MISCONCEPTIONS REGARDING SECOND HARMONIC GENERATION IN X-RAY FREE-ELECTRON LASERS

G. Geloni, E. Saldin, E. Schneidmiller and M. Yurkov
Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany

Abstract

Nonlinear generation of coherent harmonic radiation is an important option in the operation of a X-ray Free-Electron Laser facility (XFEL) since it broadens the spectral range of the facility itself, thus allowing for a wider scope of experimental applications. We find that up-to-date theoretical understanding of second harmonic generation is not correct. Derivation of correct radiation characteristics will follow our criticism. A more detailed report of our study is given in [1].

INTRODUCTION

The process of harmonic generation of coherent radiation can be considered as a purely electrodynamical one. In fact, the harmonics of the electron beam density are driven by the electromagnetic field at the fundamental frequency, but the bunching contribution due to the interaction of the electron beam with the radiation at higher harmonics can be neglected. This leads to important simplifications. Namely, the solution to the self-consistent problem for the fundamental harmonic can be used to calculate the harmonic contents of the beam current. These contents enter as known sources in the calculation of the characteristics of harmonic radiation. As a result, numerical calculations dealing with harmonic generation simply compute the solution of Maxwell equations with sources obtained by means of FEL self-consistent codes.

Non-linear generation of the second harmonic radiation, in particular, is important for extending the attainable frequency range of an XFEL facility. The subject has been a matter of theoretical studies in high-gain Self-Amplified Spontaneous Emission (SASE) FELs both for odd [3] and even harmonics [4, 5, 9], where the electrodynamical problem is dealt with. The practical interest of these studies is well underlined by both numerical analysis [6] and experiments in the infra-red and in the visible range of the electromagnetic spectrum [7, 8]. Experimental results are compared with numerical analysis and numerical analysis rely on analytical studies: this fact stresses the importance of a correct theoretical understanding of the subject. From this viewpoint we find that [4] includes arbitrary manipulations of the source terms in the paraxial wave equation, which are also proposed in [5, 9].

We find that a first incorrect step is the omission of a term depending on the gradient of the charge density. As we will see such term is responsible for a non-negligible contribution to the second harmonic field both for the horizontal and, surprisingly, for the vertical polarization component and it should not go overlooked. Moreover, the beam distribution is modelled as a collection of individual point-particles, i.e. a sum of δ-Dirac functions that is expanded in the x coordinate on the right hand side of the wave equation. Based on this manipulation, as it is discussed in [1], a main parameter is identified that has no theoretical support and will not play any role in our analysis. Also, (see, again, [1] for a detailed demonstration) the expansion of the δ-Dirac functions cannot be performed as it corresponds to an incorrect expansion of the Green's function for Maxwell equation. Finally, the estimation of the second harmonic power is based on the (arbitrarily manipulated) source term alone, without actually solving Maxwell equations. Altogether, these works predict a wrong dependence of the second harmonic field on the problem parameters. The results in [5] are extended in [9] to the case of an electron beam moving off-axis through the undulator. The authors of [9] conclude that the second harmonic power increases when the beam moves off-axis. We find that, in this case the power of the second harmonic radiation never increases: in particular, as we will see, it may only decrease or remain unvaried.

In this paper, that was inspired by a method [11] developed to deal with Synchrotron Radiation from complex setups, we present a theory of second harmonic generation for high-gain FELs. We apply a Green's function technique to solve the wave equation. Our result is used to calculate, in a specific case, properties of the second harmonic radiation such as polarization, directivity diagram and total power including proper parametric dependencies. The most surprising prediction of our theory is that the electric field is not only horizontally polarized, as it is usually assumed, but exhibits, though remaining linearly polarized, a vertical polarization component too. A more detailed report of our study is given in [1].

