Paraxial theory of sum-frequency generation by sideways alignment and phase-matching in uniaxial crystals

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A formalism in terms of Hertz potentials is presented describing sum-frequency generation in a uniaxial non-linear crystal. A scheme is proposed consisting in aligning the sideways propagation of extraordinary waves in combination with phase-matching. Simplified paraxial equations describing this situation are obtained. Particular attention is paid to the generation of second harmonics.

Keywords: Nonlinear optics; birefringence; sum-frequency generation

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1. Introduction

Sum-frequency and difference-frequency generations are important processes in nonlinear optics (see, *e.g.*, Ref. 1 and 2). The aim of the present article is to develop a formalism describing such nonlinear optical processes in terms of Hertz potentials. The first part of the article is devoted to a derivation of the equations describing the generation of higher frequencies in a uniaxial nonlinear (up to second order) crystal in the paraxial approximation. Particular attention is paid to the fact that, for extraordinary waves, the wave vectors do not coincide with the group velocity vector. This usually originates some difficulties in optical experiments and must be taken into account carefully [3]. Several experimental schemes have been proposed to take this effect into account and use it to improve the efficiency of the frequency-doubling (see Asaumi [4] and references therein). In the second part of the article, a possible scheme is proposed from a theoretical point of view for generating higher frequencies using precisely this sideways propagation. The idea is to combine phase matching, which involves wave vectors, with group velocity vectors. More specifically, the scheme consists in combining both ordinary and extraordinary beams in such a way that all three waves involved in the process are aligned in the same direction. The conditions to be fulfilled by the crystal parameters for this particular configuration are given explicitly. An analytic solution is also obtained for particular values of the amplitudes of the initial waves.

The organization of this article is as follows. In Sec. 2, a general formulation of the problem in terms of Hertz potentials is worked out following Nisbet's original treatment [5]. The results are applied in Sec. 3 to the problem of sum-frequency generation. The possible alignment of the three group velocities involved in the scheme is studied in Sec. 4. The evolution equations are presented in Sec. 5, together with a particular analytic solution. Finally, the particular case of second harmonic generation is considered in Sec. 6.

2. Propagation in a birefringent medium

Consider an anisotropic medium described by electric and magnetic field vectors, $\mathbf{E}$ and $\mathbf{B}$, and electric displacement vector $\mathbf{D}$. The Maxwell equations in the absence of free charges and currents (with magnetic permeability $\mu = 1$ and setting $c = 1$) are

$$\nabla \cdot \mathbf{B} = 0 \, , \qquad \nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0 \, , \tag{2.1}$$

$$\nabla \cdot \mathbf{D} = 0 \, , \qquad \nabla \times \mathbf{B} - \frac{\partial \mathbf{D}}{\partial t} = 0 \, . \tag{2.2}$$

The effect of the material medium can be described by a polarization vector $\mathbf{P}$ such that

$$\mathbf{D} = \mathbf{E} + 4\pi \mathbf{P},$$

the linear part being given in terms of the dyad

$$\hat{\epsilon} = \epsilon_\perp \mathbf{1} + \Delta\epsilon \, \mathbf{s} \, \mathbf{s},$$

where $\mathbf{s}$ is the optical axis of symmetry of the medium, and $\epsilon_\perp$ and $\epsilon_\parallel = \epsilon_\perp + \Delta\epsilon$ are the permeability perpendicular and parallel to this symmetry axis respectively. Then

$$\mathbf{D}(\omega, \mathbf{r}) = \hat{\epsilon}(\omega) \, \mathbf{E}(\omega, \mathbf{r}) + 4\pi \mathbf{P}^{NL}(\omega, \mathbf{r})$$

where $\mathbf{P}^{NL}$ is the non-linear contribution to the polarization vector. Here and in the following, Fourier transforms with respect to time of all quantities will be used.

Following Nisbet [5], the electromagnetic field can be described by two scalar Hertz potentials, to be called Ψ_O and Ψ_E in the present paper, and two additional scalar potentials, to be called U_O and U_E. These potentials satisfy the equations

$$\nabla_\perp U_E + \mathbf{s} \times \nabla U_O = 4\pi \mathbf{P}_\perp{}^{NL} \, , \tag{2.3}$$

$$\frac{1}{\epsilon_\perp(\omega)} \nabla \cdot \hat{\epsilon}(\omega) \cdot \nabla \, \Psi_E + \epsilon_\parallel(\omega) \omega^2 \Psi_E - \frac{\epsilon_\parallel(\omega)}{\epsilon_\perp(\omega)} \, \mathbf{s} \cdot \nabla U_E = -4\pi P_\parallel^{NL} \, , \tag{2.4}$$

$$\nabla^2\Psi_O + \epsilon_\perp(\omega)\omega^2\Psi_O + i\omega U_O = 0\ . \tag{2.5}$$

