Extended Nijboer-Zernike analysis for vectorial diffraction calculations and aberration retrieval

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OUTLINE

- What is the (extended) Nijboer-Zernike analysis?

- Axial extension of the aberrated in-focus diffraction integral to a finite focal region

- Vectorial and high-NA effects

- Future work

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What is the Nijboer-Zernike analysis?

- Complete and orthogonal representation of the wavefront aberration in the exit pupil of an optical system using circle polynomials
- Limited to a perfectly spherical support
- First proposed on the unit circle by Szego in 1919
- Introduced in optics by Zernike (1935) and Nijboer (thesis, 1942)

$$W(\rho,\vartheta) = \sum_{n,m} R_n^m(\rho)\left[a_n^m \cos(m\vartheta) + b_n^m \sin(m\vartheta)\right]$$

$$= \sum_{n,m} c_n^m R_n^{|m|}(\rho)\exp(im\vartheta) \qquad (-m_{\max} \le m \le m_{\max})$$

- Immensely popular thanks to Jim Wyant (interferometry) since 1980

Usefulness of the Nijboer-Zernike analysis

- Optical design:
  The polynomials solve the aberration balancing problem in optical design (Maréchal, Hopkins, Welford: 1940's)
- Diffraction theory:
  Calculation of diffraction patterns for small aberration values and modest defocusing (Nijboer, 1942, Nienhuis, 1943)
- Interferometry:
  Stable reconstruction of measured data;
  'fringe index' of polynomials introduced by Wyant c.s. in 1980
  (37 'first' Zernike polynomials)
- Analytic extension of (aberrated) diffraction integrals to focal *volume* and arbitrary axial position using Zernike polynomials (Janssen, 2002)

Extension through-focus N-Z analysis to high NA values

- Rigorous description of the defocus term, if necessary higher order expansion ($R_4^0(\rho)$ -polynomials etc.)

- Incorporation of vectorial description of focused field for arbitrary state of polarisation

- Inclusion of radiometric effects (Abbe or other imaging conditions)

- Treatment of new (aberrated) diffraction integrals for focal *volume* using Zernike polynomials
  (Braat, Dirksen, Janssen & van de Nes, JOSA A, Dec. 2003)

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Standard geometry of focused wave
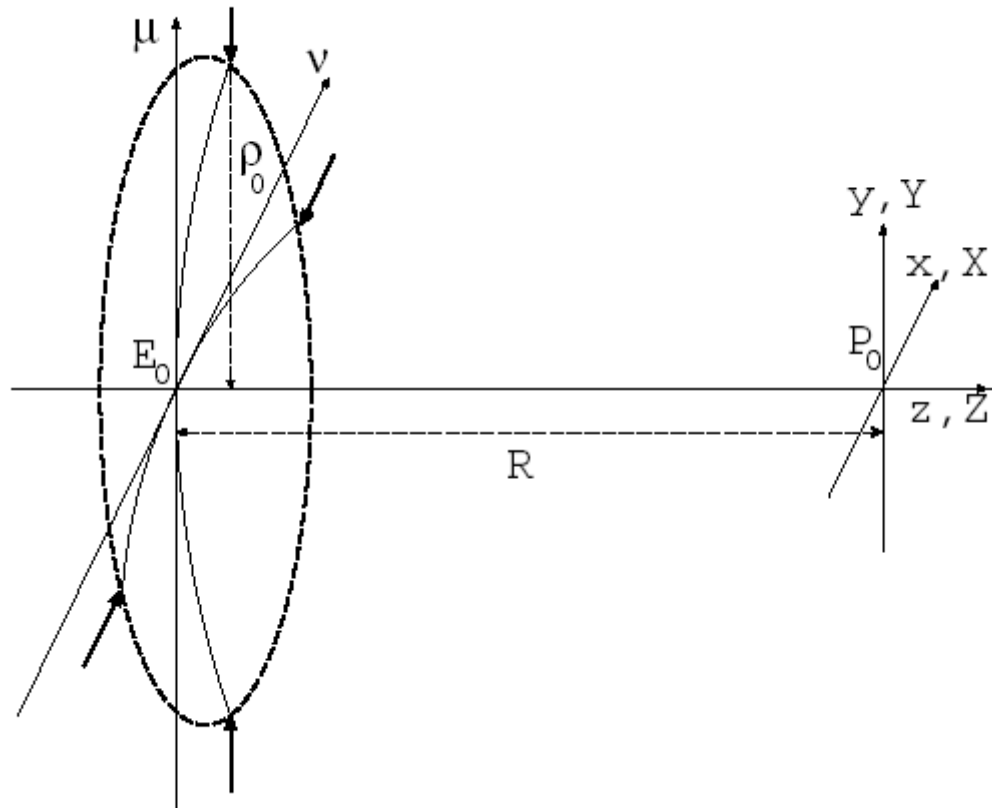
Coordinates on pupil sphere:

$$\mu + i\nu = \rho \exp(i\vartheta)$$

Coordinates in focal region:

$$r, \varphi, z$$

normalized with respect to:
λ/NA (transverse direction r)