COMPLETE ANALYSIS OF THE SECOND HARMONIC GENERATION MECHANISM

Let us consider for simplicity a beam modulated at a single frequency ω. The current density can be written as a sum of an unperturbed part independent of the modulation, $(\vec{v}/c)j_o$, and a term responsible for the beam modulation at frequency ω, whose evolution through the beamline, accounting for emittance and energy spread, is described by the function $\tilde{a}_2$, to be considered a result from an external FEL code:

$$\vec{j}(z,t,\vec{\eta}) = \frac{\vec{v}(z,\vec{\eta})}{c} j_o \left(\vec{r}_\perp - \vec{r}_\perp^{(c)}(z,\vec{\eta})\right)$$

$$\times \left\{1 + \left[\tilde{a}_2 \left(z, \vec{r}_\perp - \vec{r}_\perp^{(c)}(z,\vec{\eta})\right) \times \exp\left[i\omega \int_0^z \frac{dz'}{v_z(z',\vec{\eta})} - i\omega t\right] + \text{C.C.}\right]\right\} . \quad (1)$$

Eq. (1) has been derived in the limit $\gamma^2 \gg 1$, where $\gamma = \gamma(z)$ describes the (given) average Lorentz factor along the undulator. In the presence of energy spread the transverse size of the electron beam is assumed to be not smaller than the typical wiggling motion. Then, with accuracy $\delta\gamma/\gamma$ all particles can be considered moving coherently according to $\vec{r}_\perp^{(c)}$, which corresponds to a velocity:

$$v_z(z,\eta) = v_{z(nd)}(z)\left(1 - \frac{\eta_x^2 + \eta_y^2}{2}\right)$$
$$\vec{v}_\perp(z,\eta) = \vec{v}_{\perp(nd)}(z) + v_{z(nd)}(z)\vec{\eta} . \quad (2)$$

Here $\vec{\eta}$ is the direction of the beam deflection with respect to the undulator axis and $\vec{v}_{(nd)}$ is the velocity with no deflection. The charge density can be written as

$$\rho = \frac{j_z}{v_z} \simeq \frac{j_z}{c} , \quad (3)$$

as we will be working in the paraxial approximation. Eq. (1) and Eq. (3) give the sources for Maxwell equation. Looking for solutions in the form $\vec{E}_\perp = \tilde{\vec{E}}_\perp \exp[i\omega(z/c - t)]$ + C.C. and applying the paraxial approximation one writes the Maxwell equation as [11]:

$$\left(\nabla_\perp{}^2 + \frac{2i\omega}{c}\frac{\partial}{\partial z}\right)\tilde{\vec{E}}_\perp = \frac{4\pi}{c}\exp\left[i\omega \times \left(\int_0^z \frac{dz'}{v_z(z',\vec{\eta})} - \frac{z}{c}\right)\right]\left(\frac{i\omega}{c^2}\vec{v}_\perp - \vec{\nabla}_\perp\right) j_o \tilde{a}_2 . \quad (4)$$

We will consider the case of a planar undulator thus modelling the electron transverse motion with:

$$\vec{r}_\perp^{(c)}(z',\vec{\eta}) = \left\{\frac{K\left[\cos(k_w z') - 1\right]}{\gamma k_w} + \eta_x z'\right\}\vec{x} + \left[\eta_y z'\right]\vec{y} . \quad (5)$$

K is the deflection parameter and $k_w = 2\pi/\lambda_w$, λ_w is the undulator period. We will work in the far zone. Using a Green's function technique and the integration variable $\vec{l} = \vec{r'} - \vec{r}_\perp^{(c)}(z',\vec{\eta})$ an exact solution of Eq. (4) reads:

$$\tilde{\vec{E}}_\perp = \frac{i\omega}{c^2 z_o}\int d\vec{l} \int_{-\frac{L_w}{2}}^{\frac{L_w}{2}} dz' j_o(\vec{l})\tilde{a}_2(z',\vec{l})\exp\left[i\Phi_T\right] \times \left[\left(\frac{K}{\gamma}\sin(k_w z') + (\theta_x - \eta_x)\right)\vec{x} + (\theta_y - \eta_y)\vec{y}\right] , \quad (6)$$