In these formulas, $\nabla_\perp$ is the gradient operator in the plane perpendicular to $\mathbf{s}$. Eq. (2.3) implies

$$\nabla_\perp^2 U_E = 4\pi\ \nabla_\perp\cdot\mathbf{P}_\perp{}^{NL}\ , \tag{2.6}$$

$$\nabla_\perp^2 U_O = 4\pi\ \mathbf{s}\cdot(\nabla\times\mathbf{P}^{NL})\ , \tag{2.7}$$

which permits to decouple the potentials Ψ_O and U_O from Ψ_E and U_E.

As shown in a previous article (Hacyan and Jáuregui [6]), the advantage of this formulation is that Ψ_O and Ψ_E correspond to the potentials for the ordinary and extraordinary waves respectively. The electromagnetic field is given by

$$\mathbf{E} = -i\omega\mathbf{s}\times\nabla\Psi_O + \frac{1}{\epsilon_\perp}\nabla(\mathbf{s}\cdot\nabla\Psi_E) + \omega^2\Psi_E\ \mathbf{s} - \frac{1}{\epsilon_\perp}\nabla U_E \tag{2.8}$$

and

$$\mathbf{B} = \nabla\times[\nabla\times(\Psi_O\mathbf{s})] - i\omega\nabla\times(\Psi_E\mathbf{s})\ . \tag{2.9}$$

From these formulas, the two fundamental modes can be identified: the ordinary wave with $\mathbf{s}\cdot\mathbf{E}_O = 0$ and the extraordinary wave with $\mathbf{s}\cdot\mathbf{B}_E = 0$. The case $\mathbf{P}^{NL} = 0$ with $U_{O,E} = 0$ corresponds to the linear limit considered in Ref. 6.

The non-linear polarization vector is usually defined as

$$P_a^{NL}(\omega,\mathbf{r}) = \int d\omega_1 \int d\omega_2\ \delta(\omega-\omega_1-\omega_2) \times \chi_{abc}(\omega_1,\omega_2)E_b(\omega_1,\mathbf{r})E_c(\omega_2,\mathbf{r}) \tag{2.10}$$

in the quadratic approximation, where $\chi_{abc}(\omega_1,\omega_2)$ is the (Fourier transformed) second-order susceptibility tensor (assumed to be homogeneous).

A particularly important case is the one in which there is a discrete set of well defined frequencies ω_i, such that

$$E_a(\omega,\mathbf{r}) = \sum_i \delta(\omega-\omega_i)E_a^{(i)}(\mathbf{r})\ .$$

Then the basic equations take the form

$$\nabla_\perp U_E^{(i)}(\mathbf{r}) + \mathbf{s}\times\nabla U_O^{(i)}(\mathbf{r}) = 4\pi\mathbf{P}_\perp^{(i)}(\omega_j,\omega_k,\mathbf{r})\ , \tag{2.11}$$

and

$$-\Big[\epsilon_\parallel(\omega_i)\omega_i^2 + \frac{1}{\epsilon_\perp(\omega_i)}\nabla\cdot\widehat{\epsilon}(\omega_i)\cdot\nabla\ \Big]\Psi_E^{(i)}(\mathbf{r}) + \frac{\epsilon_\parallel(\omega_i)}{\epsilon_\perp(\omega_i)}\ \mathbf{s}\cdot\nabla U_E^{(i)}(\mathbf{r}) = 4\pi P_\parallel^{(i)}(\omega_j,\omega_k,\mathbf{r}) \tag{2.12}$$

for extraordinary waves and

$$\Big[\epsilon_\perp(\omega_i)\omega_i^2 + \nabla^2\Big]\Psi_O^{(i)}(\mathbf{r}) + i\omega_i U_O^{(i)}(\mathbf{r}) = 0 \tag{2.13}$$

for ordinary waves, where (setting $\omega_i = \omega_j + \omega_k$)

$$P_a^{(i)}(\omega_i=\omega_j+\omega_k,\mathbf{r}) = \chi_{abc}(\omega_i=\omega_j+\omega_k) \times E_b^{(j)}(\mathbf{r})E_c^{(k)}(\mathbf{r}) \tag{2.14}$$

and

$$P_a^{(j)}(\omega_j=\omega_i-\omega_k,\mathbf{r}) = \chi_{abc}(\omega_j=\omega_i-\omega_k) \times E_b^{(i)}(\mathbf{r})E_c^{(k)*}(\mathbf{r})\ . \tag{2.15}$$

