Appendix of Building an Optical Free-Electron Laser in the Traveling-Wave Thomson-Scattering Geometry

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A Electric field of a propagating Gaussian laser pulse

In order to calculate variations of laser intensity and undulator frequency in the out-of-focus geometry during the electron-laser interaction, we derive in this section an expression for the electric field distribution of a focusing laser pulse with Gaussian transverse envelope. The obtained representation of the electric field is evaluated along the electron trajectory and in the region surrounding it in order to evaluate variations of laser intensity and undulator frequency in the course of interaction. Since variations occur due to misalignment of the optical setup, resulting in nonideal orientation of pulse-front tilt and plane of optimum compression or an offset in interaction angle, the calculated variations can be compared to the limits for optical free-electron laser operation, eq. (7), which gives limits for misalignments.

By using the Rayleigh-Sommerfeld diffraction integral we obtain an analytic expression of the pulse electric field which is valid even in the proximity of the laser focus in contrast to a Fraunhofer diffraction ansatz. A Gaussian laser pulse with pulse-front tilt in the focus is in frequency domain defined as

$$\hat{E}(z=0,y,\Omega) = \epsilon(\Omega-\Omega_0)\mathrm{e}^{-\frac{y^2}{w_{0,yz}^2}}\,\mathrm{e}^{i\frac{(\Omega-\Omega_0)}{c}y\tan\alpha_{\mathrm{tilt}}}\,,$$

where the transverse profile $\exp[-y^2/w_{0,yz}^2]$ is Gaussian with a width $w_{0,yz}$ and where its spectrum $\epsilon(\Omega-\Omega_0) = \exp[-(\Omega-\Omega_0)^2\tau_0^2/4]$ is a Gaussian with Ω_0 being the central laser frequency and τ_0 the laser pulse duration. The laser pulse duration τ_0 is connected to the full duration at half maximum $\tau_{\mathrm{FWHM,I}}$ of its intensity profile by

$$\tau_0 = \frac{\tau_{\mathrm{FWHM,I}}}{\sqrt{2\ln 2}}\,.$$

Writing the phase term in the above form directly connects pulse-front tilt and angular dispersion since $\tan\alpha_{\mathrm{tilt}}(\Omega-\Omega_0)/c$ is the y-component of the wave vector for a frequency Ω (cf. (17)). The pulse propagation direction is along z.

Propagation of the pulse with the Rayleigh-Sommerfeld diffraction integral [51],[106] yields the field in a distance z from the focus

$$
\begin{aligned}
\hat{E}(z,y,\Omega) &= \epsilon(\Omega-\Omega_0)\sqrt{\frac{\Omega}{2\pi c}}\frac{\mathrm{e}^{-i\left(\frac{\Omega}{c}z-\frac{\pi}{4}\right)}}{\sqrt{z}}\int\limits_{-\infty}^{\infty}\hat{E}(z=0,y,\Omega)\mathrm{e}^{-i\frac{\Omega}{2cz}(y-\xi)^2}\,\mathrm{d}\xi \\
&= \epsilon(\Omega-\Omega_0)\sqrt{\frac{w_{0,yz}}{w_{yz}(z)}}\mathrm{e}^{-\left[y+\frac{(\Omega-\Omega_0)}{\Omega_0}z\tan\alpha_{\mathrm{tilt}}\right]^2\left[\frac{1}{w_{yz}(z)^2}+i\frac{\Omega}{2cR_{yz}(z)}\right]}\times \\
&\quad\times\mathrm{e}^{-i\frac{\Omega}{c}z+i\frac{(\Omega-\Omega_0)}{c}y\tan\alpha_{\mathrm{tilt}}+i\frac{(\Omega-\Omega_0)^2}{2\Omega_0 c}z\tan^2\alpha_{\mathrm{tilt}}+\frac{1}{2}\arctan\frac{z}{z_{\mathrm{R,yz}}}}\,,
\end{aligned}
\tag{46}
$$

