Using Hermite polynomials for effective time-dependent XFEL pulse propagation

Summer student report
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Contents.

In 2015 European X-ray Free Electron Laser (XFEL) will start operating. XFEL is a source of almost fully transverse coherent radiation. The X-ray light will be generated by Self-Amplified Spontaneous Emission (SASE), where electrons interact with the radiation that they or their neighbors emit. The result is spontaneous emission of tightly bunched packages of radiation that are amplified like laser light.

In connection with this project we need to know all the possible information about the propagation of electromagnetic wave. This work concern to propagation of the wave in free space at some range of distances.

1. Motivation.

The XFEL pulse propagated in free space from the source could be approximated by a stationary Gaussian beam only with some accuracy. For some applications (e.g. modeling of the coherent diffraction imaging experiments) time-dependent slice-by-slice propagation of SASE XFEL pulse should be done. In the article [1] was suggested a method for more accurate reproducibility of intensity's and phase's distribution.

Let us consider this method. It's known that the system of orthogonal Hermite's polynomials (details are given below) are complete in R^2 so we can use it as a basis. The beam's wave field could be expanded on a linear combination of basis's functions with some preassigned accuracy. Then we can propagate the beam's field using analytical expression for Fresnel transform. So we are able to propagate our beam at any distance with preassigned accuracy.

Another application of this algorithm is to test wave front propagation software [4]. We are able to compare the results of propagation of a linear combination of Hermite's polynomials with results of numerical propagation in the framework of Fourier optics approach.

2.Theoretical introduction.

It is well known that in paraxial approximation the evolution of a coherent light field *F(x,y,l)* under propagation in free space along the axis l is described by the parabolic equation

$$\frac{\partial^2 F}{\partial x^2} + \frac{\partial^2 F}{\partial y^2} + 2ik\frac{\partial F}{\partial l} = 0 , \quad x \in R, y \in R \qquad (2.1)$$

Here *k* is a wave number, *l* is a propagation variable, and *x,y* are transverse coordinates.

There are many solutions of the parabolic equation, but Hermite-Gaussian (HG) and Laguerre-Gaussian (LG) beams have special value among them. These solutions are described in terms of HG ana LG functions

$$H_{n,m}(r) = \sqrt{\frac{1}{\pi \cdot 2^{(n+m)} \cdot n! \cdot m!}} H_n(x) H_m(y) \qquad (n, m = 0,1\ldots) \qquad (2.2)$$

So, take to attention the weight function:

$$\iint H_{n,m}(x,y) \cdot H_{n,m}(x,y) e^{-x^2-y^2} dxdy = 1 \qquad (2.3)$$

And LG functions

$$L_{n,\pm m}(r) = \sqrt{\frac{n!}{\pi\cdot(n+m)!}}(x+iy)^m L_n^m(x^2+y^2) \qquad (n,m = 0,1\ldots) \quad (2.4)$$

Where

$$H_n(t) = (-1)^n e^{t^2} \frac{d^n}{dt^n} e^{-t^2}, \qquad (2.5)$$

$$L_n^m(t) = \frac{1}{n!} t^{-m} e^t \frac{d^n}{dt^n}(t^{n+m}e^{-t}), \qquad (2.6)$$

Analytic expression for solutions HG and LG with the usage of Fresnel transform are as follows:

$$\frac{k}{2\pi il}\iint exp\left(\frac{ik}{2l}|r-\rho|^2\right) H_{n,m}\left(\frac{\rho}{w_0}\right) d^2\rho = \frac{1}{(|\sigma|)} \exp\left(\frac{il|r^2|}{2kw_0{}^4|\sigma|^2} - i(n+m+1)\cdot \arg(\sigma)\right) H_{n,m}\left(\frac{r}{w_0|\sigma|}\right) \qquad (2.7)$$

$$\frac{k}{2\pi il}\iint exp\left(\frac{ik}{2l}|r-\rho|^2\right) L_{n,\pm m}\left(\frac{\rho}{w_0}\right) d^2\rho \frac{1}{|\sigma|} \exp(\frac{il|r^2|}{2kw_0{}^4|\sigma|^2} - i(2n+m+1)\cdot \arg(\sigma)) L_{n,\pm m}\left(\frac{r}{w_0|\sigma|}\right) \qquad (2.8)$$

When the symmetry planes of an astigmatic element and of an HG beam do not coincide, the structure of an HG beam changes radically. In this case, an HG beam is transformed into the finite sum of various HG beams

$$\iint exp\left(-i(r,\rho) + \frac{ib\psi(\rho,\theta)}{2}\right) H_{n,m}(\rho) d^2\rho = \frac{2\pi(-i)^{n+m}}{\sqrt{1+b^2}} exp\left(-\frac{ib\psi(r,\theta)}{2(1+b^2)}\right) \cdot$$

$$\sum_{k=0}^{n+m} (-1)^k e^{i(n+m-2k)arctg(b)} c_k^{(n,m)}(\theta) H_{n+m-k,k}\left(\frac{R(-\theta)r}{\sqrt{1+b^2}}\right) \qquad (2.9)$$

