

# Scalar approximation for second harmonic generation in a uniaxial crystal

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The problem of second harmonic generation in a quadratically nonlinear uniaxial crystal is considered. It is shown how a set of differential nonlinear wave equations for scalar fields at the frequencies  $\omega$  and  $2\omega$  can be derived rigorously from the Maxwell equations neglecting the effects of depolarization of interacting waves. The transition to an equivalent set of integral equations is considered in detail. It is shown that for beams with a narrow spatial spectrum the equations derived convert into the well-known contracted equations for slowly varying complex amplitudes of interacting waves. The derivation of a recurrence equation is demonstrated. This equation is proposed to be considered as an approximated (with a known accuracy) analytical solution of the scalar nonlinear problem. At the increased number of steps, it transforms into a well-known algorithm of asymptotically exact numerical solution.

## Introduction

In this paper, we consider nonmagnetic ( $\mu = 1$ ) and nonconducting ( $\sigma = 0$ ) media without free charges ( $\rho = 0$ ). The Maxwell equations corresponding to this situation can be written as

$$\operatorname{rot}\mathbf{E} = -\frac{1}{c}\frac{\partial\mathbf{H}}{\partial t}, \quad \operatorname{rot}\mathbf{H} = \frac{1}{c}\frac{\partial\mathbf{D}}{\partial t}. \quad (1)$$

We restrict our consideration to the case of quadratically nonlinear homogeneous uniaxial dielectrics, and the constitutive law for  $\mathbf{D}$  can be represented as

$$\mathbf{D} = \tilde{\varepsilon}\mathbf{E} + 4\pi\mathbf{P} = \tilde{\varepsilon}\mathbf{E} + 4\pi\tilde{\chi}\mathbf{E}\mathbf{E}, \quad (2)$$

where  $\tilde{\varepsilon}$  is the permittivity tensor (of rank 2);  $\tilde{\chi}$  is the tensor of quadratic nonlinear susceptibility (of rank 3).

The solution of Eq. (1) will be sought in the form of a sum of two monochromatic waves at the frequencies  $\omega$  and  $2\omega$ , that is,

$$\mathbf{E}(\mathbf{r}, t) = \frac{1}{2}\{\mathbf{E}_1(\mathbf{r})e^{-i\omega t} + \mathbf{E}_2(\mathbf{r})e^{-i2\omega t} + \text{c.c.}\}. \quad (3)$$

The presence of only two waves in the medium means that we deal with the scalar interaction. Assume that the primary radiation  $\mathbf{E}_1$  is an ordinary wave, while  $\mathbf{E}_2$  is an extraordinary wave. In other words, we consider the *ooe*-interaction.

Excluding  $\mathbf{H}$  from Eq. (1) and substituting it into derived equation (3), we obtain the system of statistical nonlinear wave equations

$$\operatorname{rot}\operatorname{rot}\mathbf{E}_1 - k^2\tilde{\varepsilon}(\omega)\mathbf{E}_1 = C\mathbf{P}_1, \quad (4.1)$$

$$\operatorname{rot}\operatorname{rot}\mathbf{E}_2 - (2k)^2\tilde{\varepsilon}(2\omega)\mathbf{E}_2 = 2C\mathbf{P}_2, \quad (4.2)$$

where

$$k = \omega/c; \quad C = 4\pi k^2; \quad \mathbf{P}_1 = \tilde{\chi}(\omega)\mathbf{E}_1^*\mathbf{E}_2, \quad \mathbf{P}_2 = \tilde{\chi}(2\omega)\mathbf{E}_1\mathbf{E}_1;$$

the frequency dependence of the tensors  $\tilde{\varepsilon}$  and  $\tilde{\chi}$  results from the time dispersion taken into account.<sup>1-3</sup>

A very important consequence follows directly from Eqs. (4). Any exact solution of the system of equations (4) should satisfy the condition for divergence

$$\operatorname{div}\tilde{\varepsilon}(\omega)\mathbf{E}_1 = -4\pi\operatorname{div}\mathbf{P}_1, \quad (5.1)$$

$$\operatorname{div}\tilde{\varepsilon}(2\omega)\mathbf{E}_2 = -2\pi\operatorname{div}\mathbf{P}_2. \quad (5.2)$$

The essence of the scalar approximation of interest consists in the fact that the solution of Eqs. (4) is sought in the form

$$\mathbf{E}_1(\mathbf{r}) = \mathbf{e}_1 U_1(\mathbf{r}), \quad (6.1)$$

$$\mathbf{E}_2(\mathbf{r}) = \mathbf{e}_2 U_2(\mathbf{r}), \quad (6.2)$$

where  $\mathbf{e}_1$  and  $\mathbf{e}_2$  are the constant unit vectors defined *a priori*. Correspondingly, the aim of this study is to show maximally rigorously, whenever possible, the form of the equations (differential and integral) for the scalar fields  $U_1$  and  $U_2$  from Eqs. (6).

Despite the fact that the overwhelming majority of problems of the theory of harmonics generation was considered just in the scalar approximation, a somewhat detailed discussion of the problem formulated above is unknown. Owing to the above-said and taking into account that these problems have a great methodological significance, the urgency of this study seems to be quite obvious. The transition to the scalar approximation for fields in linear uniaxial media was considered earlier.<sup>4</sup> Here it

is proposed to use nearly the same approach, only slightly modified, taking into account that conditions for divergence become inhomogeneous. In addition, this paper considers in detail the possibility of replacing the differential equations by an equivalent system of integral equations. This procedure is, essentially, quite easy, but has a great significance, because, as will be shown in Section 6, it forms a basis for obtaining an analytical solution of the scalar problem of interest.

Before discussing the subject of this paper, we would like to note a principal circumstance. The necessary scalar equations for  $U_1$  and  $U_2$  cannot be obtained through the simple substitution of Eqs. (6) into Eqs. (4), as was done in Ref. 1 for the case of plane waves. This can be demonstrated by a simplest example.

Let a medium be isotropic and linear. In this case, for the field at the frequency of the first harmonic we can find from Eqs. (4)

$$\text{rot rot } \mathbf{E}_1 - k^2 n^2 \mathbf{E}_1 = 0. \quad (7)$$

Substituting Eq. (6.1) into Eq. (7), after elementary transformations we obtain for  $U_1$

$$\left( \mathbf{e}_1 \nabla \frac{\partial U_1}{\partial x} \right) \mathbf{i} + \left( \mathbf{e}_1 \nabla \frac{\partial U_1}{\partial y} \right) \mathbf{j} + \left( \mathbf{e}_1 \nabla \frac{\partial U_1}{\partial z} \right) \mathbf{k} - \mathbf{e}_1 (\nabla^2 U_1 + k^2 n^2 U_1) = 0, \quad (8)$$

where  $\mathbf{i}$ ,  $\mathbf{j}$ ,  $\mathbf{k}$  are unit vectors of coordinate axes.

Let the field  $\mathbf{E}_1$  be linearly polarized, for example, along the axis  $X$ , that is,

$$\mathbf{e}_1 = \{1, 0, 0\}. \quad (9)$$

The substitution of Eq. (9) into Eq. (8) yields three scalar equations

$$\frac{\partial^2 U_1}{\partial x \partial y} = \frac{\partial^2 U_1}{\partial x \partial z} = \frac{\partial^2 U_1}{\partial y^2} + \frac{\partial^2 U_1}{\partial z^2} - k^2 n^2 U_1 = 0. \quad (10)$$

It is obvious that the equalities in Eq. (10) can be satisfied only if we assume that the function  $U_1(\mathbf{r})$  is independent of  $x$ , that is

$$\partial U_1 / \partial x = 0. \quad (11)$$

In other words, the field at the frequency of the first harmonic should be a cylindrical beam and, consequently, we cannot obtain a scalar equation for the three-dimensional amplitude at such an approach. It is clear that this result is a direct consequence from the condition for divergence (5.1), which takes the following form in the particular case under consideration:

$$\text{div } \mathbf{E}_1 = 0 = e_{1x} \frac{\partial U_1}{\partial x} + e_{1y} \frac{\partial U_1}{\partial y} + e_{1z} \frac{\partial U_1}{\partial z} = 0. \quad (12)$$

If we substitute the vector (9) into Eq. (12) now, then obtain the condition (11).

