

THEORETICAL COMPUTATION OF THE POLARIZATION CHARACTERISTICS OF AN X-RAY FREE-ELECTRON LASER WITH PLANAR UNDULATOR

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Abstract

We show that radiation pulses from an X-ray Free-Electron Laser (XFEL) with a planar undulator, which are mainly polarized in the horizontal direction, exhibit a suppression of the vertical polarization component of the power at least by a factor $\lambda_w^2/(4\pi L_g)^2$, where λ_w is the length of the undulator period and L_g is the FEL field gain length. We illustrate this fact by examining the XFEL operation under the steady state assumption. In our calculations we considered only resonance terms: in fact, non resonance terms are suppressed by a factor $\lambda_w^3/(4\pi L_g)^3$ and can be neglected. While finding a situation for making quantitative comparison between analytical and experimental results may not be straightforward, the qualitative aspects of the suppression of the vertical polarization rate at XFELs should be easy to observe. We remark that our exact results can potentially be useful to developers of new generation FEL codes for cross-checking their results.

INTRODUCTION

In this paper we quantify the small component of the electric field in the vertical direction in radiation pulses produced by an XFEL with horizontal planar undulator. In particular, we show that for a typical XFEL setup the horizontally polarized component of radiation is greatly dominant, and that only less than one part in a million of the total intensity is polarized in the vertical plane.

The study of XFEL polarization characteristics is obviously deeply related to the problem of electromagnetic wave amplification in XFEL, which refers to a particular class of self-consistent problems. It can be separated into two parts: the solution of the dynamical problem, i.e. finding the motion of the electrons in the beam under the action of given electromagnetic fields, and the solution of the electrodynamic problem, i.e. finding the electromagnetic fields generated by a given contribution of charge and currents. The problem is closed by simultaneous solution of the field equations and of the equations of motion.

Let us consider the electrodynamic problem more in detail. The equation for the electric field \vec{E} follows the inhomogeneous wave equation

$$c^2 \nabla^2 \vec{E} - \frac{\partial^2 \vec{E}}{\partial t^2} = 4\pi c^2 \vec{\nabla} \rho + 4\pi \frac{\partial \vec{j}}{\partial t}. \quad (1)$$

Once the charge and current densities ρ and \vec{j} are specified as a function of time and position, this equation allows one to calculate the electric field \vec{E} at each point of space and

time [1]. The current density source provides the main contribution to the radiation field in an FEL amplifier, and the contribution of the charge density source to the amplification process is negligibly small. This fact is commonly known and accepted in the FEL community.¹

Due to linearity, without the gradient term the solution of Eq. (1) exhibits the property that the radiation field \vec{E} points in the same direction of the current density \vec{j} . An important limitation of such approximation arises when we need to quantify the linear vertical field generated in the case of an XFEL with planar undulator. In the case \vec{j} points in the horizontal direction (for a horizontal planar undulator), according to Eq. (1), which is exact, only the charge term is responsible for a vertically polarized component of the field: if it is neglected, one cannot quantify the linear vertical field anymore.

Similar to the process of harmonic generation, the process of generation of the vertically polarized field component can be considered as a purely electrodynamic one. In fact, the vertically polarized field component is driven by the charge source, but the bunching contribution due to the interaction of the electron beam with the radiation generated by such source can be neglected. This leads to important simplifications. In fact, in order to perform calculations of the radiation including the vertically polarization component one can proceed first by solving the self-consistent problem with the current source only. This can either be done in an approximated way using an analytical model for the FEL process or, more thoroughly, exploiting any existing FEL code. Subsequently, the solution to the self-consistent problem can be used to calculate the first harmonic contents of the electron beam density distribution. These contents enter as known sources in our electrodynamic process, that is Eq. (1). Solution of that equation accounting for these sources gives the desired polarization characteristics.

Approximations particularly advantageous for our theoretical analysis include the modeling of the electron beam density as uniform, and the introduction of a monochromatic seed signal. Realistic conditions satisfying these assumptions are the use of a sufficiently long electron bunch with a longitudinal stepped profile and the application of a scheme in the SASE mode of operation for narrowing down the radiation bandwidth. In the framework of this model it becomes possible to describe analytically all the polarization properties of the radiation from an XFEL.

¹ However, we have been unable to find a proof of this fact in literature, except book [2] and review [3], which are only the publications, to the authors' knowledge, dealing with this issue.