Where

$$c_k^{(n,m)}(\beta) = \sqrt{\frac{(n+m-k)!k!}{n!m!}} \cos^{n-k}(\beta) \sin^{m-k}(\beta) P_k^{(n-k,m-k)}(-\cos(2\beta)) \qquad (2.10)$$

And

$$P_k^{(\mu,\nu)}(t) = \frac{(-1)^k}{2^k k!} \frac{1}{(1-t)^{k+\mu}(1+t)^{k+\nu}} \frac{d^k}{dt^k}[(1-t)^{k+\mu}(1+t)^{k+\nu}] \qquad (2.11)$$

are Jacobi polynomials.

If to define a function family

$$\mathcal{G}_{n,m}(r|a) = \sum_{k=0}^{n+m} i^k\, c_k^{(n,m)}(\alpha) H_{n+m-k,k}(r) \qquad (2.12)$$

(in some sense a unification of HG and LG beams into a common family, that were named Hermite-Laguerre-Gaussian (HLG) beams).

3. Application.

3.1 Expansion into linear combination of Hermite's polynomials.

In our case we can expand the solution of the (2.1) equation at *l = 0* as a sum:

$$F(x, y, 0) = \sum_{n,m=0}^{n,m=N,M} c_{n,m}\, H_{n,m}\left(\frac{x}{w_0}, \frac{y}{w_0}\right) \qquad (3.1),$$

where

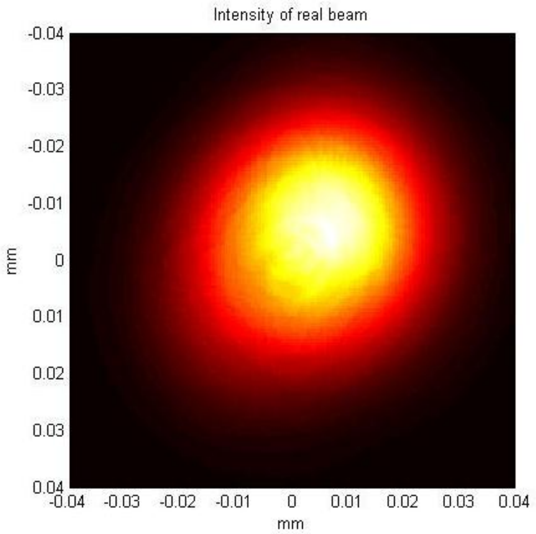
$$c_{n,m} = \iint F(x, y, 0)\, H_{n,m}\left(\frac{x}{w_0}, \frac{y}{w_0}\right) e^{-\frac{x^2}{w_0{}^2} - \frac{y^2}{w_0{}^2}} d\left(\frac{x}{w_0}\right) d\left(\frac{y}{w_0}\right) \qquad (3.2)$$

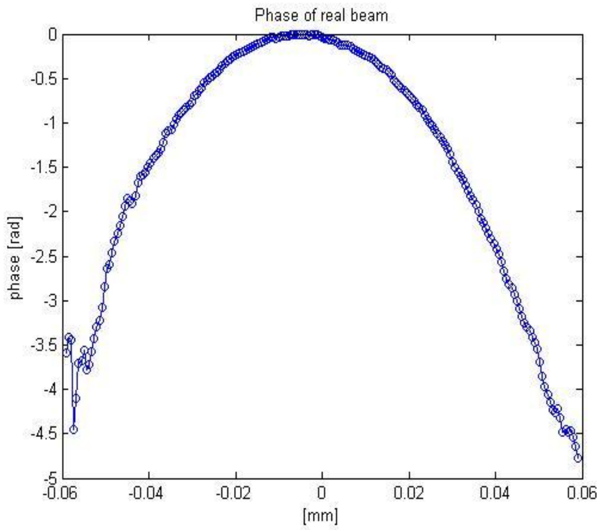
Then at arbitrary *l* the solution can be expand as:

$$F(x, y, l) = \frac{1}{|\sigma|} \exp\left(\frac{il|r^2|}{2kw_0{}^4|\sigma|^2} - i(n + m + 1) \cdot \arg(\sigma)\right) \cdot \sum_{n,m=0}^{n,m=N,M} c_{n,m}\, H_{n,m}\left(\frac{x}{w_0|\sigma|}, \frac{y}{w_0|\sigma|}\right)$$

