A new approach to optical measurements of small objects with superresolution

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ABSTRACT

The application of optical superresolution technique to measuring small particles said to be secondary light sources with various scales of sizes - from micrometers to nanometers is discussed. The concept of a separate nanosized object and theoretical approach to recognition of its sizes through the mathematical continuation of the visible angular spectrum of vector plane waves is suggested.

Keywords: nanosized objects, superresolution, secondary light sources, near-field optics

1. INTRODUCTION. IDEA AND MODEL

The to-day status of science and technology in various fields is often may be characterized as a world of very **precisely defined dimensions**. A great amount of tasks concern small and extra small elements and structures namely photomasks and compact optoelectronic devices, nanopowder particles, nanosubstrates, tools for micro and laser surgery, biomolecules, viruses, etc. In all these cases the urgency of the use of optical research methods is doubtless. However it is evident that the far-field optical microscopy offers no direct measuring technique in nanometric scale and it is necessary to take alternate means such as electron scanning microscopy techniques. Some of tasks in question accommodate the use of the latter methods but there are cases in which their application is hardly reasonable and even impossible. This concerns objects which cannot be observed with the use of electron irradiation for example biological objects accommodating only visual electromagnetic field effects, being investigated in vivo, interesting only by their optical properties, etc. So visual optics is still the reasonable choice but with request of new opportunities.

It is important that the light scattering on extra small material structures may be used according to the Babinet's principal for investigating amplitude and phase effects imposed by these structures. Hence the possibility appears of the knowledge of their dimensions as parameters of some secondary sources of light.

Nevertheless such approach inevitably will meet a great lack of necessary information for restoration subwavelength characteristics. Here the **superresolution** technique becomes very important which means the use of iterative processes and investigation of their opportunities. The next problem is a rigorous concept of diffraction on mesoscopic elements at high angles. In this case the total electromagnetic energy is distributed between the propagating and evanescent parts or in other words far and near fields.

There are theoretical and mathematical difficulties of far- and near-field phenomena representation in one model in terms of linear reversible equations. The suggested mathematical modeling is based on the superposition of solutions of Maxwell's equations enclosing linearly polarized vector plane waves in real and complex forms as functions of spatial frequencies $\left(\nu_x, \nu_y\right)$ corresponding both to the propagating $\mathbf{u}_{0ij}^{R} = \dfrac{\mathbf{k}_{ij} \times \mathbf{p}_0}{\left|\mathbf{k}_{ij} \times \mathbf{p}_0\right|}$ and evanescent $\mathbf{u}_{0ij}^{E} = \dfrac{\hat{\mathbf{k}}_{ij} \times \mathbf{p}_0}{\left|\hat{\mathbf{k}}_{ij} \times \mathbf{p}_0\right|}$ light.

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Here $\mathbf{u}_{0ij}^{R}, \mathbf{u}_{0ij}^{E}$ are the complex vector amplitudes, real $\mathbf{k}_{ij}$ and complex $\hat{\mathbf{k}}_{ij}$ denote the wave vectors corresponding to the space frequencies below and higher than $\frac{1}{\lambda}$, $\mathbf{p}_0$ is the polarization status vector.

The expression for the entire near-field distribution close to the investigated light source will be:

$$\mathbf{U}(\mathbf{r}) = \sum_i \sum_j \mathbf{B}_{ij} \mathbf{u}_{ij}(\mathbf{r}), \quad (1)$$

where $\mathbf{B}_{ij}$ – matrices of complex coefficients, $\mathbf{u}_{ij}(\mathbf{r}) = \begin{cases} \mathbf{u}_{ij}^{R}(\mathbf{r}) \\ \mathbf{u}_{ij}^{E}(\mathbf{r}) \end{cases}$, $\mathbf{u}_{ij}^{R}$ – propagating plane waves, $\mathbf{u}_{ij}^{E}$ – evanescent plane waves.