The simplicity of our model offers the opportunity for an almost completely analytical description in the case of an XFEL in the linear regime. A complete description of the operation of an XFEL can be performed only with time-dependent numerical simulation codes. Application of the numerical calculations allows one to describe the most general situation, including arbitrary electron beam quality and nonlinear effects. Finding an analytical solution is always fruitful for testing numerical simulation codes. Up to now, in conventional FEL codes the contribution of the charge source is assumed to be negligible. However, the charge term alone is responsible for the vertically polarized radiation component, which is our subject of interest. Our analytical results for the high-gain linear regime are expected to serve as a primary standard for testing future FEL codes upgrades.

Here we will report only the main results of our calculations. Details can be found in [4].

RESONANCE APPROXIMATION

Paraxial Maxwell's equations in the space-frequency domain can be used to describe radiation from ultra-relativistic electrons (see e.g. [5]). We call the Fourier transform of the real electric field in the time domain $\vec{E}_\perp(z, \vec{r}_\perp, \omega)$, where $\vec{r}_\perp = x\vec{e}_x + y\vec{e}_y$ identifies a point on a transverse plane at longitudinal position z , \vec{e}_x and \vec{e}_y being unit vectors in the transverse x and y directions. Here the frequency ω is related to the wavelength λ by $\omega = 2\pi c/\lambda$, c being the speed of light in vacuum. From the paraxial approximation follows that the electric field envelope $\vec{E}_\perp = \vec{E}_\perp \exp[-i\omega z/c]$ does not vary much along z on the scale of the reduced wavelength $\lambda/(2\pi)$. As a result, it can be shown that the following field equation holds:

$$\left(\nabla_\perp^2 + \frac{2i\omega}{c} \frac{\partial}{\partial z}\right) \vec{E}_\perp(z, \vec{r}_\perp, \omega) = -4\pi \exp\left[i \int_0^z d\bar{z} \frac{\omega}{2c\gamma_z^2(\bar{z})}\right] \left[\frac{i\omega}{c^2} \vec{v}_{o\perp} - \vec{\nabla}_\perp\right] \times \tilde{\rho}(z, \vec{r}_\perp - \vec{r}_{o\perp}(z), \omega), \quad (2)$$

where $\vec{r}_{o\perp}(z)$, $s_o(z)$ and v_o are the transverse position, the curvilinear abscissa and the velocity of a reference electron with nominal Lorentz factor γ_o that is injected on axis with no deflection and is guided by the planar undulator field. Such electron follows a trajectory specified by $\vec{r}_{o\perp}(z) = r_{ox}\vec{e}_x + r_{oy}\vec{e}_y$ with $r_{ox}(z) = K/(\gamma_o k_w) \cos(k_w z)$ and $r_{oy}(z) = 0$. Here K is the undulator parameter defined in terms of the maximum magnetic field and $k_w = 2\pi/\lambda_w$, λ_w being the undulator period. The corresponding velocity is described by $\vec{v}_{o\perp}(z) = v_{ox}\vec{e}_x + v_{oy}\vec{e}_y$. Moreover, $\gamma_z(z) = 1/\sqrt{1 - v_{oz}(z)^2/c^2}$ and $v_{oz}(z) = \sqrt{v_o^2 - v_{o\perp}(z)^2}$. Finally, $\tilde{\rho}$ is related to the Fourier transform of the macroscopic charge density, $\tilde{\rho}$, by

$$\tilde{\rho} = \tilde{\rho}(z, \vec{r}_\perp - \vec{r}_{o\perp}(z), \omega) \exp\left[i\omega \frac{s_o(z)}{v_o}\right], \quad (3)$$

s_o being the curvilinear abscissa along the trajectory.