where $w_{yz}(z)^2 = w_{0,yz}^2[1+(z/z_{\mathrm{R,yz}})^2]$ is the width of the pulse increasing with distance from the focus, $R_{yz}(z) = z[1+(z_{\mathrm{R,yz}}/z)^2]$ is the radius of phase-front curvature and $z_{\mathrm{R,yz}} = \pi w_{0,yz}^2/\lambda_{\mathrm{Laser}}$ the Rayleigh length. Angular dispersion

$$AD = \theta' = \tan(\alpha_{\mathrm{tilt}})/\Omega_0$$

causes the propagating pulse to develop spatial dispersion (SD), i.e. a separation of frequencies in its transverse cross-sectional plane. Defining the center of a frequency's spatial distribution as $y_0(z,\Omega)$, spatial dispersion is defined as the linear contribution to its expansion

$$y_0(z,\Omega) = SD(\Omega-\Omega_0)\,, \qquad \text{where} \qquad SD = \left.\frac{\mathrm{d}y_0}{\mathrm{d}\Omega}\right|_{\Omega=\Omega_0}.$$

For a Gaussian pulse y_0 and SD can be identified from the above relation for the electric field as

$$y_0(z,\Omega) = -\frac{z\tan\alpha_{\mathrm{tilt}}}{\Omega_0}(\Omega-\Omega_0) \qquad \text{and} \qquad SD(z) = -zAD\,,$$

showing that the centers of all spatial frequency distributions disperse during propagation.

In addition to the spatial separation of frequencies, they also separate temporally, i. e. the pulse develops group delay dispersion (GDD) during propagation. GDD causes an increasing phase difference between frequencies with an elongation of the pulse as a result. Terms proportional to $(\Omega-\Omega_0)^2$ in the phase φ of eq. (46) contribute to pulse elongation, since

$$GDD = \left.\frac{\mathrm{d}^2\varphi}{\mathrm{d}\Omega^2}\right|_{\Omega=\Omega_0}.$$

The major contribution to the elongation of a Gaussian pulse arises from a single phase term in (46), for which we define

$$GDD(z) = -z\frac{\Omega_0}{c}AD^2 = -\frac{z\tan^2\alpha_{\mathrm{tilt}}}{\Omega_0 c}\,.$$

Using these definitions, we calculate the electric field of the Gaussian laser pulse in time-domain by a Fourier transform

$$E(z,y,t) = \frac{1}{2\pi}\int\hat{E}(z,y,\Omega)\mathrm{e}^{i\Omega t}\mathrm{d}\Omega\,.$$

In the calculation we neglect the phase term proportional to $(\Omega-\Omega_0)^3/\Omega_0^3$, since it is a small contribution to the phase of laser pulses with several ten laser periods which we consider here. We obtain for the time domain electric field of the focusing Gaussian laser pulse

$$
\begin{aligned}
E(z,y,t) &= \sqrt{\frac{w_{0,yz}}{w_{yz}}}\mathrm{e}^{-\frac{y^2}{W_{yz}^2}}\mathrm{e}^{i\frac{\Omega_0}{c}(ct-z)}\mathrm{e}^{-i\frac{\Omega_0}{2cR_{yz}}y^2}\mathrm{e}^{i\frac{1}{2}\arctan\frac{z}{z_{\mathrm{R,yz}}}}\times \\
&\quad\times\frac{1}{\sqrt{\pi}}\left[\tau^2T^2\right]^{-\frac{1}{4}}\mathrm{e}^{-i\frac{1}{2}\arctan\left(4\frac{g}{\tau^2}\right)}\mathrm{e}^{-\frac{\tilde{L}^2}{T^2}}\mathrm{e}^{i4\frac{\left(l^2g-s^2g-ls\tau^2/2\right)}{\tau^2T^2}}
\end{aligned}
\tag{47}
$$