The use of vector representation of the light complex amplitude leads to simplified calculation procedures for rigorous far-field intensity distribution simulation. If the vector expressions for both types of plane waves are substituted into the sum (1) with taking into account that $\mathbf{k}_{ij}$ and $\hat{\mathbf{k}}_{ij}$ are the functions of spatial frequencies (ν_x, ν_y) it will be possible to use the digital Fourier transform to calculate all the components of this sum. The description of the vector amplitude distribution itself may be defined in the following form: $\mathbf{U}(\mathbf{r}) = \mathbf{S} \cdot \mathbf{u}_0$, where $\mathbf{S}$ – is the matrix model of the light source containing its dimensions, $\mathbf{u}_0$ – vector amplitude of an incident linearly polarized plane wave with the wave vector $\mathbf{k}_{00}$. Using this matrix expression together with the sum (1) and vector amplitudes of plane waves the following matrix equation may be obtained:

$$\mathbf{S} = F\left[\mathbf{P}_{ij}(\nu_x, \nu_y)\mathbf{B}_{ij}\right], \quad (2)$$

where F – direct Fourier transform operator, $\mathbf{P}_{ij}$ – a set of matrix operators of rotations according to the assumed definition of a plane wave vector amplitude, $\mathbf{B}_{ij}$ – a set of matrix coefficients, indices ij denote that the Fourier transform is taken with respect to the digitized spatial frequencies.

The matrix expression for the far-field light amplitude distribution parameters inverse to (2) is

$$\mathbf{B}_{ij} = \mathbf{P}_{ij}^{-1}(\nu_x, \nu_y) \cdot F^{-1}[\mathbf{S}], \quad (3)$$

where $\mathbf{S}$ is the mentioned matrix of the secondary light source (aperture) parameters, $\mathbf{P}_{ij}^{-1}(\nu_x, \nu_y)$ – a set of inverse matrix operators of rotations, F^{-1} – the inverse Fourier transform operator. If the amplitude of the far-field light distribution is known (which means that we know $\mathbf{B}_{ij}$) it will be possible to restore the encoded in the matrix $\mathbf{S}$ initial light field distribution dimensions by the matrix formula similar to (2). This mathematical model is an alternative to the well-known MMP-method[1] based on the superposition of spherical and dipole solutions of Maxwell's equations. Principal advantage of this model is the use of a set of reversible Fourier transformations as a nucleus of the procedure.

2. A THEORETICAL APPROACH TO MEASURINGS

To define dimensions of a subwavelength aperture we firstly have to register the far-field intensity within the solid angle of at least ±90° and after that obtain the distribution of an amplitude. Here the transformation of intensity into amplitude is suggested and after that the problems of the use of “insufficient” information are discussed.

Therefore the vector amplitude of the registered light may be described as follows:

$$U'\left(\theta_x,\theta_y\right)=\begin{pmatrix} u'_x\left(\theta_x,\theta_y\right) \\ u'_y\left(\theta_x,\theta_y\right) \\ u'_z\left(\theta_x,\theta_y\right) \end{pmatrix}=\mathbf{B}'\cdot\frac{\mathbf{k}\left(\theta_x,\theta_y\right)\times\mathbf{p}_0}{\left|\mathbf{k}\left(\theta_x,\theta_y\right)\times\mathbf{p}_0\right|}, \quad (4)$$

where $\mathbf{p}_0$ is the polarization status vector, $\mathbf{B}'=\begin{pmatrix} \sqrt{I'\left(\theta_x,\theta_y\right)} & 0 & 0 \\ 0 & \sqrt{I'\left(\theta_x,\theta_y\right)} & 0 \\ 0 & 0 & \sqrt{I'\left(\theta_x,\theta_y\right)} \end{pmatrix}$ is the diagonal matrix containing the square roots of the registered values of the angular intensity distribution.

This equation is correct in case of linear polarization and that the electric vector lies in the plane of a receiver[2]. The latter may be provided if the receiver is set at a proper angle while scanning or the investigated field is registered in the focal plane of a microobjective with high numerical aperture.

