TEM aberrations

Short introduction

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May 20, 2015

Introduction

Images of crystal defects or interfaces obtained using aberrations corrected TEM (or STEM) are free of artefacts and often allow to determine atomic column position with very high accuracy. For example:

- Delocalisation (Fresnel fringes) $\rightarrow$ spherical aberration.
- Rigid body shit $\rightarrow$ 3-fold astigmatism.

What are the aberrations? How to describe them?

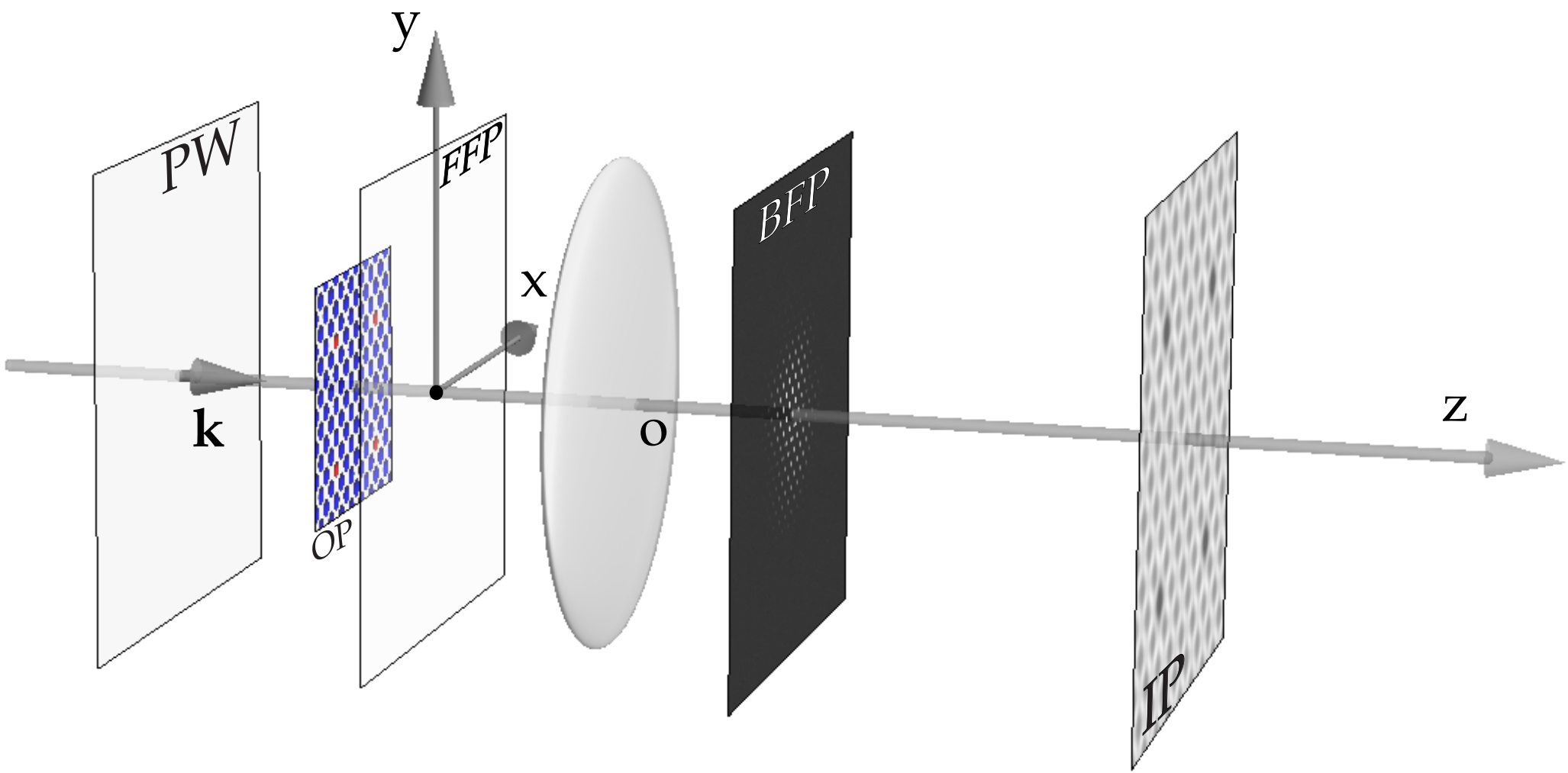
- Geometrical aberrations (image properties).
- Wavefront aberrations (transfer function properties).

What is the relationship between geometrical aberrations and wavefront aberrations?

Content

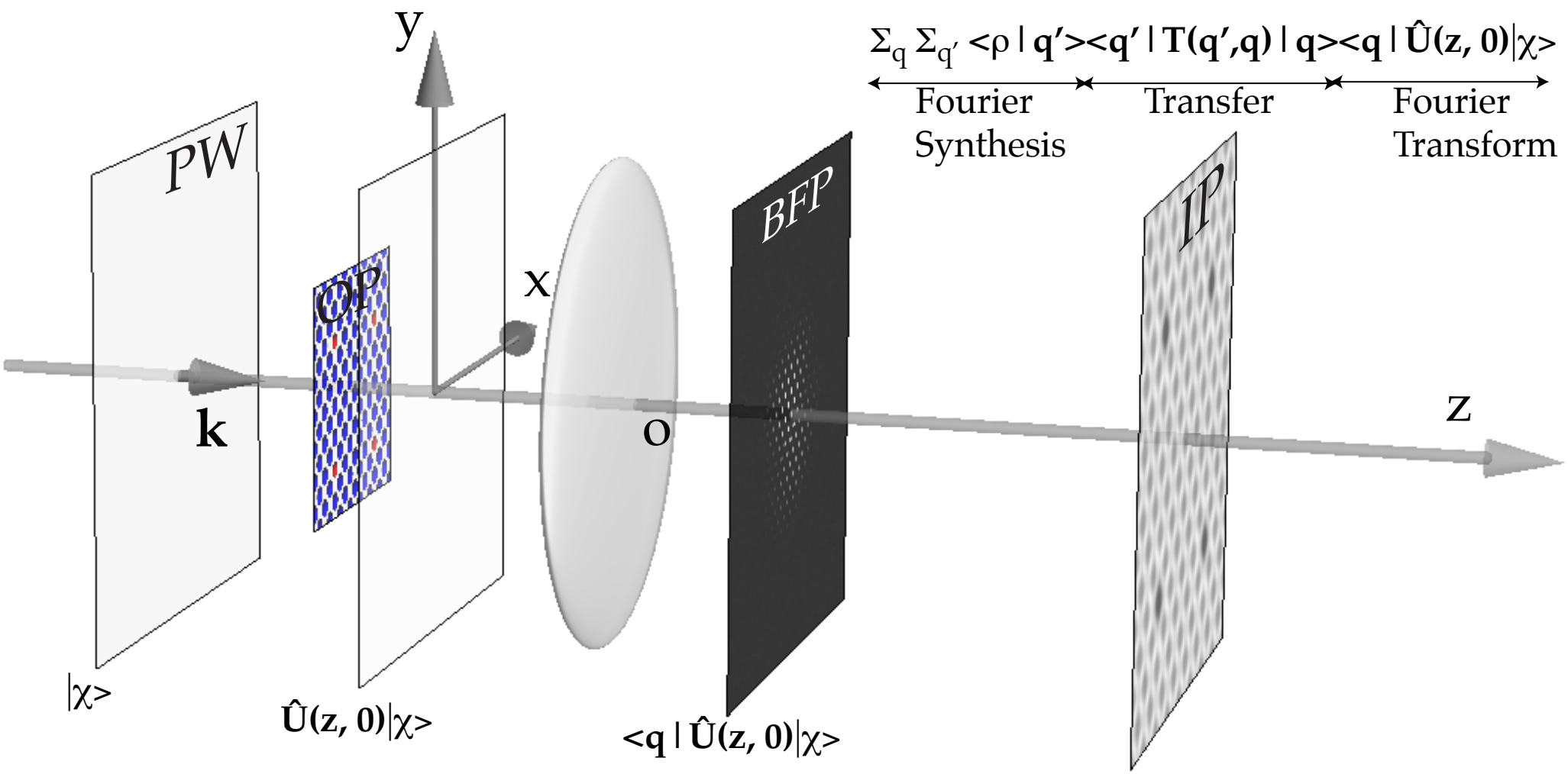
- TEM image formation
- Thin perfect lenses
- Real lenses.
- Geometrical aberrations
- Wavefront aberrations
- Problems.

TEM (very) simplified model



Modeling steps: Incident wave (PW), crystal (OP), electron-matter interaction, Fraunhofer approximation, image formation (Abbe theory), ...

Image formation modeling (HRTEM)

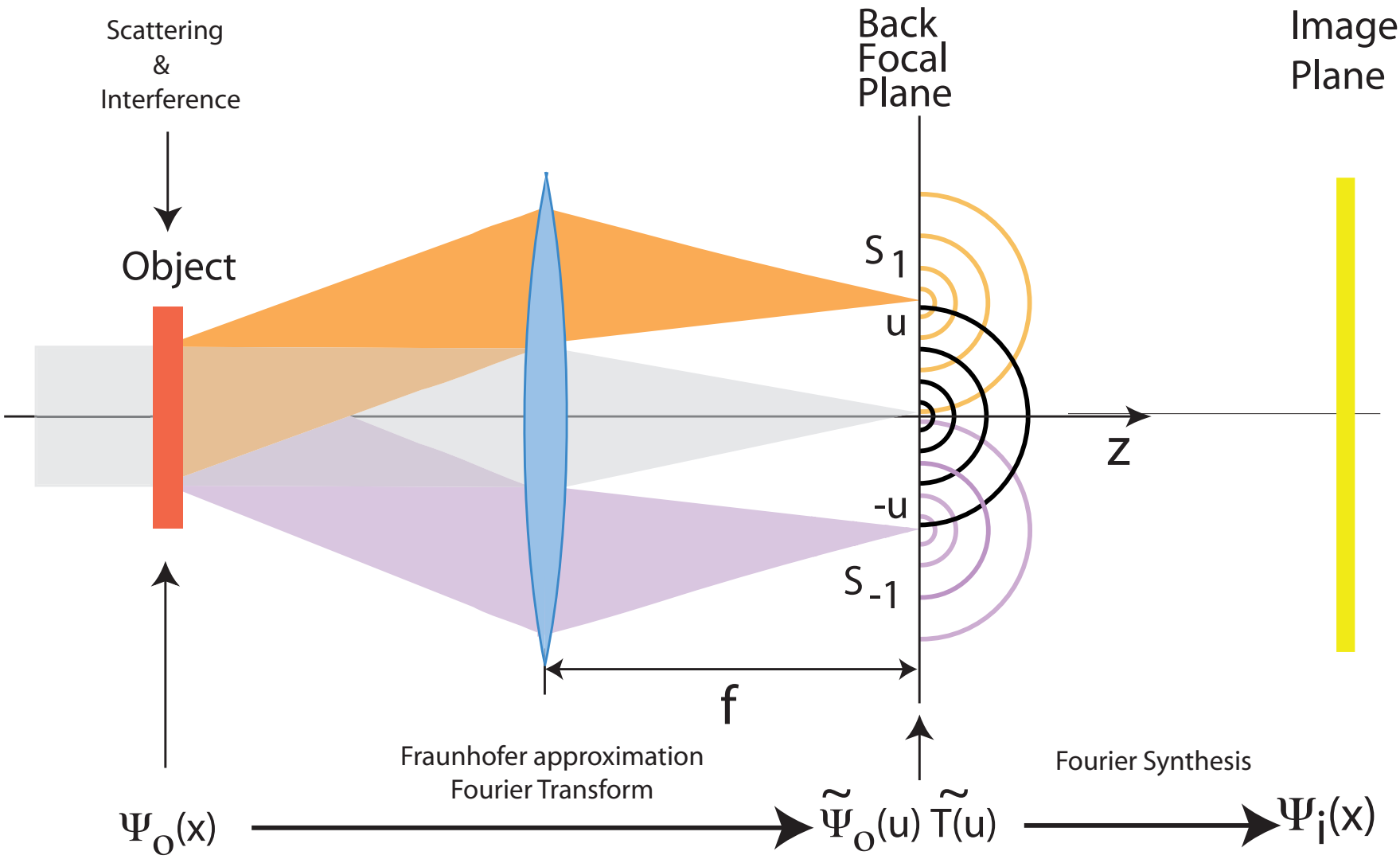


Transfer by objective lens: $< q' | T(q', q) | q >$

Image forming system has 2 properties (Abbe theory):

- Linear.
- Space invariant.

Abbe image formation



Modelling steps

In this short presentation, I'll describe using the Abbe image formation theory how the exit wave is transferred by the objective lens of this model microscope.

