DESY 05-137

DEUTSCHES ELEKTRONEN-SYNCHROTRON
in der HELMHOLTZ-GEMEINSCHAFT

DESY 05-137

August 2005

arXiv:physics/0508046 v1 8 Aug 2005

Exact Solution for the Second Harmonic Generation in XFELs

Gianluca Geloni, Evgeni Saldin, Evgeni Schneidmiller and Mikhail Yurkov
Deutsches Elektronen-Synchrotron DESY, Hamburg

ISSN 0418-9833

NOTKESTRASSE 85 - 22607 HAMBURG

Exact Solution for the Second Harmonic Generation in XFELs

Gianluca Geloni [a] Evgeni Saldin [a] Evgeni Schneidmiller [a]
Mikhail Yurkov [a]

[a] *Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany*

Abstract

The generation of harmonic radiation through a non-linear mechanism driven by bunching at fundamental frequency is an important option in the operation of high gain Free-Electron Lasers (FELs). The use of harmonic generation at a large scale facility may result in achieving shorter radiation wavelengths for the same electron beam energy. This paper describes a theory of second harmonic generation in planar undulators with particular attention to X-Ray FELs (XFELs). Our study is based on an exact analytical solution of Maxwell equations, derived with the help of the Green's function method. On the contrary, up-to-date theoretical understanding of the second harmonic generation is only limited to some estimation of the total radiation power based on the source part of the wave equation. Moreover, we find that such part of the wave equation is presented with several incorrect manipulations among which is the omission of an important contribution. Our work yields correct parametric dependencies and specific predictions of additional properties such as polarization, angular distribution of the radiation intensity and total power. The most surprising prediction is the presence of a vertically polarized part of the second harmonic radiation, whereas up-to-date understanding assumes that the field is horizontally polarized. Altogether, this paper presents the first correct theory of second harmonic generation for high gain FELs.

Key words: Free-electron Laser (FEL), X-rays, even harmonic generation
PACS: 52.35.-g, 41.75.-i

1 Introduction

In a Free-Electron Laser the electromagnetic field at the fundamental harmonic interacts with the electron beam. As a result, the beam is bunched in non-linear (sinusoidal) ponderomotive potential. When the bunching is strong enough, the beam current exhibits non-negligible Fourier components at harmonics of the fundamental as well. In the SASE case only the transverse ground mode of the fundamental harmonic survives, due to the transverse mode selection mechanism [1] in the high gain regime, and is responsible for the bunching mechanism. As a result, the nonlinear Fourier components radiate coherently and the phenomenon is referred to as (nonlinear) harmonic generation of coherent radiation.

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. In fact, in order to perform numerical analysis of the characteristics of higher harmonics radiation, one has to solve the self-consistent problem for the fundamental harmonic only. Subsequently, the solution to this problem, that must be obtained with the help of a self-consistent code, can be used to calculate the harmonic contents of the beam current. These contents enter as known sources in our electrodynamical process: solving Maxwell equations accounting for these sources gives the desired characteristics of higher harmonics radiation. As a result, simulation codes dealing with harmonic generation are not first principle codes: in fact, they simply compute the solution of Maxwell equations obtaining the proper sources by means of first-principle codes.

Non-linear generation of the second harmonic radiation, in particular, is important for extending the attainable frequency range of an XFEL facility: in fact, the high peak-brilliance increase of XFELs with respect to third generation light sources (up to eight orders of magnitude) makes the second harmonic contents of the XFEL radiation very attractive from a practical viewpoint. Moreover, it is also important in connection with experiments that make use of the fundamental harmonic only. In fact one must be able to estimate correctly the higher harmonics effects to distinguish between nonlinear phenomena induced by the fundamental and linear phenomena due to the second harmonic.

The subject has been a matter of theoretical studies in a high-gain SASE FEL both for odd [2] and even harmonics [3, 4, 8], where the electrodynamical problem is dealt with. The practical interest of these studies is well underlined by

the fact that they were followed by both numerical analysis [5] and experiments, that have been carried out in the infra-red and in the visible range of the electromagnetic spectrum [6, 7].

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. Remarkably, such understanding does not require the introduction of radically new physical mechanisms. The key ideas involved are not much different from those regarding the second harmonic generation from a single particle, treated a long time ago and presented in Synchrotron Radiation textbooks (e.g. [9, 10]). A complexity though, is constituted by the presence of many electrons involved in the radiative process, each with a given offset and phase, radiating coherently, as a whole or in part, due to the longitudinal modulation of the beam current at the second harmonic.

For a given frequency component the electromagnetic wave equation dictates both a characteristic longitudinal length (that is the radiation formation length) and a characteristic transverse length. As we will see, when the beam transverse size is smaller than the characteristic transverse length the entire electron beam behaves like a single electron and the harmonics of the beam current are simply interpretable in terms of the harmonic contents of a single particle current: in this case, all the particles act coherently and the radiated intensity scales with the square number of the electrons in the beam. When the transverse size of the beam increases and becomes much larger than the characteristic transverse length less electrons contribute collectively to the field and if the beam current remains constant the total radiated power is decreased.

The characteristic transverse length is specified in a natural way after a dimensional analysis of the problem. The first treatment [3] of non-linear generation of even harmonics does not account for the presence of such parameter, followed in this by others [4, 8]. We find that these works include arbitrary manipulations of the source terms in the paraxial wave equation. Among these, an important part of the source terms is systematically dropped. Moreover, estimations of the second harmonic power are based on the electromagnetic sources (after manipulation) while exact calculations should be based on a solution of Maxwell equations. Altogether, we find that these works predict an incorrect dependence of the second harmonic field on the problem parameters. Results of [4] are extended in [8] to the case of an electron beam moving off-axis through the undulator. One of the conclusions in [8] is that the second harmonic power increases when an angle between the beam and the undulator axis is present. We find that the power of the second harmonic radiation should never increase when such angle is present: in particular, as we will see, it is independent of it in optimal situations when the microbunching wavefront

is matched with the beam propagation.

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 in high-gain FELs. First we give, in Section 2, an exact analytical solution of the wave equation for the second harmonic generation problem. The procedure employed to derive such a solution shows the advantages of a Green's function method. In Section 3, our result is used to calculate, in a particular case, specific 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 vertically polarized component too. Following the presentation of our theory, in Section 4 we comment on the differences between our approach and the present understanding of the second harmonic generation mechanism. Finally, in Section 5, we come to conclusions.

2 Complete analysis of Second Harmonic Generation mechanism

As has been said in the Introduction, the process of (second) harmonic generation of coherent radiation is a purely electrodynamical one. First, proper initial conditions are given as input to an FEL self-consistent code, which calculates the electron beam bunching from the interaction of the beam with the first harmonic radiation. Then, the results from the self-consistent code are used as electromagnetic sources to solve the problem of second harmonic generation. For simplicity, in the following we will consider a beam modulated at a single frequency ω as the source. One may always write the longitudinal current density j_z along the undulator as a sum of an unperturbed part independent of the modulation and of the time, j_o, and a term responsible for the beam modulation, $\tilde{j}_z$, at frequency ω (perturbation):

$$j_z(z,\vec{r}_\perp,t) = j_o(z,\vec{r}_\perp) + \tilde{j}_z(z,\vec{r}_\perp,t) \ . \tag{1}$$

We assume that we can write the unperturbed part j_o as if all the particles where moving coherently, that is

$$j_o(z,\vec{r}_\perp) = j_o(\vec{r}_\perp - \vec{r}_\perp^{(c)}(z)) \ , \tag{2}$$

where $\vec{r}_\perp^{(c)}(z)$ describes the coherent motion. This assumption is always verified, for instance, in the case of a single particle, when j_o is simply a δ-Dirac function, or in the case of a monochromatic beam. If some energy spread is

present, in order for Eq. (2) to be valid we should assume that the transverse size of the electron beam is not smaller than the typical wiggling motion of the electrons. In this case, the validity of Eq. (2) has an accuracy given by the relative deviation of the particles energy form the average value, $\delta\gamma/\gamma$. Since for the FEL process $\delta\gamma/\gamma$ is, at most, of the order of the efficiency parameter, we have $\delta\gamma/\gamma \ll 1$ and Eq. (2) is valid with the same accuracy of FEL theory. However it should be noted here that the average energy of the beam is to be considered, in general, a function of the coordinate z, $\gamma = \gamma(z)$: it has to be given as a result of start-to-end simulations and considered as an input for our electromagnetic problem.

The perturbation $\tilde{j}_z$ can then be written as

$$\begin{aligned}\tilde{j}_z(z,t) = & j_o\left(\vec{r}_\perp - \vec{r}_\perp^{(c)}(z)\right) \\ & \times\left\{\tilde{a}_2\left(z,\vec{r}_\perp - \vec{r}_\perp^{(c)}(z)\right)\exp\left[i\omega\int_0^z \frac{dz'}{v_z(z')} - i\omega t\right] + \text{C.C.}\right\} \ . \end{aligned} \tag{3}$$

The function $\tilde{a}_2$ is to be considered a result from the FEL self-consistent code, and its dependence on z describes the evolution of the modulation through the beamline and accounts for emittance and energy spread effects. It should be noted that the values of $\tilde{a}_2$ are not necessarily real: in fact there can be a z-dependent phase shift with respect to the phase $\omega\int_0^z dz'/v_z(z') - \omega t$.