With the aid of the appropriate Green's function and using the far-zone approximation a solution of Eq. (2) can be found to be:

$$\vec{E}_\perp = -\frac{i\omega}{cz} \int d\vec{l} \int_{-\infty}^{\infty} dz' \tilde{\rho}(z', \vec{l}, \omega) \exp\left[i\Phi_T(z', \vec{l}, \omega)\right] \times \left[\left(\frac{K}{\gamma} \sin(k_w z') + \theta_x\right) \vec{e}_x + \theta_y \vec{e}_y\right], \quad (4)$$

where

$$\Phi_T = \omega \left\{ \frac{z'}{2\gamma^2 c} \left[1 + \frac{K^2}{2} + \gamma^2 (\theta_x^2 + \theta_y^2) \right] - \frac{K^2}{8\gamma^2 k_w c} \sin(2k_w z') - \frac{K\theta_x}{\gamma k_w c} \cos(k_w z') \right\} + \omega \left\{ \frac{K\theta_x}{k_w \gamma c} - \frac{1}{c} (\theta_x l_x + \theta_y l_y) + (\theta_x^2 + \theta_y^2) \frac{z'}{2c} \right\} \quad (5)$$

Here θ_x and θ_y indicate the observation angles x/z and y/z . Moreover, since in Eq. (4) we introduced explicitly the trajectory inside the undulator, we need to limit the integration in dz' to a proper range within the undulator. We assume that this is done by introducing a function of z' as a factor to $\tilde{\rho}$, which becomes zero outside properly defined range, thus effectively limiting the integration range in z' .

In this article we are interested in considering fields and electromagnetic sources originating from an FEL process. Imposing resonance condition between electric field and reference particle, the self-consistent FEL process automatically restricts the amplification of radiation at frequencies around the first harmonic $\omega_{1o} = 2k_w c \tilde{\gamma}_z^2$ and at emission angles $\theta_{\max}^2 \ll 1/\tilde{\gamma}_z^2$, where $\tilde{\gamma}_z^2 = \gamma^2/(1 + K^2/2)$. Our focus onto FEL emission also explains the definition in Eq. (3). In fact, introduction of $\tilde{\rho}$ is useful when $\tilde{\rho}$ is a slowly varying function of z on the wavelength scale. If the charge density distribution under study originates from an FEL process a stronger condition is satisfied, namely $\tilde{\rho}$ is slowly varying on the scale of the undulator period λ_w and, as the FEL pulse itself, is peaked around the fundamental ω_{1o} . The words 'peaked' or 'around' the fundamental mean that the bandwidth is $\Delta\omega/\omega_{1o} \ll 1$. We quantify 'how near' the frequency ω is to ω_{1o} introducing the detuning parameter $C = (\Delta\omega/\omega_{1o})k_w$, with $\Delta\omega = \omega - \omega_{1o}$. The detuning parameter C should indeed be considered as a function of z , $C = C(z)$. All other dependencies on z , for example due to the fact that the energy of particles actually deviates from γ and actually decreases during the FEL process, is accounted for in $\tilde{\rho}$. We seek to calculate the first harmonic contribution at frequencies ω around ω_{1o} , $\vec{E}_{\perp 1}$, by making use of the well-known Anger-Jacobi expansion. Invoking the FEL process allows to take the limit for $C \ll k_w$ and $\theta_{\max}^2 \ll 1/\tilde{\gamma}_z^2$. Keeping the dominant terms only we obtain

$$\vec{E}_{\perp 1} = \frac{\omega_{1o}}{cz} \exp\left[i\frac{\omega_{1o}}{2c} z(\theta_x^2 + \theta_y^2)\right]$$

$$\begin{aligned}
 & \times \left[\frac{K}{2\gamma} A_{JJ} \vec{e}_x + \frac{2K\gamma}{2+K^2} B_{JJ} \theta_x \theta_y \vec{e}_y \right] \\
 & \times \int_{-\infty}^{\infty} dl_x \int_{-\infty}^{\infty} dl_y \int_{-\infty}^{\infty} dz' \\
 & \times \exp \left[-i \frac{\omega_{1o}}{c} (\theta_x l_x + \theta_y l_y) \right] \\
 & \times \exp \left[i \frac{\omega_{1o}}{2c} (\theta_x^2 + \theta_y^2) z' \right] \tilde{\rho}(z', \vec{l}, \omega) \exp[iCz'], \quad (6)
 \end{aligned}$$

where we have defined

$$A_{JJ} = J_0 \left(\frac{K^2}{2(2+K^2)} \right) - J_1 \left(\frac{K^2}{2(2+K^2)} \right), \quad (7)$$

$$B_{JJ} = J_0 \left(\frac{K^2}{2(2+K^2)} \right) + J_1 \left(\frac{K^2}{2(2+K^2)} \right), \quad (8)$$

and $J_p(\cdot)$ indicates the Bessel function of the first kind of order p . Note that usually computer codes present the product $\tilde{\rho}(z', \vec{l}, \omega) \exp[iCz']$ combined in a single quantity typically known as the complex amplitude of the electron beam modulation with respect to the phase $\psi = k_w z' + (\omega/c)z' - \omega t$. Regarding such product as a given function allows one not to bother about a particular presentation of the beam modulation. Eq. (6) is our most general result, and is valid independently of the model chosen for the current density and the modulation. It can be used together with FEL simulation codes for detailed calculations of the evolution of the vertically polarization contribution to the FEL radiation.