Two cases:

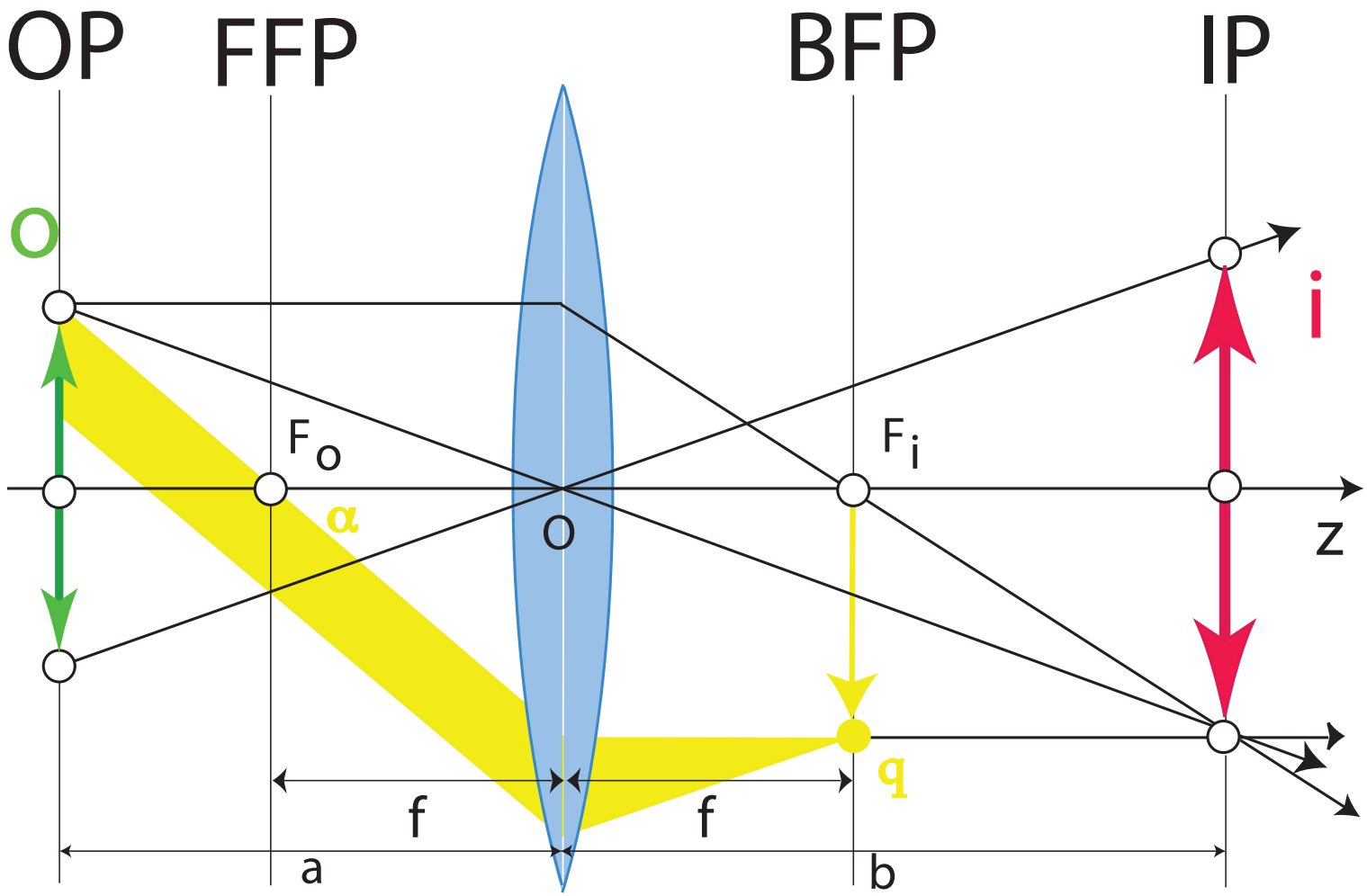
$\rightarrow$ **TEM** ($\widetilde{T}(\vec{u})$: Transfer Function):

$$\begin{aligned}\widetilde{\Psi}_i(\vec{u}) &= \widetilde{\Psi}_o(\vec{u})\widetilde{T}(\vec{u}) \\ \Psi_i(\vec{x}) &= \int \widetilde{\Psi}_o(\vec{u})\widetilde{T}(\vec{u})e^{2\pi\imath\vec{u}\cdot\vec{x}}\mathrm{d}\vec{u}\end{aligned}$$

$\rightarrow$ **STEM** ($\widetilde{OTF}(\vec{u}) = \widetilde{T}(\vec{u}) \otimes \widetilde{T}(-\vec{u})$: Optical Transfer Function):

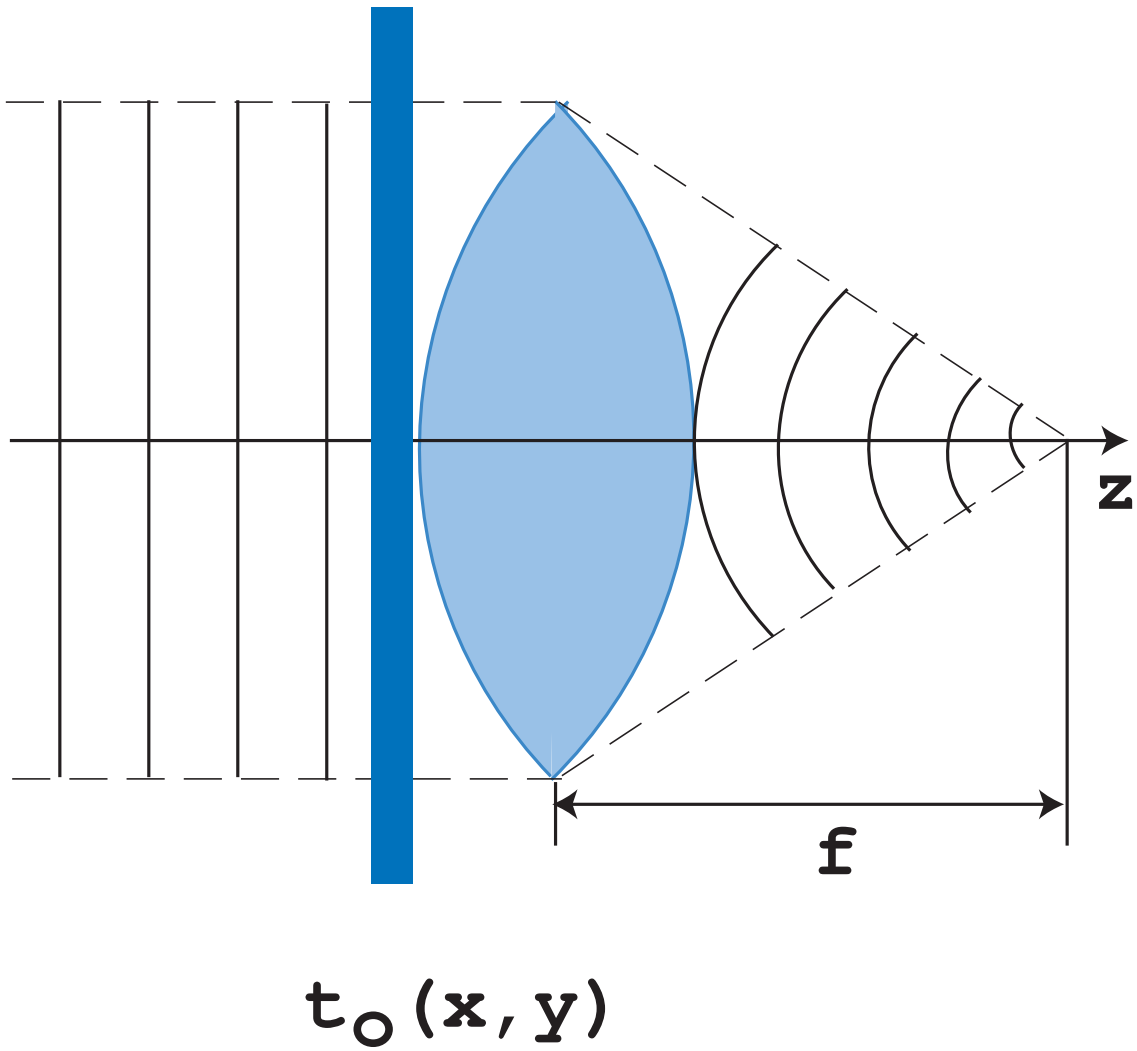
$$\begin{aligned}
I(\vec{x}) &= \langle \Psi_i(\vec{x};t)\Psi_i^*(\vec{x};t)\rangle \\
\Psi_i(\vec{x};t) &= \Psi_o(\vec{x};t) \otimes T(\vec{x}) \\
I(\vec{x}) &= \langle [\Psi_o(\vec{x};t) \otimes T(\vec{x})][\Psi_o^*(\vec{x};t) \otimes T^*(\vec{x})]\rangle && (\otimes \text{ convolution.}) \\
I(\vec{x}) &= [T(\vec{x})T^*(\vec{x})] \otimes \langle \Psi_o(\vec{x};t)\Psi_o^*(\vec{x};t)\rangle && (T(\vec{x}) \text{ is time independent.}) \\
\langle \Psi_o(\vec{x};t)\Psi_o^*(\vec{x};t)\rangle &= |\Psi_o(\vec{x})|^2 && (\text{complete spatial incoherence}) \\
I(\vec{x}) &= |\Psi_o(\vec{x})|^2 \otimes [T(\vec{x})T^*(\vec{x})] \\
I(\vec{x}) &= I_o(\vec{x}) \otimes OTF(\vec{x})
\end{aligned}$$

Paraxial optics: perfect thin lens



Principal rays of paraxial optics. Reflection (plane wave) making an angle α, where $\alpha = 2\theta_B$, corresponds to spatial frequency u.

Perfect lens: Fourier transform



It is often written that a perfect lens does a Fourier transform of the object transparency $t_o(x, y)$. Since diffraction (i.e. Fourier decomposition) occurs also without a lens, it is better to consider the lens has a mean to bring the Fraunhofer pattern (that is formed at ∞) closer to the object.