In order to correctly calculate the phase $\omega\int_0^z dz'/v_z(z') - \omega t$ in Eq. (3) one has to account for the dependence of the longitudinal velocity associated with the coherent motion, v_z on the position z. The function $v_z(z)$ can be recovered from the knowledge of $\vec{r}_\perp^{(c)}(z)$ and of the average energy of the beam $\gamma = \gamma(z)$.

If the beam is deflected of angles η_x and η_y in the horizontal and vertical direction with respect to the z axis, the velocity of the coherent motion depends also on the deflection angles. Renaming position and velocity of the coherent motion with no deflection with the subscript "(nd)" one obtains:

$$\begin{aligned} v_z(z,\eta) &= v_{z(nd)}(z)\left(1 - \frac{\eta_x^2+\eta_y^2}{2}\right) \\ \vec{v}_\perp(z,\eta) &= \vec{v}_{\perp(nd)}(z) + v_{z(nd)}(z)\vec{\eta} \ , \end{aligned} \tag{4}$$

and

$$\vec{r}_\perp^{(c)}(z,\vec{\eta}) = \vec{r}_{\perp(nd)}^{(c)}(z) + \vec{\eta}z \ . \tag{5}$$

Also $\tilde{a}_2$ will depend on $\vec{\eta}$. The exact dependence is fixed by the way the beam is prepared and should be regarded as a condition for the orientation of the

microbunching wavefront. In all generality we can write:

$$\tilde{a}_2 = \tilde{a}_2 \left(z, \vec{r}_\perp - \vec{r}_\perp^{(c)}(z, \vec{\eta}) \right) \ . \tag{6}$$

In the limit for $\gamma^2 \gg 1$, the total current density can be written as

$$\vec{j}(z,t,\vec{\eta}) = \frac{\vec{v}(z,\vec{\eta})}{c} j_o \left(\vec{r}_\perp - \vec{r}_\perp^{(c)}(z,\vec{\eta}) \right) \times \left\{ 1 + \left[\tilde{a}_2 \left(z, \vec{r}_\perp - \vec{r}_\perp^{(c)}(z,\vec{\eta}) \right) \right. \right.$$
$$\left. \left. \exp \left[i\omega \int_0^z \frac{dz'}{v_z(z',\vec{\eta})} - i\omega t \right] + \text{C.C.} \right] \right\} \ . \tag{7}$$

One can express the charge density as

$$\rho = \frac{j_z}{v_z} \simeq \frac{j_z}{c} \ , \tag{8}$$

as we will be working in the paraxial approximation.

Eq. (7) and Eq. (8) give us the expressions to be used as sources for Maxwell equation. Looking for solutions for $\vec{E}_\perp$ in the form

$$\vec{E}_\perp = \vec{\tilde{E}}_\perp \exp\left[i\omega(z/c - t) \right] + \text{C.C.} \tag{9}$$

and applying the paraxial approximation, one may write the Maxwell equation describing $\vec{\tilde{E}}_\perp$ as [11]:

$$\left({\nabla_\perp}^2 + \frac{2i\omega}{c} \frac{\partial}{\partial z} \right) \vec{\tilde{E}}_\perp = \frac{4\pi}{c} \exp \left[i \left(\Phi_s - \omega \frac{z}{c} \right) \right] \left[\frac{i\omega}{c^2} \vec{v}_\perp - \vec{\nabla}_\perp \right] j_o \tilde{a}_2 \ , \tag{10}$$

were we have put

$$\Phi_s(z,\vec{\eta}) = \omega \int_0^z \frac{dz'}{v_z(z',\vec{\eta})} \ . \tag{11}$$

With the aid of the appropriate Green's function an exact solution of Eq. (10) can be found without any extra assumption about the parameters of the problem.

$$\vec{\tilde{E}}_\perp(z_o, \vec{r}_{\perp o}) = -\frac{1}{c} \int_{-\infty}^{\infty} dz' \frac{1}{z_o - z'} \int d\vec{r'}_\perp \left[\frac{i\omega}{c^2} \vec{v}_\perp(z',\vec{\eta}) - \vec{\nabla}'_\perp \right]$$

$$\times j_o\left(\vec{r'}_\perp - \vec{r}_\perp^{(c)}(z',\vec{\eta})\right)\tilde{a}_2\left(z',\vec{r'}_\perp - \vec{r}_\perp^{(c)}(z',\vec{\eta})\right)$$
$$\exp\left\{i\omega\left[\frac{|\vec{r}_{\perp o} - \vec{r'}_\perp|^2}{2c(z_o - z')}\right] + i\left[\Phi_s(z',\vec{\eta}) - \omega\frac{z'}{c}\right]\right\} , \qquad (12)$$

where $\vec{\nabla}'_\perp$ represents the gradient operator with respect to the source point, while $(z_o, \vec{r}_{\perp o})$ indicates the observation point. Integration by parts of the gradient terms leads to

$$\tilde{\vec{E}}_\perp = -\frac{i\omega}{c^2}\int_{-\infty}^{\infty} dz' \frac{1}{z_o - z'}\int d\vec{r'}_\perp \left(\frac{\vec{v}_\perp(z',\vec{\eta})}{c} - \frac{\vec{r}_{\perp o} - \vec{r'}_\perp}{z_o - z'}\right)$$
$$\times j_o\left(\vec{r'}_\perp - \vec{r}_\perp^{(c)}(z',\vec{\eta})\right)\tilde{a}_2\left(z',\vec{r'}_\perp - \vec{r}_\perp^{(c)}(z',\vec{\eta})\right)\exp\left[i\Phi_T(z',\vec{r'}_\perp,\vec{\eta})\right] , \qquad (13)$$

where the total phase Φ_T is given by

$$\Phi_T = \left[\Phi_s - \omega\frac{z'}{c}\right] + \omega\left[\frac{|\vec{r}_{\perp o} - \vec{r'}_\perp|^2}{2c(z_o - z')}\right] . \qquad (14)$$

We will now make use of a new integration variable $\vec{l} = \vec{r'}_\perp - \vec{r}_\perp^{(c)}(z',\vec{\eta})$ so that

$$\tilde{\vec{E}}_\perp = -\frac{i\omega}{c^2}\int_{-\infty}^{\infty} dz' \frac{1}{z_o - z'}\int d\vec{l} \left(\frac{\vec{v}_\perp(z',\vec{\eta})}{c} - \frac{\vec{r}_{\perp o} - \vec{r}_\perp^{(c)}(z',\vec{\eta}) - \vec{l}}{z_o - z'}\right)$$
$$\times j_o\left(\vec{l}\right)\tilde{a}_2\left(z',\vec{l}\right)\exp\left[i\Phi_T(z',\vec{l},\vec{\eta})\right] , \qquad (15)$$

and

$$\Phi_T = \left[\Phi_s - \omega\frac{z'}{c}\right] + \omega\left[\frac{|\vec{r}_{\perp o} - \vec{r}_\perp^{(c)}(z',\vec{\eta}) - \vec{l}|^2}{2c(z_o - z')}\right] . \qquad (16)$$

We will consider the case of a planar undulator and we will be interested in the total power of the second harmonic emission and in the directivity diagram of the radiation in the far zone. Accounting for the beam deflection angles η_x and η_y we model the electron transverse motion as:

$$\vec{v}_\perp(z',\vec{\eta}) = \left[-\frac{cK}{\gamma}\sin\left(k_w z'\right) + \eta_x v_z\right]\vec{x} + \left[\eta_y v_z\right]\vec{y} , \qquad (17)$$

and

$$\vec{r}_{\perp}^{(c)}(z',\vec{\eta})+\vec{l}=\left[\frac{K}{\gamma k_w}\left(\cos\left(k_w z'\right)-1\right)+\eta_x z'+l_x\right]\vec{x}+\left[\eta_y z'+l_y\right]\vec{y}\ . \quad (18)$$

Here K is the deflection parameter and $k_w=2\pi/\lambda_w$, λ_w being the undulator period. Moreover, one has

$$\begin{aligned}\frac{c\Phi_s}{\omega}\simeq&\left(\frac{4\gamma^2}{4\gamma^2-K^2}+\frac{\eta_x^2+\eta_y^2}{2}\right)z'-\frac{K\eta_x}{k_w\gamma}\\&-\frac{K^2}{8\gamma^2 k_w}\sin\left(2k_w z'\right)+\frac{K\eta_x}{\gamma k_w}\cos\left(k_w z'\right)\ ,\end{aligned} \quad (19)$$