Now for the restored matrix $\mathbf{S}'$ we may get the following expression:

$$\mathbf{S}'=F\left[\mathbf{P}_{ij}\cdot\mathbf{B}'\right]. \quad (5)$$

The restored dimensions $\mathbf{S}'$ may differ greatly from the initial ones $\mathbf{S}$ because of the absence of direct information about the near-field distribution. The difference increases as the aperture sizes diminish. This means that the Fourier transform is applied to a part of the space frequencies spectrum and consequently the restored model of the aperture should not be correct. To solve the task of restoration an additional mathematical procedure is required.

In this stage of the work we have investigated some approaches how to construct the process of analytical continuation of the Fourier spectrum if its small part is known. Our problem differs from the most of well known superresolution examples by the fact that we don't know the input i.e. the aperture at all but only the part of its spectrum. In this case we have to make the feedback only in the spectrum space which gives an extremely ill-posed task. To make the task more steady we should use a multilevel procedure and take different functions for continuation on each level. The analysis of the problem has shown that better results may be obtained by the use of Fourier transform eigenfunctions which in one-dimensional space are known and tabulated as wave prolate (spheroidal) functions[3,4,5]. Unfortunately in the two-dimensional space these functions have not ever been used and their analytical expressions are unknown. As even for one dimension the wave prolate functions are extremely hard to be calculated[4] a new technique has been elaborated in order to make it possible to use rather effective mathematical basis for Fourier spectra continuation.

This technique encloses two steps. The first step is the partial continuation of the spectrum up to the first zeros by the use of orthogonal polynomials. The second step is the iterative continuation procedure of the spectrum upon the rest sample region using the modified Gerchberg's[6] approach. In these two steps the idea of wave prolate functions is realized not directly but through numerical algorithm which offers to obtain the optimum expansion of the spectrum by orthogonal Zernike polynomials and their analytical continuation beyond the unit circle - infinite functions with finite spectra. It is somewhat the generalization of two dimensional wave prolate functions with double orthogonality.

3. THE CONTINUATION TECHNIQUE BEYOND THE VISIBLE REGION AND PROBLEMS OF SUPERRESOLUTION.

The process of continuation itself usually is being built as the process of recognition of the input with a sequence of feedback procedures. The real examples of such kind deal either with the analytical continuation of the spectrum on the basis of the sample (Shannon's) theorem[7] or with various iterative procedures[6]. The mentioned theoretical approach with the use of one dimensional wave prolate functions with double orthogonality usually is being applied to antenna currents distributions. In case of two dimensions which is in optics this approach meets with the problem of two-dimensional basis construction and an impracticable amount of calculations.

Both approaches - the sample theorem and iterative procedures would give satisfactory results with greater or less probability but in our case it is necessary to obtain the stable information about aperture sizes. The better stableness from the use of functions with double orthogonality cannot be in question. In this work a new analytical-iterative procedure is offered. This procedure involves a step of polynomial expansion which is realized as Zernike polynomial extrapolation with new approach to calculation of polynomials beyond their orthogonality region with high accuracy. This step gives a set of orthogonal polynomial expansion coefficients which form a numerical model of the visible part of the spectrum strongly related with the model of the invisible one. With these coefficients and if the analytical expressions of the functions with double orthogonality with two dimensions were known and suitable for computing the task of restoration of subwavelength sized apertures would be solved at once. Unfortunately there are no simple analytical expressions suitable for computing to continue the spectrum in the invisible region. That is why it is reasonable to carry out a sequence of approximations in order to find the function mostly close to the part of the spectrum already defined. In this approach the use of sample functions in an iterative process has a sense of orthogonal expansion of the spectrum and should be performed more surely. The calculations taken on Pentium-166 has shown that this idea was quite correct.

After processing of the registered intensity I' and transformation of angular (θ_x, θ_y) coordinates into spatial frequencies (ν_x, ν_y) the visible part of the Fourier spectrum of the initial aperture $f^v(\nu_x, \nu_y) = Bf(\nu_x, \nu_y)$ is defined. Here B denotes that the total spectrum $f(\nu_x, \nu_y)$ is cut off by the circle $\left(-\frac{1}{\lambda} \le \sqrt{\left(\nu_x^2 + \nu_y^2\right)} \le \frac{1}{\lambda}\right)$. By the way the cutting off may be greater if smaller solid angle or numerical aperture of a microobjective are used.