Defocus parameter f in pupil:

$$\Phi_{def} = \frac{2\pi}{\lambda} z \left\{ 1 - \sqrt{1 - \rho^2 (NA)^2} \right\}$$

$$= \frac{f}{1 - \sqrt{1 - (NA)^2}} \left\{ 1 - \sqrt{1 - \rho^2 (NA)^2} \right\}$$

$$\rightarrow \quad f = \frac{2\pi}{\lambda} z \left\{ 1 - \sqrt{1 - (NA)^2} \right\}$$

Diffraction integral (scalar)

$$U(r,\varphi;f) = \frac{1}{\pi} \int_0^1 \rho \exp(if\rho^2) \left[\int_0^{2\pi} A(\rho,\vartheta) \exp\{i\Phi(\rho,\vartheta)\} \times \exp\{i2\pi r\rho \cos(\vartheta-\varphi)\} d\vartheta \right] d\rho$$

Introduction of Zernike polynomials (mapping of amplitude _and_ phase):

$$A(\rho,\vartheta) \exp\{i\Phi(\rho,\vartheta)\} = \sum_{n,m} \beta_n^m R_n^{|m|} \exp(im\vartheta)$$

Diffraction integral (scalar)

$$U(r,\varphi;f) = 2\sum_{n,m} i^m \beta_n^m V_n^m(r,f)\cos m\varphi$$

$$V_n^m(r;f) = \int_0^1 \rho \exp(if\rho^2) R_n^m(\rho) J_m(2\pi r\rho)d\rho$$

Analytic solution for the V – functions (A.J.E.M. Janssen):

$$V_n^m(r;f) = \exp(if)\sum_{l=1}^{\infty}(-2if)^{l-1}\sum_{j=0}^{p} v_{lj}\frac{J_{m+l+2j}(v)}{lv^l}; \; p=(n-m)/2, v=2\pi r$$

$$v_{lj} = (-1)^p(m+l+2j)\binom{m+j+l-1}{l-1}\binom{j+l-1}{l-1}\binom{l-1}{p-j}\Bigg/\binom{q+l+j}{l}; \quad q=(n+m)/2$$

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Diffraction integral (scalar)

In-focus Nijboer-Zernike result (1942):

$$U(r,\varphi;0) = 2\left(\frac{J_1(v)}{v} + \sum_{n,m} i^{n+1} \beta_n^m \frac{J_{n+1}(v)}{v} \cos m\varphi \right)$$

Extended (through-focus) result :

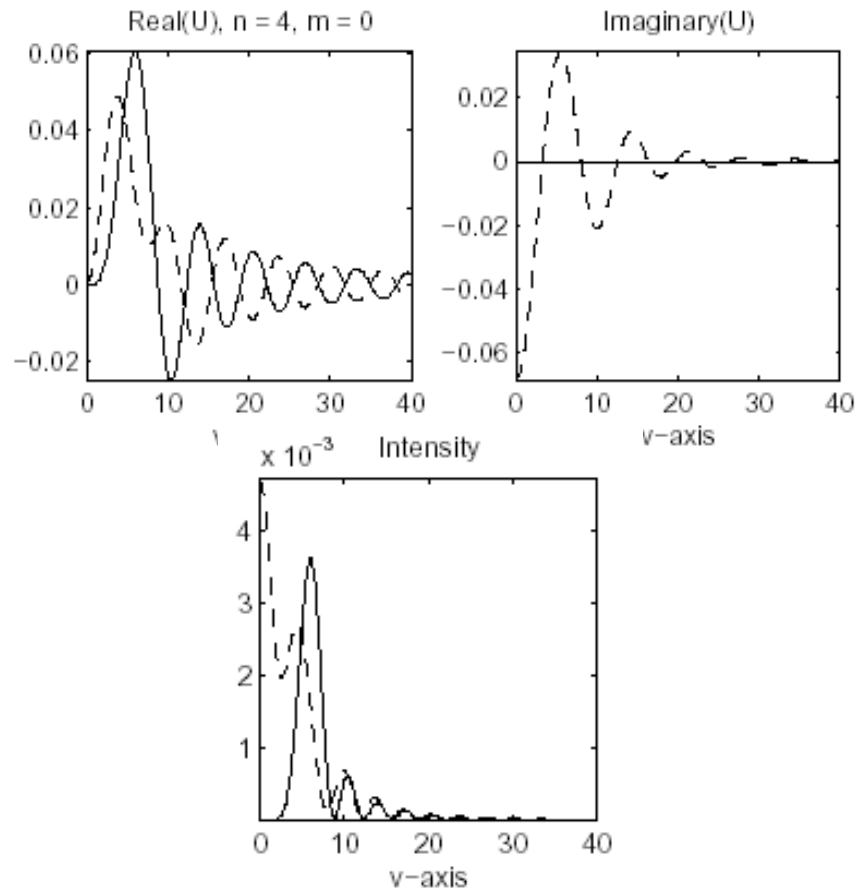$$U(r,\varphi;f) = 2\left(V_0^0(r,f) + \sum_{n,m} i^m \beta_n^m V_n^m(r,f) \cos m\varphi \right)$$
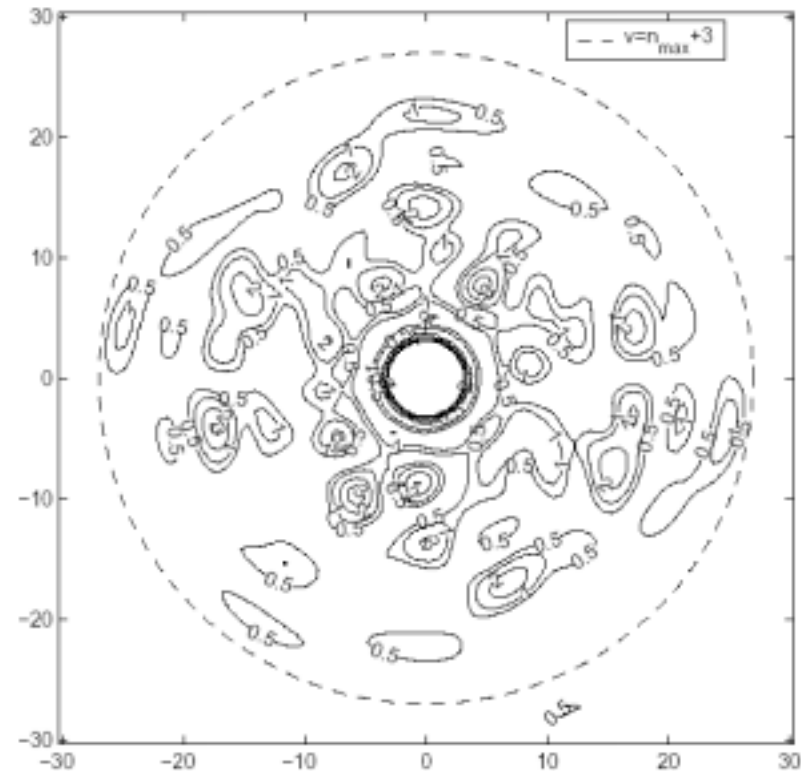
Convergence conditions:

$$L = l_{max} = 25 \qquad for :$$

$$|f| \le 2\pi, \quad v = 2\pi r \le 20, \quad 0 \le p \le q \le 6, \text{ abs. error} \le 10^{-6}$$

Some calculated patterns

Re$\{V_{4,0}\}$, Im$\{V_{4,0}\}$ and $|V_{4,0}|^2$

High-frequent pupil 'noise'; intensity pattern image plane

Extension to high-NA case

1) Correct treatment of defocus-parameter:
$$\left(u_0 = 1 - \sqrt{1 - s_0^2}\right)$$

$$\exp\left(-\frac{if}{u_0}\sqrt{1 - s_0^2\rho^2}\right)$$

2) Inclusion of 'radiometric' effect
   (aplanatic system with magnification M=0):

$$\frac{1}{\left(1 - s_0^2\rho^2\right)^{1/4}}$$

3) Finite-size point-source
   (accounted for by Gaussian pupil 'transmission'):

$$\exp\left(-\tilde{f}\,\rho^2\right)$$

   a complex defocus parameter $f_C = f + i\,\tilde{f}$
   is used!

4) Higher than quadratic effects are 'stored' in
   symmetrical polynomials of order *2n* leading
   to the formal expression at high NA:

$$\exp\left(g + f_C\rho^2\right)\sum_{k=0}^{k_{max}} h_k R_{2k}^0(\rho)$$

Extension to vectorial treatment

The Ignatowsky / Richards & Wolf treatment of the ***aberrated*** case leads to three diffraction integrals that recall the I_0-, I_1- and I_2- integrals

$$\vec{E}^x(r,\varphi; f) = -i\gamma s_0^2 \exp\left(\frac{-if}{1-\sqrt{1-s_0^2}}\right)\sum_{n,m} i^m \beta_n^{m,x} \exp(im\varphi)\times$$

$$\begin{pmatrix} V_{n,0}^m + \dfrac{s_0^2}{2}V_{n,2}^m \exp(2i\varphi) + \dfrac{s_0^2}{2}V_{n,-2}^m \exp(-2i\varphi) \\[2ex] -\dfrac{is_0^2}{2}V_{n,2}^m \exp(2i\varphi) + \dfrac{is_0^2}{2}V_{n,-2}^m \exp(-2i\varphi) \\[2ex] -is_0 V_{n,1}^m \exp(i\varphi) + is_0 V_{n,-1}^m \exp(-i\varphi) \end{pmatrix}$$

Each aberration term creates its own $V_{n,0}^m$ and $V_{n,k}^m \exp(ik\varphi)$ terms ($k = \pm 1, \pm 2$).