where

$$\Phi_T = \frac{\omega}{\omega_1}k_w z' - \frac{\omega K^2}{8\gamma^2 k_w c}\sin(2k_w z') - \frac{\omega K(\theta_x - \eta_x)}{\gamma k_w c}\cos(k_w z') + \omega\left\{\frac{K}{k_w \gamma c}(\theta_x - \eta_x) - \frac{1}{c}(\theta_x l_x + \theta_y l_y) + (\theta_x^2 + \theta_y^2)\frac{z_o}{2c}\right\} , \quad (7)$$

ω_1 being defined by

$$\omega_1^{-1} = \frac{1}{2k_w c\gamma^2}\left[1 + \frac{K^2}{2} + \gamma^2\left|\vec{\theta} - \vec{\eta}\right|^2\right] . \quad (8)$$

Here θ_x and θ_y indicate the observation angles and $L_w = N_w\lambda_w$ is the undulator length. Under the resonant approximation we will make use of the well-known expansion [12]: $\exp\left[ia\sin(\psi)\right] = \sum_{p=-\infty}^{\infty} J_p(a)\exp\left[ip\psi\right]$, J_p being the Bessel function of the first kind of order n. We will be interested in frequencies ω around the second harmonic:

$$\omega_{2o} = 4k_w c\gamma_z^2 , \quad \text{where} \quad \gamma_z^2 = \frac{\gamma^2}{1 + K^2/2} . \quad (9)$$

The second harmonic contribution $\tilde{\vec{E}}_{\perp 2}$ is then

$$\tilde{\vec{E}}_{\perp 2} = \frac{i\omega_{2o}}{c^2 z_o}\exp\left[i\frac{\omega_{2o}}{2c}z_o(\theta_x^2 + \theta_y^2)\right]\left[\mathcal{A}(\theta_x - \eta_x)\vec{x} + \mathcal{B}(\theta_y - \eta_y)\vec{y}\right]\int_{-\infty}^{\infty} dl_x dl_y dz' \tilde{\rho}^{(2)}(z',\vec{l},C) \times \exp\left[-i\frac{\omega_{2o}}{c}(\theta_x l_x + \theta_y l_y)\right] \times \exp\left\{i\frac{\omega_{2o}}{2c}\left[(\theta_x - \eta_x)^2 + (\theta_y - \eta_y)^2\right]z'\right\} . \quad (10)$$

Here we have defined

$$\mathcal{A} = 2\xi\left[J_0(\xi) - J_2(\xi)\right] + J_1(\xi) \text{ and } \mathcal{B} = J_1(\xi) , \quad (11)$$

where $\xi = K^2/(2 + K^2)$. Moreover

$$C = (\omega - \omega_{2o})/\omega_{1o} \text{ and} \quad (12)$$

$$\tilde{\rho}^{(2)} = j_o\left(\vec{l}\right)\tilde{a}_2\left(z',\vec{l}\right)\exp\left[iCz'\right]H_{L_w}(z') . \quad (13)$$

$H_{L_w}(z')$ is equal to unity over the interval $[-L_w/2, L_w/2]$ and zero everywhere else, and accounts for the fact that the integral in dz' should be performed over the undulator length. Also, the detuning parameter C should be considered as a function of z, $C = C(z)$ which can be retrieved from the knowledge of $\gamma = \gamma(z)$.

The terms in J_1 in Eq. (11) are due to the presence of the gradient term $\vec{\nabla}_\perp(j_o\tilde{a}_2)$ in Eq. (4), which has been omitted in [4, 5, 9]. The gradient term contributes for more than one fourth of the total field for the x-polarization component. Moreover, without that term, the entire contribution to the field polarized in the y direction would go overlooked.