In the case of an FEL, due to the presence of a maximum angle θ_{\max} related with the self-consistent process, the angle-integrated correction to the power from the horizontally polarized radiation component only includes the leading resonant term, and Eq. (6) can always be used to calculate such correction at the first harmonic.

ANALYTICAL CASES

We now restrict our attention to the steady-state model of an FEL amplifier. Because of the steady state assumption we restrict our attention to one single frequency. This means that, in the time domain, the electric field envelope $\vec{E}_{\perp 1}$ must correspond to a real electric field at a certain frequency $\bar{\omega} = \omega_{1o}(1 + Ck_w)$ given by $\vec{E}(z, \vec{r}_{\perp}, t) = \vec{E}_{\perp 1}(z, \vec{r}_{\perp}) \exp[i\bar{\omega}(z/c - t)] + C.C.$, where the symbol $C.C.$ indicates complex conjugation.

The power fractions into the two modes of polarization are found to be

$$W_{(\sigma, \pi)} = \frac{c}{2\pi} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy |\mathcal{E}_{\perp 1(x,y)}(z, x, y)|^2, \quad (9)$$

where

$$\vec{E}_{\perp 1}(z, \vec{r}_{\perp}, \omega) = 2\pi \vec{E}_{\perp 1}(z, \vec{r}_{\perp}) \delta(\omega - \bar{\omega}). \quad (10)$$

In order to calculate $W_{(\sigma, \pi)}$ we make use of Eq. (9). The expression for $\mathcal{E}_{\perp 1(x,y)}$ can be found in terms of $\vec{E}_{\perp 1}$ with

the help of Eq. (10). Finally, one needs to calculate $\vec{E}_{\perp 1}$, which can be done using Eq. (6).

Under the assumption of a one-dimensional steady state FEL amplifier we write the expression for the slowly-varying amplitude of the charge density as

$$\tilde{\rho}(z, \vec{r}_{\perp}, \omega) = \frac{j_o(\vec{r}_{\perp})}{v_z} 2\pi a(z) \delta(\omega - \omega_0), \quad (11)$$

where we defined the current density

$$j_o(\vec{r}_{\perp}) = -\frac{I_o}{2\pi\sigma^2} \exp\left(-\frac{r_{\perp}^2}{2\sigma^2}\right), \quad (12)$$

and where we dropped the term in $\delta(\omega + \bar{\omega})$ passing to complex notation, as done before with the field.

We will show that, typically, in the case of an XFEL with a horizontal planar undulator, only less than one part in a million of the total power at the first harmonic is polarized in the vertical direction. For some experiments even such small fraction of the π mode is of importance. The contribution of the second harmonic can be calculated using results in [6] and was studied in [4]. There it was found that the contribution from the even harmonics can be completely disregarded when the XFEL operates in linear regime. At saturation, the contribution from the second harmonic can be comparable with the first harmonic in the case when X-ray optics harmonic separation is absent.

High-gain Linear Regime

We first model the case of an FEL amplifier in the high-gain linear regime. We proceed approximating the detuning parameter C as constant along the undulator. Let us restrict, for simplicity, to the case of perfect resonance for $C = 0$. This means that from now on $\bar{\omega} = \omega_{1o}$. The high-gain asymptote of the one-dimensional steady-state theory of FEL amplifiers yields

$$a(z) = a_f \exp[(\sqrt{3} + i)z/(2L_g)], \quad (13)$$

where we set the exit of the undulator (in the linear regime) at $z = 0$ and $a_f = \text{constant}$ is the modulation level at $z = 0$. Here L_g is the field gain length. The number of undulator periods in the field gain length L_g is just $N_w = (4\pi\rho_{1D})^{-1}$, where the FEL parameter ρ_{1D} is defined in [7]. Based on Eq. (6) we obtain