where

$$
\begin{aligned}
W_{yz}^2 &= w_{yz}^2 + 4SD^2/\tau_0^2\,, \\
T^2 &= \tau^2 + 16\frac{g^2}{\tau^2}\,, \\
\tau^2 &= \tau_0^2 + 4\frac{SD^2}{w_{yz}^2}\,, \\
\tilde{L} &= l + 4\frac{sg}{\tau^2}\,, \\
l &= t + \frac{\Delta f}{c} - \frac{z}{c} + \frac{y}{c}\tan\alpha_{\text{tilt}} - \frac{y^2}{2cR_{yz}} + \frac{y}{c}\frac{\Omega_0 SD}{R_{yz}}\,, \\
s &= \frac{2ySD}{w_{yz}^2}\,, \\
g &= \frac{\Omega_0 SD^2}{2cR_{yz}} + \frac{y}{c}\frac{SD}{R_{yz}} + \frac{1}{2}GDD
\end{aligned}
$$

and at $t = 0$ the pulse is located at position $z = \Delta f$. From the above equation for the laser field some of the effects of dispersion are directly visible. The pulse width $w_{0,yz}$ increases during propagation due to SD to the value given by W_{yz} and the pulse duration τ_0 increases due to SD and GDD to T. Pulse-front tilt and curvature of the pulse-front due to focusing are included in $\tilde{L}$.

In section 3.2 we gave an expression for the total undulator frequency variation in the out-of-focus setup at the end of the interaction of electrons and laser pulse. It is derived by expanding the instantaneous undulator frequency from the middle of the interaction ($t = 0$) towards the end $t_{\text{end}} = L_{\text{int}}/2\beta_0 c$. The instantaneous undulator frequency $\tilde{\Omega}(t)$ itself is given by the time derivative of the phase $\tilde{\varphi}(z, y, t) = \operatorname{Arg} E(z, y, t)$ of the complex electric field evaluated along the electron trajectory (19)

$$
\tilde{\Omega}(t) = \frac{\mathrm{d}}{\mathrm{d}t}\tilde{\varphi}(\beta_0 ct\cos\phi + \Delta f, -\beta_0 ct\sin\phi, t)\,.
$$

Until the end of the interaction it deviates from its undisturbed value at $z = \Delta f$ by

$$
\begin{aligned}
\Delta\tilde{\Omega} &= \tilde{\Omega}(t_{\text{end}}) - \tilde{\Omega}(0) \\
&= \left[\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\varphi}(\beta_0 ct\cos\phi + \Delta f, -\beta_0 ct\sin\phi, t_{\text{end}}) - \tilde{\varphi}(\Delta f, 0, 0)\right] \\
&\approx \left[-\frac{\Omega_0}{c}\frac{y_{\text{el}}}{R_{yz}}\frac{\mathrm{d}y_{\text{el}}}{\mathrm{d}t} + \frac{c}{\Omega_0 w_{yz}^2}\frac{\mathrm{d}y_{\text{el}}}{\mathrm{d}t} - \left(\frac{1}{2} - \frac{l^2}{\tau_0^2}\right)\frac{\mathrm{d}\tilde{D}}{\mathrm{d}t} + \Delta\tilde{D}\frac{2l}{\tau_0^2}\frac{\mathrm{d}l}{\mathrm{d}t}\right]_{t=t_{\text{end}}}\,,
\end{aligned}
$$

In the order from left to right these terms originate from phase-front curvature, Gouy phase shift and the last two from group delay dispersion. For typical TWTS OFELs where the laser width $w_{yz} = L_{\text{int}}\sin\phi$ is large compared to the electron bunch width $2\sigma_{\text{b}}$, in order to achieve long interaction distances, the Gouy term is negligible. The same is possible for the dispersion terms provided dispersion compensation, e. g. by utilizing the plane of optimum compression, is applied. During the whole interaction ranging from $[-t_{\text{end}}, t_{\text{end}}]$ the normalized total change in undulator frequency is

$$
\frac{\Delta\tilde{\Omega}}{\tilde{\Omega}} = -\frac{L_{\text{int}}}{R(\Delta f)}\frac{\sin^2\phi}{(1-\beta\cos\phi)} + \frac{\cos\phi}{4\pi^2\sin^2\phi(1-\beta\cos\phi)}\frac{\lambda_{\text{Laser}}^2}{L_{\text{int}}^2}\,. \tag{48}
$$