Usually, computer codes present the functions $\tilde{a}_2$ and $\exp[iCz']$ combined in a single product, known as the complex amplitude of the electron beam modulation with respect to the phase $\psi = 2k_w z' + (\omega/c)z' - \omega t$. We will regard $\tilde{\rho}^{(2)}$ as a given function so that our description is independent on the particular presentation of the beam modulation.

We will now treat the particular case when $\gamma(z) = \bar{\gamma} =$ const, $C(z) = 0$,

$$\tilde{a}_2 = a_{2o} \exp\left[\frac{i\omega_{2o}}{c}\left(\eta_x l_x + \eta_y l_y\right)\right], \tag{14}$$

with $a_{2o} =$ const and

$$j_o\left(\vec{l}\right) = \frac{I_o}{2\pi\sigma^2}\exp\left(-\frac{l_x^2 + l_y^2}{2\sigma^2}\right), \tag{15}$$

I_o and σ being the bunch current and transverse size respectively. This corresponds to a modulation wavefront perpendicular to the beam direction of motion. Eq. (10) amounts, then, to a spatial Fourier transform and we obtain:

$$\begin{aligned}\tilde{\vec{E}}_{\perp 2} = \frac{iI_o a_{2o}\omega_{2o}L_w}{c^2 z_o}&\exp\left[i\frac{\omega_{2o}}{2c}z_o(\theta_x^2 + \theta_y^2)\right]\\ &\times\left[\mathcal{A}(\theta_x - \eta_x)\vec{x} + \mathcal{B}(\theta_y - \eta_y)\vec{y}\right]\\ \times\mathrm{sinc}&\left\{\frac{L_w\omega_{2o}}{4c}\left[(\theta_x - \eta_x)^2 + (\theta_y - \eta_y)^2\right]\right\}\\ \times\exp\left\{-\frac{\sigma^2\omega_{2o}^2}{2c^2}\right.&\left.\left[(\theta_x - \eta_x)^2 + (\theta_y - \eta_y)^2\right]\right\}.\end{aligned} \tag{16}$$

The angular distribution of intensity along the $\vec{x}$ and $\vec{y}$ polarization directions will be denoted with $I_{2(x,y)}$. Definition of normalized quantities: $\hat{\theta} = (\omega_{2o}L_w/c)^{1/2}\theta$, $\hat{\eta} = (\omega_{2o}L_w/c)^{1/2}\eta$, $\hat{l}_{x,y} = [\omega_{2o}/(cL_w)]^{1/2}l_{x,y}$ and of the Fresnel number $N = \omega_{2o}\sigma^2/(cL_w)$ give

$$\begin{aligned}I_{2(x,y)}\left(\hat{\theta}_x - \hat{\eta}_x, \hat{\theta}_y - \hat{\eta}_y\right) &= \mathrm{const}\times\left(\hat{\eta}_{x,y} - \hat{\theta}_{x,y}\right)^2\\ \times\mathrm{sinc}^2&\left\{\frac{1}{4}\left[\left(\hat{\theta}_x - \hat{\eta}_x\right)^2 + \left(\hat{\theta}_y - \hat{\eta}_y\right)^2\right]\right\}\\ \times\exp&\left\{-N\left[\left(\hat{\theta}_x - \hat{\eta}_x\right)^2 + \left(\hat{\theta}_y - \hat{\eta}_y\right)^2\right]\right\}.\end{aligned} \tag{17}$$

I_{2x} and I_{2y} have no azimuthal symmetry, contrarily with what happens for the first harmonic, where only the x polarization is present and has azimuthal symmetry [13]. The directivity diagram in Eq. (17) is plotted in Fig. 1 for different values of N as a function of $\hat{\theta}_x - \hat{\eta}_x$ at $\hat{\theta}_y - \hat{\eta}_y = 0$ for the x polarization component. The next step is the calculation of the second harmonic power for the x- and y-polarization components that is given by

$$W_{2(x,y)} = \frac{c}{2\pi}\int_{-\infty}^{\infty}dx_o\int_{-\infty}^{\infty}dy_o|\tilde{E}_{\perp x,y}(z_o, x_o, y_o)|^2 \tag{18}$$