Gaussian or geometrical optics: thick lens

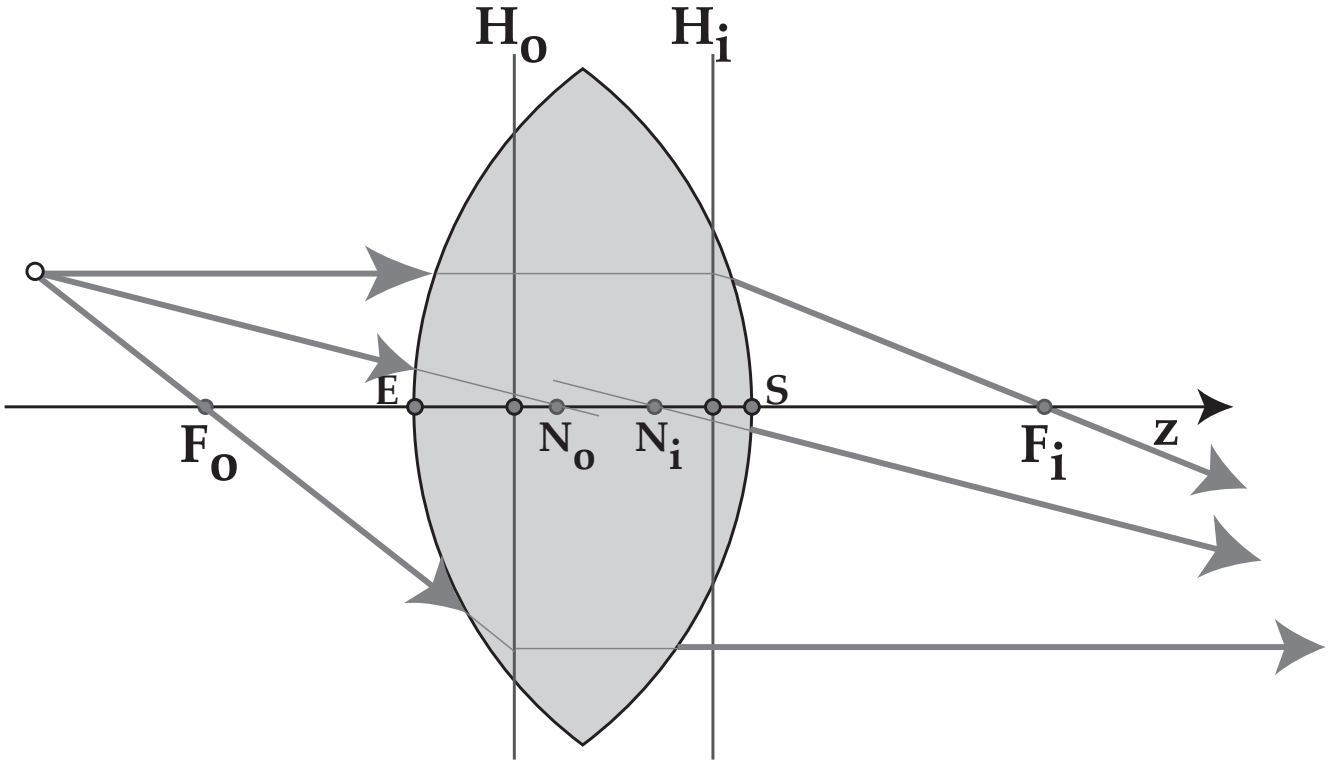
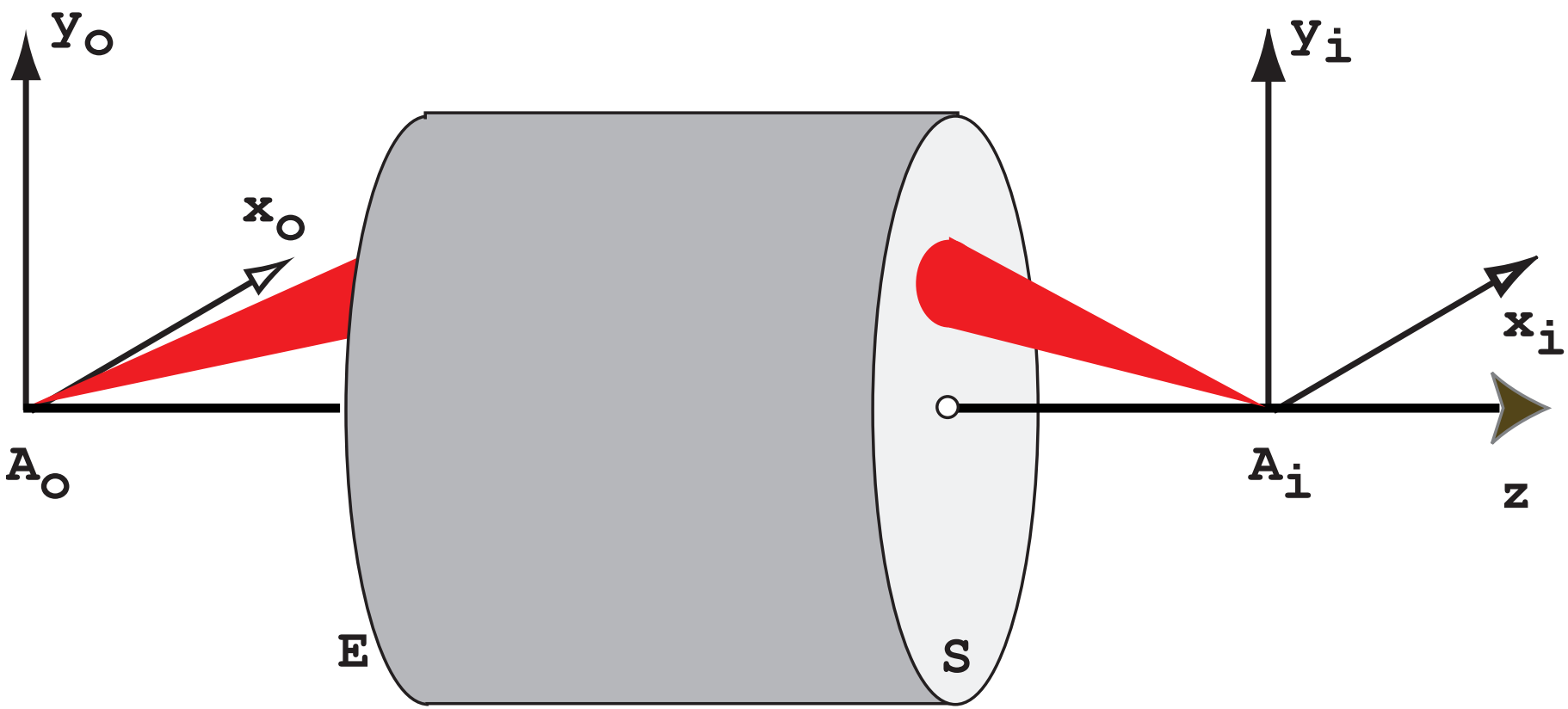


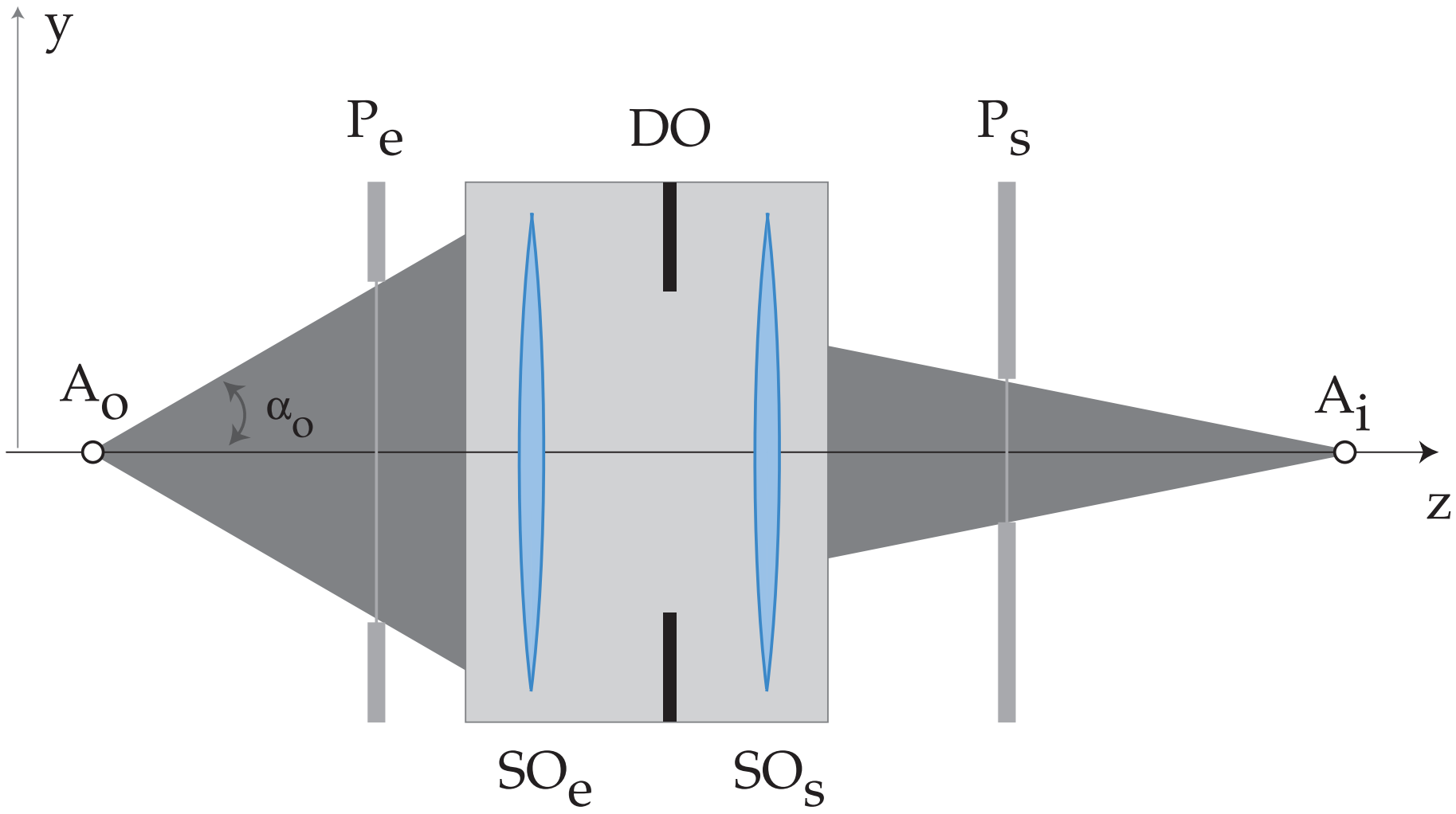
Figure: Object and image planes are conjugated (stigmatic).

Optical system



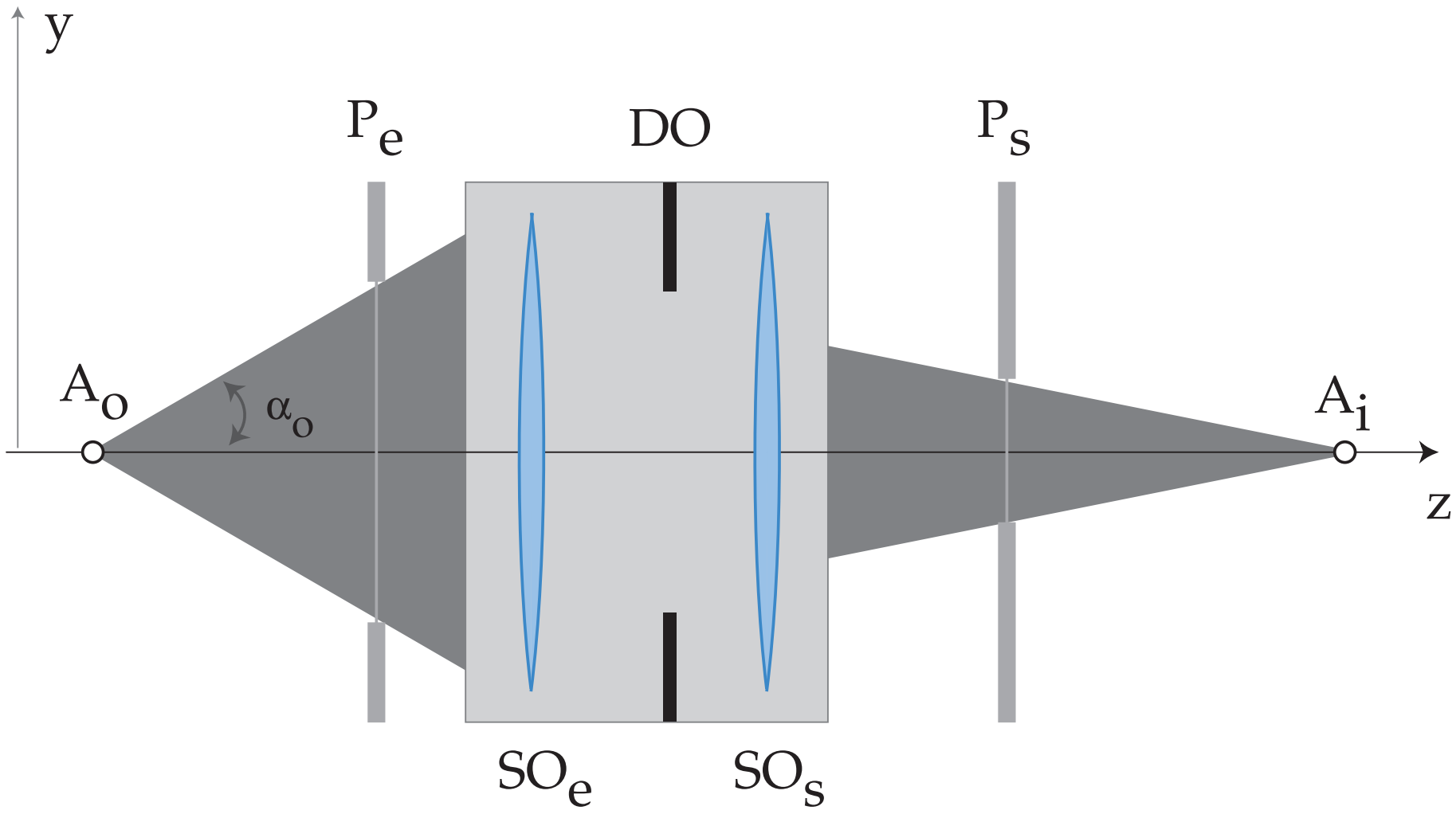
An optical system produces the image A_i of a point source object A_o. A_o and A_i are said to be conjugate. A_i is not a point since any optical system is diffraction limited. This limitation is introduced by the entrance and exit pupils of the optical system.

Pupils



Any optical system can be characterised by an entrance pupil P_e and an exit pupil P_s. The pupils are the image of the opening aperture DO by the entrance and exit optical subsystems SO_e and SO_s.

Pupils



Any optical system can be characterised by an entrance pupil P_e and an exit pupil P_s. The pupils are the image of the opening aperture DO by the entrance and exit optical subsystems SO_e and SO_s. What are P_e and P_s for a thin lens?