B Zemax macro calculating dispersion from ray path length differences

Our analytical calculations for pulse-front tilt and plane of optimum compression orientation are complemented by a Zemax calculation. To obtain pulse-front tilt angle and plane of optimum compression angle we wrote a Zemax macro that calculates time delay (TD) and group delay dispersion (GDD) from the optical path lengths for different frequencies in the setup according to eq. (44). Pulse front and plane of optimum compression orientations are found by sampling time delay and group delay dispersion along their respective planes. Along

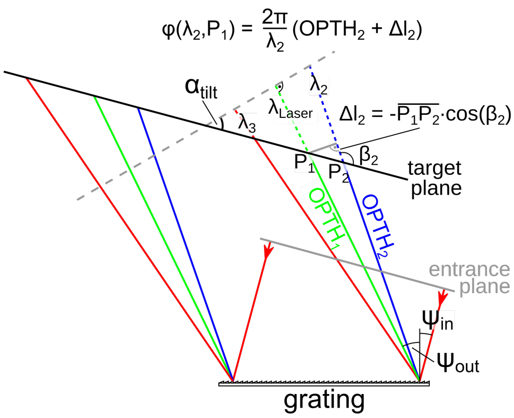

Figure 11: Optical path lengths (OPTH_i) of the wavelengths $\lambda_{\mathrm{Laser}} = \lambda_1$, λ_2 and λ_3 need to be corrected for the calculation of time delay and group delay dispersion at the position P_1 on a target plane. In this particular example, the target plane is the pulse front which encloses the angle α_{tilt} with the phase front of the central laser wave.

the pulse front time delay is constant and along the plane of optimum compression group delay dispersion is constant.

The definitions of TD and GDD require to calculate derivatives of the optical phase at a certain point. These derivatives are calculated from the optical phases of three different waves at this point of interest, where the three plane waves with wavelengths $\lambda_2 < \lambda_1 = \lambda_{\mathrm{Laser}} < \lambda_3$ start with equal phase at some entrance plane before the first optical element of the setup. Their phase ϕ_i at the point of interest is calculated from the distance DIST_i which is covered by their phase front during propagation from the entrance plane to the point of interest in the target plane, $\phi_i = (2\pi/\lambda_i)\mathrm{DIST}_i$, as it is sketched in fig. 11.

When using optical path lengths provided by Zemax to calculate TD and GDD, one needs to take into account that these path lengths OPTH_i are given for every wavelength until it stops at the target plane. Therefore, the path lengths OPTH_i need to be corrected since they are not equal to DIST_i if there are dispersive optical elements in the setup.