We will now introduce the far zone approximation. Substitution of Eq. (19), Eq. (18) and Eq. (17) in Eq. (13) yields the field contribution calculated along the undulator:

$$\begin{aligned}\tilde{\vec{E}}_{\perp}=&\frac{i\omega}{c^2 z_o}\int d\vec{l}\int_{-L_w/2}^{L_w/2}dz' j_o\left(\vec{l}\right)\tilde{a}_2\left(z',\vec{l}\right)\exp\left[i\Phi_T\right]\\&\times\left[\left(\frac{K}{\gamma}\sin\left(k_w z'\right)+\left(\theta_x-\eta_x\right)\right)\vec{x}+\left(\theta_y-\eta_y\right)\vec{y}\right]\ ,\end{aligned} \quad (20)$$

where

$$\begin{aligned}\Phi_T=&\omega\left\{\frac{z'}{2\gamma^2 c}\left[1+\frac{K^2}{2}+\gamma^2\left(\left(\theta_x-\eta_x\right)^2+\left(\theta_y-\eta_y\right)^2\right)\right]\right.\\&\left.-\frac{K^2}{8\gamma^2 k_w c}\sin\left(2k_w z'\right)-\frac{K(\theta_x-\eta_x)}{\gamma k_w c}\cos\left(k_w z'\right)\right\}\\&+\omega\left\{\frac{K}{k_w\gamma c}(\theta_x-\eta_x)-\frac{1}{c}(\theta_x l_x+\theta_y l_y)+(\theta_x^2+\theta_y^2)\frac{z_o}{2c}\right\}\ .\end{aligned} \quad (21)$$

Here θ_x and θ_y indicate the observation angles x_o/z_o and y_o/z_o. Moreover, the integration is performed in from $-L_w/2$ to $L_w/2$ in dz', $L_w=N_w\lambda_w$ being the undulator length. In fact, working under the resonance approximation in the limit for $N_w\gg 1$ allows us to neglect contributions outside the undulator [11].

We will make use of the well-known expansion (see [12])

$$\exp\left[ia\sin\left(\psi\right)\right]=\sum_{p=-\infty}^{\infty}J_p(a)\exp\left[ip\psi\right]\ , \quad (22)$$

where J_p indicates the Bessel function of the first kind of order n.

We will be interested in frequencies around the second harmonic:

$$\omega_{2o} = 4k_w c\gamma_z^2 \ , \tag{23}$$

where

$$\gamma_z^2 = \frac{\gamma^2}{1 + K^2/2} \ . \tag{24}$$

Indicating with $\widetilde{\vec{E}}_{\perp 2}$ the second harmonic contribution calculated at frequencies around ω_{2o} one obtains

$$\begin{aligned}
\widetilde{\vec{E}}_{\perp 2} = & \frac{i\omega_{2o}}{c^2 z_o} \int_{-\infty}^{\infty} dl_x \int_{-\infty}^{\infty} dl_y \int_{-L_w/2}^{L_w/2} dz' j_o\left(\vec{l}\right) \tilde{a}_2\left(z', \vec{l}\right) \exp[i\Phi_o] \\
& \times \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} J_m(u) J_n(v) \exp\left[\frac{in\pi}{2}\right] \\
& \times \left\{ \left[-i\frac{K}{2\gamma} \left(\exp\left\{i[R_\omega + 1]k_w z'\right\} - \exp\left\{i[R_\omega - 1]k_w z'\right\} \right) \right.\right. \\
& \left.\left. + (\theta_x - \eta_x) \exp\left\{iR_\omega k_w z'\right\} \right] \vec{x} + \left[(\theta_y - \eta_y) \exp\left\{iR_\omega k_w z'\right\} \right] \vec{y} \right\} \ ,
\end{aligned} \tag{25}$$

where

$$R_\omega = \frac{\omega}{\omega_1} - n - 2m \ , \tag{26}$$

with

$$\omega_1^{-1} = \frac{1}{2k_w c\gamma^2} \left\{ 1 + \frac{K^2}{2} + \gamma^2 \left[(\theta_x - \eta_x)^2 + (\theta_y - \eta_y)^2 \right] \right\} \ . \tag{27}$$

Moreover

$$u = \frac{\omega_{2o}}{\omega_1} \frac{K^2 \left[1 - K^2/(4\gamma^2)\right]}{4\left\{1 + \frac{K^2}{2} + \gamma^2 \left[(\theta_x - \eta_x)^2 + (\theta_y - \eta_y)^2 \right] \right\}}, \tag{28}$$

$$v = \frac{\omega_{2o}}{\omega_1} \frac{2K\gamma \left[1 - K^2/(4\gamma^2)\right] (\theta_x - \eta_x)}{1 + \frac{K^2}{2} + \gamma^2 \left[(\theta_x - \eta_x)^2 + (\theta_y - \eta_y)^2 \right]} \tag{29}$$

and

$$\Phi_o = \omega_{2o} \left[\frac{K}{k_w \gamma c} (\theta_x - \eta_x) - \frac{1}{c} (\theta_x l_x + \theta_y l_y) + \frac{z_o}{2c} (\theta_x^2 + \theta_y^2) \right] \ . \tag{30}$$

In the limit for $N_w \gg 1$ and if $\tilde{a}_2$ does not vary much in z' over a period of the undulator λ_w the fast oscillations in the exponential function in the integrand of Eq. (25) tend to suppress the integral unless $R_\omega = 0$, $R_\omega = -1$ or $R_\omega = 1$, that is when at least one of the exponential function is simply unity. If $\omega = \omega_2$ this corresponds to $n = 2 - 2m$, $n = 3 - 2m$ and $n = 1 - 2m$ respectively. Neglecting all other terms and imposing $\omega = \omega_2 + \Delta\omega_2$ we obtain

$$\begin{aligned}
\widetilde{\vec{E}}_{\perp 2} = & \frac{i\omega_{2o}}{c^2 z_o} \int_{-\infty}^{\infty} dl_x \int_{-\infty}^{\infty} dl_y \int_{-L_w/2}^{L_w/2} dz' j_o\left(\vec{l}\right) \tilde{a}_2\left(z', \vec{l}\right) \exp[i\Phi_o] \exp\left\{i\frac{\Delta\omega_2}{\omega_1} k_w z'\right\} \\
& \times \sum_{m=-\infty}^{\infty} \left\{ \left[-i\frac{K}{2\gamma} \left(J_m(u) J_{3-2m}(v) \exp\left\{\frac{i[3-2m]\pi}{2}\right\} \right.\right.\right. \\
& \left. -J_m(u) J_{1-2m}(v) \exp\left\{\frac{i[1-2m]\pi}{2}\right\} \right) \\
& \left. + (\theta_x - \eta_x) J_m(u) J_{2-2m}(v) \exp\left\{\frac{i[2-2m]\pi}{2}\right\} \right] \vec{x} \\
& \left. + \left[(\theta_y - \eta_y) J_m(u) J_{2-2m}(v) \exp\left\{\frac{i[2-2m]\pi}{2}\right\} \right] \vec{y} \right\} . \qquad (31)
\end{aligned}$$

For any value of K and $\theta_x - \eta_x$ much smaller than $1/\gamma_z$, v is a small parameter and only the smallest indexes in the Bessel functions $J_q(v) \sim v^q$ in Eq. (25) give non negligible contribution. As a result, Eq. (25) can be drastically simplified. One can write (compare, for instance, with [11]):

$$\begin{aligned}
\widetilde{\vec{E}}_{\perp 2} = & \frac{i\omega_{2o}}{c^2 z_o} \left[\mathcal{A}(\theta_x - \eta_x)\vec{x} + \mathcal{B}(\theta_y - \eta_y)\vec{y}\right] \int_{-\infty}^{\infty} dl_x \int_{-\infty}^{\infty} dl_y \int_{-L_w/2}^{L_w/2} dz' \exp\left[i\Phi_o\right] \\
& \times j_o\left(\vec{l}\right) \tilde{a}_2\left(z', \vec{l}\right) \exp[iCz'] \exp\left\{i2\gamma_z^2 \left[(\theta_x - \eta_x)^2 + (\theta_y - \eta_y)^2\right] k_w z'\right\} \qquad (32)
\end{aligned}$$

where we have defined

$$\mathcal{A} = \frac{2K^2}{2+K^2} \left[J_0\left(\frac{K^2}{2+K^2}\right) - J_2\left(\frac{K^2}{2+K^2}\right) \right] + J_1\left(\frac{K^2}{2+K^2}\right) , \qquad (33)$$

$$\mathcal{B} = J_1\left(\frac{K^2}{2+K^2}\right) , \qquad (34)$$

we have used the fact that

$$\frac{\Delta\omega_2}{\omega_1} = 2\gamma_z^2 \left[(\theta_x - \eta_x)^2 + (\theta_y - \eta_y)^2\right] + C , \qquad (35)$$