3. Sum-frequency generation

Consider a typical problem of sum-frequency generation. Suppose an ordinary and an extraordinary waves, of frequencies ω_1 and ω_2 respectively, combine inside the crystal to generate an extraordinary wave of frequency $\omega_3 = \omega_1 + \omega_2$. Let ψ_i be the Hertz potential corresponding to frequencies ω_i, and U_i the associated auxiliary potentials. Accordingly the basic equations take the form:

$$\Big[\omega_1^2\epsilon_\perp(\omega_1) + \nabla^2\ \Big]\Psi_1(\mathbf{r}) = -i\omega_1 U_1(\mathbf{r})\ , \tag{3.1}$$

$$\Big[\omega_2^2\epsilon_\perp(\omega_2)\epsilon_\parallel(\omega_2) + \nabla\cdot\widehat{\epsilon}(\omega_2)\cdot\nabla\Big]\Psi_2(\mathbf{r}) = \epsilon_\parallel(\omega_2)\mathbf{s}\cdot\nabla U_2(\mathbf{r}) - 4\pi\epsilon_\perp(\omega_2)P_\parallel^2(\omega_2{=}\omega_3{-}\omega_1,\mathbf{r}), \tag{3.2}$$

$$\Big[\omega_3^2\epsilon_\perp(\omega_3)\epsilon_\parallel(\omega_3) + \nabla\cdot\widehat{\epsilon}(\omega_3)\cdot\nabla\ \Big]\Psi_3(\mathbf{r}) = \epsilon_\parallel(\omega_3)\mathbf{s}\cdot\nabla U_3(\mathbf{r}) - 4\pi\epsilon_\perp(\omega_3)P_\parallel^3(\omega_3{=}\omega_1{+}\omega_2,\mathbf{r}), \tag{3.3}$$

and

$$\nabla_\perp^2 U_1 = 4\pi\ \mathbf{s}\cdot[\nabla\times\mathbf{P}_\perp^1(\omega_1=\omega_3-\omega_2,\mathbf{r})]\ , \tag{3.4}$$

$$\nabla_\perp^2 U_2 = 4\pi\ \nabla_\perp\cdot\mathbf{P}^2(\omega_2=\omega_3-\omega_1,\mathbf{r})\ , \tag{3.5}$$

$$\nabla_\perp^2 U_3 = 4\pi\ \nabla_\perp\cdot\mathbf{P}^3(\omega_3=\omega_1+\omega_2,\mathbf{r})\ , \tag{3.6}$$

where

$$\begin{aligned} P_a^1(\omega_1{=}\omega_3{-}\omega_2,\mathbf{r}) &= \chi_{abc}(\omega_1{=}\omega_3{-}\omega_2)E_b^3(\mathbf{r})[E_c^2(\mathbf{r})]^* \\ P_a^2(\omega_2{=}\omega_3{-}\omega_1,\mathbf{r}) &= \chi_{abc}(\omega_2{=}\omega_3{-}\omega_1)E_b^3(\mathbf{r})[E_c^1(\mathbf{r})]^* \\ P_a^3(\omega_3{=}\omega_1{+}\omega_2,\mathbf{r}) &= \chi_{abc}(\omega_3{=}\omega_1{+}\omega_2)E_b^1(\mathbf{r})E_c^2(\mathbf{r}). \end{aligned} \tag{3.7}$$

As a next step, let us assume that the potentials have the form

$$\psi_i = A_i(\mathbf{r})e^{i\mathbf{k}_i\cdot\mathbf{r}} \tag{3.8}$$

where

$$\mathbf{k}_1^2 = \epsilon_\perp(\omega_1)\ \omega_1^2 \tag{3.9}$$

and

$$\mathbf{k}_j\cdot\widehat{\epsilon}(\omega_j)\cdot\mathbf{k}_j = \epsilon_\perp(\omega_j)\mathbf{k}_{j\perp}^2 + \epsilon_\parallel(\omega_j)\mathbf{k}_{j\parallel}^2 = \epsilon_\perp(\omega_j)\epsilon_\parallel(\omega_j)\ \omega_j^2\ , \tag{3.10}$$

for $j = 2, 3$, and also

$$U_1 = u_1(\mathbf{r})e^{i(\mathbf{k}_3-\mathbf{k}_2)\cdot\mathbf{r}} , \tag{3.11}$$

$$U_2 = u_2(\mathbf{r})e^{i(\mathbf{k}_3-\mathbf{k}_1)\cdot\mathbf{r}} , \tag{3.12}$$

$$U_3 = u_3(\mathbf{r})e^{i(\mathbf{k}_1+\mathbf{k}_2)\cdot\mathbf{r}} . \tag{3.13}$$

In the above equations, $A_i(\mathbf{r})$ and $u_i(\mathbf{r})$ are slowly varying functions of $\mathbf{r}$.

