ch. 2*, Nauka, Moscow.

Smirnov, Y., Schürmann, H. & Shestopalov, Y. (2005). Propagation of TE-waves in cylindrical nonlinear dielectric waveguides, *Physical Review E* 71: 0166141–10.

Vainstein, L. (1988). *Electromagnetic Waves*, Radio i Svyas, Moscow. In Russian.

Vinogradova, M., Rudenko, O. & Sukhorukov, A. (1990). *Wave Theory*, Nauka, Moscow.

Yatsyk, V. (2006). Diffraction by a layer and layered structure with positive and negative susceptibilities of Kerr-nonlinear media, *Usp. Sovr. Radioelektroniki* 8: 68–80.

Yatsyk, V. (2007). About a problem of diffraction on transverse non-homogeneous dielectric layer of Kerr-like nonlinearity, *Int. J. Electromagnetic Waves and Electronic Systems* 12(1): 59–69.

Yatsyk, V. (June 21-26, 2010). Generation of the third harmonic at the diffraction on nonlinear layered structure, *International Kharkov Symposium on Physics and Engineering of Microwaves, Millimeter and Submillimeter Waves (MSMW-2010)*, Kharkov, Ukraine, pp. A–20:1–3.

Yatsyk, V. (September 21-24, 2009). Problem of diffraction on nonlinear dielectric layered structure. Generation of the third harmonic, *International Seminar/Workshop on Direct and Inverse Problems of Electromagnetic and Acoustic Wave Theory (DIPED-2009)*, IAPMM, NASU, Lviv, Ukraine, pp. 92–98.
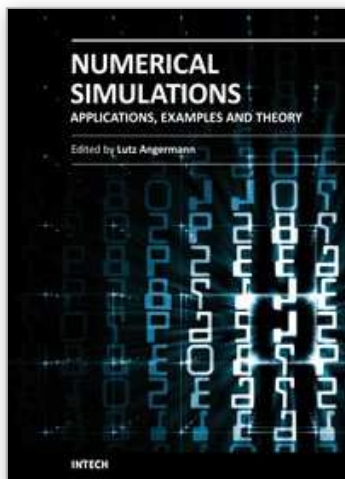
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