It is convenient to present the expressions for W_{2x} and W_{2y} in a dimensionless form. After appropriate normalization they both are function of one dimensionless parameter:

$$\hat{W}_{2x} = \hat{W}_{2y} = F_2(N) = \ln\left(1 + \frac{1}{4N^2}\right). \tag{19}$$

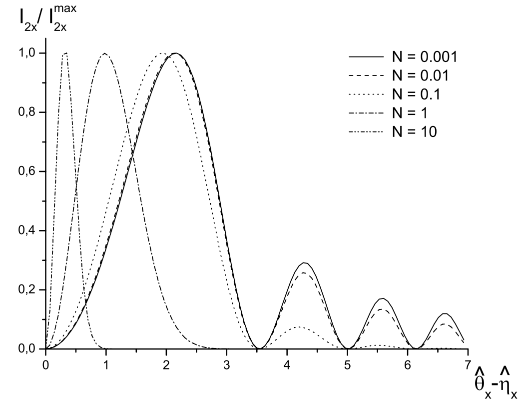

Figure 1: Plot of the directivity diagram for the radiation intensity as a function of $\hat{\theta}_x - \hat{\eta}_x$ at $\hat{\theta}_y - \hat{\eta}_y = 0$ for the x-polarization component, for different values of N.

Here $\hat{W}_{2x} = W_{2x}/W_{ox}^{(2)}$ and $\hat{W}_{2y} = W_{2y}/W_{oy}^{(2)}$ are the normalized powers. The normalization constants $W_{ox}^{(2)}$ and $W_{oy}^{(2)}$ are given by

$$\begin{pmatrix} W_{ox}^{(2)} \\ W_{oy}^{(2)} \end{pmatrix} = \begin{pmatrix} \mathcal{A}^2 \\ \mathcal{B}^2 \end{pmatrix} W_b\left[\frac{a_{2o}^2}{2\pi}\right]\left[\frac{I_o}{\gamma I_A}\right], \tag{20}$$

where $W_b = m_e c^2\gamma I_o/e$ is the total power of the electron beam and $I_A = m_e c^3/e \simeq 17$ kA is the Alfven current.

The logarithmic divergence in $F_2(N)$ in the limit for $N \ll 1$ imposes a limit on the meaningful values of N. On the one hand, the characteristic angle $\hat{\theta}_{\max}$ associated with the intensity distribution is given by $\hat{\theta}^2_{\max} \sim 1/N$. On the other hand, the expansion of the Bessel function used in our derivation is valid only as $\hat{\theta}^2 \leq N_w$. As a result we find that Eq. (19) is valid only up to values of N such that $N \geq N_w^{-1}$. As $N < N_w^{-1}$ the dimensionless problem parameter N is smaller than the accuracy of the resonance approximation scaling as N_w^{-1}. In this situation our electrodynamic description does not distinguish anymore between a beam with finite transverse size and a point-like particle and, for estimations, we should make the substitution $\ln(N) \longrightarrow \ln(N_w^{-1})$.

The first harmonic study in [13] refers to a modulation wavefront orthogonal to the direction of propagation of the beam exactly as here and results have been presented in dimensionless form, which allows direct comparison between the powers of the second and of the first harmonic:

$$\frac{W_2(N)}{W_1(N)} = \frac{1}{(2\pi)^3 N_w}\frac{2 + K^2}{K^2}\frac{a_{2o}^2}{a_{1o}^2}\frac{\mathcal{A}^2 + \mathcal{B}^2}{A_{JJ}^2}\frac{F_2(N)}{F_1(N)}, \tag{21}$$