Thus, our statement that we are not interesting in the wave polarization, that is, use the approximations (6), turns out to be insufficient for obtaining the scalar equations for  $U_1$  and  $U_2$  directly from the Maxwell equations in the general case. Some intermediate vector equations are required for the formally rigorous transition to the scalar approximation. The search for such equations at the frequencies of the first and second harmonics is the particular goal of this paper.

## 1. Coordinate systems

The axis  $Z$  of the Cartesian coordinate system is directed along the optical axis of a uniaxial crystal. The axes  $X$  and  $Y$  are believed to coincide with the crystallographic axes. Since the values of components of the tensor  $\tilde{\chi}$  are usually presented just for this coordinate system, the system will be referred to as  $\chi$ -coordinates for definiteness.

The direction of propagation of the laser beam (direction along the longitudinal axis of the beam) is determined by the vector  $\mathbf{s}$ . The problem of interest is to find the second-harmonic (SH) field formed by the laser beam, whose vector  $\mathbf{s}$  makes an arbitrary angle  $\theta$  with the optical axis of the crystal and an arbitrary angle  $\varphi$  with other crystallographic axis, for example,  $X$  in the general case. It is convenient to solve this problem in a different coordinate system, which will be referred to as  $\varepsilon$ -coordinates. The axis  $X$  of the latter is directed along the optical axis, while the axes  $Y$  and  $Z$  are oriented so that the vector  $\mathbf{s}$  lies in the plane  $XZ$ . For nonzero components of the permittivity tensor in the  $\varepsilon$ -coordinates, we have

$$\varepsilon_{11} = n_e^2 \neq \varepsilon_{22} = \varepsilon_{33} = n_o^2, \quad (13)$$

where  $n_o$  and  $n_e$  are the main refractive indices of the uniaxial crystal.

The relation between the  $\chi$ - and  $\varepsilon$ -coordinates has the following form:

$$\left. \begin{aligned} x_\varepsilon &= z_\chi \\ y_\varepsilon &= \sin \varphi x_\chi - \cos \varphi y_\chi \\ z_\varepsilon &= \cos \varphi x_\chi + \sin \varphi y_\chi \end{aligned} \right\}. \quad (14)$$

Finally, consider the system of  $E$ -coordinates, in which the axis  $Z$  is directed along the vector  $\mathbf{s}$ , while two other axes are oriented so that the optical axis ( $\mathbf{o}$ ) lies in the plane  $XZ$ . In this case, we obtain that

$$\mathbf{o} = \{\sin \theta, 0, \cos \theta\}. \quad (15)$$

The relation between the  $\varepsilon$ - and  $E$ -coordinates is described by the equations

$$\left. \begin{aligned} x_\varepsilon &= \sin \theta x_E + \cos \theta z_E \\ y_\varepsilon &= y_E \\ z_\varepsilon &= -\cos \theta x_E + \sin \theta z_E \end{aligned} \right\}, \quad (16)$$

and the  $\chi$ - and  $E$ -coordinates are related as follows:

$$\left. \begin{aligned} x_E &= -\cos\theta \cos\varphi x_\chi - \cos\theta \sin\varphi y_\chi + \sin\theta z_\chi \\ y_E &= \sin\varphi x_\chi - \cos\varphi y_\chi \\ z_E &= \sin\theta \cos\varphi x_\chi + \sin\theta \sin\varphi y_\chi + \cos\theta z_\chi \end{aligned} \right\} \quad (17)$$

Upon the change of the coordinate systems, the components of the tensors  $\tilde{\epsilon}$  and  $\tilde{\chi}$  should be transformed:

$$\epsilon'_{jn} = \sum_{\alpha,\gamma} \frac{\partial x'_j}{\partial x_\alpha} \frac{\partial x'_n}{\partial x_\gamma} \epsilon_{\alpha\gamma}; \quad (18.1)$$

$$\chi'_{ijk} = \sum_{\alpha,\beta,\gamma} \frac{\partial x'_i}{\partial x_\alpha} \frac{\partial x'_j}{\partial x_\beta} \frac{\partial x'_k}{\partial x_\gamma} \chi_{\alpha\beta\gamma}. \quad (18.2)$$

In particular, using Eqs. (13), (16), and (18.1), for components of the  $\tilde{\epsilon}$  tensor in the  $E$ -coordinates we find

$$\begin{aligned} \epsilon_{11} &= n_o^2 b = n_o^2 (c^2 + \beta^2 s^2), \quad \epsilon_{22} = n_o^2, \quad \epsilon_{33} = n_o^2 a = n_o^2 (s^2 + \beta^2 c^2), \\ \epsilon_{13} = \epsilon_{31} &= n_o^2 cs(\beta^2 - 1) = n_o^2 a\rho, \quad \epsilon_{12} = \epsilon_{21} = \epsilon_{32} = \epsilon_{23} = 0, \end{aligned} \quad (19)$$

where  $s \equiv \sin(\theta)$ ;  $c \equiv \cos(\theta)$ ;  $\beta = n_e/n_o$ ;  $\rho = cs(\beta^2 - 1)/a$  is the birefringence angle. It should be also noted that  $n^e(\theta) = n_e/\sqrt{a}$  is the refractive index in the direction of the first harmonic, that is, at the angle  $\theta$  to the optical axis.

## 2. Scalar approximation for the ordinary wave at the first harmonic frequency

Let us write Eq. (4.1) in the  $E$ -coordinate system. The index  $E$  is omitted for simplicity. By definition,<sup>4</sup> the  $o$ -wave should not have a projection of the vector  $\mathbf{E}$  on the optical axis. In the  $E$ -coordinate system (see Eq. (15)), this is equivalent to fulfillment of the condition

$$sE_x + cE_z = 0, \quad (20)$$

where  $s = \sin(\theta)$ ;  $c = \cos(\theta)$ .

Using Eqs. (19) and (20), we find

$$\begin{aligned} \tilde{\epsilon}\mathbf{E}_1 &= \mathbf{i}(\epsilon_{11}E_{1x} + \epsilon_{13}E_{1z}) + \mathbf{j}\epsilon_{22}E_{1y} + \mathbf{k}(\epsilon_{13}E_{1x} + \epsilon_{33}E_{1z}) = \\ &= n_o^2 \left\{ \mathbf{i}E_{1x} \left[ c^2 + \beta^2 s^2 - \frac{s}{c} cs(\beta^2 - 1) \right] + \mathbf{j}E_{1y} + \right. \\ &\quad \left. + \mathbf{k}E_{1z} \left[ -\frac{c}{s} cs(\beta^2 - 1) + s^2 + \beta^2 c^2 \right] \right\} = n_o^2 \mathbf{E}_1. \end{aligned} \quad (21)$$

This means that for the  $o$ -wave the conditions for divergence (5.1) can be written in the form

$$\text{div}\mathbf{E}_1 = -\frac{4\pi}{n_o^2} \text{div}\mathbf{P}_1. \quad (22)$$

Substituting Eq. (22) in Eq. (4.1), we obtain that any exact solution of Eq. (4.1) should also be a solution of the equation

$$\nabla^2 \mathbf{E}_1 + k_1^2 \mathbf{E}_1 = -C\mathbf{P}_1 - \frac{4\pi}{n_o^2} \text{grad div}\mathbf{P}_1, \quad (23)$$

where  $k_1 = kn_o(\omega)$ .

It is important to note that the inverse proposition is not valid in the general case. The exact solution of Eq. (23) does not need to be simultaneously the exact solution of Eq. (4.1), and this manifests itself in the failure of equality (22). The conclusion formulated is, quite obviously, the direct consequence of the fact that condition (22) was assumed to hold *a priori* when deriving Eq. (23).