$$\begin{pmatrix} W_{\sigma} \\ W_{\pi} \end{pmatrix} = W_o \begin{pmatrix} A_{JJ}^2 \rho_{1D}^{-1} G_{\sigma}(N) \\ B_{JJ}^2 \rho_{1D} G_{\pi}(N) \end{pmatrix}, \quad (14)$$

where

$$\begin{aligned}
 G_{\sigma}(N) &= \frac{1}{2\sqrt{3}} \exp[(1 - i\sqrt{3})N] \{ \pi \\
 &+ \pi \exp[2i\sqrt{3}N] - i \exp[2i\sqrt{3}N] \text{Ei}(N(-1 - i\sqrt{3})) \\
 &+ i \text{Ei}(iN(i + \sqrt{3})) \} \quad (15)
 \end{aligned}$$

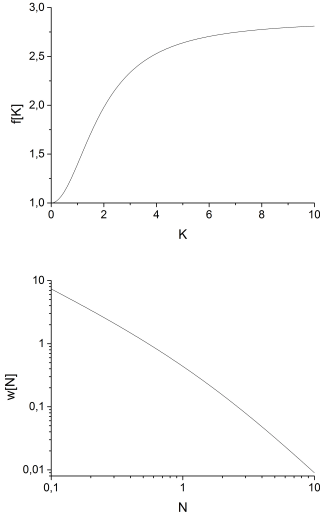


Figure 1: Illustration of the behavior of $f(K)$ (left) and $w(N)$ (right).

$$G_{\pi}(N) = \frac{1}{6} \left\{ \frac{3}{N} - (-3i + \sqrt{3}) \exp[(1 + i\sqrt{3})N] \right. \\ \times [\pi - i\text{Ei}((-1 - i\sqrt{3})N)] - (3i + \sqrt{3}) \\ \left. \times \exp[(1 - i\sqrt{3})N] [\pi + i\text{Ei}(i(i + \sqrt{3})N)] \right\} \quad (16)$$

and

$$W_o = W_b a_f^2 \left(\frac{I_o}{\gamma I_A} \right) \left(\frac{K^2}{2 + K^2} \right) \quad (17)$$

where $W_b = m_e c^2 \gamma I_o / e$ is the total power of the electron beam and $N = \omega_{1o} \sigma^2 / (c L_w)$ is the diffraction parameter (or Fresnel number) with $L_w = L_g$ in our case.

The ratio between the fractions radiated in the two modes of polarization is therefore conveniently expressed as a function of three separate factors:

$$\frac{W_{\pi}}{W_{\sigma}} = f(K) g(N_w) w(N) \quad (18)$$

with

$$f(K) = \frac{B_{JJ}^2}{A_{JJ}^2}, g(\rho_{1D}) = \rho_{1D}^2, w(N) = \frac{G_{\pi}(N)}{G_{\sigma}(N)}. \quad (19)$$

The first factor, $f(K)$, is only a function of the undulator K parameter and is plotted in Fig. 1. The second factor, $g(\rho_{1D})$ scales as the inverse number of undulator periods squared, and is a signature of the fact that the gradient term in the equation for the electric field scales as the inverse number of undulator periods. The third factor, $w(N)$, is only a function of the diffraction parameter that is, once the

wavelength and the undulator length are fixed, a function of the electron beam size only. It is also plotted in Fig. 1. It is unity for values of the diffraction parameter around unity, but it quickly decreases for larger values of N . The power fraction radiated in the π mode increases drastically with the photon energy, partly due to a larger number of undulator period per field gain-length, but mainly because of a larger diffraction parameter.

As an example we consider a 250 pC electron beam at a photon energy of about 9 keV for the SASE2 line of the European XFEL, at the electron energy of 17.5 GeV. Here $K \approx 3.6$, the peak current is about 5 kA, and the rms sizes of the electron beam in the horizontal and vertical directions are about $\sigma_x \approx 15 \mu\text{m}$ and $\sigma_y \approx 18 \mu\text{m}$ respectively. For our purposes of exemplification we consider a round beam with $\sigma = 16 \mu\text{m}$. The peak current density can then be estimated as $I_o / (2\pi\sigma^2)$. Finally, the undulator period is $\lambda_w = 40 \text{ mm}$. From these numbers we obtain the parameter $\rho_{1D} \approx 8 \cdot 10^{-4}$. Plugging these numbers in Eq. (18) and remembering the definition in Eq. (19) we obtain $f(K) \approx 2.5$, $g(\rho_{1D}) \approx 6.4 \cdot 10^{-7}$, $N \approx 3$ and $w(N) \approx 0.072$, so that the overall ratio $W_{\pi}/W_{\sigma} \approx 1.13 \cdot 10^{-7}$.