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New integral *V* to be treated

Old $V_n^m(r,f)$ - integral (scalar treatment)

$$V_n^m(r,f) = \int_0^1 \exp\left[if\rho^2\right] R_n^{|m|}(\rho) J_m(2\pi r\rho)\, \rho d\rho$$

New $V_{n,j}^m(r,f)$ - integral (vectorial treatment) :

$$V_{n,j}^m(r,f) = \int_0^1 \rho^{|j|}\left(1+\sqrt{1-s_0^2\rho^2}\right)^{-|j|+1} \exp\left[\frac{if}{1-\sqrt{1-s_0^2}}\left(1-\sqrt{1-s_0^2\rho^2}\right)\right] \times$$

$$R_n^{|m|}(\rho) J_{m+j}(2\pi r\rho)\, \rho d\rho$$

The second integral can be treated using the analytic series expansion

solution of $V_n^m(r,f)$

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Results of analytic vectorial analysis (no aberrations)
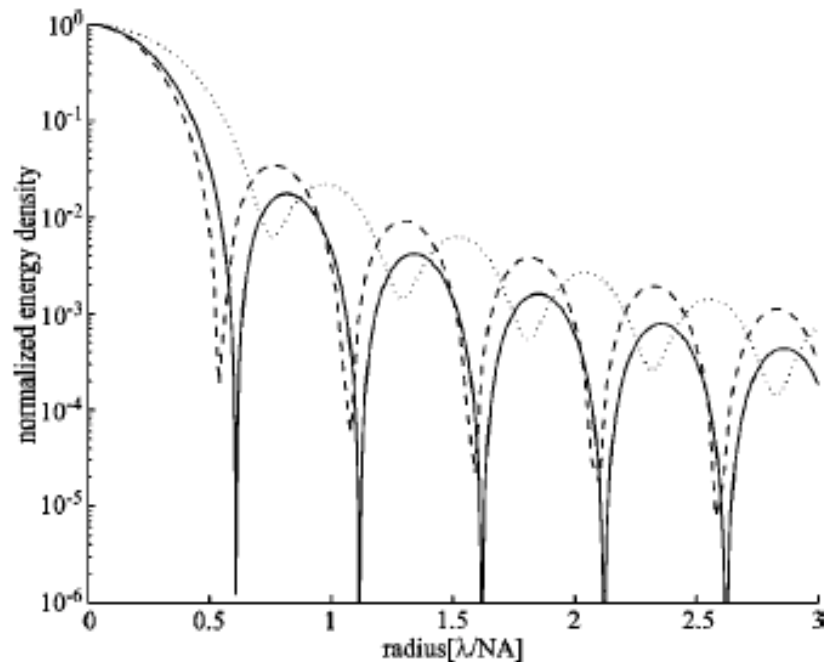

Fig. 3. Comparison of the energy density function in the high-NA focus ($f = 0$) and the scalar Airy distribution as a function of the radial coordinate r. The energy density function in the cross section $\theta = 0$ is represented by the dotted curve, and the one in the cross section $\theta = \pi/2$ by the dashed curve. The scalar Airy distribution is shown by the solid curve. The fact that the dashed high-aperture curve does not reach very low levels is due to the sampling density used in plotting this curve.

Comparison of scalar (Airy-disc) intensity cross-section and vectorial cases:

- $\theta = 0$
- $\theta = \pi/2$

Introduction of aberrations

The complex pupil function is written as

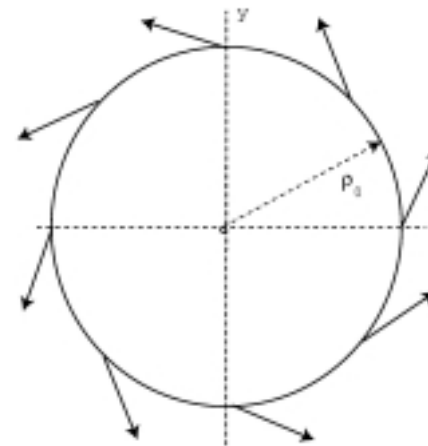$$B^x(\rho,\vartheta) = A^x(\rho,\vartheta)\exp\left[i2\pi W(\rho,\vartheta)\right]$$

$$B^y(\rho,\vartheta) = A^y(\rho,\vartheta)\exp\left[i2\pi W(\rho,\vartheta)+i\varepsilon(\rho,\vartheta)\right]$$

A is the transmission function, W the wavefront aberration and ε the (phase) birefringence

Special types of polarisation : RADIAL

$$A^x = A_0\cos(\vartheta+\vartheta_0)$$

$$A^y = A_0\sin(\vartheta+\vartheta_0)$$

Radiometric effect and Zernike expansion

The complex pupil function including the radiometric effect is written as

$$B_R^x(\rho,\vartheta) = \frac{B^x(\rho,\vartheta)}{\left(1 - s_0^2 \rho^2\right)^{1/4}} \exp\left[i2\pi W(\rho,\vartheta)\right] = \sum_{n,m} \beta_n^{m,x} R_n^{|m|}(\rho) \exp\left[im\vartheta\right]$$

s_0 is the numerical aperture; m runs from $-m_{\max}$ to $+m_{\max}$.