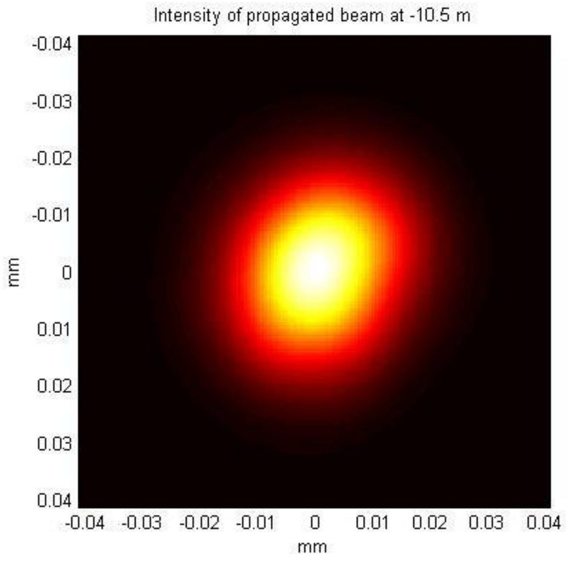
(3.3)

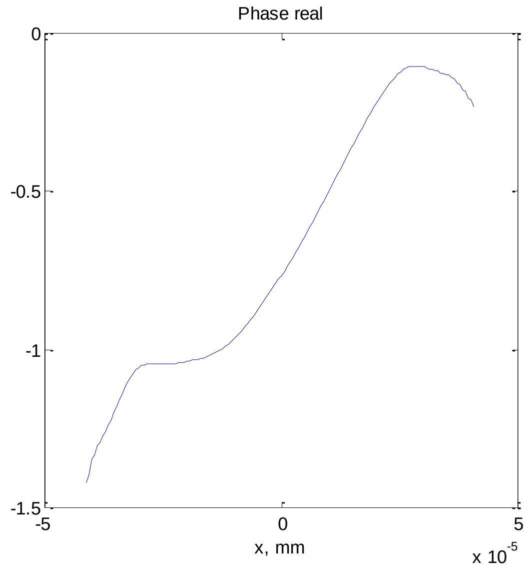
We have an output of FAST [4] code that is a field's distribution (matrix of complex numbers) at some distance from source:



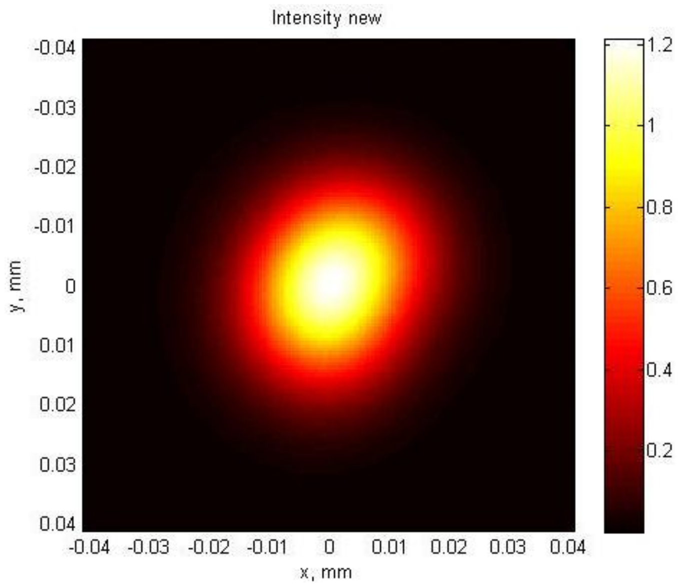


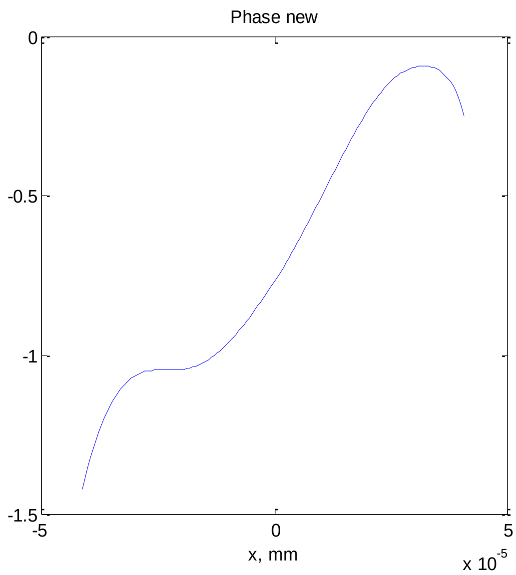
First of all, we need to define field distribution at l=0. We are able to make back propagation and to determine what the distance to source is (more details are in 3.2).