For the vector function  $\mathbf{E}_1(\mathbf{r})$  to be the exact solution of the Maxwell equations [or wave equation (4.1)], it is necessary and sufficient for  $\mathbf{E}_1$  to be the exact solution of Eq. (23) and to exactly meet condition (22). Actually, in the most general case,  $\mathbf{E}_1$  can be presented in the form

$$\mathbf{E}_1(\mathbf{r}) = \mathbf{e}_1(\mathbf{r})U_1(\mathbf{r}), \quad (24)$$

where

$$e_{1j}(\mathbf{r}) = E_{1j}(\mathbf{r})/U_1(\mathbf{r}), \quad j = x, y, z.$$

In this case, equations (22) and (23) make four scalar equations sufficient for unambiguous determination of four unknown scalar functions  $U_1(\mathbf{r})$  and  $e_{1j}(\mathbf{r})$ .

Assume that determination of the exact form of the functions  $e_{1j}(\mathbf{r})$  is a secondary problem. Thus, in place of the exact solution of Eq. (24), we will search for an approximate solution of the form (6.1), that is, restrict ourselves by determination of only one scalar function  $U_1(\mathbf{r})$ . With this formulation of the problem (search for the solution in the scalar approximation), one equation (23) is already insufficient. To make sure, substitute Eq. (6.1) into Eq. (23), multiply the both sides of the equation scalarly by  $\mathbf{e}_1$ , and obtain the equation for the scalar field at the first harmonic (FH) frequency:

$$\nabla^2 U_1 + k_1^2 U_1 = -C\mathbf{e}_1\mathbf{P}_1 - \frac{4\pi}{n_o^2} \mathbf{e}_1 \text{grad div}\mathbf{P}_1. \quad (25)$$

If all  $\chi_{ijk} = 0$ , then equation (25) is transformed into the Helmholtz equation, being the basic equation for the field in a homogeneous isotropic medium.

Here we do not discuss how strongly  $U_1$  from Eq. (25) differs from the function  $|\mathbf{E}_1| = \sqrt{E_{1x}^2 + E_{1y}^2 + E_{1z}^2}$ , obtained as a solution of Eq. (4.1). Taking into account this circumstance, but keeping in mind that there is no other principal inconsistency in the reasoning presented, we call this

procedure of transition to the scalar approximation formally rigorous.

Let us specify the form of the vectors  $\mathbf{e}_1$  and  $\mathbf{e}_2$  from Eq. (6) taking into account that the field  $\mathbf{E}_1$  should be an ordinary wave, while  $\mathbf{E}_2$  should be an extraordinary wave:

$$\mathbf{e}_1 = \{0, 1, 0\}, \mathbf{e}_2 = \{1, 0, 0\}. \tag{26}$$

In the  $E$ -coordinates, vectors (26) determine polarization of the plane  $o$ - and  $e$ -waves propagating along the axis  $Z$  (the tilt of the vector  $\mathbf{e}_2$  due to birefringence is ignored).

Using Eq. (26), we find

$$\mathbf{P}_1 = \tilde{\chi}(\omega)\mathbf{E}_1\mathbf{E}_2 = \mathbf{p}_o P_o, \tag{27}$$

where

$$\mathbf{p}_o = \{\mathbf{i}\chi_{121} + \mathbf{j}\chi_{221} + \mathbf{k}\chi_{321}\}; P_o = U_1^* U_2;$$

$\mathbf{i}, \mathbf{j}, \mathbf{k}$  are unit vectors of the  $E$ -coordinates.

Upon substitution of Eq. (27) into Eq. (25), we obtain

$$\nabla^2 U_1 + k_1^2 U_1 = F_1(\mathbf{r}), \tag{28}$$

where

$$F_1(\mathbf{r}) = 2k_1\sigma_1 P_o - \frac{4\pi}{n_o^2} \left\{ \chi_{121} \frac{\partial^2 P_o}{\partial x \partial y} + \chi_{221} \frac{\partial^2 P_o}{\partial y^2} + \chi_{321} \frac{\partial^2 P_o}{\partial y \partial z} \right\};$$

$$\sigma_1 = -\frac{2\pi k_1}{n_o^2} \chi_{221}$$

is the nonlinear coupling coefficient.

Equation (28) is the most general form of representation of the scalar equation for the ordinary wave at the FH frequency.

Using a KDP as an example, we illustrate how the nonlinear coupling coefficient is specified. In the  $\chi$ -coordinates, the following coefficients are nonzero in crystals of this symmetry<sup>1</sup>:

$$\chi_{123} = \chi_{132} = \chi_{213} = \chi_{231} \approx \chi_{312} = \chi_{321} \approx d_{36}.$$

Substituting these values in Eq. (18.2) and using Eq. (17), we find that in Eq. (28)  $\chi_{221} = -d_{36} \sin(\theta) \sin(2\varphi)$ . The equation for the nonlinear coupling coefficient is transformed into the well-known equation presented in all corresponding papers (see, for example, Refs. 1 and 2).

### 3. Scalar approximation for the extraordinary wave of the second harmonic

Write Eq. (4.2) in the  $\varepsilon$ -coordinates ( $\varepsilon$  is omitted). By definition,<sup>4</sup> the field of the  $e$ -wave should not have a projection of the vector  $\mathbf{H}$  on the optical axis. Consequently:

$$H_{2x} = \frac{1}{i2k} \left( \frac{\partial E_{2z}}{\partial y} - \frac{\partial E_{2y}}{\partial z} \right) = 0. \tag{29}$$

From Eq. (29) we obtain

$$\frac{\partial^2 E_{2z}}{\partial y \partial z} = \frac{\partial^2 E_{2y}}{\partial z^2}, \frac{\partial^2 E_{2z}}{\partial y^2} = \frac{\partial^2 E_{2y}}{\partial y \partial z}. \tag{30}$$

Upon differentiation of Eq. (5.2), three additional equations are obtained, which have the following form taking into account Eq. (30):

$$\frac{\partial^2 E_{2y}}{\partial x \partial y} + \frac{\partial^2 E_{2z}}{\partial x \partial z} = -\beta^2 \frac{\partial^2 E_{2x}}{\partial x^2} - \frac{2\pi}{n_{2o}^2} \frac{\partial}{\partial x} \text{div} \mathbf{P}_2,$$

$$\frac{\partial^2 E_{2x}}{\partial x \partial y} = -\frac{1}{\beta^2} \left( \frac{\partial^2 E_{2y}}{\partial y^2} + \frac{\partial^2 E_{2y}}{\partial z^2} \right) - \frac{2\pi}{n_{2e}^2} \frac{\partial}{\partial y} \text{div} \mathbf{P}_2, \tag{31}$$

$$\frac{\partial^2 E_{2x}}{\partial x \partial z} = -\frac{1}{\beta^2} \left( \frac{\partial^2 E_{2z}}{\partial y^2} + \frac{\partial^2 E_{2z}}{\partial z^2} \right) - \frac{2\pi}{n_{2e}^2} \frac{\partial}{\partial z} \text{div} \mathbf{P}_2,$$

where  $n_{2o}$  and  $n_{2e}$  are the main refractive indices at the frequency  $2\omega$ ;  $\beta = n_{2e}/n_{2o}$ .