Within this same approximation:

$$\mathbf{E}_1 \simeq \omega_1 \, \mathbf{s} \times \mathbf{k}_1 A_1(\mathbf{r})e^{i\mathbf{k}_1\cdot\mathbf{r}} \tag{3.14}$$

and

$$\mathbf{E}_j \simeq \left[\omega_j^2\mathbf{s} - \frac{1}{\epsilon_\perp(\omega_j)}(\mathbf{s}\cdot\mathbf{k}_j)\mathbf{k}_j\right]A_j(\mathbf{r}) \; e^{i\mathbf{k}_j\cdot\mathbf{r}} - \frac{1}{\epsilon_\perp(\omega_j)}\nabla U_j \; . \tag{3.15}$$

for $j = 1, 2$. The last term in the above equation is quadratic in the electromagnetic field; to be consistent, it must be neglected when evaluating the polarization vector up to second order. Accordingly:

$$\begin{aligned}
\mathbf{P}_1(\omega_1 = \omega_3 - \omega_2, \mathbf{r}) &= \mathbf{p}_1 \; A_3(\mathbf{r})A_2^*(\mathbf{r})e^{i(\mathbf{k}_3-\mathbf{k}_2)\cdot\mathbf{r}} \; , \\
\mathbf{P}_2(\omega_2 = \omega_3 - \omega_1, \mathbf{r}) &= \mathbf{p}_2 \; A_3(\mathbf{r})A_1^*(\mathbf{r})e^{i(\mathbf{k}_3-\mathbf{k}_1)\cdot\mathbf{r}} \; , \\
\mathbf{P}_3(\omega_3 = \omega_1 + \omega_2, \mathbf{r}) &= \mathbf{p}_3 \; A_1(\mathbf{r})A_2(\mathbf{r})e^{i(\mathbf{k}_1+\mathbf{k}_2)\cdot\mathbf{r}} \; ,
\end{aligned} \tag{3.16}$$

where the vectors $\mathbf{p}_i$ are given in terms of χ_{abc}, $\mathbf{s}$ and $\mathbf{k}_i$ as

$$\begin{aligned}
p_{1,a} &= \chi_{abc}(\omega_1 = \omega_3 - \omega_2) \; e_{3,b} \; e_{2,c} \; , \\
p_{2,a} &= \chi_{abc}(\omega_2 = \omega_3 - \omega_1) \; e_{3,b} \; e_{1,c} \; , \\
p_{3,a} &= \chi_{abc}(\omega_3 = \omega_1 + \omega_2) \; e_{1,b} \; e_{2,c} \; ,
\end{aligned} \tag{3.17}$$

with

$$\mathbf{e}_1 = \omega_1 \mathbf{s} \times \mathbf{k}_1 \; , \tag{3.18}$$

$$\mathbf{e}_j = \omega_j^2\mathbf{s} - \frac{1}{\epsilon_\perp(\omega_j)}(\mathbf{s}\cdot\mathbf{k}_j)\mathbf{k}_j \; , \tag{3.19}$$

for $j = 2, 3$.

The basic Eqs. (3.1) to (3.6) now take the form

$$\nabla^2 A_1 + 2i\mathbf{k}_1 \cdot \nabla A_1 = -i\omega_1 u_1 e^{-i\Delta\mathbf{k}\cdot\mathbf{r}}, \tag{3.20}$$

$$\nabla \cdot \hat{\epsilon}(\omega_2) \cdot \nabla A_2 + 2i\mathbf{k}_2 \cdot \hat{\epsilon}(\omega_2) \cdot \nabla A_2 = \Big[\, i\epsilon_\parallel(\omega_2) \, \mathbf{s} \cdot (\mathbf{k}_3 - \mathbf{k}_1)u_2 - 4\pi\epsilon_\perp(\omega_2)p_{2\parallel}A_1^*A_3\Big]e^{-i\Delta\mathbf{k}\cdot\mathbf{r}} \; , \tag{3.21}$$