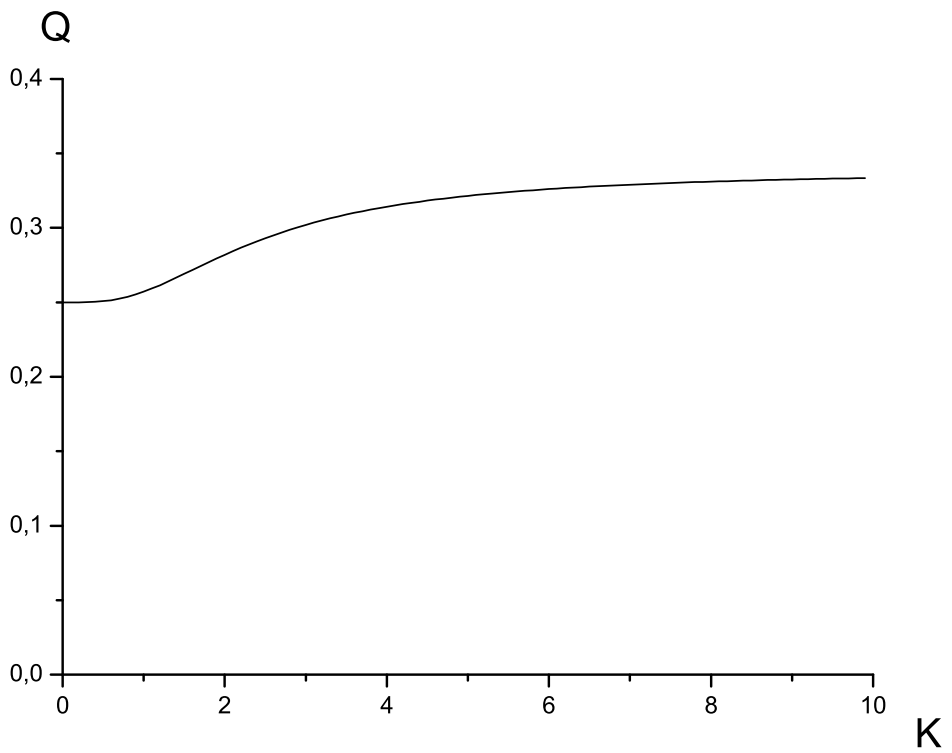

Fig. 1. Illustration of the behavior of the ratio $Q(K)$ between the second harmonic field contribution due to the gradient of the density part of the source and the contribution due to the current part of the source.

with

$$C = \frac{\omega - \omega_{2o}}{\omega_{1o}} \tag{36}$$

and, under the resonant approximation, we have

$$\Phi_o = \frac{\omega_{2o}}{c}\left[-(\theta_x l_x + \theta_y l_y) + \frac{z_o}{2}(\theta_x^2 + \theta_y^2)\right] \ . \tag{37}$$

The detuning parameter C should indeed be considered as a function of z, $C = C(z)$ which can be retrieved from the knowledge of $\gamma = \gamma(z)$.

It is important to see that the terms in J_1 in Eq. (33) and Eq. (34) are due to the presence of the gradient term in $\vec{\nabla}_\perp(j_o \tilde{a}_2)$ in Eq. (10), which has been omitted in [3] and later on in [4, 8]. We find that, without the gradient, term one would recover results quantitatively incorrect for the x-polarization component. In Fig. 1 we plotted the ratio between the contribution of the radiation

field due to the gradient of the density part of the source and the contribution due to the current part of the source for the x-polarization component. This is a function $Q(K)$ of the K parameter only and it can be written as

$$Q = \frac{\tilde{E}_{\perp 2g}}{\tilde{E}_{\perp 2c}} = \frac{2+K^2}{2K^2} J_1\left(\frac{K^2}{2+K^2}\right) \Big/ \left[J_0\left(\frac{K^2}{2+K^2}\right) - J_2\left(\frac{K^2}{2+K^2}\right)\right] \ , \tag{38}$$

where the subscript "g" stands for "gradient and "c" stands for "current". As it can be seen from Fig. 1, the gradient term always contributes for more than one fourth of the total field, independently of the values of K. Also, if the gradient term is omitted, the entire contribution to the field polarized in the y direction would go overlooked. The inclusion of the gradient term in the source part of the wave equation should not be considered as a peculiarity of the second harmonic generation mechanism. In Synchrotron Radiation theory from bending magnets, for instance, the presence of such a source term is customary and it is responsible, as here, for part of the horizontally polarized field and for the entire vertically polarized field. Moreover, the gradient term is always associated with an integration by part, and therefore is always accompanied with the gradient of the Green's function, which is responsible for a term proportional to the observation angle $\theta_{x,y}$.

Eq. (32) can be also written as:

$$\begin{aligned}\tilde{\vec{E}}_{\perp 2} = & \frac{i\omega_{2o}}{c^2 z_o} \exp\left[i\frac{\omega_{2o}}{2c} z_o(\theta_x^2+\theta_y^2)\right] \left[\mathcal{A}(\theta_x-\eta_x)\vec{x} + \mathcal{B}(\theta_y-\eta_y)\vec{y}\right] \\ & \times \int_{-\infty}^{\infty} dl_x \int_{-\infty}^{\infty} dl_y \int_{-\infty}^{\infty} dz' \exp\left[-i\frac{\omega_{2o}}{c}\left(\theta_x l_x + \theta_y l_y\right)\right] \\ & \times \exp\left\{i\frac{\omega_{2o}}{2c}\left[(\theta_x-\eta_x)^2 + (\theta_y-\eta_y)^2\right] z'\right\} \tilde{\rho}^{(2)}(z', \vec{l}, C) \ , \end{aligned} \tag{39}$$

where we have defined $\tilde{\rho}$ as

$$\tilde{\rho}^{(2)}(z', \vec{l}, C) = j_o\left(\vec{l}\right) \tilde{a}_2\left(z', \vec{l}\right) \exp\left[iCz'\right] H_{L_w}(z') \ , \tag{40}$$

$H_{L_w}(z')$ being a function equal to unity over the interval $[-L_w/2, L_w/2]$ and zero everywhere else. Its introduction simply amounts to a notational change. Namely it accounts for the fact that the integral in dz' is performed over the undulator length in Eq. (32), while it is performed from $-\infty$ to ∞ in Eq. (39). It should be noted that, usually, computer codes do not present the functions $\tilde{a}_2$ and $\exp[iCz']$ separately as we did, but rather they combine them in a single product, usually known as the complex amplitude of the electron beam modulation with respect to the phase $\psi = 2k_w z' + (\omega/c)z' - \omega t$. Regarding $\tilde{\rho}^{(2)}$

as a given function allows one not to bother about a particular presentation of the beam modulation.

Eq. (32) or, equivalently, Eq. (39) are our most general result, and are valid independently on the model chosen for the current density and the modulation. It is interesting to note here that, when one writes Eq. (32) in the form of Eq. (39), one obtains an expression which is *formally* similar to the spatial Fourier transform of $\tilde{\rho}^{(2)}(z', \vec{l}, C)$ with respect to z' and $\vec{l}$. There are two problems though: first, $\tilde{\rho}^{(2)}$ is a function of $\vec{\eta}$, which appears in the conjugate variable to z' and, second, if $\gamma = \gamma(z)$ one has $\omega_{2o} = \omega_{2o}(z)$.

3 Analysis of a simple model

Let us treat a particular case. Namely, let us consider the case when we can consider $\gamma(z) = \bar{\gamma} = \text{const}$, when $C(z) = 0$ and

$$\tilde{\rho}^{(2)}(z, \vec{l}) = j_o\left(\vec{l}\right) a_{2o} \exp\left[i\frac{\omega_{2o}}{c}\left(\eta_x l_x + \eta_y l_y\right)\right] H_{L_w}(z) \ , \tag{41}$$

with $a_{2o} = \text{const}$ and

$$j_o\left(\vec{l}\right) = \frac{I_o}{2\pi\sigma^2} \exp\left(-\frac{l_x^2 + l_y^2}{2\sigma^2}\right) \ , \tag{42}$$

I_o and σ being the bunch current and transverse size respectively.