The mathematical equations showing the process of continuation may be given as follows:

the **first step** (Zernike extrapolation) -

$$f^{v+}(\nu_x^+, \nu_y^+) = \sum_i \sum_j P_{ij}(\nu_x^+, \nu_y^+) C_{ij}, \tag{6}$$

where C_{ij} are the Zernike polynomial expansion coefficients defined from the equation

$$f^v(\nu_x, \nu_y) = \sum_i \sum_j P_{ij}(\nu_x, \nu_y) C_{ij}. \tag{7}$$

Here $P_{ij}(\nu_x, \nu_y)$ are the Zernike polynomials orthogonal on the region $\left(-\frac{1}{\lambda} \le \sqrt{\left(\nu_x^2 + \nu_y^2\right)} \le \frac{1}{\lambda}\right)$ and $\left(\nu_x^+, \nu_y^+\right)$ are the coordinates of points in the region greater than the initial visible space. The dimensions of this new region may be 1.5, 2., 3 and more times larger. In order to maintain the correctness of this task a new approach to the polynomial extrapolation is suggested. The polynomials should not be conventionally Zernike but have to be built as special orthogonal polynomials with variable properties of orthogonality. Such polynomials were elaborated in the St.-Petersburg Institute of Fine Mechanics and Optics in 1983 in order to enrich the properties of Zernike polynomials by new numerical advantages[8]. The coefficients C_{ij} may be defined from (7) which is in the visible region by the very stable standard Gram-Schmidt procedure.

The result of the first step is the extended "visible" region in order to run the superresolution procedure under promoted conditions. Consequently one of the well-known iterative procedures[9,10] may be taken to finish the continuation. Thus the **second step** is formulated as follows:

a) $$s_e^{(p)}(x, y) = F\left[f^v\left(\nu_x, \nu_y\right)\right], \tag{8}$$

where $s_e^{(p)}(x,y)$ is the preliminary estimation of the input. This estimation is being analyzed in order to find the smallest region Ω_s enclosing all the points where the values of the signal exceed a taken numerical threshold s_0. The signal $s_e^{(p)}(x,y)$ within Ω_s is denoted as $Qs_e^{(p)}$ and the first estimation of the spectrum will be

$$f_e(\nu_x,\nu_y) = F^{-1}\left[Qs_e^{(p)}(x,y)\right]; \qquad (9)$$

$$s_e^{(s)}(x,y) = F\left[f_e(\nu_x^{\,+},\nu_y^{\,+}) + f^{\nu}(\nu_x^{\,-},\nu_y^{\,-})\right],$$

where $s_e^{(s)}(x,y)$ is the secondary estimation of the input, $(\nu_x^{\,-},\nu_y^{\,-})$ define the points of the "visible" part of the spectrum (polynomial extrapolation) and $(\nu_x^{\,+},\nu_y^{\,+})$ define the points of the rest area. Then $s_e^{(s)}(x,y)$ should be substituted instead of $s_e^{(p)}(x,y)$ into (9) and the iterative cycle is to be continued.

The process is going on until the value of

$$\left(\iint_{\Omega_e}\left|f_m(\nu_x^{\,-},\nu_y^{\,-}) - f^{\nu+}(\nu_x^{\,-},\nu_y^{\,-})\right|^2 d\omega\right) \Big/ \iint_{\Omega_e}\left|f^{\nu+}(\nu_x^{\,-},\nu_y^{\,-})\right|^2 d\omega$$

becomes less than a chosen tolerance ε which usually depends on the numerical threshold s_0 and $f_m(\nu_x^{\,-},\nu_y^{\,-})$ being the spectrum of the m-th estimation of the input.

This approach has been tested for various apertures with different dimensions and for various sets of orthogonal polynomials in order to optimize the process. The numerical calculations have shown that this technique may give very promising results.