$$\nabla \cdot \hat{\epsilon}(\omega_3) \cdot \nabla A_3 + 2i\mathbf{k}_3 \cdot \hat{\epsilon}(\omega_3) \cdot \nabla A_3 = \Big[\, i\epsilon_\parallel(\omega_3) \, \mathbf{s} \cdot (\mathbf{k}_1 + \mathbf{k}_2)u_3 - 4\pi\epsilon_\perp(\omega_3)p_{3\parallel}A_1A_2\Big]e^{i\Delta\mathbf{k}\cdot\mathbf{r}} \; , \tag{3.22}$$

where $\Delta\mathbf{k} = \mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3$, and

$$-(\mathbf{k}_{3\perp} - \mathbf{k}_{2\perp})^2 u_1 = 4\pi i \, [\mathbf{s} \times (\mathbf{k}_3 - \mathbf{k}_2)] \cdot \mathbf{p}_{1\perp} \; A_2^* A_3 \tag{3.23}$$

$$-(\mathbf{k}_{3\perp} - \mathbf{k}_{1\perp})^2 u_2 = 4\pi i \; (\mathbf{k}_{3\perp} - \mathbf{k}_{1\perp}) \cdot \mathbf{p}_{2\perp} \; A_1^* A_3 \; , \tag{3.24}$$

and

$$-(\mathbf{k}_{1\perp} + \mathbf{k}_{2\perp})^2 u_3 = 4\pi i \; (\mathbf{k}_{1\perp} + \mathbf{k}_{2\perp}) \cdot \mathbf{p}_{3\perp} \; A_1 A_2 \; , \tag{3.25}$$

within the same approximation (that is, keeping only terms of order $\mathbf{k}^2$).

3.1. Phase matching

The phase matching condition is $\mathbf{k}_3 = \mathbf{k}_1 + \mathbf{k}_2$, in which case the above equations somewhat simplify:

$$\nabla^2 A_1 + 2i\mathbf{k}_1 \cdot \nabla A_1 = -i\omega_1 u_1, \tag{3.26}$$

$$\nabla \cdot \hat{\epsilon}(\omega_2) \cdot \nabla A_2 + 2i\mathbf{k}_2 \cdot \hat{\epsilon}(\omega_2) \cdot \nabla A_2 = i\epsilon_\parallel(\omega_2) \, \mathbf{s} \cdot \mathbf{k}_2 u_2 - 4\pi\epsilon_\perp(\omega_2)p_{2\parallel}A_1^*A_3 \; , \tag{3.27}$$

$$\nabla \cdot \hat{\epsilon}(\omega_3) \cdot \nabla A_3 + 2i\mathbf{k}_3 \cdot \hat{\epsilon}(\omega_3) \cdot \nabla A_3 = i\epsilon_\parallel(\omega_3) \, \mathbf{s} \cdot \mathbf{k}_3 u_3 - 4\pi\epsilon_\perp(\omega_3)p_{3\parallel}A_1A_2 \; , \tag{3.28}$$

and

$$\begin{aligned}
-(\mathbf{k}_{1\perp})^2 u_1 &= 4\pi i \; (\mathbf{s} \times \mathbf{k}_1) \cdot \mathbf{p}_1 A_2^* A_3 \; , \\
-(\mathbf{k}_{2\perp})^2 u_2 &= 4\pi i \; \mathbf{k}_2 \cdot \mathbf{p}_{2\perp} A_1^* A_3 \; , \\
-(\mathbf{k}_{3\perp})^2 u_3 &= 4\pi i \; \mathbf{k}_3 \cdot \mathbf{p}_{3\perp} A_1 A_2 \; .
\end{aligned} \tag{3.29}$$

Now, if no absorption is present, we have the following general relations:

$$\chi_{abc}^*(\omega_3 = \omega_1 + \omega_2) = \chi_{bca}(\omega_1 = \omega_3 - \omega_2) = \chi_{cab}(\omega_2 = \omega_3 - \omega_1)$$

(Kleinman [7]). Eqs. (3.17) then imply

$$\mathbf{e}_1 \cdot \mathbf{p}_1 = \mathbf{e}_2 \cdot \mathbf{p}_2 = \mathbf{e}_3 \cdot \mathbf{p}_3^* \equiv -C \; . \tag{3.30}$$