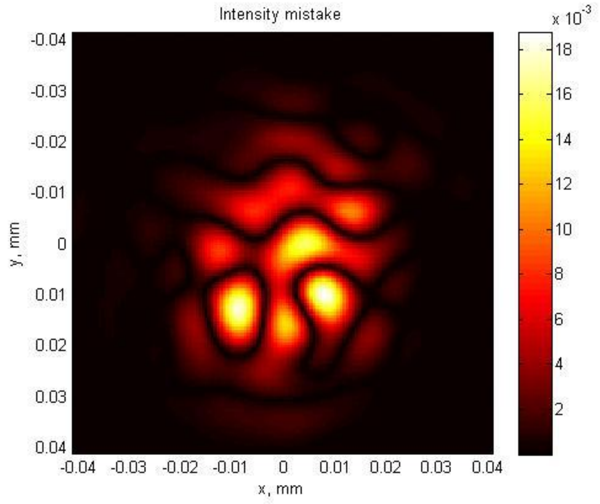


After the expansion into the finite sum of Hermite’s polynomials (the quantity of polynomials is 15x15 = 225) we obtained:
:

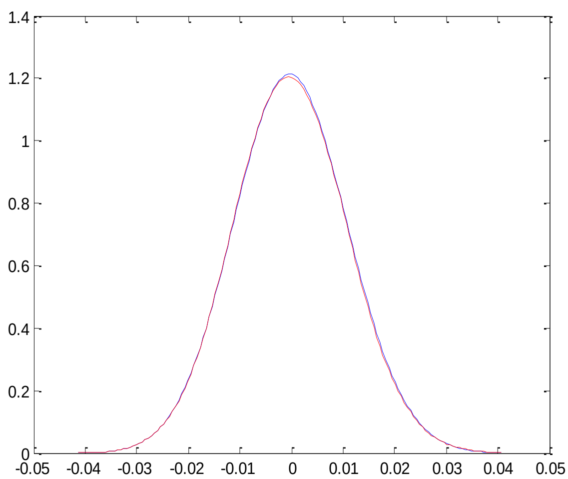


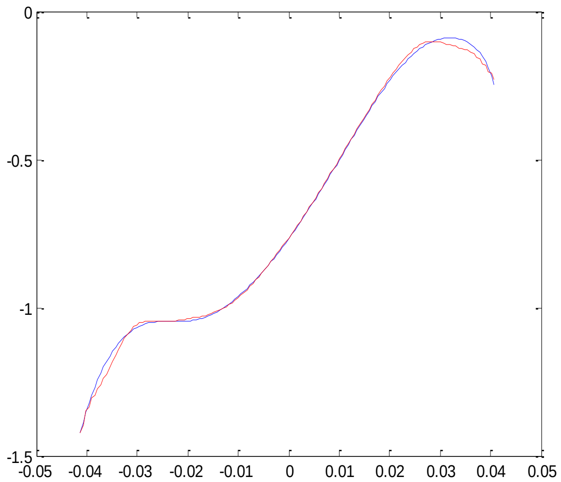


The difference between the function and its expansion into finite sum:



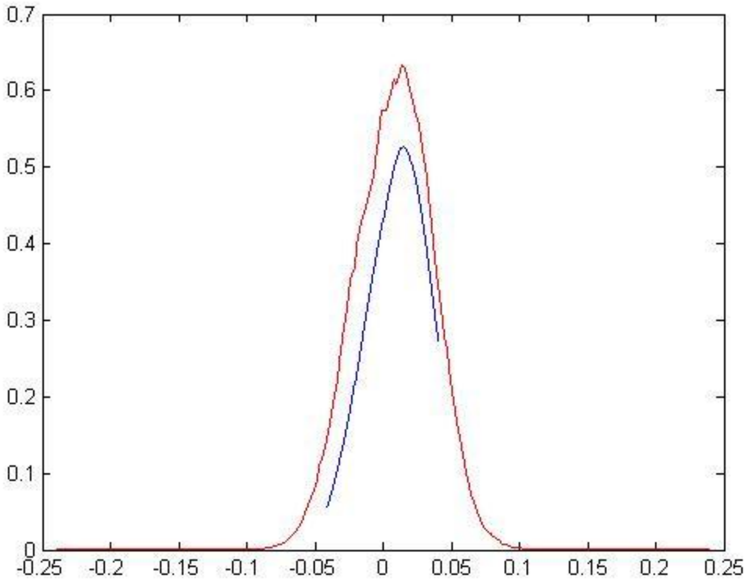
Central sections of intensity and phase (red line – input data) :





After propagation the results are not so satisficed.