After substitution of Eqs. (29) and (31) in Eq. (4.2) (see Ref. 4), it becomes clear that any exact solution of Eq. (4.2) should also satisfy the equation

$$\nabla_{\beta}^2 \mathbf{E}_2 + k_{2e}^2 \mathbf{E}_2 = -2C \mathbf{P}_{\beta} - \frac{2\pi}{n_{2o}^2} \text{grad div} \mathbf{P}_2, \tag{32}$$

where

$$\mathbf{P}_2 = \{P_{2x}, P_{2y}, P_{2z}\}, \mathbf{P}_{\beta} = \{P_{2x}, \beta^2 P_{2y}, \beta^2 P_{2z}\};$$

$$\nabla_{\beta}^2 = \beta^2 \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}; k_{2e} = 2kn_{2e}.$$

Now we substitute Eq. (6.2) into Eq. (32) and after scalar multiplication by  $\mathbf{e}_2$  obtain the equation

$$\nabla_{\beta}^2 U_2 + k_{2e}^2 U_2 = -2C \mathbf{e}_2 \mathbf{P}_{\beta} - \frac{2\pi}{n_{2o}^2} \mathbf{e}_2 \text{grad div} \mathbf{P}_2, \tag{33}$$

which is the sought scalar approximation for Eq. (4.2) written in the  $\varepsilon$ -coordinate system.

Refer now to the  $E$  coordinate system, in which the vector  $\mathbf{e}_2$  has, as we decided above, the form (26), and

$$\mathbf{P}_2 = \tilde{\chi}(2\omega)\mathbf{E}_1\mathbf{E}_1 = \mathbf{p}_e P_e, \tag{34}$$

where

$$P_e = U_1^2(\mathbf{r}); \mathbf{p}_e = \{\mathbf{i}\chi_{122} + \mathbf{j}\chi_{222} + \mathbf{k}\chi_{322}\};$$

$\mathbf{i}, \mathbf{j}, \mathbf{k}$  are unit vectors of  $E$  coordinates.

It follows from Eqs. (34) and (26) that

$$\mathbf{e}_2 \text{grad div} \mathbf{P}_2 = \chi_{122} \frac{\partial^2 P_e}{\partial x^2} + \chi_{222} \frac{\partial^2 P_e}{\partial x \partial y} + \chi_{322} \frac{\partial^2 P_e}{\partial x \partial z}. \tag{35}$$

Now determine vectors  $\mathbf{e}_2$  and  $\mathbf{P}_2$  in the  $\varepsilon$ -coordinate system. Using Eq. (16), we find

$$\mathbf{e}_2 = \mathbf{i}s - \mathbf{k}c; \tag{36.1}$$

$$\mathbf{P}_2 = U_1^2(\mathbf{r}) \{\mathbf{i}(s\chi_{122} + c\chi_{322}) + \mathbf{j}\chi_{222} + \mathbf{k}(-c\chi_{122} + s\chi_{322})\}, \tag{36.2}$$

where, as above,  $s = \sin\theta$ ,  $c = \cos\theta$ , and  $\mathbf{i}, \mathbf{j}, \mathbf{k}$  are unit vectors of the  $\epsilon$ -coordinate system.

Taking into account Eq. (36), for the scalar product  $\mathbf{e}_2\mathbf{P}_\beta$  from Eq. (33) we have

$$\begin{aligned} \mathbf{e}_2\mathbf{P}_\beta &= U_1^2(\mathbf{r})[s(c\chi_{122} + c\chi_{322}) - c\beta^2(-c\chi_{122} + s\chi_{322})] = \\ &= a\chi_{122} - a\rho\chi_{322}, \end{aligned} \quad (37)$$

where the coefficients  $a$  and  $\rho$  are determined in Eq. (19).

To find the sought equation for the scalar field  $U_2$  of the second harmonic, we write Eq. (33) using Eq. (16) in the  $E$ -coordinates, substitute Eqs. (35) and (37) into the equation derived, and obtain

$$\left( \frac{\partial^2}{\partial z^2} + 2\rho \frac{\partial^2}{\partial x \partial z} + \frac{b}{a} \frac{\partial^2}{\partial x^2} + \frac{1}{a} \frac{\partial^2}{\partial y^2} + k_2^2 \right) U_2 = F_2(\mathbf{r}), \quad (38)$$

where the parameter  $b$  is determined in Eq. (19), and  $k_2$  is determined in Eq. (29);

$$\begin{aligned} F_2(\mathbf{r}) &= 2k_2\sigma_2 a P_e + 2C a \rho \chi_{322} P_e - \\ &- \frac{2\pi}{n_o^2} \left( \chi_{122} \frac{\partial^2}{\partial x^2} + \chi_{222} \frac{\partial^2}{\partial x \partial y} + \chi_{322} \frac{\partial^2}{\partial x \partial z} \right) P_e; \\ \sigma_2 &= - \frac{\pi k_2}{(n_e^2)^2} \chi_{122} \end{aligned}$$

is the second nonlinear coupling coefficient.

Equation (38) in its content is a full analog of Eq. (28), but for the  $e$ -wave at the double frequency. It should be also noted that the structures of these equations coincide completely if we assume  $\beta = 1$  (isotropic medium) in Eq. (38). Repeating the procedure used in Section 2, we obtain that  $\sigma_2$  from Eq. (38) in the KDP crystal depends on  $\chi_{122} = d_{36} \sin(\theta) \sin(2\varphi)$ , that is, we again have the well-known equation for the nonlinear coupling coefficient.

Thus, the main results from Sections 2 and 3 can be formulated as follows. If, according to the conditions of the problem, the approximate representations (6) + (26) for the FH and SH fields are declared suitable, then Eqs. (28) and (38) (written in the  $E$ -coordinates in this case) form the system of differential equations for determination of the amplitudes  $U_1$  and  $U_2$  from Eq. (6). This system is the sought scalar approximation of the rigorous problem determined by the wave equations (4).

### 4. Integral equations for first and second harmonics

Consider the transition to the integral equation for the scalar field  $U_2$  of the second harmonic. For the field of the first harmonic, all the calculations are quite analogous and simpler.

We refer to the  $\epsilon$ -coordinate system and introduce the Green's function  $g_e(\mathbf{r}, \mathbf{r}_0)$ , which is the solution of the equation

$$\nabla_\beta^2 g_e + k_{2e}^2 g_e = -4\pi\delta(\mathbf{r} - \mathbf{r}_0), \quad (39)$$

where  $\nabla_\beta^2$  and  $k_{2e}$  are determined in Eq. (32).

It can be easily shown that the solution of Eq. (39) has the form

$$g_e(\mathbf{r}, \mathbf{r}_0) = \frac{1}{\beta} \frac{e^{ik_{2e}R'}}{R'}, \quad (40)$$

where

$$\begin{aligned} R' &= \sqrt{\frac{(x-x_0)^2}{\beta^2} + (y-y_0)^2 + (z-z_0)^2}; \\ \beta &= n_{2e}(2\omega) / n_{2o}(2\omega). \end{aligned}$$

Multiply Eq. (33) by  $g_e$  and Eq. (39) by  $U_2$ , subtract the latter from the former, and integrate the result over an arbitrary volume  $V$  bounded by the closed surface  $S$ . As a result, for an arbitrary internal observation point  $\mathbf{r}_0$  is

$$\begin{aligned} U_2(\mathbf{r}_0) &= \frac{1}{4\pi} \int_V (g_e \nabla_\beta^2 U_2 - U_2 \nabla_\beta^2 g_e) dV - \\ &- \frac{1}{4\pi} \int_V F_2(\mathbf{r}) g_e(\mathbf{r}, \mathbf{r}_0) dV, \end{aligned} \quad (41)$$

where  $F_2(\mathbf{r})$  is used to designate the right-hand side of Eq. (33).

In Eq. (41), pass to the new coordinates

$$x' = x/\beta, \quad y' = y, \quad z' = z \quad (42)$$

and for the first integral ( $I(\mathbf{r}_0)$ ) in the right-hand side of Eq. (41) have (dashes are omitted)

$$I(\mathbf{r}_0) = \frac{1}{4\pi} \int_V (g_e \nabla^2 U_2 - U_2 \nabla^2 g_e) \beta dV. \quad (43)$$

Here, the explicit form of  $g_e$  can be found from Eq. (40) using Eq. (42), and  $dV_\epsilon = dx_\epsilon dy_\epsilon dz_\epsilon$  should be replaced with  $\beta dx' dy' dz' = \beta dV'$ .