With this last condition, it follows after some lengthy but straightforward algebra [taking relations (3.10) into account] that the basic equations (3.26-3.28) take the form

$$\nabla^2 A_1 + 2i\mathbf{k}_1 \cdot \nabla A_1 = \frac{4\pi}{|\mathbf{k}_{1\perp}|^2} \, C A_2^* A_3 \; , \tag{3.31}$$

$$\nabla \cdot \hat{\epsilon}(\omega_2) \cdot \nabla A_2 + 2i\mathbf{k}_2 \cdot \hat{\epsilon}(\omega_2) \cdot \nabla A_2 = \frac{4\pi}{|\mathbf{k}_{2\perp}|^2}\, \epsilon_\parallel(\omega_2)\epsilon(\omega_2)\, C A_1^* A_3 \,, \quad (3.32)$$

$$\nabla \cdot \hat{\epsilon}(\omega_3) \cdot \nabla A_3 + 2i\mathbf{k}_3 \cdot \hat{\epsilon}(\omega_3) \cdot \nabla A_3 = \frac{4\pi}{|\mathbf{k}_{3\perp}|^2}\, \epsilon_\parallel(\omega_3)\epsilon(\omega_3)\, C^* A_1 A_2 \,. \quad (3.33)$$

4. Sideways alignment

Suppose we want to generate a frequency $\omega_3 = \omega_1 + \omega_2$. Since rays 2 and 3 are extraordinary, they do not propagate along $\mathbf{k}_2$ and $\mathbf{k}_3$, but rather along the directions $\hat{\epsilon}(2) \cdot \mathbf{k}_2$ and $\hat{\epsilon}(3) \cdot \mathbf{k}_3$ respectively, due to the sideways effect (see *e.g.*, Ref. 8). It it then possible to choose the directions of propagations in such a way that the three rays propagates along the same direction, *in addition* to the phase matching condition. This can be achieved setting

$$\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 \,,$$
$$\hat{\epsilon}(2) \cdot \mathbf{k}_2 = \epsilon_\perp(2)\mathbf{k}_{2\perp} + \epsilon_\parallel(2) k_{2\parallel}\mathbf{s} = \alpha \mathbf{k}_1 \quad (4.1)$$
$$\hat{\epsilon}(3) \cdot \mathbf{k}_3 = \epsilon_\perp(3)\mathbf{k}_{3\perp} + \epsilon_\parallel(3) k_{3\parallel}\mathbf{s} = \beta \mathbf{k}_1$$

(in this section, we set $\epsilon(\omega_i) \rightarrow \epsilon(i)$ in order to lighten the notation). This system of linear equations admits non-trivial solutions if the proportionality constants α and β take the values:

$$\alpha = \frac{\epsilon_\parallel(2)\epsilon_\perp(2)\Delta\epsilon(3)}{D}$$
$$\beta = \frac{\epsilon_\parallel(3)\epsilon_\perp(3)\Delta\epsilon(2)}{D} \,, \quad (4.2)$$

where

$$D \equiv \epsilon_\perp(3)\Delta\epsilon(2) - \epsilon_\perp(2)\Delta\epsilon(3). \quad (4.3)$$

Furthermore, it is evident that the three ray vectors $\mathbf{k}_i$ and the optical axis $\mathbf{s}$ must be in the same plane.

Dividing the wave vectors into components perpendicular and parallel to $\mathbf{s}$, we have additionally the conditions

$$k_{1\perp}^2 + k_{1\parallel}^2 = \epsilon_\perp(1)\, \omega_1^2 \,, \quad (4.4)$$

$$\frac{k_{2\perp}^2}{\epsilon_\parallel(2)} + \frac{k_{2\parallel}^2}{\epsilon_\perp(2)} = \omega_2^2 \,, \quad (4.5)$$

$$\frac{k_{3\perp}^2}{\epsilon_\parallel(3)} + \frac{k_{3\parallel}^2}{\epsilon_\perp(3)} = \omega_3^2 \,, \quad (4.6)$$

and since

$$k_{2\perp} = \frac{\alpha}{\epsilon(2)} k_{1\perp} \,, \quad k_{2\parallel} = \frac{\alpha}{\epsilon_\parallel(2)} k_{1\parallel} \,,$$

$$k_{3\perp} = \frac{\beta}{\epsilon(3)} k_{1\perp} \,, \quad k_{3\parallel} = \frac{\beta}{\epsilon_\parallel(3)} k_{1\parallel} \,,$$

it follows from (4.5) that

$$\Delta\epsilon(2) k_{1\perp}^2 = \Big(\frac{\omega_2 D}{\Delta\epsilon(3)}\Big)^2 - \epsilon_\perp(1)\epsilon_\perp(2)\omega_1^2 \,, \quad (4.7)$$

$$\Delta\epsilon(2) k_{1\parallel}^2 = -\Big(\frac{\omega_2 D}{\Delta\epsilon(3)}\Big)^2 + \epsilon_\perp(1)\epsilon_\parallel(2)\omega_1^2 \,. \quad (4.8)$$