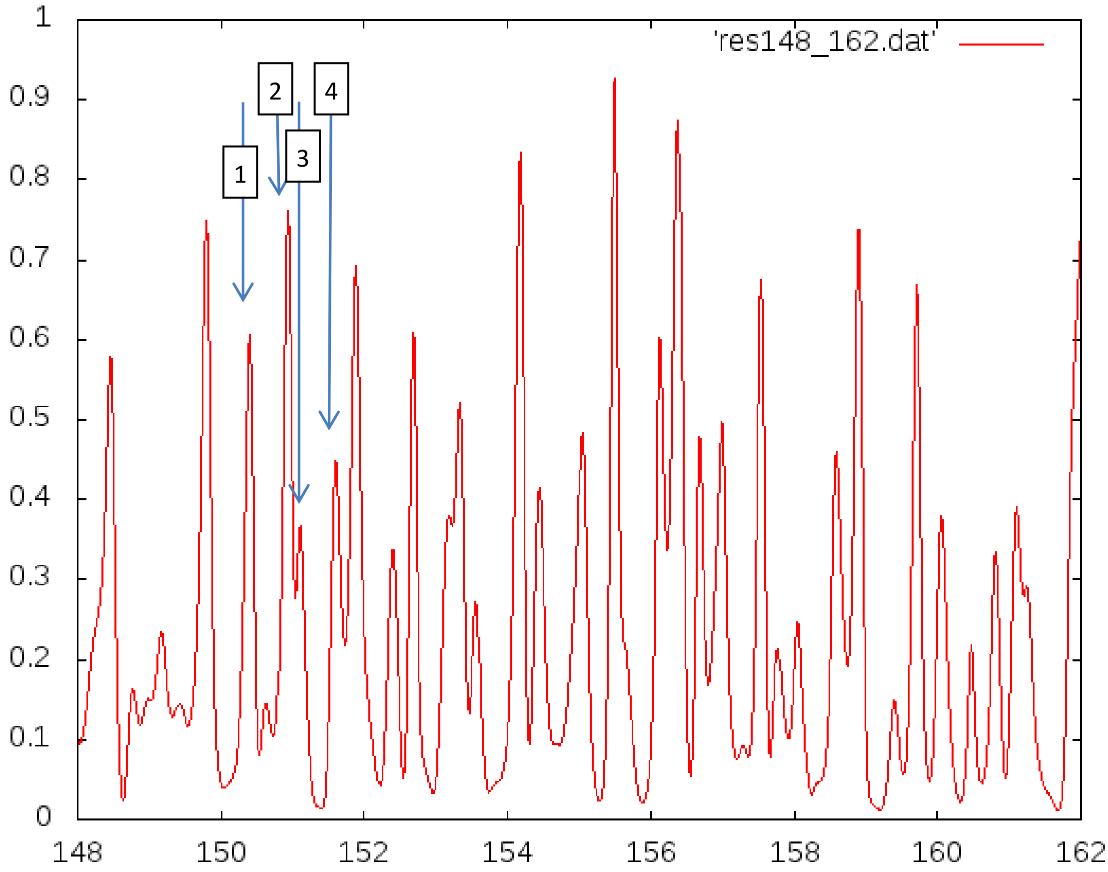
Central section of intensity (red line – input data) :



3.2 Back propagation.

Let us consider the field's distribution in some slice and propagate it back. The distance to source we can estimate by phase's behavior (!!!) in significant area (where the intensity is different from 0). At distance l = 0 the phase change its convexity. Shifts of the distance to source between slices in one spike and between neighboring spikes evidence about the degree of coherence.

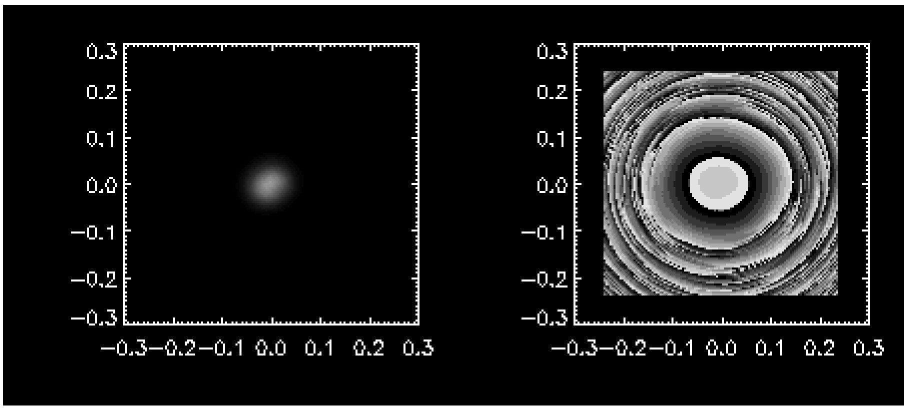
Let us see on one-dimensional distribution of intensity (we examined only indicated fragments):