Aberrations: how to define them

Some light rays emitted by object point A_o do not reach the image at point A_i.

Position of $A_i \longrightarrow$ intersection of the reference light ray (non deviated) and the image plane.

The image of a point source is a **spot** whose shape and intensity depend of the quality of the optical system.

Two types of aberrations:

1. Monochromatic.
2. Chromatic (λ dependent).

Monochromatic aberrations

In order to evaluate the monochromatic aberrations one must define a function characteristic of the optical system.

This function will depend on:

1. The selected reference planes.
2. The optical path followed by the light ray.

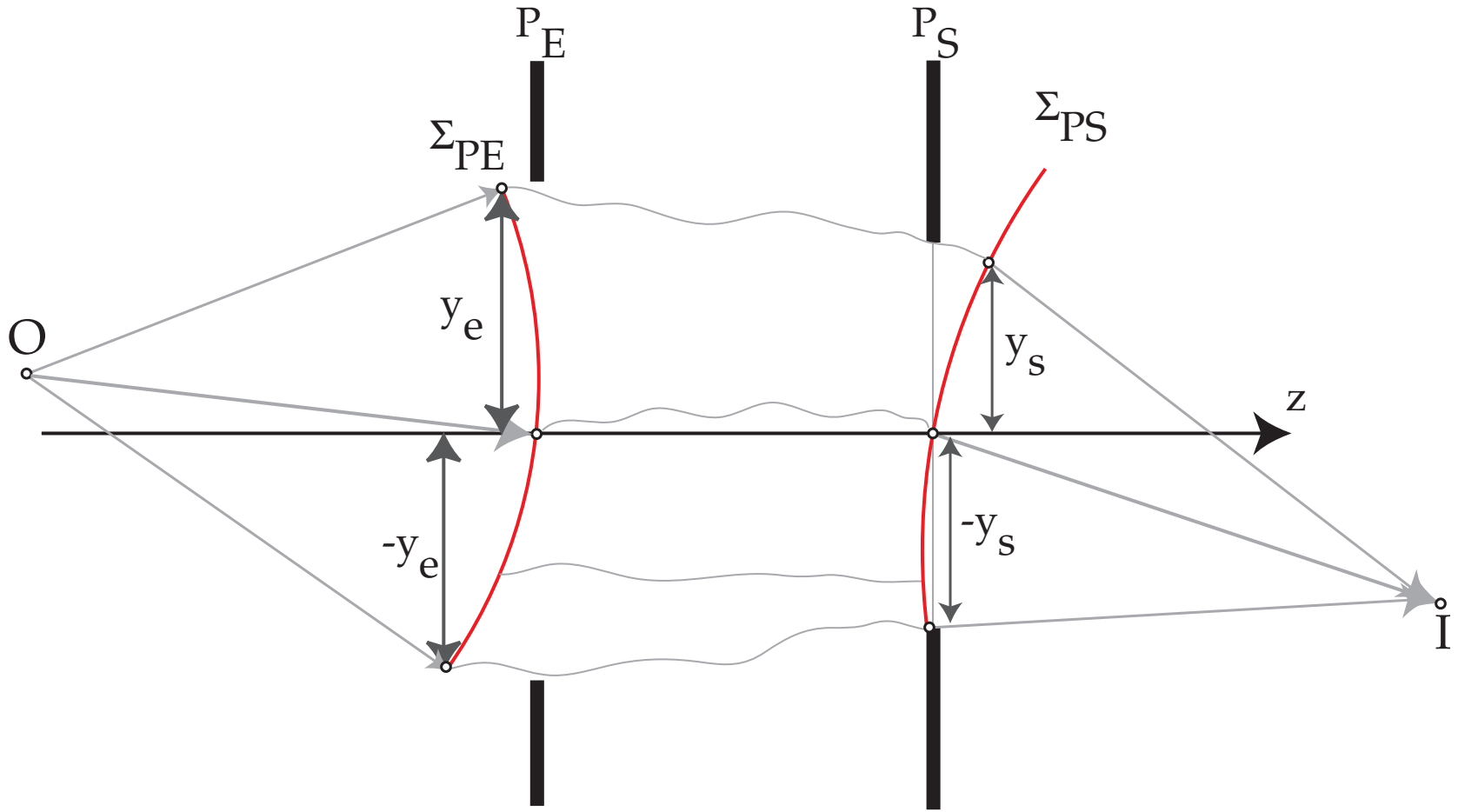
Optical path: length

The important feature is the optical path length (OPL).

$$OPL(P_1P_2) = \int_{P_1}^{P_2} n(\overrightarrow{r})\, ds$$

1. OPL is measured in meters ($n(\vec{r}) = \frac{c}{v(\vec{r})}$ has no unit).
2. OPL is proportional to the time spent by the light ray to travel from P_1 to P_2.
3. Surface of constant OPL $\longrightarrow$ wavefront (surface of constant travel time).
4. OPL is measured from the entrance pupil P_E to the exit pupil P_S.

Optical Path Length: OPL

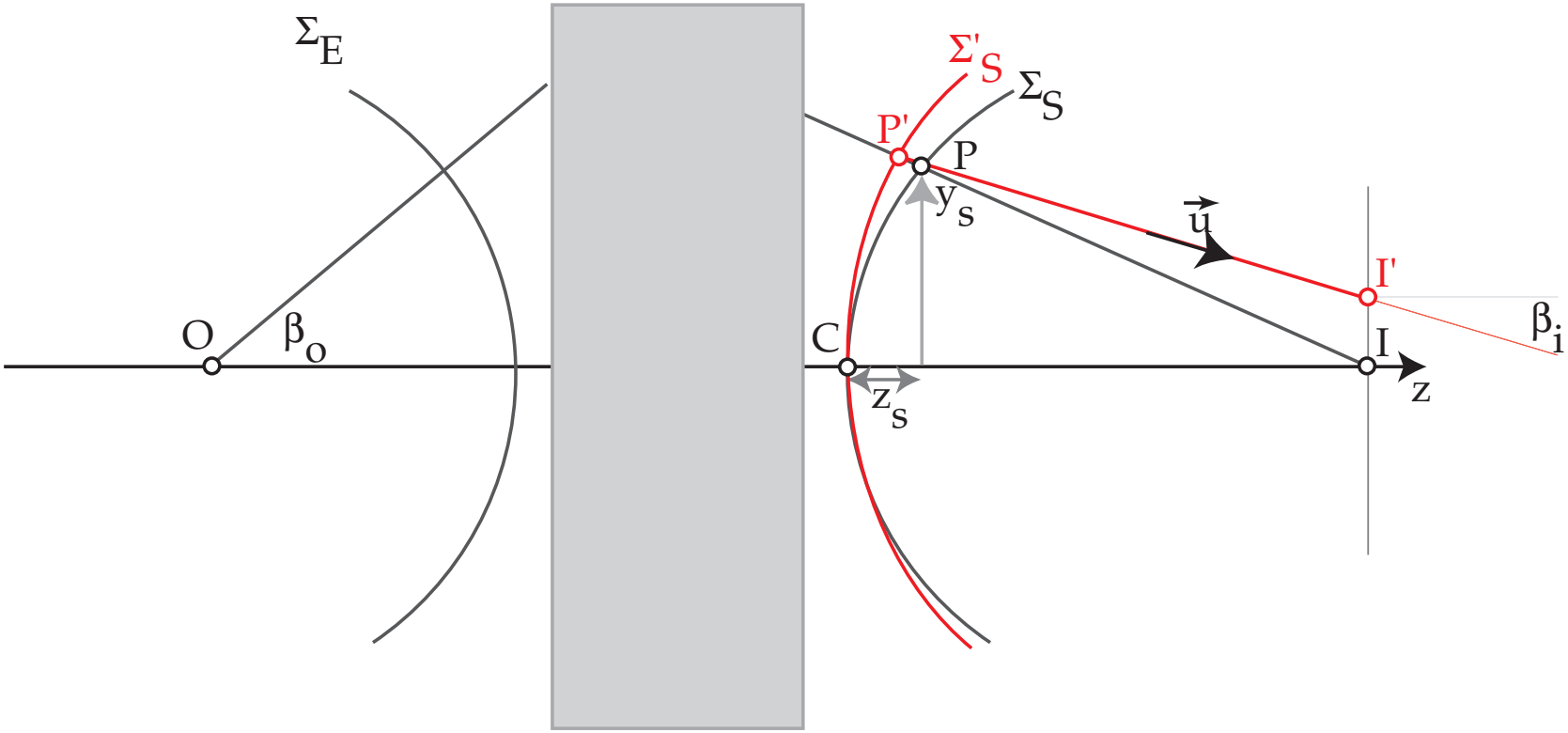


- Before P_E the reference wavefront Σ_{PE} is spherical (point source at O).
- After P_S the reference wavefront Σ_{PS} is spherical (converges towards I).

For a perfect optical system, both the entrance Σ_{PE} and exit Σ_{PS} wavefronts are spherical. The Optical Path Length form O to I is independent of the path.

Difference of OPL: OPD

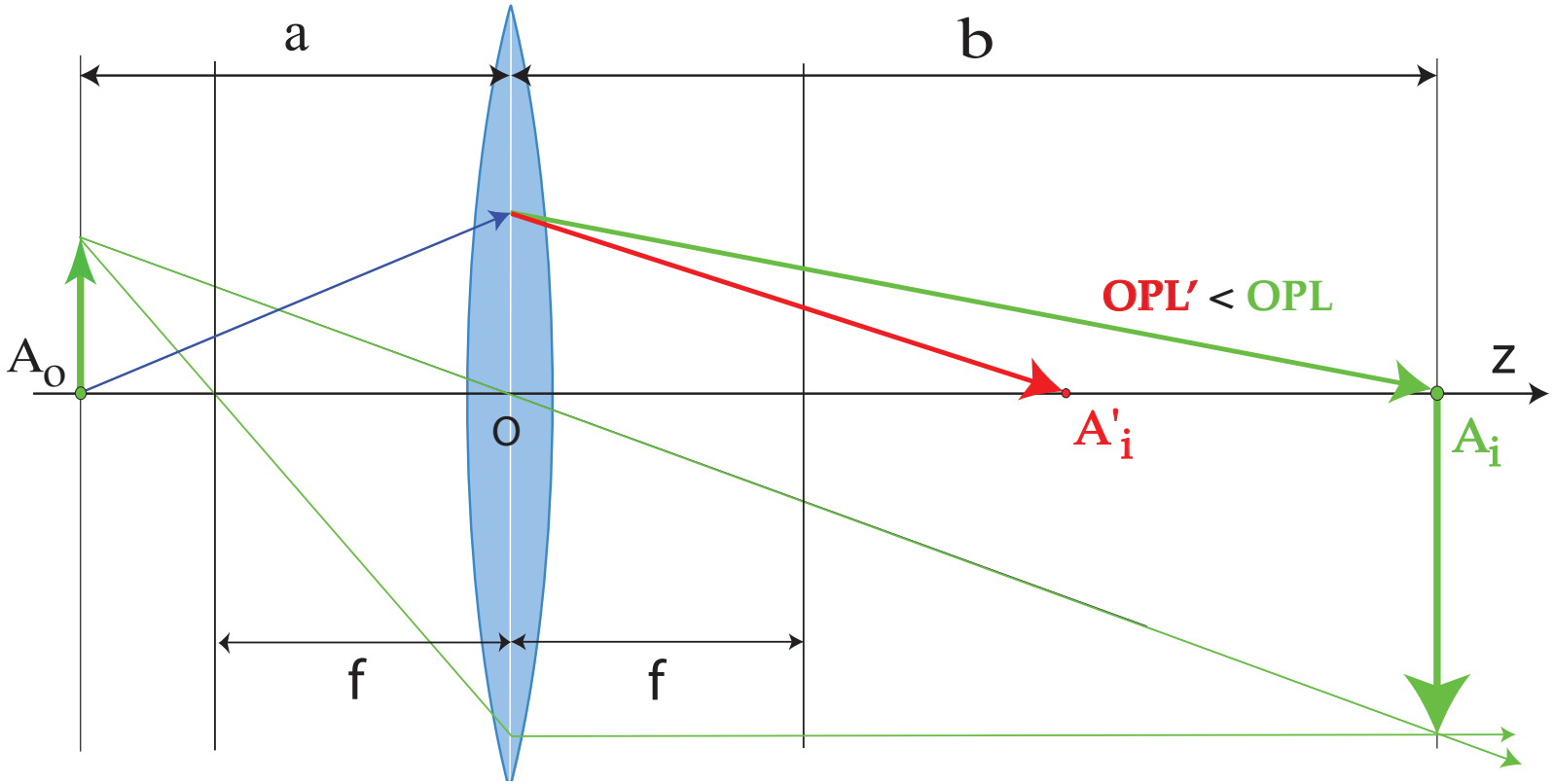
The OPD measure the deviation of a wavefront from a perfect spherical wavefront (vacuum or homogenous medium).
At the exit pupil P_S, the spherical wavefront converging towards **I** defines the reference wavefront.