The $\beta_n^{m,x}$ are calculated as usually following

$$\beta_n^{m,x} = \frac{n+1}{\pi} \int_0^1 \int_0^{2\pi} \frac{B^x(\rho,\vartheta)}{\left(1 - s_0^2 \rho^2\right)^{1/4}} R_n^{|m|}(\rho) \exp\left[-im\vartheta\right] \rho\, d\rho\, d\vartheta$$
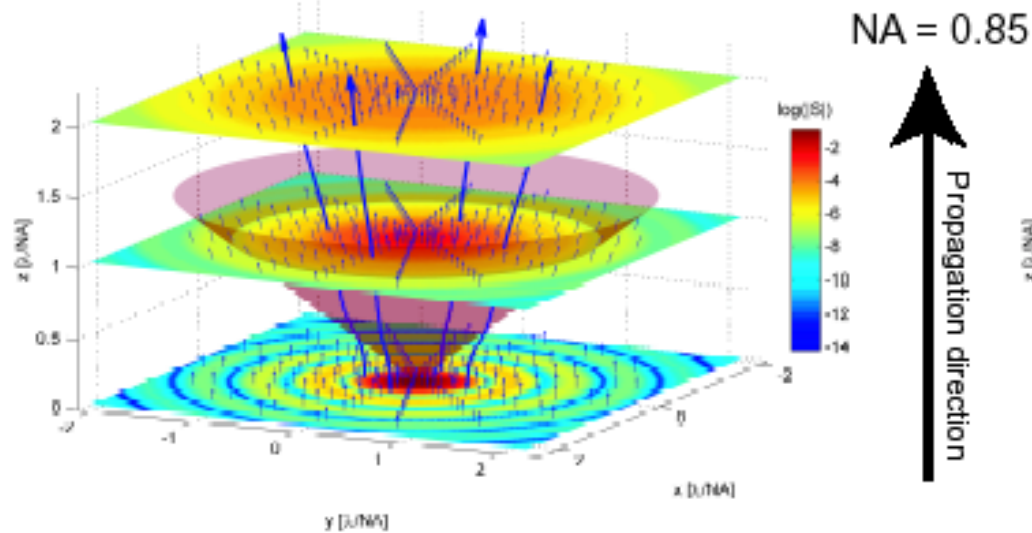
with normalisation according to

$$\int_0^1 R_{n'}^{|m|}(\rho) R_n^{|m|}(\rho) \rho\, d\rho = \frac{\delta_{nn'}}{2(n+1)}$$
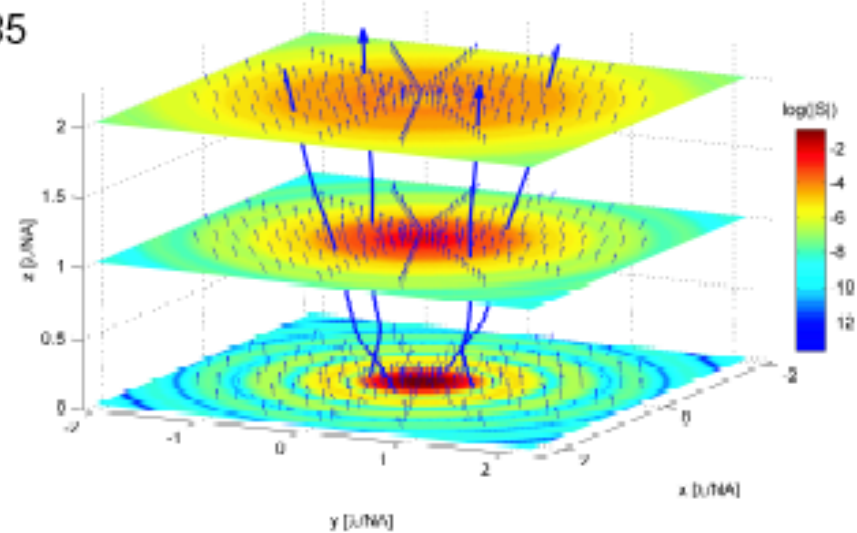
Results of analytic vectorial analysis

Tracing the EM energy flow field through the focal region
(using the analytic expression for the Poynting vector)

Linearly polarised light

Right circularly polarized light

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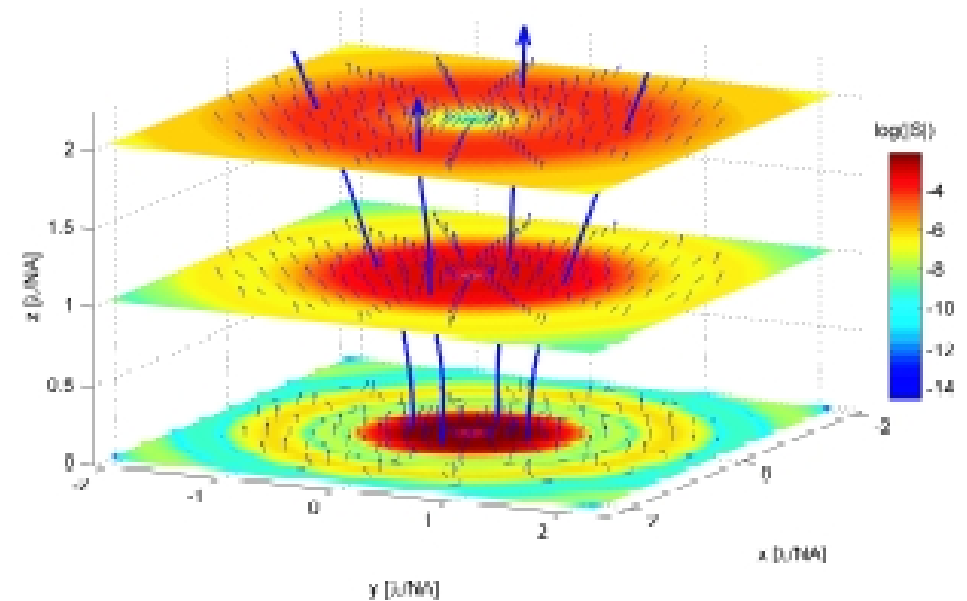
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Results of analytic vectorial analysis