From (4.6) it also follows that

$$\Delta\epsilon(3) k_{1\perp}^2 = \Big(\frac{\omega_3 D}{\Delta\epsilon(2)}\Big)^2 - \epsilon_\perp(1)\epsilon_\perp(3)\omega_1^2 \,, \quad (4.9)$$

$$\Delta\epsilon(3) k_{1\parallel}^2 = -\Big(\frac{\omega_3 D}{\Delta\epsilon(2)}\Big)^2 + \epsilon_\perp(1)\epsilon_\parallel(3)\omega_1^2 \,. \quad (4.10)$$

Accordingly, the following relation is necessary for consistency:

$$\epsilon(1)\omega_1^2 = D\Big(\frac{\omega_3^2}{\Delta\epsilon(2)} - \frac{\omega_2^2}{\Delta\epsilon(3)}\Big) \,, \quad (4.11)$$

besides, of course, $\omega_1 + \omega_2 = \omega_3$.

From the above formulas, it follows with some lengthy but straightforward algebra that the angle θ_1 between $\mathbf{k}_1$ and $\mathbf{s}$ are given by the following equivalent formulas:

$$\sin^2\theta_1 = \frac{k_{1\perp}^2}{k_{1\parallel^2}} = \frac{1}{\epsilon_\perp(1)\Delta\epsilon(2)}\Big(\frac{\omega_2 D}{\omega_1\Delta\epsilon(3)}\Big)^2 - \frac{\epsilon_\perp(2)}{\Delta\epsilon(2)}$$
$$= \frac{1}{\epsilon_\perp(1)\Delta\epsilon(3)}\Big(\frac{\omega_3 D}{\omega_1\Delta\epsilon(2)}\Big)^2 - \frac{\epsilon_\perp(3)}{\Delta\epsilon(3)}$$
$$= \frac{[\omega_2\Delta\epsilon(2)]^2\epsilon_\perp(3) - [\omega_3\Delta\epsilon(3)]^2\epsilon_\perp(2)}{\Delta\epsilon(2)\Delta\epsilon(3)\,[\omega_3^2\Delta\epsilon(3) - \omega_2^2\Delta\epsilon(2)]} \,. \quad (4.12)$$

The consistency conditions for these equations (since $1 > \sin^2\theta > 0$) are

$$\Big[\omega_3\Delta\epsilon(3)\Big]^2 \epsilon_\parallel(2) > (<) \Big[\omega_2\Delta\epsilon(2)\Big]^2 \epsilon_\parallel(3) \quad (4.13)$$

if $\omega_3^2\Delta\epsilon(3) > (<) \omega_2^2\Delta\epsilon(2)$.

5. Evolution equations

Equations (3.31-3.33) simplify considerably under the assumption that the only relevant spatial variations are along $\mathbf{k}_1$. Choosing the z axis along that direction, it follows that

$$\frac{d}{dz}A_1 = C_1 A_2^* A_3,$$
$$\frac{d}{dz}A_2 = C_2 A_1^* A_3, \quad (5.1)$$
$$\frac{d}{dz}A_3 = -\, C_3^* A_1 A_2 \,,$$

where, using (4.1) and (4.2),

$$C_1 = \frac{4\pi}{2ik_1|\mathbf{k}_{\perp 1}|^2} C \quad (5.2)$$

$$C_2 = \frac{D^3}{\epsilon_\parallel^2(2)\Delta\epsilon^3(3)} C_1 \quad (5.3)$$

$$C_3 = \frac{D^3}{\epsilon_\parallel^2(3)\Delta\epsilon^3(2)} C_1 \,. \quad (5.4)$$

Notice that all three coefficients C_1, C_2 and C_3 are complex, but have the same phase.

From the above equations it follows that there is a conserved quantity:

$$\frac{d}{dz}\Big(C_2C_3^*|A_1|^2 + C_3C_1^*|A_2|^2 - C_1C_2^*|A_3|^2\Big) = 0\ , \quad (5.5)$$

which is the Manley-Rowe relation [9].

A particular solution of Eqs. (5.1) is

$$A_1 = a_1e^{i\delta}\,\mathrm{sech}(\gamma z)$$

$$A_2 = a_2e^{i\delta}\,\mathrm{sech}(\gamma z)$$

$$A_3 = a_3e^{i\delta}\tanh(\gamma z)\ ,$$

where δ is the common phase of C_i and a_i are real coefficients. Since the amplitudes of A_1 and A_2 are given as initial conditions, the amplitude A_3 of the generated wave follows from the relation

$$a_3 = -|C_3|a_2a_2\gamma^{-1}, \quad (5.6)$$

with

$$\gamma^2 = |C_1||C_3|a_2^2 = |C_2||C_3|a_1^2. \quad (5.7)$$

Thus the additional condition $|C_1|/|C_2| = a_1^2/a_2^2$ must be fulfilled for the above analytic solution to be valid. The ratio $|C_1|/|C_2|$ follows directly from Eqs. (5.2) and (5.3).