By Green's theorem, for Eq. (43) we have

$$I(\mathbf{r}_0) = \frac{1}{4\pi} \int_S \left( g_e \frac{\partial U_2}{\partial \mathbf{n}} - U_2 \frac{\partial g_e}{\partial \mathbf{n}} \right) \beta dS, \quad (44)$$

where  $\mathbf{n}$  is the external normal to the surface  $S$  bounding the volume  $V$ .

As  $S$ , select the plane  $Z_E = 0$  of the  $E$ -coordinate system closed by a hemisphere of finite radius in the region  $Z_E > 0$ . The integral over the hemisphere is neglected by common reasons,<sup>3,5</sup> and we conclude that the surface  $S$  in Eq. (44) is the plane  $Z_E = 0$ .

Using Eq. (16), we find that in the  $\epsilon$ -coordinates the position of the external normal to  $S$  is determined as

$$\mathbf{n} = \{-c, 0, -s\}, \quad (45.1)$$

while in the coordinates (42)

$$\mathbf{n} = \{-c/\beta, 0, -s\}, \quad (45.2)$$

where, as above,  $s = \sin\theta$ ,  $c = \cos\theta$ .

Now substitute Eq. (45.2) in Eq. (44). Then

$$I(\mathbf{r}_0) = \frac{1}{4\pi} \int_S \left[ -g_e(c/\beta) \frac{\partial U_2}{\partial x} - g_e s \frac{\partial U_2}{\partial z} + U_2(c/\beta) \frac{\partial g_e}{\partial x} + U_2 s \frac{\partial g_e}{\partial z} \right] \beta dS. \quad (46)$$

In Eq. (46), return to the  $\varepsilon$ -coordinates and take into account that

$$dS' \sim dx'dy' \rightarrow \frac{1}{\beta} dx_\varepsilon dy_\varepsilon \sim \frac{1}{\beta} dS_\varepsilon, \quad (47)$$

then substitute the result in Eq. (41) and obtain

$$U_2(\mathbf{r}_0) = -\frac{1}{4\pi} \int_V F_2(\mathbf{r}) g_e(\mathbf{r}, \mathbf{r}_0) dV + \frac{1}{4\pi} \int_S \left[ -g_e c \frac{\partial U_2}{\partial x} - g_e s \frac{\partial U_2}{\partial z} + U_2 c \frac{\partial g_e}{\partial x} + U_2 s \frac{\partial g_e}{\partial z} \right] dS. \quad (48)$$

Write Eq. (48) in the  $E$ -coordinates, taking into account that from Eq. (16)

$$\frac{\partial}{\partial x_\varepsilon} = s \frac{\partial}{\partial x_E} + c \frac{\partial}{\partial z_E}, \quad \frac{\partial}{\partial z_\varepsilon} = -c \frac{\partial}{\partial x_E} + s \frac{\partial}{\partial z_E},$$

and finally obtain

$$U_2(\mathbf{r}_0) = -\frac{1}{4\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx dy \int_0^{\infty} F_2(\mathbf{r}) g_e(\mathbf{r}, \mathbf{r}_0) dz + \frac{1}{4\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left( U_2 \frac{\partial g_e}{\partial z} - g_e \frac{\partial U_2}{\partial z} \right)_{z=0} dx dy, \quad (49)$$

where  $g_e$  is the function (40) written in the  $E$ -coordinates and having the form<sup>4</sup>:

$$g_e(\mathbf{r}, \mathbf{r}_0) = \frac{\sqrt{a}}{\beta} \frac{e^{ik_2 R'}}{R'}; \quad (50)$$

$$R' = \sqrt{\frac{a^2}{\beta^2} (x - x_0 + \rho z_0 - \rho z)^2 + (y - y_0)^2 + (z - z_0)^2};$$

$k_2$  was determined in Eq. (29).

Equation (49) written in the  $E$ -coordinates is the integral equivalent of the differential equation (38). Quite analogously, but without invoking the additional coordinate system (42), it can be shown that the differential equation (28) is equivalent to the integral equation, which in the  $E$ -coordinates is

$$U_1(\mathbf{r}_0) = \frac{1}{4\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left[ g_o \frac{\partial U_1}{\partial z} - U_1 \frac{\partial g_o}{\partial z} \right]_{z=0} dx dy - \frac{1}{4\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx dy \int_0^{z_0} F_1(\mathbf{r}) g_o(\mathbf{r}, \mathbf{r}_0) dz, \quad (51)$$

where  $F_1$  was determined in Eq. (28);

$$g_o(\mathbf{r}, \mathbf{r}_0) = e^{ik_1 R} / R; \quad (52)$$

$$R = \sqrt{(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2};$$

$k_1$  is determined in Eq. (23).

In Eq. (49), the surface integral is calculated on the plane  $Z = 0$ . This allows us to somewhat simplify the final result<sup>6</sup> by using

$$G_e(\mathbf{r}, \mathbf{r}_0) = g_e(\mathbf{r}, \mathbf{r}_0) - g_{2m}(\mathbf{r}, \mathbf{r}_0) \quad (53)$$

in place of  $g_e(\mathbf{r}, \mathbf{r}_0)$ . In Eq. (53),  $g_{2m} = g_e(x, y, -z, \mathbf{r}_0)$ , which also is a rigorous solution of Eq. (39).

Substituting  $G_e$  in Eq. (49), we make sure that under the sign of the volume integral the following functions appear

$$F_2 g_e \sim e^{i(2k_1 - k_2)z}, \quad F_2 g_{2m} \sim e^{i(2k_1 + k_2)z}. \quad (54)$$

Taking into account that  $k_{1z}$  and  $k_{2z}$  are very large,  $F_2 g_{2m}$  from Eq. (54) turns out to be a fast oscillating function of the variable  $z$ , and the integral of this function with respect to  $dz$  can be neglected.

Thus, invoking Eq. (53) and the analogous function for the  $o$ -wave:

$$G_o(\mathbf{r}, \mathbf{r}_0) = g_o(\mathbf{r}, \mathbf{r}_0) - g_{1m}(\mathbf{r}, \mathbf{r}_0), \quad (55)$$

where  $g_{1m}(\mathbf{r}, \mathbf{r}_0) = g_o(x, y, -z, \mathbf{r}_0)$ , we obtain in place of Eqs. (49) and (51) respectively

$$U_1(\mathbf{r}_0) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left( U_1 \frac{\partial g_o}{\partial z} \right)_{z=0} dx dy - \frac{1}{4\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx dy \int_0^{z_0} F_1(\mathbf{r}) g_o(\mathbf{r}, \mathbf{r}_0) dz, \quad (56.1)$$

$$U_2(\mathbf{r}_0) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left( U_2 \frac{\partial g_e}{\partial z} \right)_{z=0} dx dy - \frac{1}{4\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx dy \int_0^{z_0} F_2(\mathbf{r}) g_e(\mathbf{r}, \mathbf{r}_0) dz, \quad (56.2)$$

where  $F_1$  and  $F_2$ , determined in Eqs. (28) and (38), are equal to zero outside the crystal; the observation plane  $z = z_0$  is internal with respect to the crystal, that is,

$$0 \leq z_0 \leq L. \quad (57)$$

Equations (56) are just the required system of integral equations for the scalar amplitudes  $U_1$  and  $U_2$  of the field at the FH and SH frequencies. When deriving equation (56), we assume implicitly that the following conditions are met:

1. The laser beam radius in the crystal should be much smaller than the transversal dimensions of the crystal itself. This allows us to use infinite limits in the integrals with respect to  $dx dy$  from Eq. (56).

2. Refraction of the fields at the entrance and exit sides of the crystal is ignored, that is, both the boundary conditions and the solution (56) are believed to be defined inside the crystal.