This particular case corresponds to a modulation wavefront perpendicular to the beam direction of motion. In this case Eq. (39) can be written as

$$\begin{aligned}\tilde{\vec{E}}_{\perp 2} = & \frac{i a_{2o}\omega_{2o}}{c^2 z_o} \exp\left[i\frac{\omega_{2o}}{2c} z_o(\theta_x^2 + \theta_y^2)\right] \left[\mathcal{A}(\theta_x - \eta_x)\vec{x} + \mathcal{B}(\theta_y - \eta_y)\vec{y}\right] \\ & \times \int_{-\infty}^{\infty} dl_x \int_{-\infty}^{\infty} dl_y \int_{-\infty}^{\infty} dz' \exp\left\{-i\frac{\omega_{2o}}{c}\left[\left(\theta_x - \eta_x\right) l_x + \left(\theta_y - \eta_y\right) l_y\right]\right\} \\ & \times \exp\left\{i\frac{\omega_{2o}}{2c}\left[\left(\theta_x - \eta_x\right)^2 + \left(\theta_y - \eta_y\right)^2\right] z'\right\} j_o\left(\vec{l}\right) H_{L_w}(z')\end{aligned} \tag{43}$$

and amounts, indeed to the spatial Fourier transform of $j_o\left(\vec{l}\right) H_{L_w}(z')$. We obtain straightforwardly:

$$\tilde{\vec{E}}_{\perp 2} = \frac{i I_o a_{2o}\omega_{2o} L_w}{c^2 z_o} \exp\left[i\frac{\omega_{2o}}{2c} z_o(\theta_x^2 + \theta_y^2)\right] \left[\mathcal{A}(\theta_x - \eta_x)\vec{x} + \mathcal{B}(\theta_y - \eta_y)\vec{y}\right]$$

$$\times \mathrm{sinc}\left\{\frac{L_w\omega_{2o}}{4c}\left[(\theta_x-\eta_x)^2+(\theta_y-\eta_y)^2\right]\right\}$$
$$\times \exp\left\{-\frac{\sigma^2\omega_{2o}^2}{2c^2}\left[(\theta_x-\eta_x)^2+(\theta_y-\eta_y)^2\right]\right\} . \quad (44)$$

If the beam is prepared in a different way so that, for instance, the modulation wavefront is not orthogonal to the direction of propagation of the beam, Eq. (39) retains its validity. However it should be noted that, in this case, Eq. (39) is not, in general, a Fourier transform. It is if $\gamma(z) = \bar{\gamma} = \text{const}$ and $\tilde{\rho}^{(2)}$ includes a phase factor of the form $\exp\left[i\alpha\vec{\eta}\cdot\vec{l}\right]$. The case $\alpha = 1$ has just been treated. The case $\alpha = 0$ corresponds, instead, to a modulation wavefront orthogonal to the z axis and *not* to the direction of propagation.

Going back to our particular case in Eq. (44), a subject of particular interest is the angular distribution of the radiation intensity along the $\vec{x}$ and $\vec{y}$ polarization directions which will be denoted with $I_{2(x,y)}$. Upon introduction of normalized quantities:

$$\hat{\theta} = \sqrt{\frac{\omega_{2o}L_w}{c}}\theta = \sqrt{8\pi N_w}\gamma_z\theta$$
$$\hat{\eta} = \sqrt{\frac{\omega_{2o}L_w}{c}}\eta = \sqrt{8\pi N_w}\gamma_z\eta$$
$$\hat{l}_{x,y} = \sqrt{\frac{\omega_{2o}}{cL_w}}l_{x,y} = \sqrt{8\pi N_w}\frac{\gamma_z}{L_w}l_{x,y} \quad (45)$$

and of the Fresnel number:

$$N = \frac{\omega_{2o}\sigma^2}{cL_w} , \quad (46)$$

one obtains

$$I_{2(x,y)}\left(\hat{\theta}_x-\hat{\eta}_x,\hat{\theta}_y-\hat{\eta}_y\right) = \text{const}\times\left(\hat{\eta}_{x,y}-\hat{\theta}_{x,y}\right)^2$$
$$\times\mathrm{sinc}^2\left\{\frac{1}{4}\left[\left(\hat{\theta}_x-\hat{\eta}_x\right)^2+\left(\hat{\theta}_y-\hat{\eta}_y\right)^2\right]\right\}$$
$$\times\exp\left\{-N\left[\left(\hat{\theta}_x-\hat{\eta}_x\right)^2+\left(\hat{\theta}_y-\hat{\eta}_y\right)^2\right]\right\} . \quad (47)$$

Note that in the limit for $N \ll 1$, Eq. (47) restitutes the directivity diagram for the second harmonic radiation from a single particle. In agreement with Synchrotron Radiation textbooks [9, 10] none of the polarization components of $I_{2(x,y)}$ has azimuthal symmetry, contrarily with what happens for the first harmonic, where only the x polarization is present and is endowed with azimuthal symmetry.

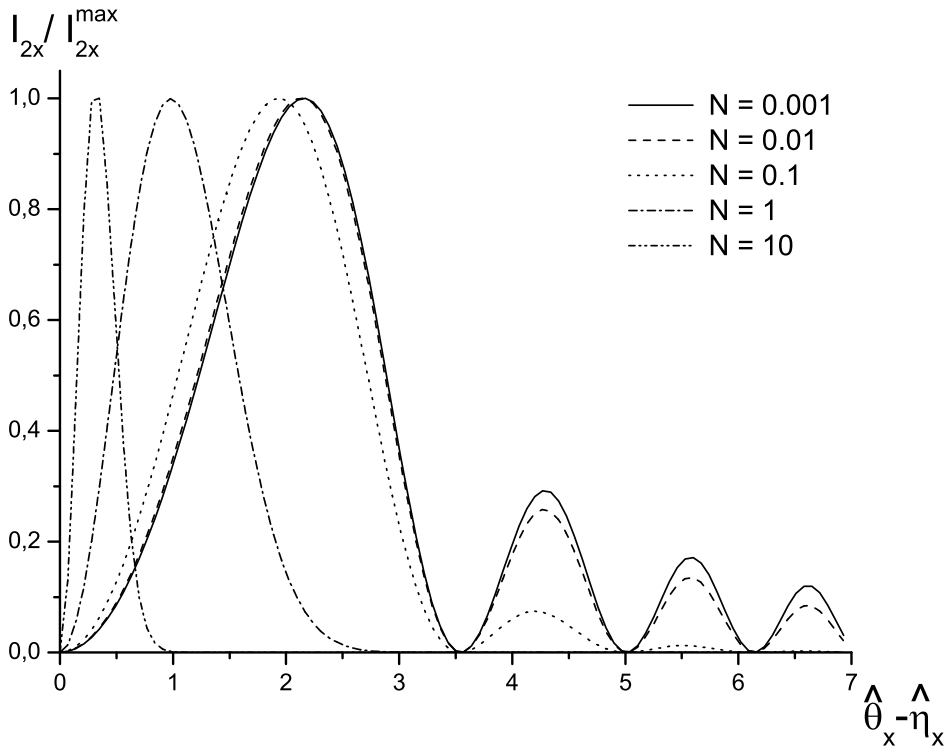

Fig. 2. Plot of the directivity diagram for the radiation intensity as a function of $\hat{\theta}_x - \hat{\eta}_x$ at $\hat{\theta}_y - \hat{\eta}_y = 0$ for the horizontal polarization component, for different values of N.

As an example, the directivity diagram in Eq. (47) is plotted in Fig. 2 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 horizontal polarization component.

The next step is the calculation of the second harmonic power. The power for the x- and y-polarization components of the second harmonic radiation are given by

$$W_{2(x,y)} = \frac{c}{4\pi} \int_{-\infty}^{\infty} dx_o \int_{-\infty}^{\infty} dy_o \overline{|E_{\perp x,y}(z_o, x_o, y_o, t)|^2}$$
$$= \frac{c}{2\pi} \int_{-\infty}^{\infty} dx_o \int_{-\infty}^{\infty} dy_o |\tilde{E}_{\perp x,y}(z_o, x_o, y_o)|^2 \ , \quad (48)$$

where $\overline{(...)}$ denotes averaging over a cycle of oscillation of the carrier wave.

We will still consider the model specified by Eq. (41) and Eq. (42) with $C = 0$. It is convenient to present the expressions for W_{2x} and W_{2y} in a dimension-

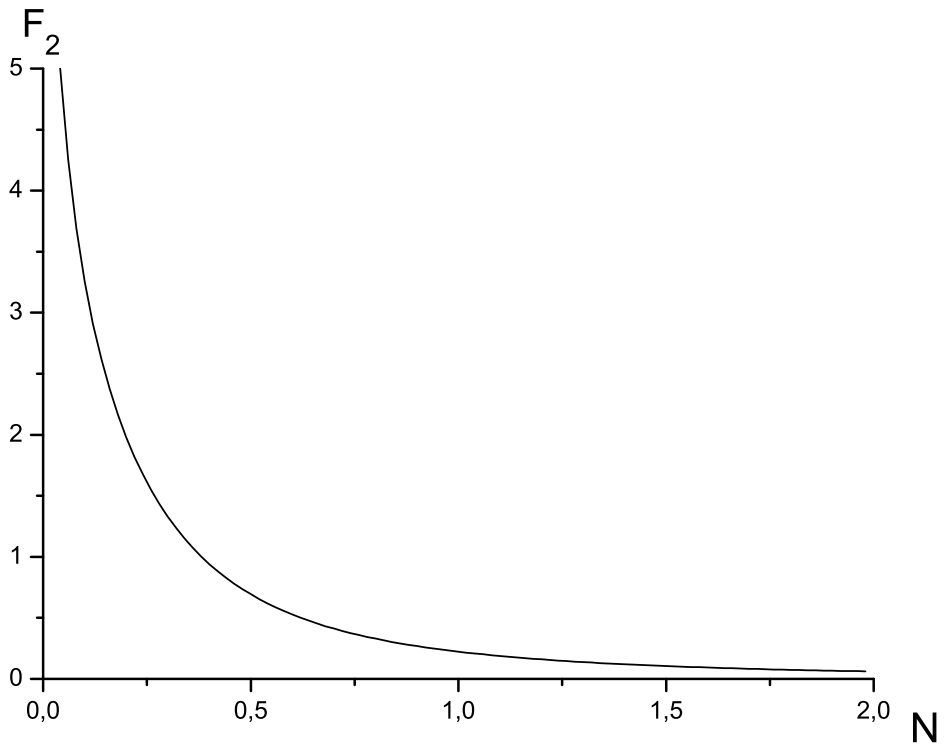

Fig. 3. Illustration of the behavior of $F_2(N)$.