4. NUMERICAL RESULTS

The suggested technique is illustrated by the examples of sizes recognition where the final error is quite negligible while the spectrum continuation is too long. The figures 1 and 9 show the taken initial apertures. The figures 3,4 and 11,12 show the primary extension of the spectra by Zernike polynomial extrapolation - too long from the traditional point of view. The horizontal axis here is marked in degrees corresponding to especially spatial frequencies that is why only for the visible region there are realistic angular values. The figures 5,6 and 13,14 show the final spectra obtained without and after the use of preliminary polynomial extrapolation. The figures 7,8 and 15,16 display restored apertures without and after polynomial extrapolation and figures 2,10 refer to uncharacterized restored shapes without any iteration.

It is important that what we can see on figs. 3 and 11 is a very short part of the whole Fourier spectrum. This is the only data that may be registered and we have to take all the necessary information out of it. The following polynomial extension is surprisingly 4 times larger than the visible region and provides much better initial conditions for the finishing iterative continuation.

We may surely say that the suggested approach is quite promising to construct a new measuring process. The next step of this work is to understand the noise sensitivity and conditioning degree of this task being applied to realistic data.

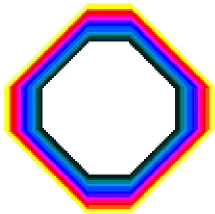

Fig. 1 Aperture 150×150 nm^2

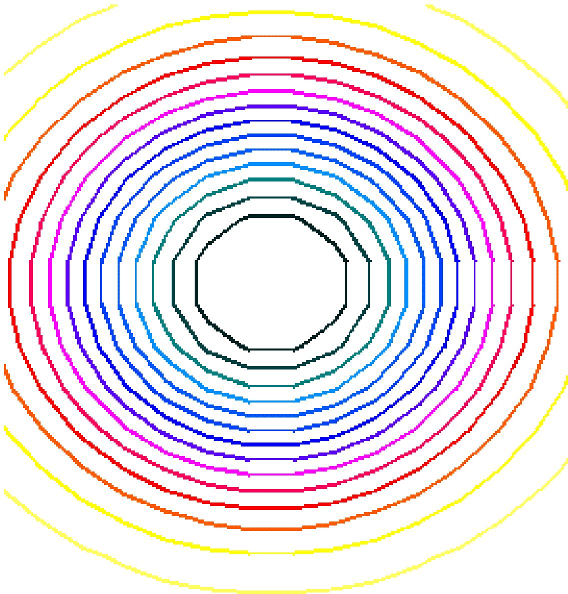

Fig. 2 Restored aperture without iterations

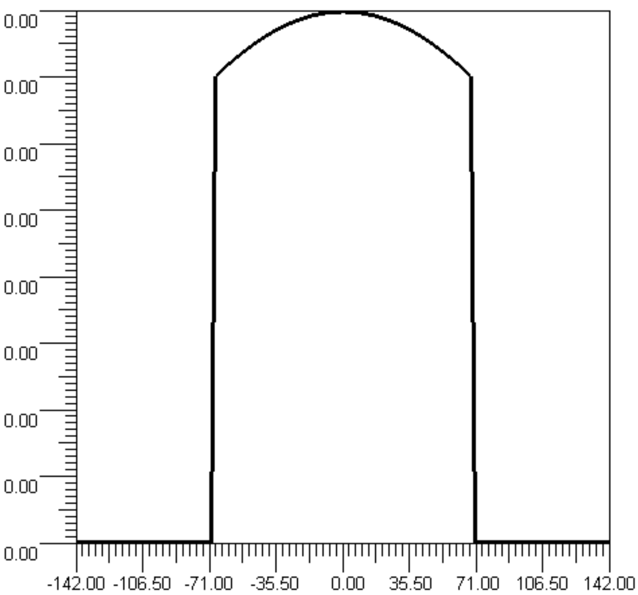

Fig. 3 The cross sections of the visible part of the spectrum (scaled within ± 142°).