3. Reflection from the crystal exit side and wave backscattering are neglected, which allows Eq. (56) to be used for any internal plane.<sup>7</sup>

Note also that in the paraxial approximation (see Section 5) equation (56) can be easily generalized to the case  $z_0 > L$  [Refs. 8 and 9]. However, within the framework of this paper, this possibility is not of principal interest, and we restrict our consideration to the scopes determined by the inequality (57).

### 5. Equations for SHG in the paraxial approximation

Assume that the nonlinear crystal is a slightly anisotropic medium, while the laser radiation is represented by a slightly divergent beam, that is,

$$|\rho| \sim |\alpha| \sim \mu \ll 1, \tag{58}$$

where  $\alpha$  is the beam divergence;  $\rho$  is the birefringence angle determined in Eq. (19).

Condition (58) is sufficient<sup>3</sup> for

$$\left| \frac{x-x_0}{z-z_0} \right| \sim \left| \frac{y-y_0}{z-z_0} \right| \sim \mu \ll 1. \tag{59}$$

to be true in Eq. (56).

In this case, for parameters of Eq. (56) we obtain<sup>4</sup>:

$$\begin{aligned} R &= (z_0 - z) + \frac{(x-x_0)^2 + (y-y_0)^2}{2(z_0 - z)} + O(\mu^3, \mu^4, \dots), \\ R' &= (z_0 - z) + \frac{(x-x_0 + \rho z_0 - \rho z)^2 + (y-y_0)^2}{2(z_0 - z)} + O(\mu^3, \mu^4, \dots), \\ a \sim b \sim \beta &\approx 1 + O(\mu, \mu^2, \dots), \end{aligned} \tag{60}$$

where  $O(\mu, \mu^2, \mu^3, \dots)$  are values of the orders of  $\mu, \mu^2, \mu^3$ , etc.

Another decisive indicator of the paraxial approximation is the validity of representation of the fields  $U_1$  and  $U_2$  of interest in the form of quasiplane waves:

$$U_{1,2}(\mathbf{r}) = A_{1,2}(\mu x, \mu y, \mu^2 z) e^{ik_1 z}, \tag{61}$$

where  $\mu$  is the small parameter of Eq. (58).

Using Eq. (61) for  $F_1$  and  $F_2$ , we obtain from Eq. (58):

$$\begin{aligned} F_1 &= 2k_1 \sigma_1 A_1^* A_2 e^{i(k_2 - k_1)z} + O(\mu, \mu^2, \dots), \\ F_2 &= 2k_2 \sigma_2 A_1^2 e^{i2k_2 z} + O(\mu, \mu^2, \dots). \end{aligned} \tag{62}$$

Substitute Eqs. (60)–(62) in Eq. (56) and remain the terms up to the second order of smallness inclusive in the exponents. For terms outside the exponents, we remain by zero order of smallness. As a result, in place of Eq. (56) we have the following system of integral equations for the complex amplitudes  $A_1$  and  $A_2$  from Eq. (61):

$$\begin{aligned} A_1(\mathbf{r}_0) &= \frac{ik_1}{2\pi z_0} \times \\ &\times \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} A_1(x, y) \exp \left[ ik_1 \frac{(x-x_0)^2 + (y-y_0)^2}{2z_0} \right] dx dy - \\ &- i\sigma_1 \int_0^{z_0} dz \left[ -\frac{ik_1}{2\pi(z_0 - z)} \right] e^{i\Delta k z} \times \\ &\times \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} A_1^*(\mathbf{r}) A_2(\mathbf{r}) \exp \left[ ik_1 \frac{(x-x_0)^2 + (y-y_0)^2}{2(z_0 - z)} \right] dx dy, \end{aligned} \tag{63.1}$$

$$\begin{aligned} A_2(\mathbf{r}_0) &= \frac{ik_2}{2\pi z_0} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} A_2(x, y) \times \\ &\times \exp \left[ ik_2 \frac{(x-x_0 + \rho z_0)^2 + (y-y_0)^2}{2z_0} \right] dx dy - \\ &- i\sigma_2 \int_0^{z_0} dz \left[ -\frac{ik_2}{2\pi(z_0 - z)} \right] e^{-i\Delta k z} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} A_1^2(\mathbf{r}) \times \\ &\times \exp \left[ ik_2 \frac{(x-x_0 + \rho z_0 - \rho z)^2 + (y-y_0)^2}{2(z_0 - z)} \right] dx dy, \end{aligned} \tag{63.2}$$

where  $A_1(x, y)$  and  $A_2(x, y)$  are the boundary conditions determined at the entrance into the crystal and inside the crystal.

The direct substitution demonstrates clearly that the integral equations (63) are equivalent to the following differential equations:

$$\left[ \frac{\partial}{\partial z} + \frac{1}{2ik_1} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \right] A_1 = -i\sigma_1 A_1^* A_2 e^{-i\Delta k z}, \tag{64.1}$$

$$\left[ \frac{\partial}{\partial z} + \rho \frac{\partial}{\partial x} + \frac{1}{2ik_2} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \right] A_2 = -i\sigma_2 A_1^2 e^{-i\Delta k z}. \tag{64.2}$$

Equations (64) are called contracted (or parabolic), and just they are the basic ones in the theory of harmonic generation.<sup>1–3</sup>

### 6. Asymptotically exact solution of the system of integral equations

If to differentiate the left-hand and right-hand sides of Eq. (56) with respect to  $z_0$ , then the system of equations can be obtained in the form, for which the efficient method of numerical calculation has been developed.<sup>10</sup> Without consideration of this approach, called the method of separation by physical properties, let us try to derive the analogous result for our particular problem from simple physical reasoning. To do this, the basic principles of the perturbation method are needed,<sup>3</sup> which, in turn, also is a method for solution of the nonlinear problem.

Represent the system of equations (56) in the form

$$\begin{aligned} U_1(x, y, L) &= U_{1\text{lin}}(x, y, L) + \sigma \hat{L}_1 U_{1(\mathbf{r})}^* U_2(\mathbf{r}), \\ U_2(x, y, L) &= U_{2\text{lin}}(x, y, L) + \sigma \hat{L}_2 U_1^2(\mathbf{r}), \end{aligned} \tag{65}$$

where  $L$  is the length of the crystal;  $U_{1\text{lin}}$  and  $U_{2\text{lin}}$  are solutions of the corresponding linear problems for the fields at the exit from the crystal (they coincide with the integrals over plane in Eqs. (56));  $\hat{L}_1$  and  $\hat{L}_2$  are volume integrals from Eqs. (56), and it is assumed for simplicity that  $\sigma_1 \approx \sigma_2 \approx \sigma$ .

Equations (65) are solved with the boundary conditions, determined at the entrance into the crystal:

$$U_1(x, y, 0) = U_{10}(x, y), \quad U_2(x, y, 0) = U_{20}(x, y). \quad (66)$$

It is obvious that at the given conditions (66) the functions  $U_{1\text{lin}}$  and  $U_{2\text{lin}}$  should also be considered as known.