less form. After appropriate normalization they both are a function of one dimensionless parameter only:

$$\hat{W}_{2x} = \hat{W}_{2y} = F_2(N) = \ln\left(1 + \frac{1}{4N^2}\right) . \tag{49}$$

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

$$\begin{pmatrix} W_{ox}^{(2)} \\ W_{oy}^{(2)} \end{pmatrix} = \begin{pmatrix} \mathcal{A}^2 \\ \mathcal{B}^2 \end{pmatrix} \frac{a_{2o}^2 I_o^2}{2\pi c} . \tag{50}$$

For practical purposes it is convenient to express Eq. (50) in the form:

$$\begin{pmatrix} W_{ox}^{(2)} \\ W_{oy}^{(2)} \end{pmatrix} = \begin{pmatrix} \mathcal{A}^2 \\ \mathcal{B}^2 \end{pmatrix} W_b \left[\frac{a_{2o}^2}{2\pi}\right] \left[\frac{I_o}{\gamma I_A}\right] , \tag{51}$$

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 function $F_2(N)$ is plotted in Fig. 3. 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 in Eq. (32) is valid only as $\hat{\theta}^2 \lesssim N_w$. As a result we find that Eq. (49) is valid only up to values of N such that $N \gtrsim N_w^{-1}$. However, in the case $N < N_w^{-1}$ we deal with a situation when the dimensionless problem parameter N is smaller than the accuracy of the resonance approximation $\sim N_w^{-1}$. 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 $\ln(N) \longrightarrow \ln(N_w^{-1})$.

We will now compare our results for the second harmonic with already known results for the first. The case treated in [13] corresponds to a modulation wavefront orthogonal to the direction of propagation, exactly as specified here for the second harmonic (i.e. perfect resonance with Eq. (41) and Eq. (42) valid) and allows direct comparison of results. The outcomes of [13] have been presented, similarly to what has been done here for the second harmonic, in dimensionless form. After appropriate normalization, one finds:

$$\hat{W}_1(N) = \frac{W_1}{W_o^{(1)}} = F_1(N) = \frac{2}{\pi}\left[\arctan\left(\frac{1}{N}\right) + \frac{N}{2}\ln\left(\frac{N^2}{N^2+1}\right)\right] \ , \qquad (52)$$

where the normalization factor $W_o^{(1)}$ is given by

$$W_o^{(1)} = W_b \left[2\pi^2 a_{1o}^2\right]\left[\frac{I_o}{\gamma I_A}\right]\left[\frac{K^2}{2+K^2}\right] N_w A_{JJ}^2 \ , \qquad (53)$$

A_{JJ} being given by

$$A_{JJ} = J_0\left(\frac{K^2}{4+2K^2}\right) - J_1\left(\frac{K^2}{4+2K^2}\right) \ . \qquad (54)$$

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]. It should also be noted that all N in Eq. (52) are multiplied by a factor $1/2$ with respect to what is reported in [13]. This is because we are referring all results to the Fresnel number for the second harmonic.

The function $F_1(N)$ is plotted in Fig. 4. We can compare more quantitatively the normalized power for the second and for the first harmonic:

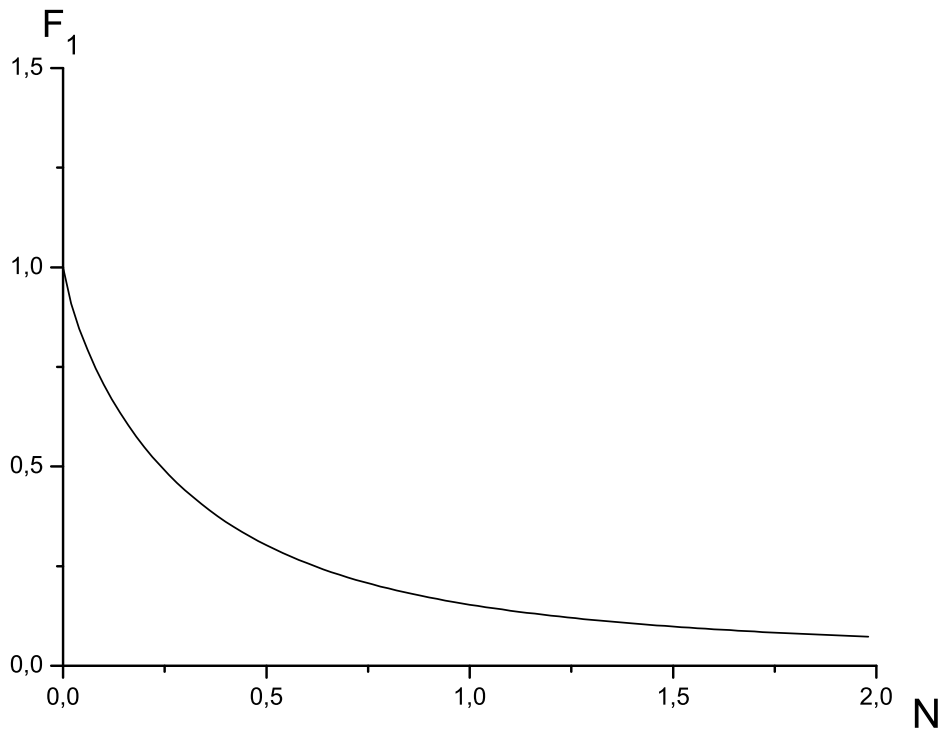

Fig. 4. Illustration of the behavior of $F_1(N)$.

$$\frac{F_2(N)}{F_1(N)} = \frac{\pi}{2}\left[\frac{\ln\left(1+\frac{1}{4N^2}\right)}{\arctan\left(\frac{1}{N}\right)+\frac{N}{2}\ln\left(\frac{N^2}{N^2+1}\right)}\right] , \tag{55}$$

while, from a practical viewpoint, the comparison between the real powers is equal to

$$\frac{W_2}{W_1} = \frac{W_{ox}^{(2)}+W_{oy}^{(2)}}{W_o^{(1)}}\frac{F_2(N)}{F_1(N)} = \frac{1}{(2\pi)^3 N_w}\frac{2+K^2}{K^2}\frac{a_{2o}^2}{a_{1o}^2}\frac{\mathcal{A}^2+\mathcal{B}^2}{A_{JJ}^2}\frac{F_2(N)}{F_1(N)} . \tag{56}$$

It is interesting to calculate Eq. (55) in the limit $N \gg 1$. We have

$$\frac{F_2(N)}{F_1(N)} \longrightarrow \frac{\pi}{4N} \quad \text{at} \quad N \gg 1 . \tag{57}$$

In Fig. 5 we plot the behavior of F_2/F_1 as a function of N and its asymptotic, $\pi/(4N)$, for $N \gg 1$.

Finally, it is possible to study the ratio between the second harmonic power due to the y vertical and the x horizontal polarization components, that is only

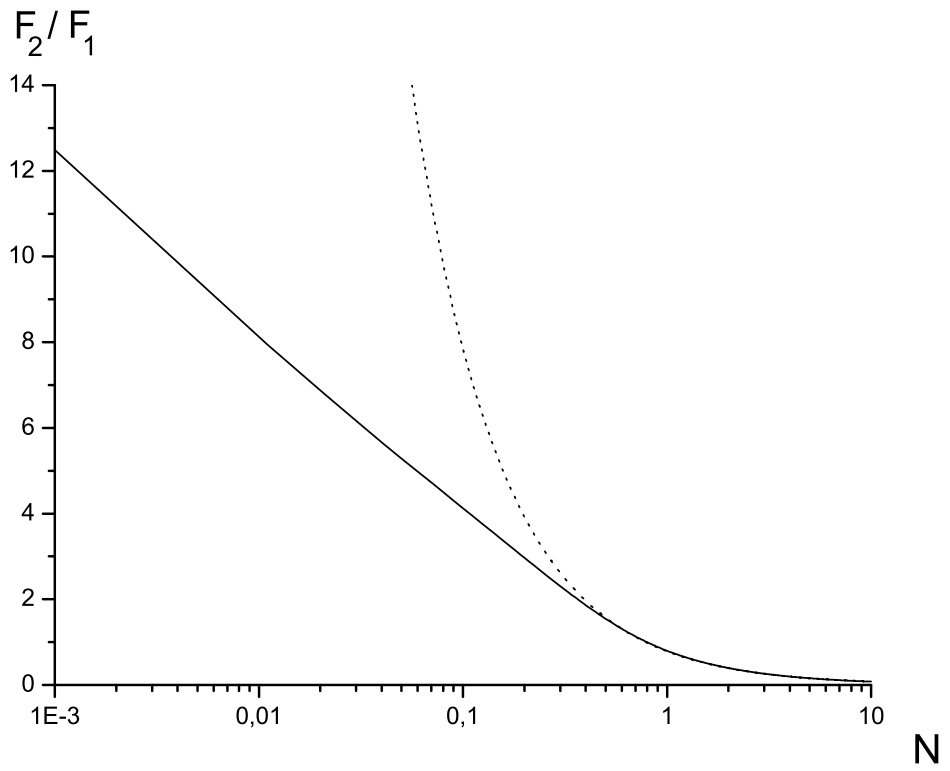

Fig. 5. Solid line: illustration of the behavior of F_2/F_1 as a function of N. Dashed line: its asymptotic, $\pi/(4N)$, for $N \gg 1$.