Accordingly, a compensation calculation is part of the script to obtain correct values for TD and GDD. This compensation calculations requires information about the propagation direction ($\pm z$) of the pulse at the final plane which is an input parameter of the script. This script is loosely based on the script provided in Ref. [107]. Note, the variable `bandw` in the script is not meant to be the laser bandwidth. It rather specifies the range between the wavelengths λ_2 and λ_3 which needs to be small since the error of the derivative approximation is proportional to it.

```
!*****************************************************************************
! Zemax macro to compute the angular dispersion and
! group delay dispersion of a laser pulse.
!
!
! Klaus Steiniger, 2016
! Last review 28 Jun 2017
!

!*****************************************************************************
! Constants and input parameter
!
pi = 4*ATAN(1)
cspeed = 0.299792458     # [cspeed] = 1E9 * m / s = mm / ps

INPUT "Central Wavelength of laser in micrometer", lambda0
PRINT "Central Laser wavelength [mum] = ", lambda0          #[lambda] = 1E-6 m

bandw = 0.001*lambda0
```

```
nlambda = 3 #odd number!
dlambda = bandw/(nlambda-1)

INPUT "Surface at which to calculate dispersion", NSURF
PRINT "NSUR = ", NSURF

INPUT "Propagation direction at plane of measurement? (z = 1, -z = -1)", coord_sys

PRINT ""

SETSYSTEMPROPERTY 201, nlambda

!********************************************************************************
! Set wavelengths for dispersion calculation
!
SETSYSTEMPROPERTY 202, 1, lambda0
VEC1(1) = lambda0                    # Vector of the wavelengths which are
                                     # propagated through the setup
                                     # [VEC1] = 1E-6 m

K=-INTE(.5*nlambda)

! Set wavelength smaller than central
!
FOR J, 2, INTE(.5*nlambda) + 1, 1
    lambda = lambda0 + K*dlambda
    SETSYSTEMPROPERTY 202, J, lambda
    VEC1(J) = lambda
    K = K+1
NEXT

K = K+1 # leave out center frequency in frequency calculation

! Set wavelength larger than central
!
FOR J, INTE(.5*nlambda) + 2, nlambda, 1
    lambda = lambda0 + K*dlambda
    SETSYSTEMPROPERTY 202, J, lambda
    VEC1(J) = lambda
    K = K+1
NEXT

!********************************************************************************
! Calculate Dispersions
!
PRINT ""

PRINT "Entrance pupil coordinate py, y-coordinate at plane[mm], TD[ps], GDD[fs^2]"

transv_samples = 3  # Refactor to an input value if necessary

!*** Produce container ***
DECLARE PHASES, DOUBLE, 1, 1000     # container for optical phase
DECLARE TD, DOUBLE, 1, 1000         # container for time delay
DECLARE GDD, DOUBLE, 1, 1000        # container for group delay dispersion

!*** Sample over multiple ray starting positions across the entrance pupil ***
```

```
!***
For L, 1, transv_samples, 1
    !*** Equally distribute the starting positions ***
    py = -1 + (L-1)*2/(transv_samples - 1)

    FOR J, 1, nlambda, 1
        RAYTRACE 0, 0, 0, py, J
        !-----------------------------------------------------------------------
        ! Calculate compensation of optical path length for rays of different
        ! frequency than the central frequency.
        !
        ! For the calculation of dispersion, the optical path length
        ! of a ray must be measured until its phase-front overlaps with the
        ! point of dispersion measurement.
        ! That is, at the position where the central frequency ray hits the
        ! measurement plane in Zemax.
        ! Since Zemax calculates optical path lengths of rays until they hit
        ! the measurement plane, the optical path length of
        ! non-central-frequency rays needs to be corrected.
        ! Which is done in the following.
        !
        ! Assumes that propagation is in vacuum (n=1)
        ! Sign of compensation depends on the propagation direction with
        ! respect to coord.-system in the measurement plane.
        !
        ypos = RAYY(NSURF)
        IF (J==1) THEN plane_intercept_c = ypos
        plane_intercept_difference = ypos - plane_intercept_c
        opth_compensation = plane_intercept_difference * RAYM(NSURF)
        path_length =  OPTH(NSURF) - coord_sys*opth_compensation
                                        # OPTH returns the path in millimeter
                                        # [path_length] = 1E-3 m
        PHASES(J) = 2*PI*path_length/VEC1(J)
                                        # Phase from optical path along the ray
                                        # VEC1 is wavelength in microns
                                        # [PHASES] = 1E3
    NEXT

    dlambda = -lambda0*lambda0/(2*pi*cspeed)        # [dlambda] = 1E-21 m s
    ddlambda = -lambda0 * dlambda /(pi*cspeed)      # [ddlambda] = 1E-36 m s**2

    FOR J, 2, INTE(.5*nlambda) + 1, 1
        h = VEC1(1)-VEC1(J)                             # [h] = 1E-6 m
        !-----------------------------------------------------------------------
        ! optical phase derivatives with respect to frequency (TD and GDD)
        !
        dphase = (PHASES(nlambda+2-J)-PHASES(J))/2/h    # [dphase] = 1E9 / m
        ddphase = (PHASES(nlambda+2-J)-2*PHASES(1)+PHASES(J))/h/h
                                                    # [ddphase] = 1E15 / m**2
        TD(J) = dphase*dlambda                      # [TD] = 1E-12 s = ps
        GDD(J) = ddphase*dlambda*dlambda + dphase*ddlambda
                                                    # [GDD] = 1E-27 s**2
        PRINT py, ", ", plane_intercept_c, ", ", TD(J), ", ", GDD(J)*1E3
    NEXT
NEXT
```