Rewrite Eqs. (65) as follows:

$$V_1(x, y, L) = V_{1\text{lin}}(x, y, L) + \mu \hat{L}_1 \frac{1}{L} V_1^*(\mathbf{r}) V_2(\mathbf{r}), \quad (67)$$

$$V_2(x, y, L) = V_{2\text{lin}}(x, y, L) + \mu \hat{L}_2 \frac{1}{L} V_1^2(\mathbf{r}),$$

where

$$A_0 = U_{1,2} / A_0; \quad (V_{1,2})_{\text{lin}} = (U_{1,2})_{\text{lin}} / A_0;$$

$A_0$  is the maximal value of the function  $U_{10}(x, y)$ ;  $\mu$  is a dimensionless parameter determined by the equation

$$\mu = \sigma L A_0. \quad (68)$$

If

$$\mu \ll 1, \quad (69)$$

then the solution of Eq. (67) should be searched in the form

$$V_1 = V_{10} + \mu V_{11} + \mu^2 V_{12} + \dots, \quad (70)$$

$$V_2 = V_{20} + \mu V_{21} + \mu^2 V_{22} + \dots$$

Substitute Eq. (70) in Eq. (67) and equalize the coefficients of  $\mu$  to the same power. Then in the zero approximation (unperturbed, linear problem), the solution can be written in the form  $V_{10} = V_{1\text{lin}}$ ,  $V_{20} = V_{2\text{lin}}$ , then the functions

$$V_1 = V_{10} + \mu V_{11} = V_{1\text{lin}} + \mu \hat{L}_1 \frac{1}{L} V_{1\text{lin}}^* V_{2\text{lin}}, \quad (71)$$

$$V_2 = V_{20} + \mu V_{21} = V_{2\text{lin}} + \mu \hat{L}_2 \frac{1}{L} V_{1\text{lin}}^2$$

are solutions of Eq. (67) in the first approximation. It can be easily shown how the approximations of higher orders look, but we restrict our consideration to Eqs. (71), which take the following forms in the initial designations

$$\begin{aligned} U_1 &= U_{1\text{lin}} + \sigma \hat{L}_1 U_{1\text{lin}}^* U_{2\text{lin}}, \\ U_2 &= U_{2\text{lin}} + \sigma \hat{L}_2 U_{1\text{lin}}^2. \end{aligned} \quad (72)$$

Approximation (72) is used most often along with the assumption that the function  $V_{20}$  from Eq. (70) is zero (the SH field is absent at the entrance to the crystal). Thus, in Eq. (72)  $U_1 = U_{1\text{lin}}$  (the FH field does not undergo the nonlinear perturbation), and we come to the so-called approximation of the given field, which is widely used<sup>1-3</sup> to describe the low-efficiency generation of harmonics.

Another quite important aspect should be noted. Designate the exact solution of the nonlinear problem as  $(U_{1,2})_E$ , and the solution in the first approximation [that is, Eq. (72)] as  $(U_{1,2})_F$ . It can be easily shown that the use of the approximation (72) gives the following errors in the calculation of interacting fields

$$\eta_{1,2} = [(U_{1,2})_E - (U_{1,2})_F] / (U_{1,2})_E \sim \mu^2, \quad (73)$$

where  $\mu$  is determined by Eq. (68).

Taking into account the above-said, let us pass to the direct goal of this Section. Let us divide virtually the nonlinear crystal into  $N$  layers by planes normal to the longitudinal axis, such gaining  $N + 1$  planes:

$$z = z_k = (k - 1)\Delta, \quad \Delta = L / N, \quad k = 1, 2, N + 1. \quad (74)$$

Assume that the solution of Eq. (65) for an arbitrary plane  $z = z_k$  appeared to be known in some way, as well as the functions

$$U_1(x, y, z_k) = U_{1,k}(x, y), \quad U_2(x, y, z_k) = U_{2,k}(x, y), \quad (75)$$

and our task is to find  $U_1$  and  $U_2$  on the plane  $z = z_{k+1}$  (that is, to determine  $U_{1,k+1}$  and  $U_{2,k+1}$ ) using Eq. (75) as new boundary conditions.

It is clear that such an "intermediate" task is not simpler than the initial one, because it is still reduced to the solution of the same equations (65), but with other boundary conditions. It is quite another matter that selecting the value of  $N$  in Eq. (74) large enough, we can satisfy the following condition with any required accuracy

$$\mu_k = (\sigma \Delta A_{0k}) = (\sigma \frac{L}{N} A_{0k}) \ll 1, \quad (76)$$

where  $A_{0k}$  is the maximal value of  $U_{1,k}(x, y)$ , consequently, we can obtain sufficiently good approximation for  $U_{1,k+1}$  and  $U_{2,k+1}$  using Eq. (72).

Using this feasibility, we find that

$$\begin{aligned} U_{1,k+1}(x, y, z_{k+1}) &= U_{1\text{lin},k}(x, y, z = \Delta) + U_{1\text{nonl},k}(x, y, z = \Delta), \\ U_{2,k+1}(x, y, z_{k+1}) &= U_{2\text{lin},k}(x, y, z = \Delta) + U_{2\text{nonl},k}(x, y, z = \Delta), \end{aligned} \quad (77)$$

where

$$\begin{aligned}
 U_{1lin,k}(\mathbf{r}_0) &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} U_{1,k}(x,y) \left[ \frac{\partial g_o(\mathbf{r}, \mathbf{r}_0)}{\partial z} \right]_{z=0} dx dy, \\
 U_{2lin,k}(\mathbf{r}_0) &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} U_{2,k}(x,y) \left[ \frac{\partial g_e(\mathbf{r}, \mathbf{r}_0)}{\partial z} \right]_{z=0} dx dy, \\
 U_{1nonl,k}(\mathbf{r}_0) &= \sigma \hat{L}_1 U_{1lin,k}^* U_{2lin,k} = \\
 &= -\frac{1}{4\pi} \int_0^{z_0} dz \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} F_1 [U_{1lin,k}^*(\mathbf{r}), U_{2lin,k}(\mathbf{r})] g_o(\mathbf{r}, \mathbf{r}_0) dx dy, \\
 U_{2nonl,k}(\mathbf{r}_0) &= \sigma \hat{L}_2 U_{1lin,k}^2 = \\
 &= -\frac{1}{4\pi} \int_0^{z_0} dz \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} F_2 [U_{1lin,k}^2(\mathbf{r})] g_e(\mathbf{r}, \mathbf{r}_0) dx dy; \\
 \mathbf{r} &= \{x, y, z\}, \quad \mathbf{r}_0 = \{x_0, y_0, z_0\};
 \end{aligned}$$

$z$  and  $z_0$  vary between 0 and  $\Delta$ ; the explicit forms of  $F_1$  and  $F_2$  are given in Eqs. (28) and (38), respectively.

Formula (77) is recursion for determining the solution of the system of equations (65) on any plane  $z = z_k$  inside the nonlinear crystal. Actually, at the first step ( $k = 1$ ) we use the boundary conditions (66), that is, assume that

$$\begin{aligned}
 U_{1,1}(x, y, z_1 = 0) &= U_{10}(x, y), \\
 U_{2,1}(x, y, z_1 = 0) &= U_{20}(x, y)
 \end{aligned} \tag{78}$$

and determine  $U_{1,2}(x, y, z_2)$  and  $U_{2,2}(x, y, z_2)$  using Eqs. (77) and (78). Then, upon substitution of these equations in Eq. (77) as the following boundary conditions, we find the solution of the problem on the plane  $z = z_3$ , and so on. As a result, having repeated this process  $N$  times, we determine the functions

$$U_{1,N+1}(x, y, z_{N+1}) = U_1(x, y, L)$$

and

$$U_{2,N+1}(x, y, z_{N+1}) = U_2(x, y, L),$$

that is, the sought equations for the scalar fields  $U_1$  and  $U_2$  at the exit from the nonlinear crystal.

Estimate the error inevitably arising with the use of Eq. (77). Referring to Eq. (73), we notice that, replacing the rigorous solution by the approximate one (72) at every step, we neglect the terms proportional to  $\mu_k^2$  from Eq. (76). Thus, as a result, after the required  $N$  steps, we lose the values of the order of

$$\begin{aligned}
 \sum_{k=1}^N \mu_k^2 &\leq N(\mu_{k,max})^2 = N(\sigma \Delta A_0)^2 = N \left( \sigma \frac{L}{N} A_0 \right)^2 = \\
 &= \frac{(\sigma L A_0)^2}{N} = \frac{\mu^2}{N}.
 \end{aligned} \tag{79}$$

It follows from Eq. (79) that, selecting the number  $N$  large enough, we can always reduce the error introduced by Eq. (77) to the required minimum.

Thus, we can state that the problem is solved in the formally methodological aspect. Equation (77) is just the sought analytical solution of the system of nonlinear equations represented as a recurrence equation. At the given finite value of  $N$ , the solution is approximate and its accuracy is determined by Eq. (79). If  $N$  tends to infinity, then the error of calculations tends to zero, and this makes Eq. (77) the asymptotically exact solution of the nonlinear problem.