a function of the K parameter and is simply given by the ratio $R = W_{2y}/W_{2x}$:

$$R(K) = \frac{W_{2y}}{W_{2x}} = \frac{\mathcal{A}^2(K)}{\mathcal{B}^2(K)} \ . \tag{58}$$

A plot of $R(K)$ is given in Fig. 6. As it is seen the relative magnitude scales from 4% in the case $K \ll 1$ till about 6% in the limit $K \gg 1$: as one can see, the vertical polarization component of the radiation depends quite weakly on the K parameter. 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 wavelength range, the reflection coefficients of many materials (e.g. SiC, that is widely used for mirrors) exhibit a complicated behavior, and there may be even an order of magnitude difference depending on the polarization of the radiation. It should be noted that $R(K)$ is independent of the particular model chosen for the beam modulation as it is easy to understand inspecting Eq. (32). It is also important to remark the fact that the second harmonic radiation from a planar undulator is linearly polarized, since vertical and horizontal polarization components are characterized

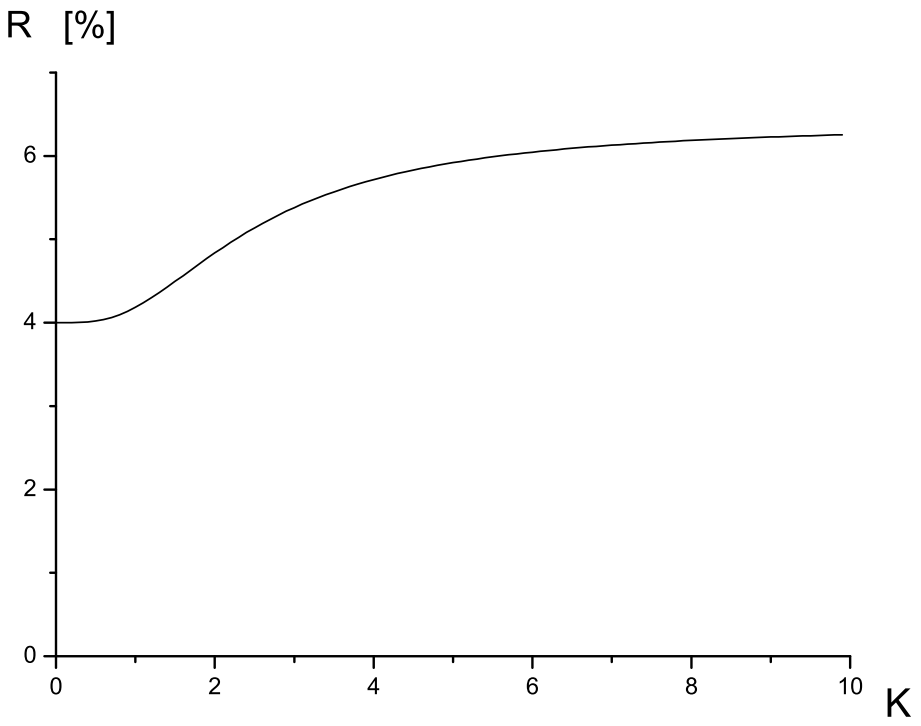

Fig. 6. Illustration of the behavior of the ratio between the second harmonic power due to the y vertical and the x horizontal polarization components, $R(K)$.

by the same phase factor. This fact is well-known in Synchrotron Radiation theory for a single particle and it is true for any observation angle and any harmonic of the radiation from a planar undulator [10] in contrast, for instance, to the case of bending magnet radiation, when vertical and horizontal polarization components exhibit a relative $\pi/2$ phase shift, indicating circular polarization.

An important comment to what has been done before is needed. We calculated the electric field, the angular intensity distribution and the power for the second harmonic making a particular assumption about the electron beam modulation in Eq. (41). This amounts to consider the modulation wavefront orthogonal to the direction of propagation of the beam. The same assumption has been implicitly done calculating the first harmonic power (the expression in [13] has been used, which does not account for deflection angles). In this particular case 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 the more general situation we find that the second harmonic power can be independent of the beam deflection angle (like in the situation treated by us) or can decrease due to the presence of extra oscillating factors in $\vec{l}$ in Eq. (39). On the contrary, in [8], an increase of the total power is reported due to the presence of deflection

angles.

4 Discussion

After the presentation of our theory has been given, in this Section we want to discuss in a more detailed way the differences between our approach and the currently accepted treatment of the problem of second harmonic generation.

It is worth to begin summarizing the steps which led us to our main results. First, we started from the wave equation assuming that the electromagnetic sources are given externally by some code calculating the electron beam bunching at the second harmonic. Second, after applying the ultrarelativistic approximation ($\gamma^2 \gg 1$) and the resonance approximation ($N_w \gg 1$), both non-restrictive ones, we solved exactly the wave equation using the Green's function method. Third, we calculated the angular distribution of intensity assuming a given beam modulation and we derived an expression for the total power radiated at the second harmonic by integrating the expression for the angular distribution of intensity. Finally we compared the expression for the second harmonic power with the analogous expression for the first harmonic.

In [3] and later on in [4, 8] the ultrarelativistic and the resonance approximation were used too, but several steps were performed on the wave equation which we find incorrect. First, the gradient term in the source part of the wave equation is overlooked. Second, the particles trajectory in the transverse x direction is expanded (we will comment on this later on), and because of that the Fresnel number N is not identified as the main physical parameter of the problem. Third, after these manipulations, the wave equation is not solved but, rather, the second harmonic power is estimated in the following way: (a) the squared of the (manipulated) source parts of the wave equation for the second harmonic is calculated; (b) the squared of the source parts for the first [8] or the third [3, 4] harmonic is calculated; (c) the ratio between the square of the source parts for the second and either the first [8] or the third [3, 4] is taken. As a result, magnitude of the second harmonic power and polarization characteristics are predicted that are in disagreement with what we have found. In [8], further notions regarding the case of deflection angle between the beam and the undulator axis are introduced. We already expressed our critical view on this last conclusion at the end of the previous Section. Let us briefly comment on the other points mentioned above by analyzing more in detail the approach followed in [3, 4, 8].

As has been already said, we find that neglecting the gradient term in the wave equation is not correct. As we have seen in Section 2 such term is responsible for a contribution to the total intensity for the second harmonic both for the

horizontal and for the vertical polarization components and, indeed, it cannot be neglected. Doing so would result in any case in an overall incomplete result: namely one would obtain only part of the horizontally polarized component of the field.

Going further with the derivation in [3, 4, 8], the motion of the electrons in the x-direction is written as a sum of a fast oscillation due to the undulating motion and a slow motion due to the betatron functions. On the y-direction instead, only the slow motion due to betatron functions is present. The beam distribution is then considered as a collection of individual point-particles, i.e. a sum of δ-Dirac functions. For the i-th electron one may write

$$x_i'(z) = \bar{x}_i(z) + \Delta x_i(z) \tag{59}$$

and

$$y_i'(z) = \bar{y}_i(z) \ , \tag{60}$$

where $\Delta x_i(z)$ describes the fast oscillation, while $\bar{x}_i(z)$ and $\bar{y}_i(z)$ describe the slow motion.