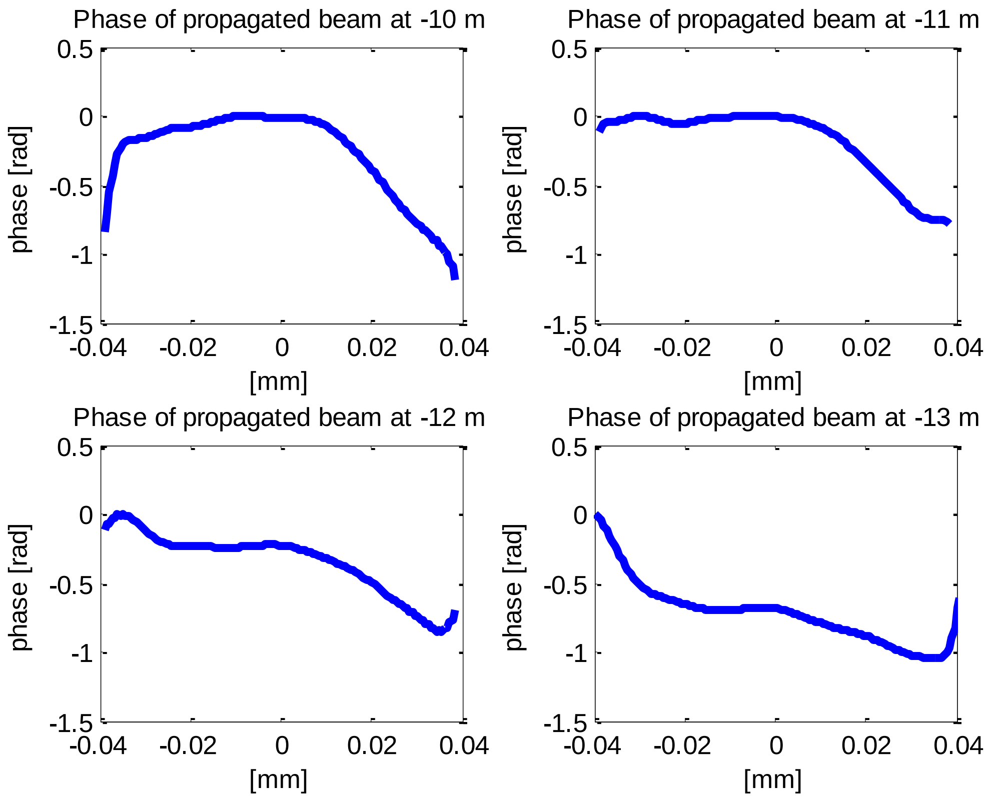
Firstly, we will analyse the data of slices of the same spike.

Input data:

1). T=151.613fs (spike3)

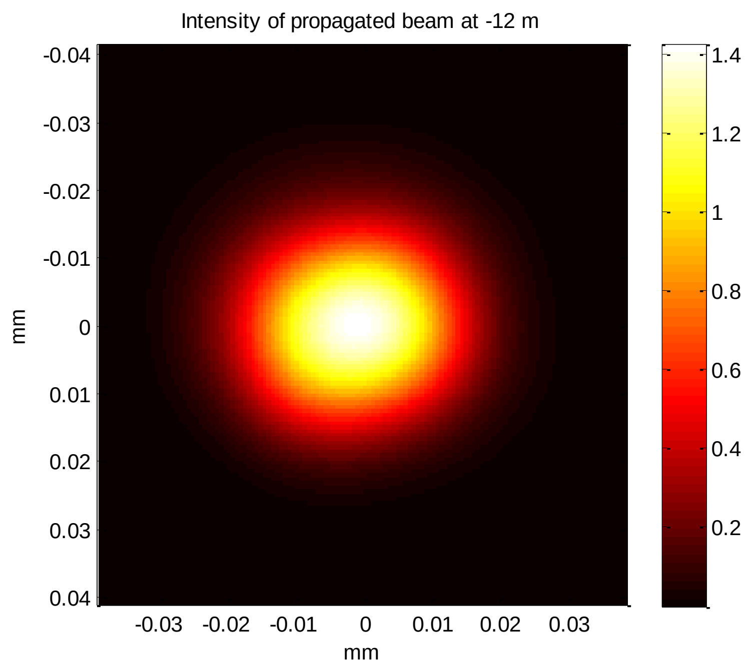


After back propagation:

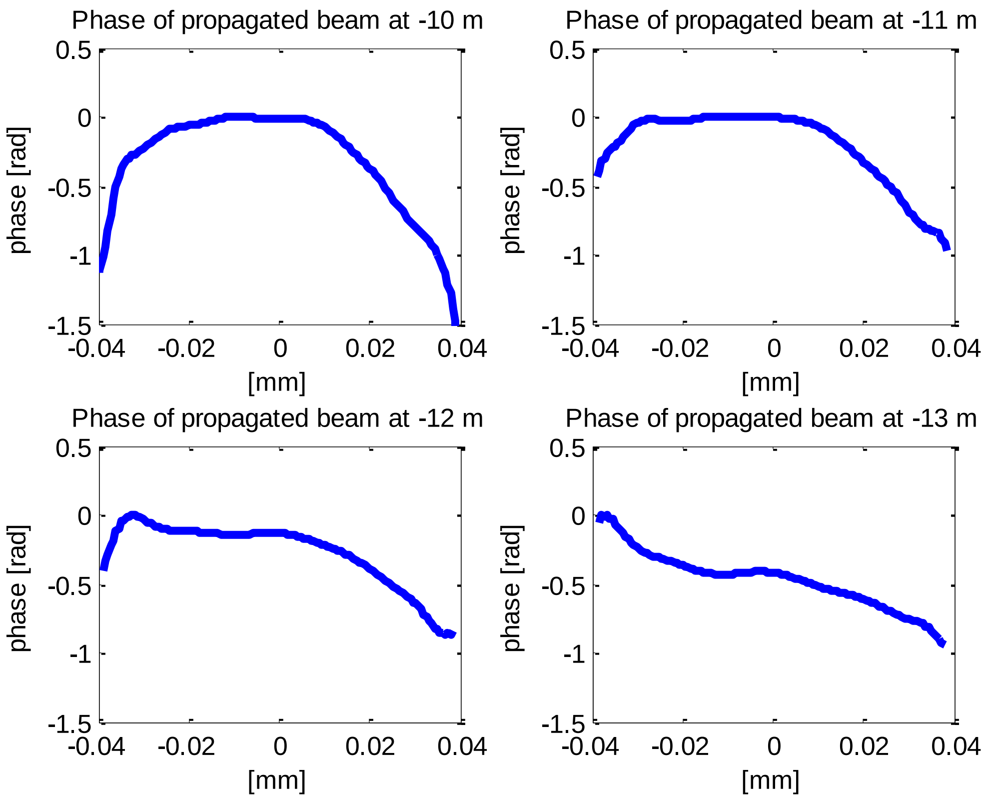


The criteria of choice of “optimal” length to sourse – is the best correspondence to line (linear approximation). In this case l = 12m.

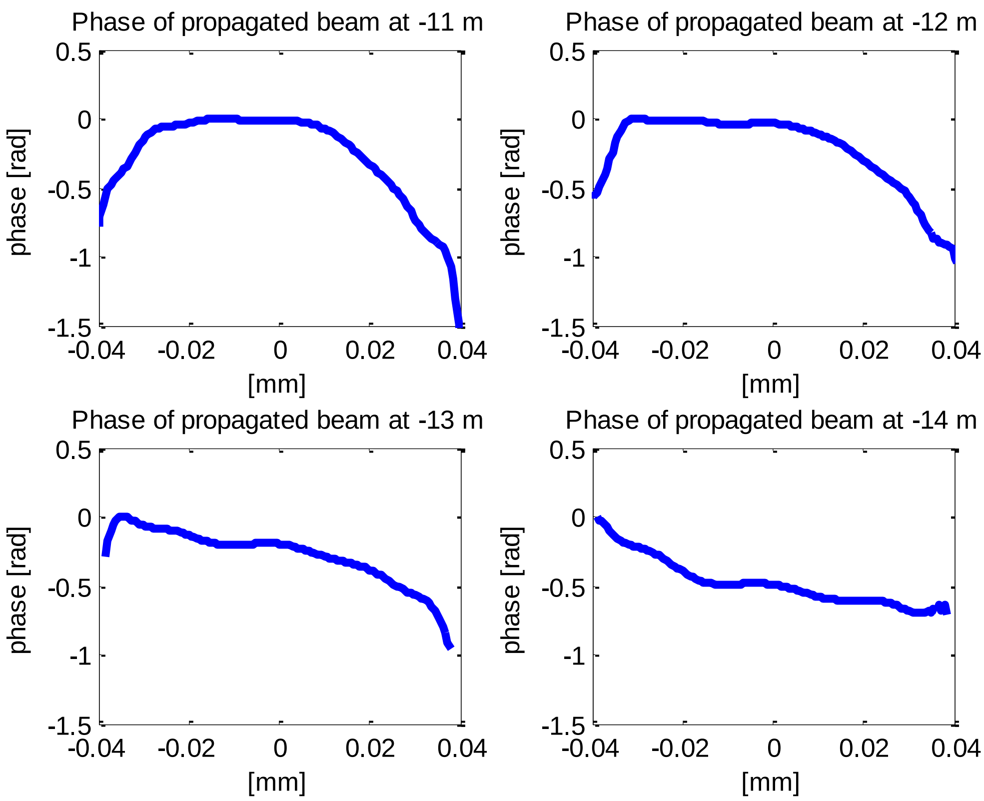
The distribution of intensity at “optimal” length:



2).T=151.627fs (the second slice from the same spike3)



3).T=151.640fs (the third slice from the same spike3)



With our degree of accuracy we can say that the distance to source does not change in one and the same spike.

Let us see the next spikes:

4). T=150.400 – 8.5 (spike1)

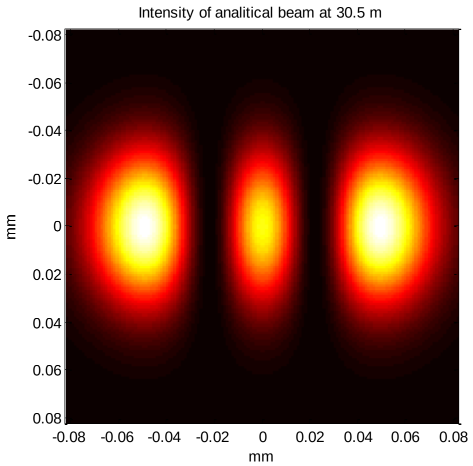
5). T=150.893fs – 11m (spike2)