Constant Density Modulation

In analogy with the previous paragraph, we now proceed to study the case of a constant density modulation along an undulator of fixed length L_w , imitating the behavior of an FEL at saturation. We can still set $C(z) = 0$. At variance with the previous model we now write

$$\tilde{\rho}(z, \vec{l}) = j_o(\vec{l}) 2\pi a_f H_{L_g}(z) \delta(\omega - \omega_{1o}). \quad (20)$$

Here $a_f = \text{const}$, $H_{L_w}(z) = 1$ for z in the range $(-L_w/2, L_w/2)$ and zero otherwise, with L_w the undulator length, and j_o is defined as in Eq. (12). One finds

$$\begin{pmatrix} W_{\sigma} \\ W_{\pi} \end{pmatrix} = W_o \begin{pmatrix} A_{JJ}^2 (4\pi N_w) F_{\sigma}(N) \\ B_{JJ}^2 (4\pi N_w)^{-1} F_{\pi}(N) \end{pmatrix}, \quad (21)$$

where

$$F_{\sigma}(N) = \arctan\left(\frac{1}{2N}\right) + N \ln\left(\frac{4N^2}{4N^2 + 1}\right), \quad (22)$$

$$F_{\pi}(N) = \frac{1}{N(1 + 4N^2)}, \quad (23)$$

and where parameters N and W_o are defined above.

Similarly as before, the ratio between the two fractions radiated into the two modes of polarization is conveniently expressed as a function of three separate factors:

$$\frac{W_{\pi}}{W_{\sigma}} = f(K) g(N_w) h(N) \quad (24)$$

with

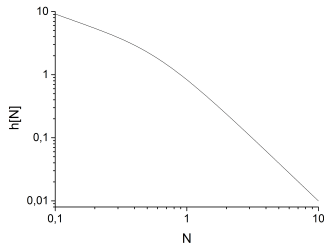


Figure 2: Illustration of the behavior of $h(N)$.

$$f(K) = \frac{B_{JJ}^2}{A_{JJ}^2}, g(N_w) = \frac{1}{(4\pi N_w)^2}, h(N) = \frac{F_\pi(N)}{F_\sigma(N)}. \quad (25)$$

The function f has been defined in the previous paragraph. Concerning the second factor g , we have an expression which is similar to that in Eq. (19). The only difference is that here we replaced ρ_{1D} with $(4\pi N_w)^{-1}$, with N_w the number of undulator periods in the undulator. The number of undulator periods in a field gain length is just $N_w = (4\pi\rho_{1D})^{-1}$, and therefore the second factor in Eq. (24) just amounts to ρ_{1D}^2 for an undulator length $L_w = L_g$, L_g being, as before, the field gain length. By setting the undulator length equal to the field gain length the two models can be directly compared by studying $w(N)$ as defined in Eq. (19) and $h(N)$ defined in Eq. (25). We plot $h(N)$ explicitly in Fig. 2. As one can see it differs from Fig. 1, due to the different model used.

Considering the same example made in the previous paragraph we find again $f(K) \simeq 2.5$, $g(\rho_{1D}) \simeq 6.4 \cdot 10^{-7}$, $N \simeq$

3. Plugging the value for N into Eq. (25) we obtain $h(N) \simeq 0.097$, so that the overall ratio $W_\pi/W_\sigma \simeq 1.5 \cdot 10^{-7}$.

The case of a constant density modulation treated in this paragraph not only pertains an FEL at saturation, but also the case of spontaneous emission in an undulator. A major difference compared to the FEL case is that the FEL process limits the detuning to values $C \ll k_w$ and the angle of interest up to θ_{\max} . Such limitations are not automatically present in the case of spontaneous emission. However, if we limit the acceptance angle of the spontaneous emission to θ_{\max} and we assume the undulator length of order of the FEL gain length, we expect the same ratio of the fractions radiated in the two modes of polarization found in Eq. (24).

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