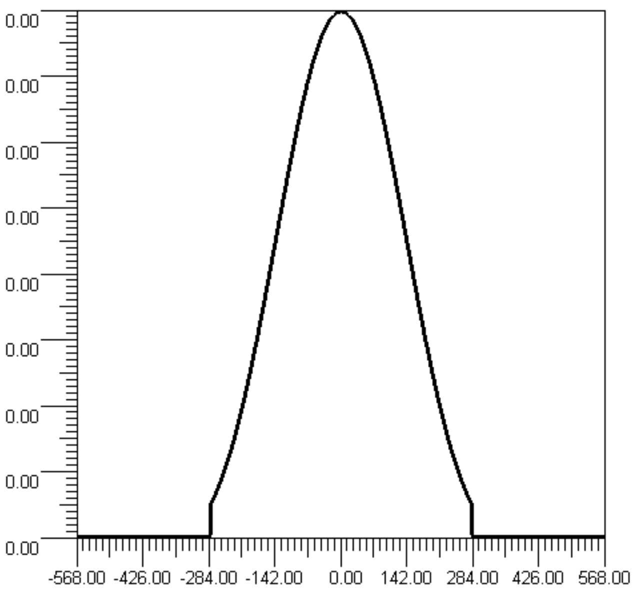

Fig. 4 The cross sections of the Zernike extrapolation beyond the visible region (scaled within ± 568°).

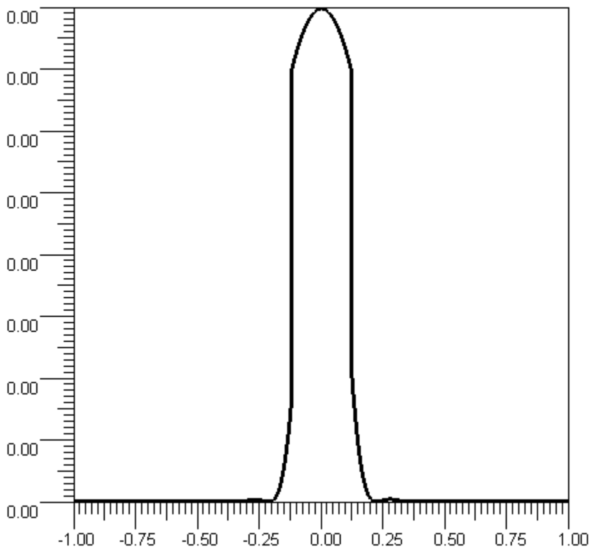

Fig. 5 Final spectrum without polynomial extrapolation (in relative frequency coordinates)

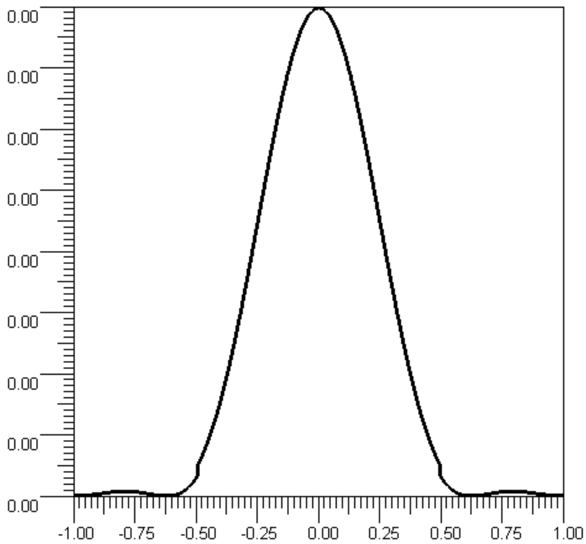

Fig. 6 Final spectrum after polynomial extrapolation (in relative frequency coordinates)