Tracing the EM energy flow field through the focal region
(using the analytic expression for the Poynting vector)

Orbital angular momentum (l=1)   OAM (l=1) + right circularly polarised light

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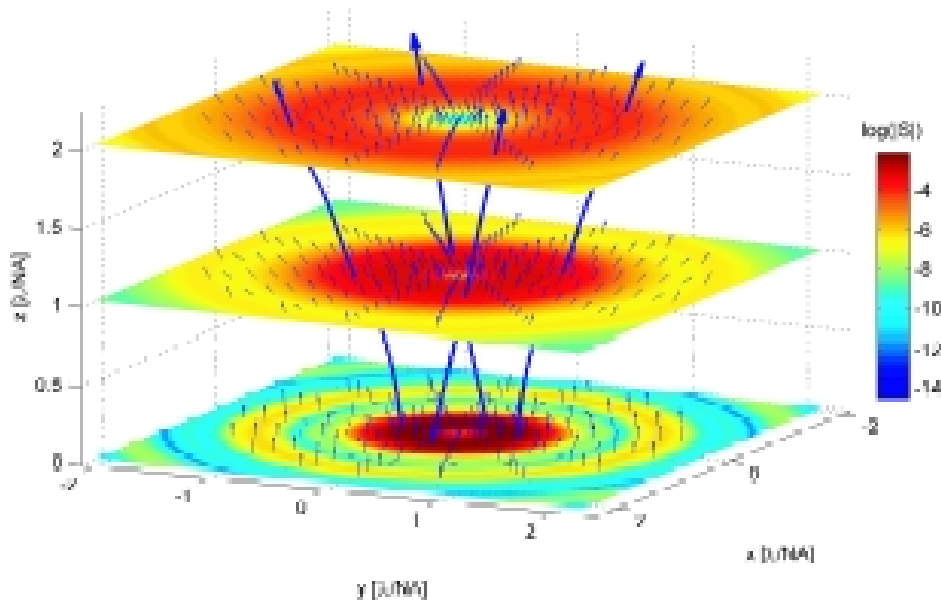
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Results of analytic vectorial analysis

Tracing the EM energy flow field through the focal region
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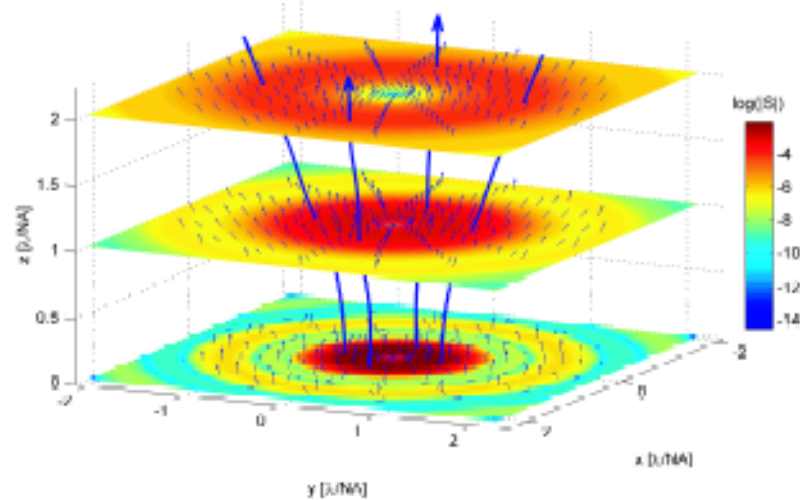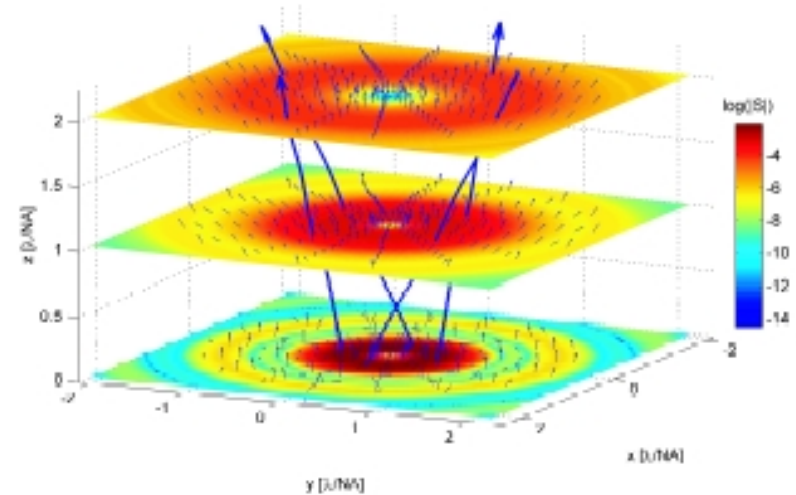
Orbital angular momentum (l=1)
+ right circular polarisation