6. Second harmonic generation

Let us consider as a further example the generation of second harmonics by non-linear effects. Usually, under appropriate conditions, an ordinary wave of frequency ω gives rise to an extraordinary wave of frequency 2ω. Accordingly, the process is described by the equations given above, with the following identification: $\mathbf{k}_1$ and $\mathbf{k}_2$ correspond to the ordinary and extraordinary rays respectively, both with frequency ω, and $\mathbf{k}_3$ corresponds to the extraordinary wave of frequency 2ω, that is: $\omega_1 = \omega_2 \equiv \omega$ and $\omega_3 = 2\omega$.

In order to further lighten the notation, let us redefine $\epsilon_\perp(\omega) \equiv \epsilon$ and $\epsilon_\perp(2\omega) \equiv \bar{\epsilon}$, and similarly for $\Delta\epsilon$ and $\epsilon_\|$.

Then, according to the consistency condition (4.11):

$$\epsilon = D\Big(\frac{4}{\Delta\epsilon} - \frac{1}{\Delta\bar{\epsilon}}\Big), \quad (6.1)$$

from where it follows, using the definition of D, that

$$\frac{\epsilon}{\bar{\epsilon}} = 1 - \Big[\frac{\Delta\epsilon}{2\Delta\bar{\epsilon}} - 1\Big]^2 \quad (6.2)$$

and therefore

$$D = \frac{\bar{\epsilon}\Delta\epsilon^2}{4\Delta\bar{\epsilon}}. \quad (6.3)$$

It also follows from (6.2) that

$$0 < \frac{\Delta\epsilon}{\Delta\bar{\epsilon}} < 4\ . \quad (6.4)$$

This inequality must be satisfied in order to have triple alignment of the velocity vectors.

Also

$$\sin^2\theta_1 = \frac{\Delta\epsilon^2\bar{\epsilon} - 4\epsilon\Delta\bar{\epsilon}^2}{\Delta\epsilon\Delta\bar{\epsilon}(4\Delta\bar{\epsilon} - \Delta\epsilon)}. \quad (6.5)$$

Thus, if the optical axis $\mathbf{s}$ makes an angle ϕ with the unit normal vector to the surface of the crystal, then according to Snel's law,

$$\sin\iota = \sqrt{\epsilon}\sin(\theta_1 - \phi), \quad (6.6)$$

where ι is the incidence angle to which the impinging ray must be directed in order to have a phase-matching assisted by sideway alignment. Equation (6.4) must be satisfied.

The evolution of the field is given by Eqs. (5.1) with its coefficient given by

$$C_2 = \frac{\bar{\epsilon}^3}{\epsilon_\|^2}\Big(\frac{\Delta\epsilon}{2\Delta\bar{\epsilon}}\Big)^6 C_1\ ,$$

$$C_3 = \frac{\bar{\epsilon}^3}{\bar{\epsilon}_\|^2}\Big(\frac{\Delta\epsilon}{2\Delta\bar{\epsilon}}\Big)^6 C_1\ . \quad (6.7)$$

7. Concluding remarks

The formalism presented in this paper can be applied to other processes, such as difference-frequency generation and parametric down-conversion (to be considered in a forthcoming publication). As for the particular scheme of sideways alignment herein proposed, it is left as a proposal to find crystals with the appropriate parameters, and to check its validity experimentally.

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1. R.W. Boyd, *Nonlinear optics* (Academic Press; 3rd ed. 2008).
2. G. New, *Introduction to nonlinear optics* (Cambridge U. Press 2011).
3. R. Danielius, A. Piskarskas, P. Di Trapani, A. Andreoni, C. Solcia, and P. Foggi, *Opt. Lett.* **21** (1996) 973.
4. K. Asaumi, *App. Opt.* **37** (1998) 555.
5. A. Nisbet, *Proc. Roy. Soc.* **A 240** (1957) 375.
6. S. Hacyan and R. Jáuregui, *J. Opt. A: Pure Appl. Opt.* **11** (2009) 085204.
7. D.A. Kleinman, *Phys. Rev.* **126** (1962) 1977.
8. S. Hacyan, *J. Opt. Soc. Am.* **A 27** (2010) 602.
9. J.M. Manley and H.E. Rowe, *Proc. IRE* **47** (1959) 2115.