where

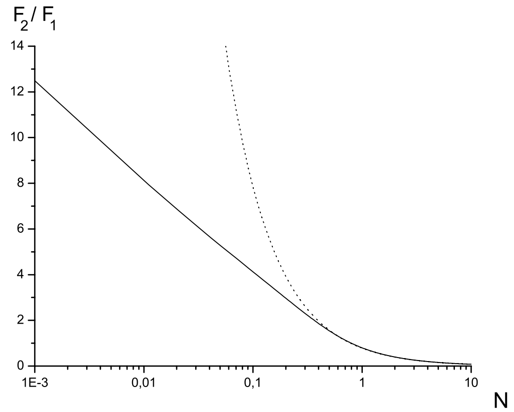

Figure 2: Solid line: F_2/F_1 as a function of N. Dashed line: its asymptotic, $\pi/(4N)$, for $N \gg 1$.

$$F_1(N) = \frac{2}{\pi}\left[\arctan\left(\frac{1}{N}\right) + \frac{N}{2}\ln\left(\frac{N^2}{N^2+1}\right)\right] \quad (22)$$

and $A_{JJ} = J_0(\xi/2) - J_1(\xi/2)$. Here a_{1o} is the analogous of a_{2o} for the first harmonic. For notational reasons, a_{1o} is one half of the original modulation level $a_{\rm in}$ in Eq. (27) of [13]. Moreover, all N in Eq. (22) are multiplied by a factor $1/2$ with respect to [13], since N is defined for the second harmonic. In Fig. 2 we plot the behavior of F_2/F_1 as a function of N and its asymptotic, $\pi/(4N)$, for $N \gg 1$.

The knowledge of the polarization contents of the radiation, even if relatively small as in this case, can be important from an experimental viewpoint. For example, in the VUV range, the reflection coefficients of many materials (e.g. SiC, that is widely used for mirrors) exhibit a complicated behavior, and there may be differences of even an order of magnitude depending on the polarization of the radiation. A study of $R(K) = W_{2y}/W_{2x} = \mathcal{A}^2(K)/\mathcal{B}^2(K)$ shows that the relative magnitude of the y and the x polarization components of the second harmonic power ranges from 4% at $K = 0$ to about 6% in the limit $K \gg 1$. Note that $R(K)$ is independent of the particular model chosen for the beam modulation and that the second harmonic radiation is linearly polarized.

It is important to remark that we have treated a particular situation when the modulation wavefront is orthogonal to the direction of propagation of the beam. We have seen that the total power of the second harmonic radiation does not depend on the deflection angles η_x and η_y. In general, the second harmonic power can be independent of the beam deflection angle (like in this case) or can decrease due to the presence of extra oscillating factors in $\vec{l}$ in Eq. (10). On the contrary in [9], an increase of the total power is reported, due to deflection angles: we find that such conclusion does not correspond to physical reality.

CONCLUSIONS

In this paper we addressed the mechanism of second harmonic generation in Free-Electron Lasers. We find that available theoretical treatments of this phenomenon consist of estimations based on arbitrary manipulations of the source term of the wave equation that describes the electrodynamical problem.

By solving analytically the wave equation with the help of the Green's function technique we derived an exact expression for the field of the second harmonic emission. We limited ourselves to the steady-state case which is close to practice in High-Gain Harmonic Generation (HGHG) schemes but, for the rest, we did not make restrictive approximations. Our solution of the wave equation may therefore be considered as a basis for the development of numerical codes dealing with second harmonic emission which should be using as input data the electron beam bunching for the second harmonic, as calculated by self-consistent FEL codes.

In general, the second harmonic field presents both horizontal and vertical polarization components and the electric field is linearly polarized. We calculated analytically the directivity diagram and the power associated with the second harmonic radiation assuming a particular beam modulation case. We expect that these expressions may be useful for cross-checking of numerical results.

A more detailed report of our study is given in [1].

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