All the δ-Dirac in the x coordinate on the right hand side of Maxwell equation are subsequently expanded as

$$\delta(x_i - \bar{x}_i(z) - \Delta x_i(z)) \simeq \delta(x_i - \bar{x}_i(z)) - \Delta x_i(z)\delta'(x_i - \bar{x}_i(z)) \ , \tag{61}$$

based on the only assumption that the transverse beam dimension is much larger than the wiggling amplitude of the electron motion. It should be noted that, based on this assumption, the ratio between the wiggling amplitude and the transverse beam dimensions, $K/(\gamma k_w \sigma) \ll 1$, is identified as the main physical parameter of the theory and is denoted as the coupling strength of the second harmonic emission. In contrast with this we have found that the exact solution of the wave equation depends on the Fresnel number, but not on the coupling strength (see, for instance, Eq. (47)). In this regard it is suggestive to write $1/N = L_w c/(\sigma^2 \omega)$ as $1/N = [K/(\gamma k_w \sigma)]^2 \times \pi N_w (2 + K^2)/(4K^2)$. As $K/(\gamma k_w \sigma)$ assumes a fixed value (for instance, much smaller than unity according to the assumption above), our Fresnel number can assume any value, depending on the number of undulator periods N_w. If, on the one hand, $N \gg 1$ we have a behavior $F_2(N) \sim 1/(4N^2) \propto N_w^2$ so that $F_2(N)/F_1(N) \propto N_w$ as has been seen in Eq. (57) and therefore the ratio W_2/W_1 is independent on N_w as one can see from Eq. (56). On the other hand, if $N \ll 1$ we obtain $F_2(N) \sim \ln[1/(4N^2)] \sim$ const so that $F_2(N)/F_1(N)$ is independent on N_w while $W_2/W_1 \propto N_w^{-1}$. On the contrary, being based on the coupling strength

parameter only, current understandings of the second harmonic mechanism predict that W_2/W_1 is always independent on N_w.

Finally we find that, from a mathematical viewpoint, the expansion in Eq. (61) constitutes an incorrect manipulation of the right hand side of Maxwell equation and. To show this, we simply need to consider the mathematical structure of the wave equation. For any polarization component we are dealing with a differential equation:

$$\mathcal{L}\tilde{E}_{x,y}(x,y,z) = f_{x,y}(z)\sum_i \delta(x_i - \bar{x}_i(z) - \Delta x_i(z))\delta(y_i - \bar{y}_i(z)) \ , \tag{62}$$

with

$$\mathcal{L} = \left(\nabla_\perp{}^2 + \frac{2i\omega}{c}\frac{\partial}{\partial z}\right) \ , \tag{63}$$

where $f_{x,y}(z)$ is a function containing the appropriate phase factor. This is essentially equivalent to our starting equation, Eq. (10), the only differences being that the sources are presented in a different way and that, at that stage, we had already assumed that the transverse beam dimensions are not smaller than the wiggling amplitude of the electron motion.

The problem with the expansion in Eq. (61) is that $\Delta x_i = \Delta x_i(z)$ is a function of the longitudinal coordinate and that the Green's function for the wave equation depends on both longitudinal and transverse coordinates. Let us see this point in more detail. If we call with $G(z_o - z', x_o - x', y_o - y')$ the Green's function of the operator $\mathcal{L}$ we have

$$\begin{aligned}\tilde{E}_{x,y}(z_o, x_o, y_o) = &\int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dy' \int_{-\infty}^{\infty} dz' \ G(z_o - z', x_o - x', y_o - y') \\ &\times f_{x,y}(z')\delta(x' - \bar{x}(z') - \Delta x(z'))\delta(y' - \bar{y}(z)) \ ,\end{aligned} \tag{64}$$

that is

$$\begin{aligned}\tilde{E}_{x,y}(z_o, x_o, y_o) = &\int_{-\infty}^{\infty} dz' G(z_o - z', x_o - \bar{x}(z') - \Delta x(z'), y_o - \bar{y}(z')) \\ &\times f_{x,y}(z') \ .\end{aligned} \tag{65}$$

It follows that the expansion of the δ-Dirac in Eq. (61) is mathematically equivalent to the expansion of the Green's function G in $\Delta x_i(z')$ around $x_o - \bar{x}_i(z')$; however under the only assumptions $\bar{x}_i(z') \gg \mid \Delta x_i(z') \mid$ and $\bar{y}_i(z') \gg \mid$

$\Delta x_i(z')$ | we cannot expand the Green's function in $\Delta x_i(z')$ around $x_o - \bar{x}_i(z')$. In fact we have that

$$\begin{aligned} & G(z_o - z', x_o - \bar{x}_i(z') - \Delta x_i(z'), y_o - \bar{y}(z')) \\ & \neq G(z_o - z, x_o - \bar{x}_i(z'), y_o - \bar{y}_i(z')) \\ & -\Delta x_i(z') \frac{dG(z_o - z', \xi, y_o - \bar{y}_i(z'))}{d\xi} \mid_{\xi = x_o - \bar{x}_i(z')} \quad , \end{aligned} \tag{66}$$

because G is simultaneously a function of z not only through $\Delta x_i(z')$, $\bar{x}_i(z')$ and $\bar{y}_i(z')$ but also through $z_o - z'$.

5 Conclusions

In this paper we addressed the mechanism of second harmonic generation in Free-Electron Lasers.

We found that an early treatment of this phenomenon [3] is based on arbitrary manipulations of the source term of the wave equation, which describes the electrodynamical part of the problem. First, an important part of the source term is neglected and, second, an expansion of the particles trajectory in the transverse horizontal direction is performed, while we find that there is no ground for such a step. Moreover, this leads to the identification of the ratio between the amplitude of the electron wiggling motion in the (planar) undulator and the electron beam transverse size as the main physical parameter, while such parameter does not play any role in our theory. The same steps were also followed in [4, 8]. After these manipulations, the wave equation is not solved but, rather, an estimation of the second harmonic power is given by calculating the squared of the manipulated source parts in the wave equation for the second and either for the first [8] or the third [3, 4] harmonic and, subsequently, taking the ratio between the squared of the second harmonic source part and either the squared of the first or the third. Finally in [8] it is introduced the notion of a second harmonic power increasing when a deflection angle between the beam trajectory and the undulator z direction is present. On the contrary, we find that such power can only decrease or, at most, be independent of the deflection angle, depending on how the beam modulation is prepared.

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. This solution of the wave equation may therefore be used 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.

We found that, in general, the second harmonic field presents both horizontal and vertical polarization components and that the electric field is linearly polarized, while the relative magnitude of the power associated to the vertical polarization component to that associated to the horizontal polarization component is a function of the undulator deflection parameter only. Using our result 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.

In this paper, we presented a theory of the second harmonic generation mechanism in XFELs and pointed out several notions on such mechanism which we consider incorrect. In this regard, it should be noted that some of them appear to go beyond the subject of harmonic generation itself. In fact we have seen that these notions imply an increase of the second harmonic power when an angle between the beam direction and the undulator axis is present, as if this was a general property depending on Maxwell equations. In other words, it looks like the solution of Maxwell equations for any electron beam in an undulator would yield a non-trivial dependence on the angle between the trajectory and the undulator axis. If so, this conclusion should be valid, in particular, for a single particle as well. We find that this is not correct: in fact, for a single particle in a undulator the dependence of the electric field on the angle between the average direction of the particle and the undulator axis, $\eta_{x,y}$, is simply related to the chosen reference system, i.e., usually, one with the z axis aligned with the undulator axis. A simple rotation of an angle $\eta_{x,y}$ to a system with the z axis aligned with the electron average velocity would give a result independent on such angle. This means that the basic characteristics of undulator radiation, in particular the intensity distribution at fixed frequency and the spectrum at fixed observation angle $\theta_{x,y}$, depend on the combination $(\theta_{x,y} - \eta_{x,y})$ only. In other words the presence of an angle $\eta_{x,y}$ between the electron direction and the undulator axis has the only effect of introducing a rotation in the expression of the electric field otherwise leaving unvaried all its characteristics, including its resonance frequency.

6 Acknowledgements

The authors wish to thank Martin Dohlus (DESY) for useful discussions and Josef Feldhaus (DESY) for his interest in this work.

References

[1] E. Saldin, E. Schneidmiller and M. Yurkov, The Physics of Free Eelectron Lasers, Springer, 2000

[2] Z. Huang and K. Kim, Phys. Rev. E, 62, 5 (2000)

[3] M. Schmitt and C. Elliot, Phys. Rev. A, 34, 6 (1986)

[4] Z. Huang and K. Kim, Nucl. Instr. and Meth. in Phys. Res. A 475, 112 (2001)

[5] H. Freund, S. Biedron and S. Milton., Nucl. Instr. and Meth. in Phys. Res. A 445, 53 (2000)

[6] A. Tremaine et al., Phy. Rev. Lett. 88, 204801 (2002)

[7] S. Biedron et al. Nucl. Instr. Meth. A 483, 94 (2002)

[8] Z. Huang and S. Reiche, Proceedings of the FEL 2004 Conference, Trieste, Italy

[9] H. Wiedemann, Synchrotron Radiation, Springer-Verlag, Germany (2003)

[10] Undulators, Wigglers and their applications, Edited by H. Onuki and P. Ellaume, Taylor & Francis (2003)

[11] G. Geloni, E. Saldin, E. Schneidmiller and M. Yurkov, Paraxial Green's functions in Synchrotron Radiation theory, DESY 05-032, ISSN 0418-9833 (2005)

[12] D. Alferov, Y.A. Bashmakov et al. Sov. phys. - Tech. Phys. 18, 1336 (1974)

[13] E. Saldin et al. Nucl. Instr. Meth. A 539, 499 (2005)