Orbital angular momentum (l=1)
+ left circular polarisation

How to obtain a parametric expression for the field density in the imaging volume?

$$w_E = \frac{\varepsilon_0}{4} n_r^2 |E|^2 = \frac{\varepsilon_0}{4} n_r^2 \left\{ E_1 E_1^* + E_2 E_2^* + E_3 E_3^* \right\} \text{with} :$$

$$\vec{E}^x(r,\varphi;f) = -i\gamma s_0^2 \exp\left(\frac{-if}{1-\sqrt{1-s_0^2}} \right) \sum_{n,m} i^m \beta_n^{m,x} \exp(im\varphi) \times$$

$$\left(
\begin{array}{l}
V_{n,0}^m + \dfrac{s_0^2}{2} V_{n,2}^m \exp(2i\varphi) + \dfrac{s_0^2}{2} V_{n,-2}^m \exp(-2i\varphi) \\[2ex]
- \dfrac{is_0^2}{2} V_{n,2}^m \exp(2i\varphi) + \dfrac{is_0^2}{2} V_{n,-2}^m \exp(-2i\varphi) \\[2ex]
- is_0 V_{n,1}^m \exp(i\varphi) + is_0 V_{n,-1}^m \exp(-i\varphi)
\end{array}
\right)$$

$dW_{\exp} = \dfrac{\partial w_E}{\partial t} \Delta t$ is the quantity that determines the resist exposure per unit volume in time Δt!

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Extended Nijboer-Zernike Analysis (vectorial)
IISB Fraunhofer Lithography Workshop
17-19 September 2004

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Basic term in the expression for the exposure

$$G_{kl}(r,\varphi;f) =$$

$$\sum_{n,m} i^m \alpha_n^m V_{n,k}^m \exp(im\varphi)\exp(ik\varphi) \times \sum_{n',m'} i^{-m'} \beta_{n'}^{m'} V_{n',l}^{m'*} \exp(-im'\varphi)\exp(-il\varphi) =$$

$$\sum_{n',m'} \exp\{i(m-m')\pi/2\}\exp\{i(m-m'+k-l)\varphi\}\alpha_n^m \beta_{n'}^{m'*} V_{n,k}^m(r,f) V_{n',l}^{m'*}(r,f)$$

Small β - approximation (dominating β_0^0 - coefficient)

$$G_{kl}(r,\varphi;f) = e^{i(k-l)\varphi} \sum_{\nu=0}^{\nu_{\max}} \sum_{\mu=-\mu_{\max}(\nu)}^{+\mu_{\max}(\nu)} \left\{ \begin{array}{l} e^{-i\mu\pi/2} e^{-i\mu\varphi} \alpha_0^0 \beta_\nu^{\mu*} V_{0,k}^0(r,f) V_{\nu,l}^{\mu*}(r,f) + \\ (1-\varepsilon_{\nu\mu}) e^{+i\mu\pi/2} e^{+i\mu\varphi} \alpha_\nu^\mu \beta_0^{0*} V_{\nu,k}^\mu(r,f) V_{0,l}^{0*}(r,f) \end{array} \right\}$$

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Representation of light intensity (fully polarised case)

$$\beta_n^{m,x} = a\beta_n^m$$

$$\beta_n^{m,y} = b\beta_n^m$$

$$(|a|^2 + |b|^2 = 1 \text{ for normalisation purposes})$$

$$w_E(r,\varphi;f) = \frac{\varepsilon_0 n_r^2 s_0^2}{4}
\begin{bmatrix}
G_{00}(\beta,\beta) + \\
s_0^2\left\{\left[|a|^2 - |b|^2\right]\mathrm{Re}\left\{G_{0,2}(\beta,\beta)\right\} - 2\mathrm{Re}(ab^*)\mathrm{Im}\left\{G_{0,2}(\beta,\beta)\right\}\right\} + \\
s_0^2\left\{\left[|a|^2 - |b|^2\right]\mathrm{Re}\left\{G_{0,-2}(\beta,\beta)\right\} + 2\mathrm{Re}(ab^*)\mathrm{Im}\left\{G_{0,-2}(\beta,\beta)\right\}\right\} + \\
\frac{s_0^4}{2}\left\{\left[1 - 2\mathrm{Im}(ab^*)\right]G_{2,2}(\beta,\beta) + \left[1 + 2\mathrm{Im}(ab^*)\right]G_{-2,-2}(\beta,\beta)\right\} + \\
s_0^2\left\{\left[1 - 2\mathrm{Im}(ab^*)\right]G_{1,1}(\beta,\beta) + \left[1 + 2\mathrm{Im}(ab^*)\right]G_{-1,-1}(\beta,\beta)\right\} + \\
-2s_0^2\left\{\left[|a|^2 - |b|^2\right]\mathrm{Re}\left\{G_{+1,-1}(\beta,\beta)\right\} + 2\mathrm{Re}(ab^*)\mathrm{Im}\left\{G_{+1,-1}(\beta,\beta)\right\}\right\}
\end{bmatrix}$$