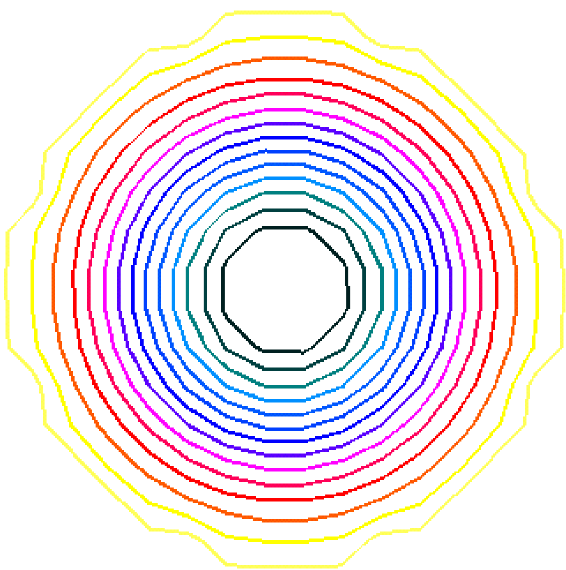

Fig. 7 Restored aperture without Zernike extrapolation

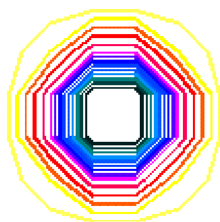

Fig. 8 Restored aperture with Zernike extrapolation and the following iterative continuation

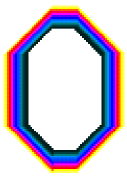

Fig. 9 Aperture 150×250 nm^2

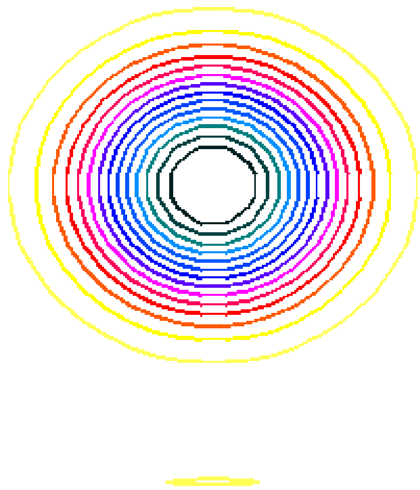

Fig. 10 Restored aperture without iterations

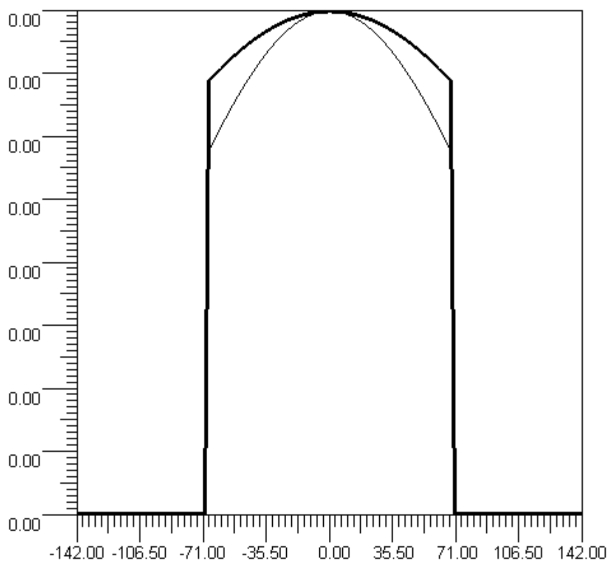

Fig. 11 The cross sections of the visible part of the spectrum (scaled within ± 142°).

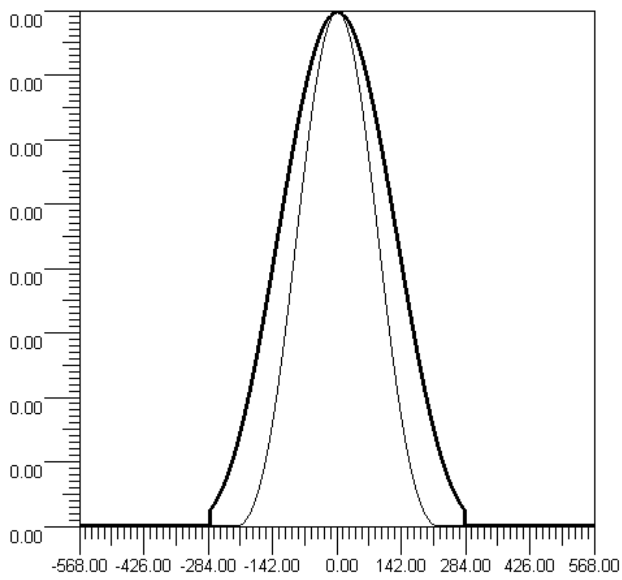

Fig. 12 The cross sections of the Zernike extrapolation beyond the visible region (scaled within ± 568°).