In the presence of aberrations the wavefront Σ'_S is no more spherical. The Optical Path Dinference (distance between the deformed Σ'_S and spherical waveform Σ_S) introduced the phase shift:

$$\delta\phi = e^{2\pi\imath\frac{OPD(x_S,y_S)}{\lambda}}$$

OPD: spherical aberration

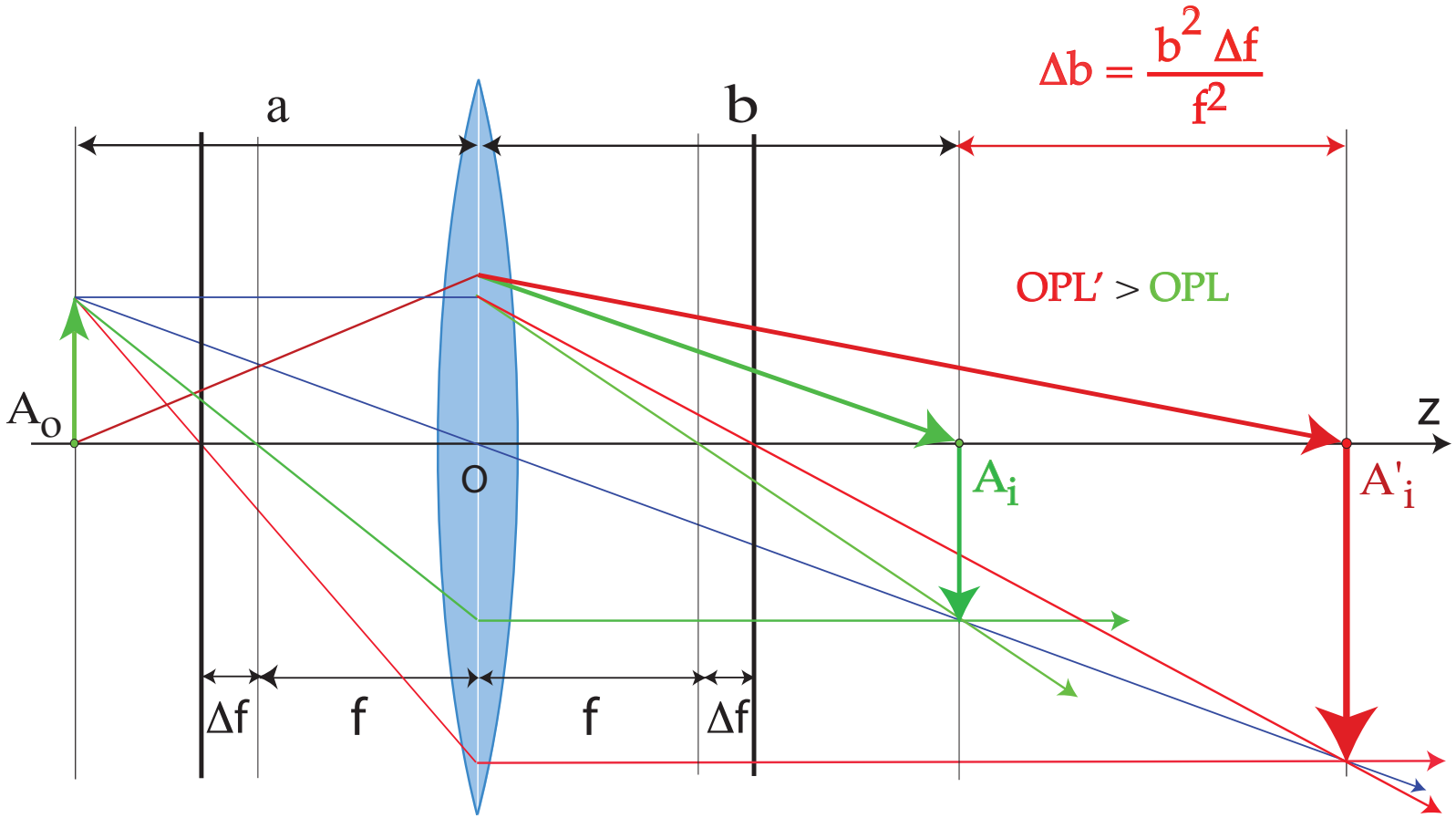


In presence of spherical aberration, the optical path length (OPL') form A_o to A'_i is smaller than OPL from A_o to A_i. The wavefront at A'_i is out-of-phase by[1]:

$$e^{-2\pi i \frac{C_s \lambda^3 (\vec{q}.\vec{q})^2}{4}}$$

[1] With our plane wave choice $e^{-2\pi \imath \vec{q}.\vec{r}}$.

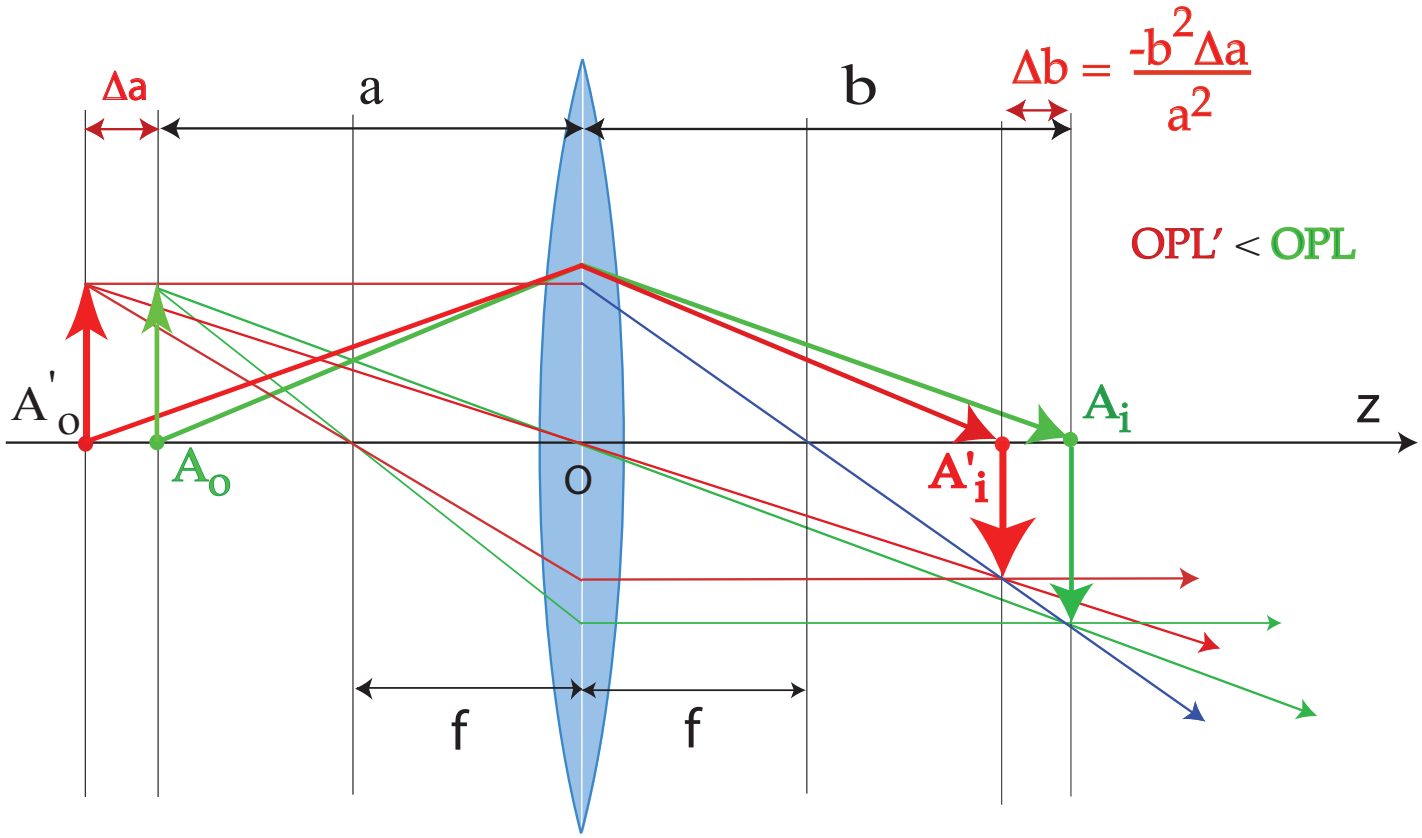
OPD: underfocus



Underfocus weakens the objective lens, i.e. increases **f**. As a consequence the OPL from A_o to A'_i is larger:

$$e^{2\pi i \frac{\Delta f \lambda (\vec{q}\cdot\vec{q})}{2}}$$

OPD: eccentricity



On the contrary keeping **f** constant and moving the object by Δa decreases the OPL.

Transfer function $T(\vec{q})$

$$T(\vec{q}) = e^{\chi(\vec{q})} = \cos(\chi(\vec{q})) + i \underbrace{\sin(\chi(\vec{q}))}_{\text{Contrast transfer function}}$$

$$\chi(\vec{q}) = \pi \left[W_{20}\, \lambda\, \vec{q}.\vec{q} + W_{40} \frac{\lambda^3\, (\vec{q}.\vec{q})^2}{2} + ... \right]$$

Where:

- W_{20} : defocus (z)
- W_{40}: spherical aberration (C_s)

At present TEM and STEM aberration correctors only correct axial aberrations, i.e. aberrations that affect images of point sources located on the optical axis.

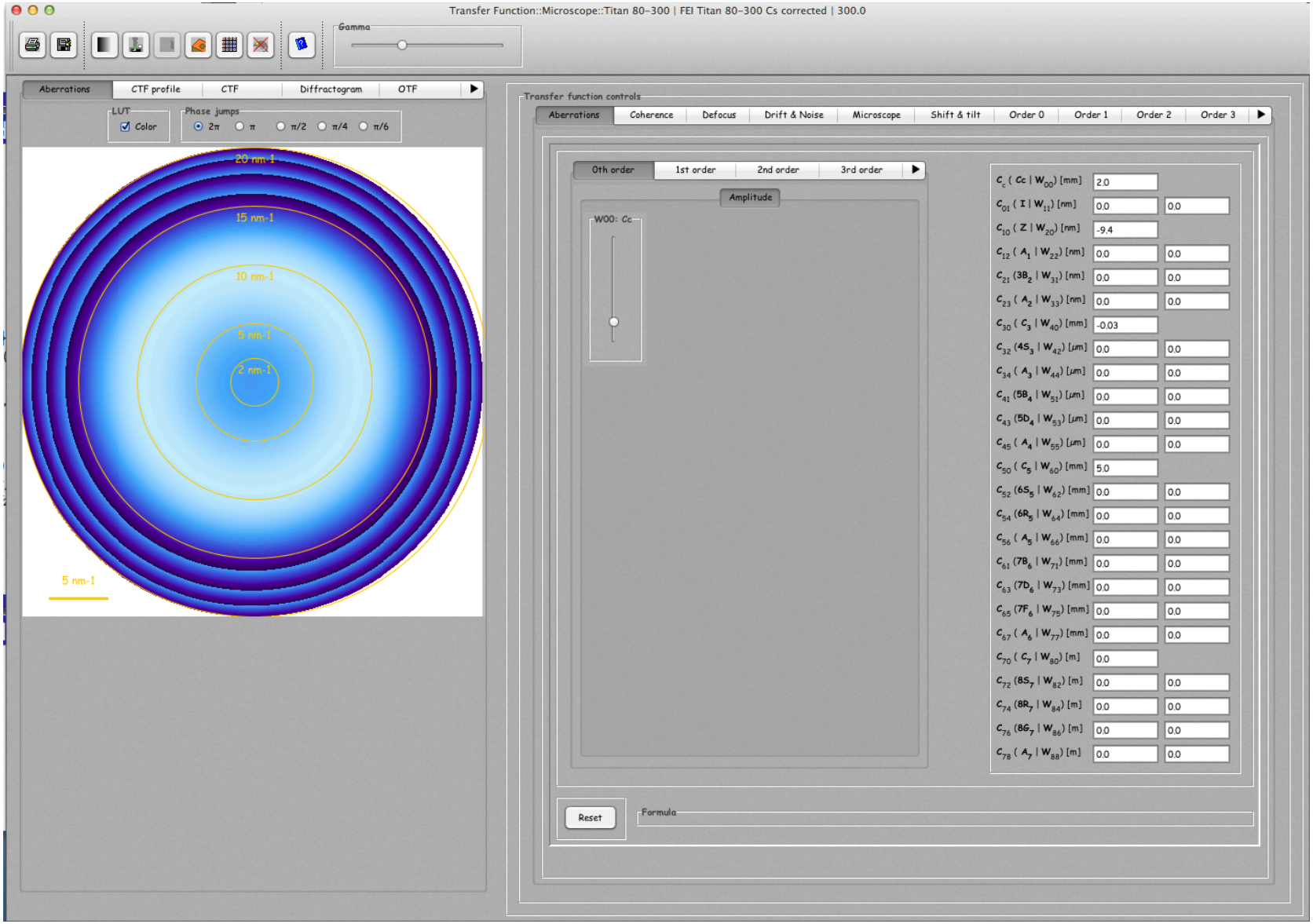
Wavefront aberrations to 6th order (cartesian coordinates)