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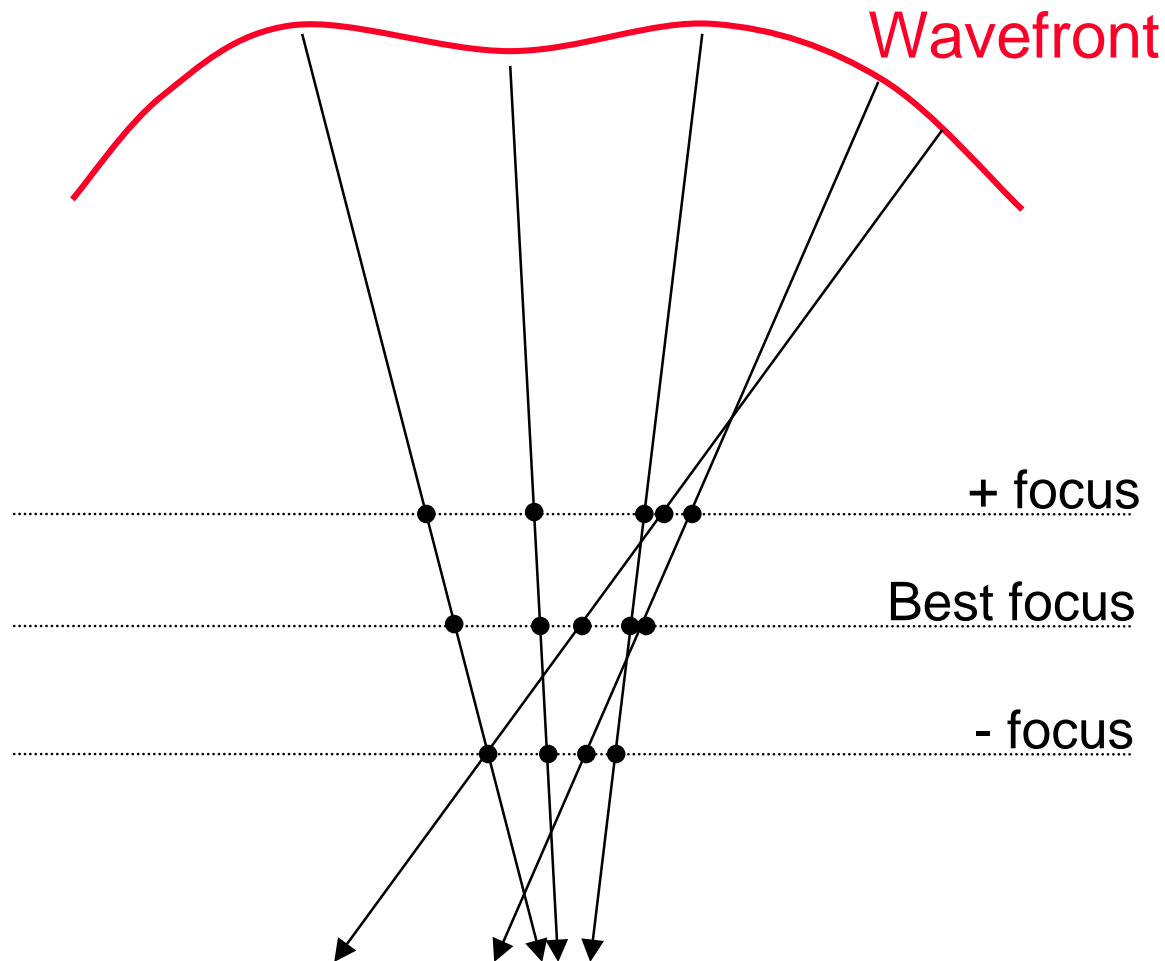Technische Universiteit Delft

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Strehl intensity

On $-$ axis (Srehl) intensity using β - type expansion

$$A_S = \frac{1}{\pi} \int_0^{2\pi} \int_0^1 B(\rho, \vartheta) \rho \, d\rho \, d\vartheta =$$

$$\frac{1}{\pi} \int_0^{2\pi} \int_0^1 \sum_{n,m} \beta_n^m R_n^m (\rho) \exp(im\vartheta) \rho \, d\rho \, d\vartheta =$$

$$\sum_{n,m} \beta_n^m \frac{1}{\pi} \int_0^{2\pi} \int_0^1 R_n^m (\rho) \exp(im\vartheta) \rho \, d\rho \, d\vartheta = \beta_0^0$$

$$\rightarrow I_S = \left| \beta_0^0 \right|^2 \quad \text{(scalar approximation)}$$

With the radiometric effect included in the Zernike expansion,

the relation remains true also in the vectorial case!

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Complex pupil function reconstruction remains possible in the vectorial case?

Wavefront

Intuitive picture of aberration retrieval

+ focus

Best focus

- focus

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Further developments

- Complex amplitude retrieval of the pupil function at large NA should remain possible thanks to the parametric description of the intensity distribution in the focal volume using the Zernike ß-expansion and the extended Nijboer-Zernike theory applied to the vectorial diffraction.

- Much of the numerical work in solving the system of equations for the ß-coefficients has to be done only once and the results can be tabulated and stored for further use.

- Simultaneous retrieval of aberration and birefringence possible?