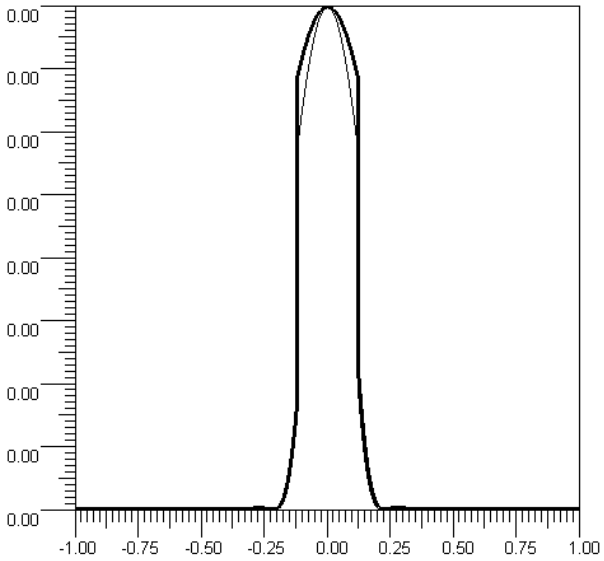

Fig. 13 Final spectrum without polynomial extrapolation (in relative frequency coordinates)

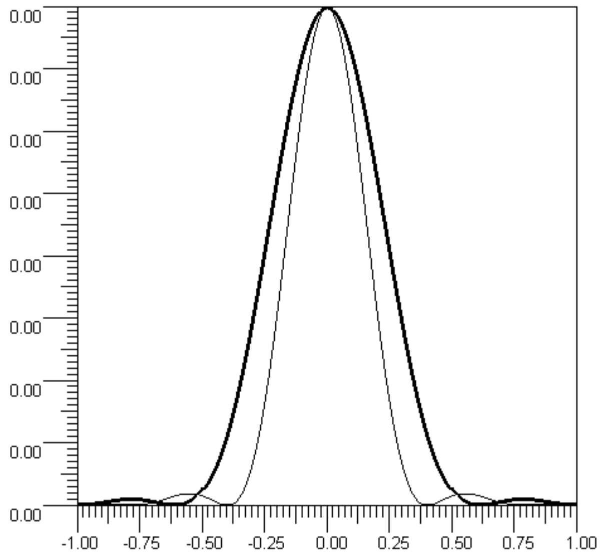

Fig. 14 Final spectrum after polynomial extrapolation (in relative frequency coordinates)

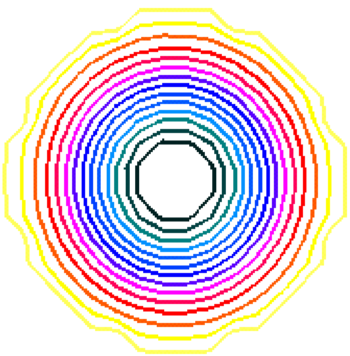

Fig. 15 Restored aperture without Zernike extrapolation

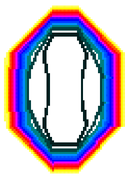

Fig. 16 Restored aperture with Zernike extrapolation and the following iterative continuation

5. CONCLUSION

One of the important results of this work is that the inverse task is being solved by a set of standard algorithms - Fast Fourier Transform (FFT), Matrix Operations, Gram-Schmidt Orthogonalization. The use of such procedures greatly simplifies the calculations and at the same time diminishes the probable error. That is why there is a great certainty of successful real data processing. It is also favorable that orthogonal polynomials may accommodate an errorless long extrapolation provided that they are in a proper use. The whole process offers to define a very capacious information of the initial object or boundary structure.

Moreover it should be noted that such model and technique offers grounds of thoughts both in extra sized measurements and in optical image processing at all especially for unresolved structures and we may quite assume that the limits of optical resolution are still far away.

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