$\{z, \pi\left(u^2+v^2\right)\lambda\}$ (*defocus*)
$\{W(1,1), 2\pi(u\cos(\phi(1,1)) + v\sin(\phi(1,1)))\}$
$\{W(2,2), \pi\lambda((u-v)(u+v)\cos(2\phi(2,2)) + 2uv\sin(2\phi(2,2)))\}$
$\{W(3,1), \frac{2}{3}\pi\left(u^2+v^2\right)\lambda^2(u\cos(\phi(3,1)) + v\sin(\phi(3,1)))\}$
$\{W(3,3), \frac{2}{3}\pi\lambda^2\left(u\left(u^2-3v^2\right)\cos(3\phi(3,3)) - v\left(v^2-3u^2\right)\sin(3\phi(3,3))\right)\}$
$\left\{W(4,0), \frac{1}{2}\pi\left(u^2+v^2\right)^2\lambda^3\right\}$ (3rd *order spherical aberration or* C_3)
$\{W(4,2), \frac{1}{2}\pi\left(u^2+v^2\right)\lambda^3((u-v)(u+v)\cos(2\phi(4,2)) + 2uv\sin(2\phi(4,2)))\}$
$\{W(4,4), \frac{1}{2}\pi\lambda^3\left(\left(u^4-6v^2u^2+v^4\right)\cos(4\phi(4,4)) + 4u(u-v)v(u+v)\sin(4\phi(4,4))\right)\}$
$\left\{W(5,1), \frac{2}{5}\pi\left(u^2+v^2\right)^2\lambda^4(u\cos(\phi(5,1)) + v\sin(\phi(5,1)))\right\}$
$\{W(5,3), \frac{2}{5}\pi\left(u^2+v^2\right)\lambda^4\left(u\left(u^2-3v^2\right)\cos(3\phi(5,3)) - v\left(v^2-3u^2\right)\sin(3\phi(5,3))\right)\}$
$\{W(5,5), \frac{2}{5}\pi\lambda^4\left(u\left(u^4-10v^2u^2+5v^4\right)\cos(5\phi(5,5)) + v\left(5u^4-10v^2u^2+v^4\right)\sin(5\phi(5,5))\right)\}$
$\left\{W(6,0), \frac{1}{3}\pi\left(u^2+v^2\right)^3\lambda^5\right\}$ (5th *order spherical aberration or* C_5)
$\left\{W(6,2), \frac{1}{3}\pi\left(u^2+v^2\right)^2\lambda^5((u-v)(u+v)\cos(2\phi(6,2)) + 2uv\sin(2\phi(6,2)))\right\}$
$\{W(6,4), \frac{1}{3}\pi\lambda^5\left(\left(u^6-5v^2u^4-5v^4u^2+v^6\right)\cos(4\phi(6,4)) + 4uv\left(u^4-v^4\right)\sin(4\phi(6,4))\right)\}$
$\{W(6,6), \frac{1}{3}\pi\lambda^5\left(\left(u^6-15v^2u^4+15v^4u^2-v^6\right)\cos(6\phi(6,6)) + 2uv\left(3u^4-10v^2u^2+3v^4\right)\sin(6\phi(6,6))\right)\}$

jems describes wavefront aberrations to order 8 [2].

[2] urlhttp://cimewww

jems


Transfer Function::Microscope::Titan 80-300 | FEI Titan 80-300 Cs corrected | 300.0
Gamma
Aberrations
CTF profile
CTF
Diffractogram
OTF
LUT
Color
Phase jumps
2π
π
π/2
π/4
π/6
20 nm-1
15 nm-1
10 nm-1
5 nm-1
2 nm-1
5 nm-1
Transfer function controls
Aberrations
Coherence
Defocus
Drift & Noise
Microscope
Shift & tilt
Order 0
Order 1
Order 2
Order 3
0th order
1st order
2nd order
3rd order
Amplitude
W00: Cc
Reset
Formula

OPD calculation: coordinates system

2 reference planes:

- Coordinates system attached to the reference sphere Σ_{P_S} of the exit pupil P_S.
- Coordinates system in the image plane $(Ox_iy_iz_i)$.
- Reference ray $\longrightarrow$ principal ray through the nodal points of the optical system.
- Reference ray defines reference points on Σ_{P_S} and $(Ox_iy_iz_i)$.
- Distribution of the light rays around the reference points defines the aberrations associated with the reference light ray.

Aberration (ϵ_x, ϵ_y) associated to a ray

For (x_i, y_i) coordinates of image reference point I, the aberration of a ray of coordinates (x, y) in the image plane:

$$\begin{pmatrix} \epsilon_x \\ \epsilon_y \end{pmatrix} = \begin{pmatrix} x - x_i \\ y - y_i \end{pmatrix}$$

Calculation of aberrations (ϵ_x, ϵ_y) with:
Characteristic function $\longrightarrow$ OPL $\longrightarrow$ OPD $\longrightarrow$ aberrations.

Characteristic function

Aberrations of optical system calculated using a characteristic function. Defined using:

1. between 2 points conjugated points (objet and image) of position $\overrightarrow{a_o}$ and $\overrightarrow{a_i}$.
2. Optical path between these points is $V(\overrightarrow{a_o}, \overrightarrow{a_i})$.
3. V defines a field of geometrical rays.
4. Knowing V is enough to fully describe the optical system (ray tracing).

Optical path $\longrightarrow$ extremum

Fermat principle $\longrightarrow$ optical path between 2 points is an extremum.

A very small perturbation of the coordinates $\delta \overrightarrow{a_i}$ of the image point increases the OPL by:

$$V(\overrightarrow{a_i} + \delta \overrightarrow{a_i}, \overrightarrow{a_o}) - V(\overrightarrow{a_i}, \overrightarrow{a_o}) = \delta \overrightarrow{a_i} \nabla V$$

$$n_i \overrightarrow{u} \delta \overrightarrow{a_i} = \delta \overrightarrow{a_i} \nabla V$$

where $\overrightarrow{u}$ unit vector parallel to $\delta \overrightarrow{a_i}$.

At image point I

Since $\delta \overrightarrow{a_i}$ is arbitrary:

$$n_i \overrightarrow{u} = \nabla V$$

With the director cosines $(\alpha_i, \beta_i, \gamma_i)$ of $\overrightarrow{u}$ at the image point $\overrightarrow{a_i}$:

$$n_i \alpha_i = \frac{\partial V}{\partial x_i}$$
$$n_i \beta_i = \frac{\partial V}{\partial y_i}$$
$$n_i \gamma_i = \frac{\partial V}{\partial z_i}$$

Wavefront $\rightarrow$ geometrical aberrations

Relationship between wavefront aberrations given by characteristic function defined on sphere attached to exit pupil and position of intersection of light ray with image plane. Calculation done for object on optical axis O_z.

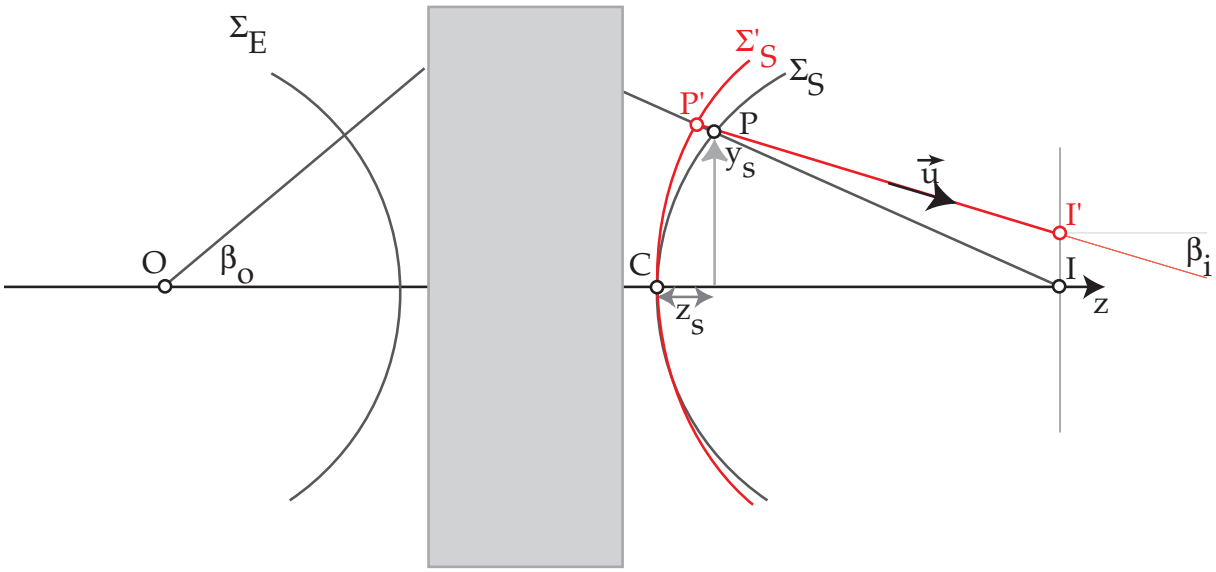


Figure: Coordinates on the reference sphere Σ_S.

P' of (x_s, y_s) on reference sphere Σ_S. $W(x_s, y_s) = n_i \overline{P'P}$ (wavefront aberration) = wavefront deformation at P' = OPL from P' to P.

Transverse geometric aberrations

Image I' does not coincide with I.

Displacement from I to I', $\overrightarrow{\epsilon} = (\epsilon_x, \epsilon_y) =$ geometrical aberration $\overrightarrow{\epsilon}$.

$\overrightarrow{\epsilon}$ function of (x_s, y_s).

$\Longrightarrow$ wavefront and transverse geometric aberrations depend on the position of P on Σ_S.

The characteristic function V $\Longrightarrow$ provides the relationship between wavefront and transverse geometric aberrations.

OPL (optical path) from P to I is $V(I, P)$. W at (x_s, y_s):

$$W(x_s, y_s) = V(I, P) - V(I, P') = V(I, C) - V(I, P')$$

P and C on same reference wavefront and $V(I, P') = V(x_s, y_s, z_s)$ with

$z_s = z_s(x_s, y_s)$.

$\frac{\partial W(x_s,y_s)}{\partial x_s}$ and $\frac{\partial W(x_s,y_s)}{\partial y_s}$ calculations

Differentiating $W(x_s, y_s)$ $(V(I, C) = n_i R = cste)$:

$$\frac{\partial W}{\partial x_s} = -\frac{\partial V}{\partial x_s} - \frac{\partial V}{\partial z_s}\frac{\partial z_s}{\partial x_s}$$
$$\frac{\partial W}{\partial y_s} = -\frac{\partial V}{\partial y_s} - \frac{\partial V}{\partial z_s}\frac{\partial z_s}{\partial y_s}$$

With x_s, y_s and z_s from the reference sphere equation:

$$x_s^2 + y_s^2 + (R - z_s)^2 = R^2$$

With $\frac{\partial z_s}{\partial x_s} = \frac{x_s}{R-z_s}$ and $\frac{\partial z_s}{\partial y_s} = \frac{y_s}{R-z_s}$ and the cosine directors:

$$\begin{pmatrix} \alpha_i \\ \beta_i \\ \gamma_i \end{pmatrix} \simeq \frac{1}{R} \begin{pmatrix} \epsilon_x - x_s \\ \epsilon_y - y_s \\ R - z_s \end{pmatrix}$$

$$\frac{1}{n_i}\frac{\partial W}{\partial x_s} = -\left(\alpha_i + \frac{\gamma_i x_s}{R - z_s}\right)$$
$$\frac{1}{n_i}\frac{\partial W}{\partial y_s} = -\left(\beta_i + \frac{\gamma_i y_s}{R - z_s}\right)$$

Wavefront aberration $\Longrightarrow$ transfer function

$$\epsilon_x = -\frac{R}{n_i}\frac{\partial W}{\partial x_s}$$
$$\epsilon_y = -\frac{R}{n_i}\frac{\partial W}{\partial y_s}$$

When the geometrical aberration is known (from ray tracing) the wavefront

aberration is obtained by integration of the transverse geometric aberration on the reference sphere:

$$\frac{R}{n_i}(W_B - W_A) = \int_A^B (\epsilon_x dx_s + \epsilon_y dy_s)$$

Geometrical aberrations: Seidel coefficients

We are free to set the reference plane at different places. Placing them at the object and image plane we can define the geometric aberrations as functions of the object position and the angle of the light ray to the optical axis.
We introduce a complex notation for the calculation of the geometrical aberrations:

- $\overrightarrow{x_o}$ object position.
- $\overrightarrow{x_i}$ image position.

$$\overrightarrow{x} = \begin{pmatrix} x \\ y \end{pmatrix} = (x + \imath y)$$

The optical system is again characterized by the entrance and exit pupils PE and PS. The image $\vec{x_i}$ is a function of $\vec{x_o}$ and of the angle to the optical axis $\vec{\alpha_o}$ of the light rays:

$$\vec{\alpha} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = (\alpha + \imath\beta)$$

où α et β sont les angles des rayons incidents avec les plans O_{xz} et O_{yz} respectivement.