Despite the proposed approach assumes the use of a computer, we are inclined to believe that equations (77) are just the approximate solution of the system of equations, rather than the algorithm for numerical calculations. In our opinion, the argument in favor of the above-said is that, unlike the classical numerical methods (for example, proposed in Ref. 9), equations (77) keep the physical meaning and practical significance even when  $N$  is equal to unity. Moreover, we can point out the situations (for example, if the value of  $A_0$  in Eq. (67) is rather small), when at  $N = 1$  equations (77) turn out to be a good approximation to the exact solution.

It should be noted once again that equations (77) have only methodological significance. It is quite difficult to use them as an algorithm for practical estimation at  $N > 1$ . Therefore, to simplify the problem, let us get rid of integrals entering into the equation for nonlinear additions. For this purpose, we use the general physical reasons not related to the theory of numerical methods and consider the situation when the number  $N$  is large enough.

It can be easily shown that in Eqs. (77) the condition  $z_0 \rightarrow 0$  ( $N \rightarrow \infty$ ) transforms the exponents from  $g_o(\mathbf{r}, \mathbf{r}_0)$  and  $g_e(\mathbf{r}, \mathbf{r}_0)$  into the fast oscillating functions of  $x$  and  $y$  compared to  $F_1(\mathbf{r})/R$  and  $F_2(\mathbf{r})/R'$ . This means that the integrals over  $dx$  and  $dy$  can be estimated asymptotically by using the method of stationary phase.<sup>5</sup> As a result, for nonlinear additions from Eqs. (77) we obtain

$$\begin{aligned}
 U_{1nonl,k}(\mathbf{r}_0) &= -\frac{i}{2k_1} \times \\
 &\times \int_0^{z_0} F_1 [U_{1lin,k}^*(x_{1k}, y_{1k}, z), U_{2lin,k}(x_{1k}, y_{1k}, z)] e^{ik_1(z_0-z)} dz, \tag{80} \\
 U_{2nonl,k}(\mathbf{r}_0) &= -\frac{i}{2k_2} \int_0^{z_0} F_2 [U_{1lin,k}^2(x_{2k}, y_{2k}, z)] e^{ik_2(z_0-z)} dz,
 \end{aligned}$$

where for the points of stationary phase we have

$$x_{1k} = x_0, \quad y_{1k} = y_0 \quad \text{и} \quad x_{2k} = x_0 - \rho z_0 + \rho z, \quad y_{2k} = y_0.$$

The physical meaning of these actions is absolutely clear. When calculating the nonlinear additions, we neglected the diffraction. It is obvious that the smaller the distance  $\Delta$ , at which the nonlinear interaction occurs, the more accurate is the approximation.

Depending on the required accuracy, many versions of Eqs. (80) simplification can be proposed. We use the most rough approximation, but leading to the simplest final results.

The integrals in the right-hand side of Eqs. (80) can be considered as functions  $\Phi_{1,2}(z_0)$ . Represent this functions as an expansion into the Taylor series in the vicinity of the point  $z_0 = 0$ . After elementary transformations, restricting the consideration to the first nonzero terms of the series, we obtain

$$\Phi_{1,2}(z_0) = \int_0^{z_0} F_{1,2}(z_0, z) dz \approx z_0 [F_{1,2}(z_0, z = z_0)]_{z_0=0}. \quad (81)$$

Using Eq. (81), for Eqs. (80) we have

$$U_{1\text{nonl},k}(\mathbf{r}_0) = -\frac{iz_0}{2k_1} F_1[U_{1,k}^*(x_0, y_0, z_k) U_{2,k}(x_0, y_0, z_k)], \quad (82)$$

$$U_{2\text{nonl},k}(\mathbf{r}_0) = -\frac{iz_0}{2k_2} F_2[U_{1,k}^2(x_0, y_0, z_k)],$$

in which it is taken into account that

$$U_{1\text{lin},k}(x, y, 0) = U_{1,k}(x, y, z_k),$$

$$U_{2\text{lin},k}(x, y, 0) = U_{2,k}(x, y, z_k)$$

obviously follows from Eqs. (75) and (77).

The physical meaning of approximation (82) is also undoubted. The transition to Eqs. (82) means that the fields  $U_{1,k}$  and  $U_{2,k}$  do not change at the distance  $z_0$ , that is, within one step. In other words, the use of Eqs. (82) means that the approximation of plane waves (or, more precisely, beams with the plane phase front) is used to calculate nonlinear additions. The asymptotic (at  $\Delta \rightarrow 0$ ) accuracy of this approximation was discussed earlier.<sup>8</sup>

We substitute Eqs. (82) into Eqs. (77) and obtain the required simplified version of the recurrence equation:

$$U_{1,k+1}(x, y, z_{k+1}) = U_{1\text{lin},k}(x, y, z = \Delta) - \frac{i\Delta}{2k_1} F_1[U_{1,k}^*(x, y, z_k) U_{2,k}(x, y, z_k)], \quad (83)$$

$$U_{2,k+1}(x, y, z_{k+1}) = U_{2\text{lin},k}(x, y, z = \Delta) - \frac{i\Delta}{2k_1} F_2[U_{1,k}^2(x, y, z_k)].$$

The final equations (83) turned out to coincide exactly with the result, obtained by the method of separation by physical properties proposed in Ref. 9 and applied directly to the system of, generally speaking, initial differential equations. Since the errors arising with the use of equations of the form (83) have been analyzed in detail in Ref. 9, we do not dwell on this issue here.

Comparing the recurrence equations (77) and (83) or two algorithms for solution of the same system of equations, one can easily notice their principal difference. At the fixed value of  $N$ , the accuracy of solution of Eqs. (83) is already independent of the amplitude of the FH field, which is characteristic of the Eqs. (77) solution. It is quite clear, because both approximations (80) and (82) remain valid for any amplitudes of the interacting fields, if  $z_0$  is short enough. Since the use of these approximations is true only at a rather small step, equations (83) lose the physical meaning at  $N \rightarrow 1$ . It was just what we kept in mind when spoke about the different methodological contents of the proposed approach (77) and already known approach (83).

## Conclusions

In this paper, the transition to the scalar approximation is demonstrated using the problem on SHG at the scalar *ooe*-interaction of waves in a quadratically nonlinear crystal as an example. It should be noted that the methodological basis for this transition, as well as in the problem on the linear field, is formed by the general definitions for ordinary and extraordinary waves<sup>4</sup> propagating in a uniaxial medium. Thus, it seems quite obvious that all the above-said can be generalized to any kinds of nonlinear processes proceeding in a uniaxial medium, that is, to the cases when the electromagnetic radiation can exist only in the form of *o*- or *e*-wave. In this case, as well as in the situation considered, any nonlinear problem of this type is reduced to the system similar to Eqs. (56). It is clear that the number of integral equations and the form of integrands ( $F_j$ ) vary depending on the particular type of a nonlinear process under consideration.

Rather rigorous derivation of the analytical solutions for the scalar amplitudes of the interacting waves (and the corresponding systems of differential and integral equations) directly from the Maxwell equations in this paper is, in our opinion, of undoubted methodological significance. It is not so obvious whether the use of equations of the form (56) makes practical sense within the framework of the scalar theory or the paraxial approximation, that is, well-known equations (63), is sufficient. It is clear that as the divergence of the laser beam increases, the contribution of the terms neglected during the derivation of the parabolic equations [in the first turn, with the expansions (62) in mind] increases. In this sense, equations (56) should seemingly provide a more accurate solution of the problem.

However, at the same time, it should be kept in mind that with the increase of the radiation divergence the possibility of using the scalar approximation, that is, representations (6), becomes less obvious. In our opinion, the unambiguous answer to this question can be obtained only in the presence of rigorous solution of the principally vector problem, which is beyond the scope of this paper.

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