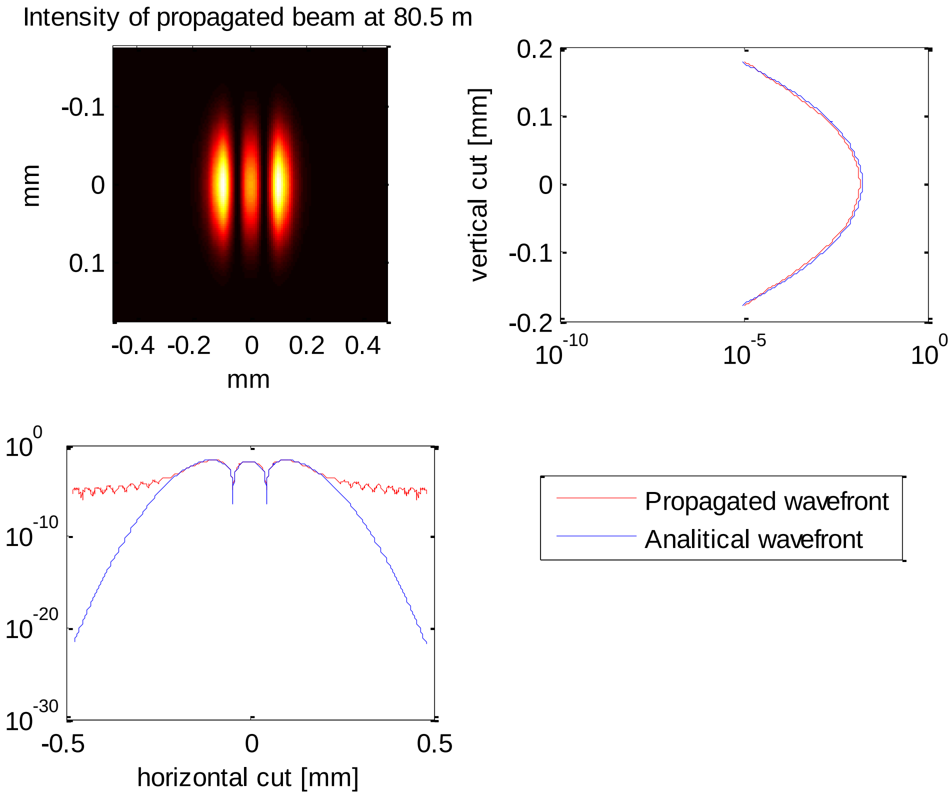
6). T=151.867fs – 9m (spike4)

As we can estimate the distance between different spikes varies from spike to spike but within the limits of 10%.

3.3 Propagation of the single Hermite's polynom.

We took the single Hermite's polynomial of the oder n = 2, m = 0 at l = 30.5, and propagate it (using "SRWLib")





As we see the structure of this polynomial is saved.

4.Results and discussions.

To sum up: we can expand the field distribution with any preassigned accuracy at l = 0, but the problem of its propagation is still open. We can make some assumptions why it is so:

- inaccurate determination of plane l = 0 (the distance of input data's back propagation)
- inappropriate values of beam's parameters (for example, w_0 – the minimum spot size of the beam, that was originally determined for Gaussian beam)

Another part of work connected with back propagation could help us to understand the degree of source's coherence and if it is possible to use "wave-front-propagation" in "SRWLib" – program.

5.Acknowledgements.

I would like to thank my supervisors Liubov Samoylova and Harald Sinn for support, time spending and sharing their knowledge. Thanks to them I learnt a lot of new things either in wave optic's theory or in practical application in computer simulation. Also I would like to thank all the people who made this Summer Student Program possible. It were great experience and unforgettable summer.

6.References.

[1]. E.G. Abramochkin, "Hermite-Laguerre-Gaussian functions", Vestnik Samarskogo gos. universiteta, 2001, p.19-41 (in Russian) and E.G. Abramochkin, E.V. Razueva, V.G.Volostnikov, "Hermite–Laguerre–Gaussian beams in astigmatic optical systems", Vestnik Samarskogo gos. universiteta, 2001, p.103-121
(in English: http://www.spie.org.ua/Final_Article/23-174-185.pdf)

[2]. General astigmatic transform of Hermite–Laguerre–Gaussian beams Eugeny Abramochkin, Evgeniya Razueva, and Vladimir Volostnikov, JOSA A, Vol. 27, Issue 11, pp. 2506-2513 (2010)

[3]. [SRWLib] L. Samoylova, A. Buzmakov, G. Geloni, O. Chubar, H. Sinn "Cross-platform wave optics software for XFEL applications", Proceedings SPIE, SPIE San Diego (2011)

[4]. [FAST] Saldin, E., Schneidmiller, E. and Yurkov, M., "FAST: A three-dimensional time-dependent FEL simulation code," Nucl. Instrum. Methods A 429, 233–237 (1999)