Seidel coefficients

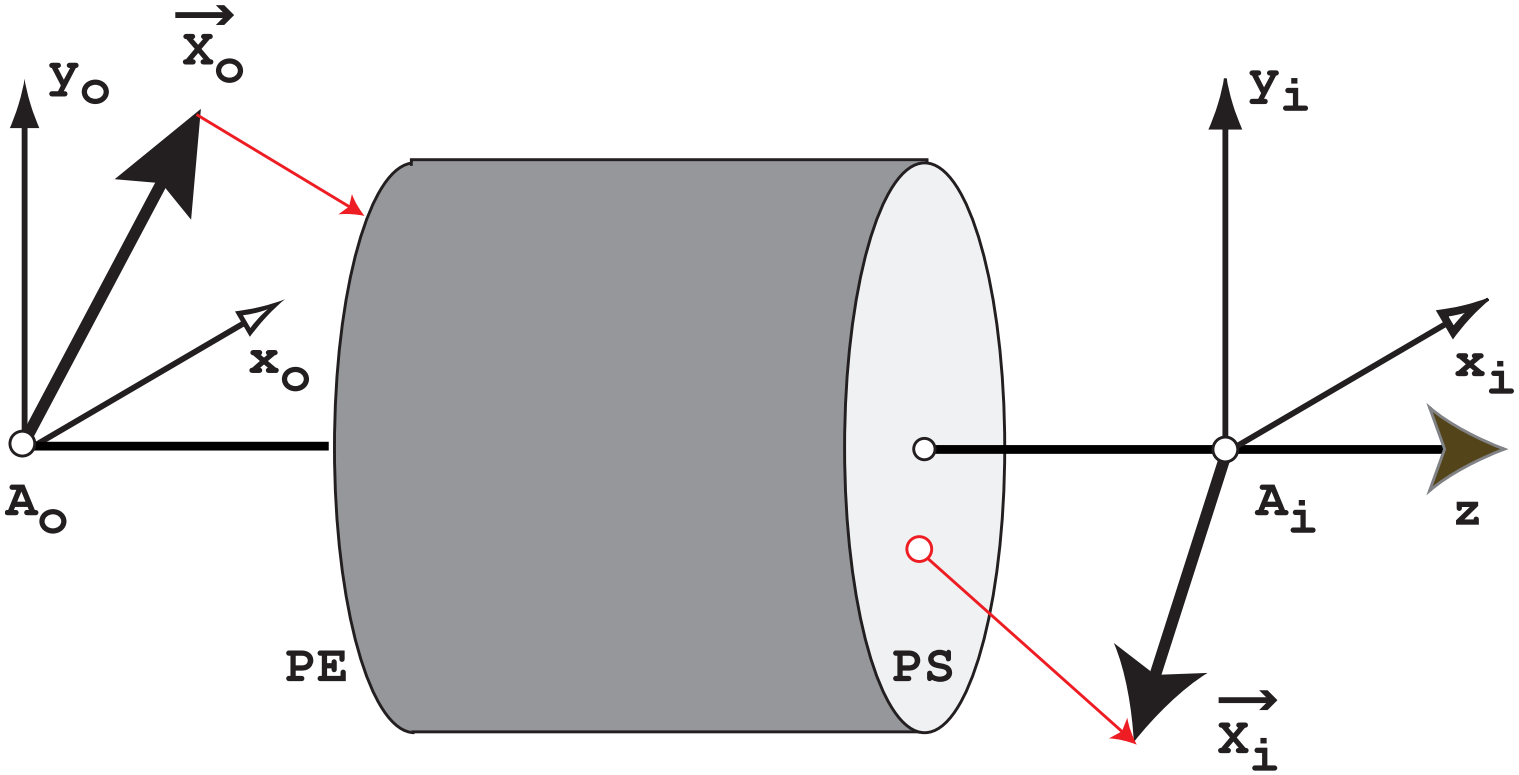


Figure: Object and image planes are conjugated.

Image $\vec{x_i}$ depend on $\vec{x_o}$ and on $\vec{\alpha_o}$. This function is developed in a Taylor series in x, y, α and β.

Seidel polynomial

The Taylor development is written using the complex notation for $\vec{x_o}$ and $\vec{\alpha_o}$ and their complex conjugates $\vec{x_o^*}$ et $\vec{\alpha_o^*}$:

$$\vec{x_i} = \sum_{\mu\nu kl} C_{\mu\nu kl} \vec{x_o^\mu} \vec{x_o^{*\nu}} \vec{\alpha_o^k} \vec{\alpha_o^{*l}}$$

The optical system is centered with rotational symmetry $\Longrightarrow$ change of object orientation $\vec{x_o}$ to $\vec{x_o}e^{\imath\theta}$ and $\vec{\alpha_o}$ to $\vec{\alpha_o}e^{\imath\theta}$ $\longrightarrow$ rotation of the image $\vec{x_i}$ to $\vec{x_i}e^{\imath\theta}$.

$$\overrightarrow{x_i}\, e^{\imath\theta} = \sum_{\mu\nu kl} C_{\mu\nu kl} \overrightarrow{x_o^{\mu}}\, \overrightarrow{x_o^{*\nu}}\, \overrightarrow{\alpha_o^{k}}\, \overrightarrow{\alpha_o^{*l}}\, e^{\imath\theta(\mu-\nu+k-l)}$$

Thus:

$$\mu - \nu + k - l = 1$$

or:

$$\mu + k = \nu + l + 1$$

Only odd **m** terms since:

$$m = \mu + \nu + k + l = 2\left(\nu + l\right) + 1$$

Order 1

The order 1 (linear approximation) $\vec{x}$ and $\vec{\alpha}$ is obtained for $\mathbf{m = 1}$, $\nu + l = 0$ et $\mu + k = 1$, possible only when si:

1. $\mu = 1$, $\nu = 0$, k = 0, l = 0.
2. $\mu = 0$, $\nu = 0$, k = 1, l = 0.

The image $\vec{x_i}$ is proportional to $\vec{x_o}$:

$$\overrightarrow{x_i} = C_{1000}\overrightarrow{x_o} + C_{0010}\overrightarrow{\alpha_o}$$

Order 1 $\Longrightarrow$ paraxial approximation

Since $\vec{x_o}$ et $\vec{x_i}$ are conjugated $C_{0010} = 0$ (every ray emitted at $\vec{x_o}$ and transmitted by the optical system reaches $\vec{x_i}$ independent of its angle to the optical axis). This provides the paraxial approximation:

$$\vec{x_i} = C_{1000}\vec{x_o} = G_t\vec{x_o}$$

There is no order 2 terms.

Order 3

For $\mathbf{m = 3}$, $\nu + l = 1$ and $\mu + k = 2$, there 6 non zero terms of the Taylor development. Their coefficients are the Seidel coefficients.
The departure from the paraxial approximation $\Delta \overrightarrow{x_i}$ is describing order three aberrations.
The departure is:

$$\begin{aligned}
\Delta \overrightarrow{x_i} &= \overrightarrow{x_i} - G_t \overrightarrow{x_o} \\
&= C_{0021} \overrightarrow{\alpha_o}^2 \overrightarrow{\alpha_o}^* \\
&+ C_{1011} \overrightarrow{x_o} \overrightarrow{\alpha_o} \overrightarrow{\alpha_o}^* + C_{0120} \overrightarrow{x_o}^* \overrightarrow{\alpha_o}^2 \\
&+ C_{2001} \overrightarrow{x_o}^2 \overrightarrow{\alpha_o}^* \\
&+ C_{1110} \overrightarrow{x_o} \overrightarrow{x_o}^* \overrightarrow{\alpha_o} \\
&+ C_{2100} \overrightarrow{x_o}^2 \overrightarrow{x_o}^*
\end{aligned}$$

Ordre 3: monochromatic aberrations

$$
\begin{aligned}
\Delta \overrightarrow{x_i} &= C_{0021} |\overrightarrow{\alpha_o}|^2 \overrightarrow{\alpha_o} \\
&+ C_{1011} \overrightarrow{x_o} |\overrightarrow{\alpha_o}|^2 + C_{0120} \overrightarrow{x_o}^* \overrightarrow{\alpha_o}^2 \\
&+ C_{2001} \overrightarrow{x_o}^2 \overrightarrow{\alpha_o}^* \\
&+ C_{1110} |\overrightarrow{x_o}|^2 \overrightarrow{\alpha_o} \\
&+ C_{2100} |\overrightarrow{x_o}|^2 \overrightarrow{x_o}
\end{aligned}
$$

Monochromatic aberrations

1. Spherical aberration depends on $|\vec{\alpha_o}|^2$ and $\vec{\alpha_o}$: $C_{0021}|\vec{\alpha_o}|^2\vec{\alpha_o}$.
2. Coma aberration depends on $\vec{x_o}$, $\vec{x_o}^*$, $|\vec{\alpha_o}|^2$ and $\vec{\alpha_o}^2$: $C_{1011}\vec{x_o}|\vec{\alpha_o}|^2 + C_{0120}\vec{x_o}^*\vec{\alpha_o}^2$.
3. 3rd astigmatism depends on $\vec{x_o}^2$ and $\vec{\alpha_o}^*$: $C_{2001}\vec{x_o}^2\vec{\alpha_o}^*$.
4. Field curvature depends on $|\vec{x_o}|^2$ and $\vec{\alpha_o}$: $C_{1110}|\vec{x_o}|^2\vec{\alpha_o}$.
5. Distortion depends on $|\vec{x_o}|^2$ and $\vec{x_o}$: $C_{2100}|\vec{x_o}|^2\vec{x_o}$.

Seidel coefficients: polar form

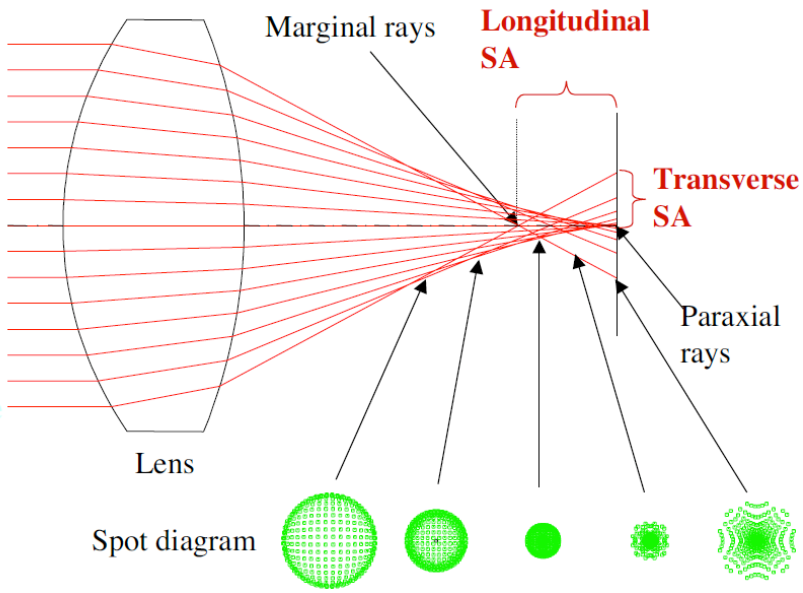
In polar form where $\vec{x_o}$ and $\vec{\alpha_o}$ are repalced by: $x_o = r_o e^{\imath\theta_o}$ et $\alpha_o = \rho_o e^{\imath\phi_o}$ the 6 Seidel coefficients are:

$$\begin{aligned}\Delta\overrightarrow{x_i} &= C_{0021}\rho_o^3 e^{i\phi_o} + C_{1011} r_o \rho_o^2 e^{i\theta_o} + C_{0120} r_o \rho_o^2 e^{i(2\phi_o - \theta_o)} \\ &+ C_{2001} r_o^2 \rho_o e^{\imath(2\theta_o - \phi_o)} + C_{1110} r_o^2 \rho_o e^{\imath\phi_o} + C_{2100} r_o^3 e^{\imath\theta_o}\end{aligned}$$

Knowing the Seidel coefficients the wavefront aberrations and the transfer function are easily calculated. In fact, nowadays, only axial aberrations are corrected since at high magnification the object is pretty close to the optical axis.

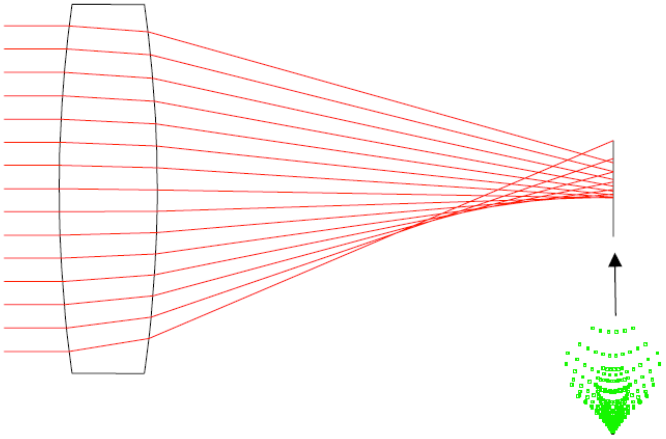
Spherical aberration

- Spherical Aberration
- Coma
- Astigmatism
- Field Curvature
- Distortion

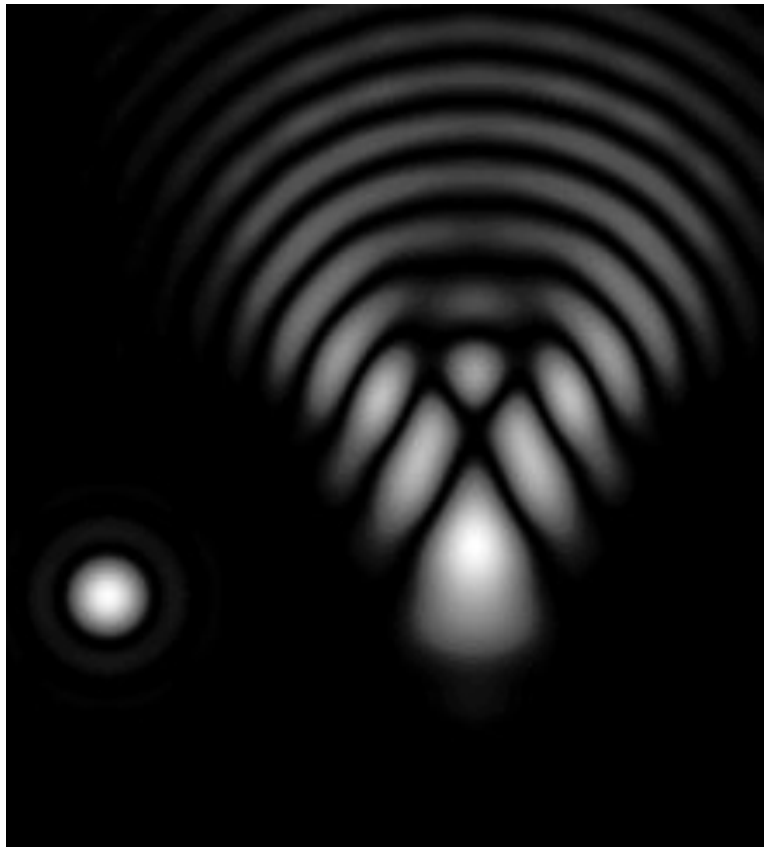


Coma

- Spherical Aberration
- Coma
- Astigmatism
- Field Curvature
- Distortion

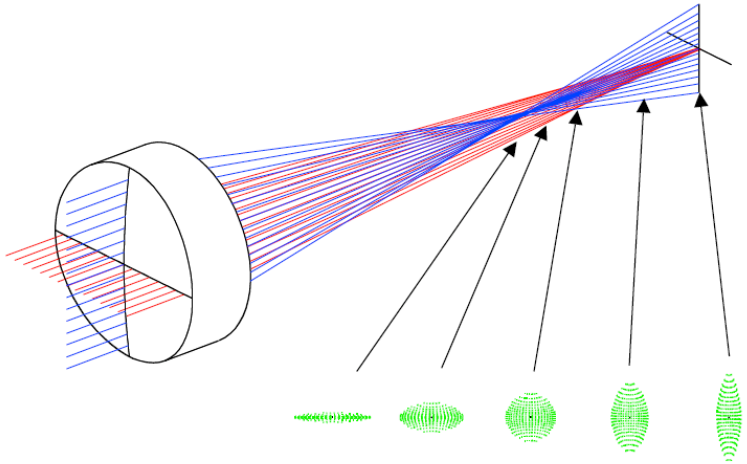


Coma



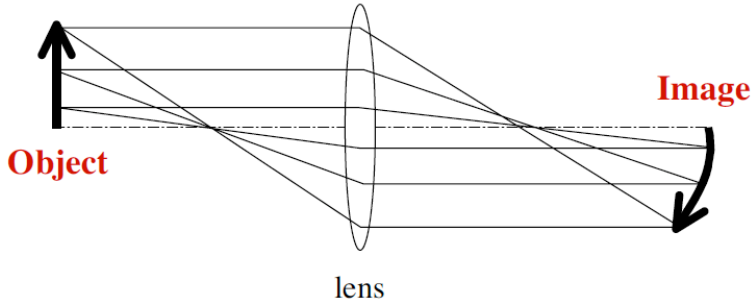
Astigmatism

- Spherical Aberration
- Coma
- Astigmatism
- Field Curvature
- Distortion



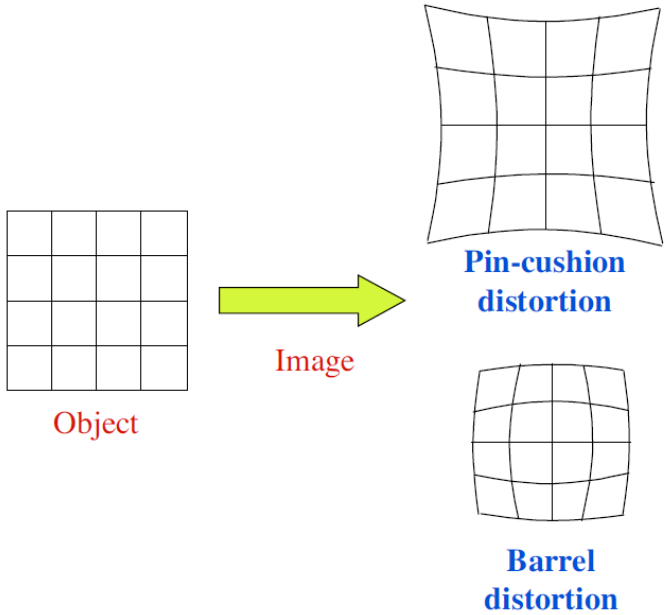
Field curvature

- Spherical Aberration
- Coma
- Astigmatism
- **Field Curvature**
- Distortion



Distortion

- Spherical Aberration
- Coma
- Astigmatism
- Field Curvature
- Distortion



Example: spherical aberration

The spherical aberration is the most important aberration in microscopy. When the object is located on the optical axis $\vec{x_o}$ and $\vec{x_i}$ are nulls.

$$\Delta\vec{x_i} = C_{0021}\,\rho_o^3\,e^{\imath\phi_o}$$

Writing $\Delta r_i = |\Delta\vec{x_i}|$ and ρ the maximum of ρ_o:

$$\Delta r_i = C_{0021}\,\rho_o^3$$

We see that C_{0021} has a length dimension that is written:

$$C_{0021} = |G_t|\,C_s$$

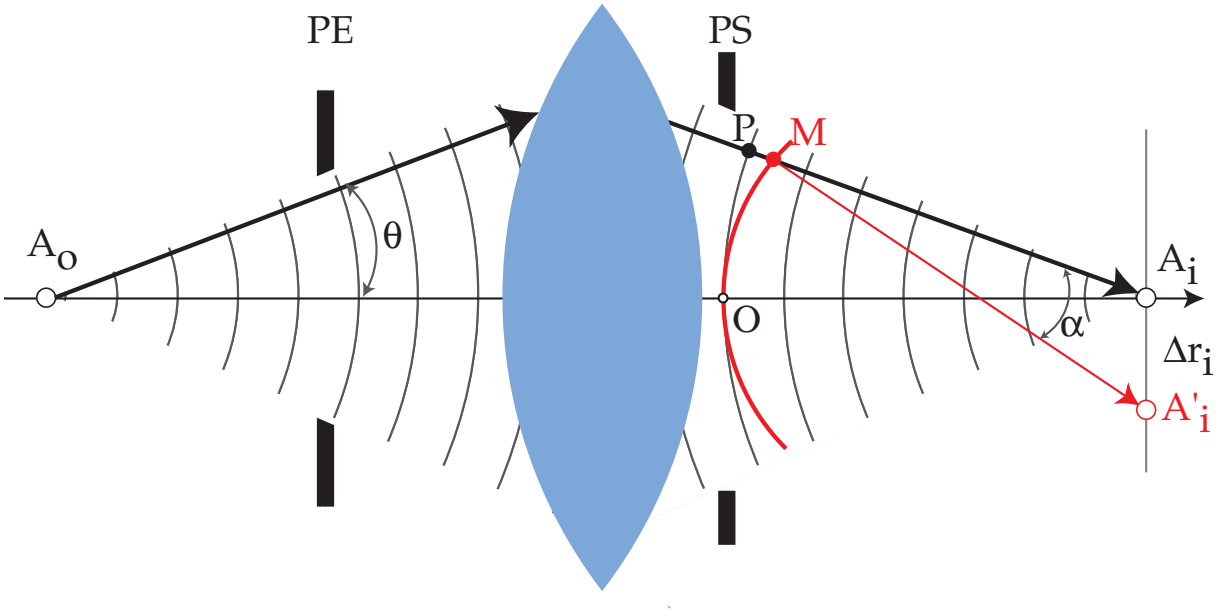
C_s is the spherical aberration coefficient and the object displacement is:

$$\Delta r_i = |G_t|\,C_s\,\rho^3$$

Spherical aberration: OPD

The phase change $W_{C_s}(\rho)$ due to spherical aberration is calculated by considering the optical path difference, OPD, between a gaussian ray (paraxial) and the ray submitted to the aberration.

Spherical aberration: OPD



$$\Delta r_i = |G_t| C_s \rho^3$$

Spherical aberration: OPL

Reference spherical wavefront OP in the exit pupil plane PS converges to the ideal image point A_i.
Wavefront OM, deformed by the spherical aberration, converges to point A'_i.
2 types of spherical aberration:

1. Transverse.
2. Longitudinal.

Spherical aberration: OPD

The rays PA_i and MA'_i are perpendicular to the wavefronts OP and OM.

$$OPD = W(\rho) = \overline{PM}$$

Phase change $\chi(\rho)$:

$$\chi(\rho) = \frac{2\pi}{\lambda} W(\rho)$$

With $G_t = \frac{z_i}{f}$ and $\rho = \frac{r}{f}$ where r = distance from P to the optical axis O_z:

$$\Longrightarrow \Delta r_i = z_i \, C_s \, \frac{r^3}{f^4}$$

With $\frac{\Delta r_i}{z_i} = \frac{\partial W}{\partial \theta}$:

$$W(\theta) = \frac{1}{z_i} \int \Delta r_i dr = \frac{1}{z_i} \int_0^\theta z_i \, C_s \, \frac{r^3}{f^4} dr = C_s \frac{\theta^4}{4}$$

Finally with Bragg law $2\theta_B \approx \lambda u \Longrightarrow \theta \approx \lambda u$ with u spatial frequency:

$$\chi_{C_s}(u) = 2\pi \frac{C_s \lambda^3 u^4}{4}$$

Defocus Δz

When the object is slightly out of the object plane, Δz, the phase change $\chi_{\Delta z}$ due to Fresnel propagation over the small distance Δz is:

$$\chi_{\Delta z} = -2\pi \frac{\Delta z \lambda u^2}{2}$$

Optical system: transfer function

The transfer function in the Abbe image formation model that modifies the phase of the diffracted beams is:

$$\widetilde{TF}(u) = \exp\left[2\pi\imath\left(\frac{C_s\,\lambda^3\,u^4}{4} - \frac{\Delta z\,\lambda\,u^2}{2}\right)\right]$$

where u spatial frequency of the object.

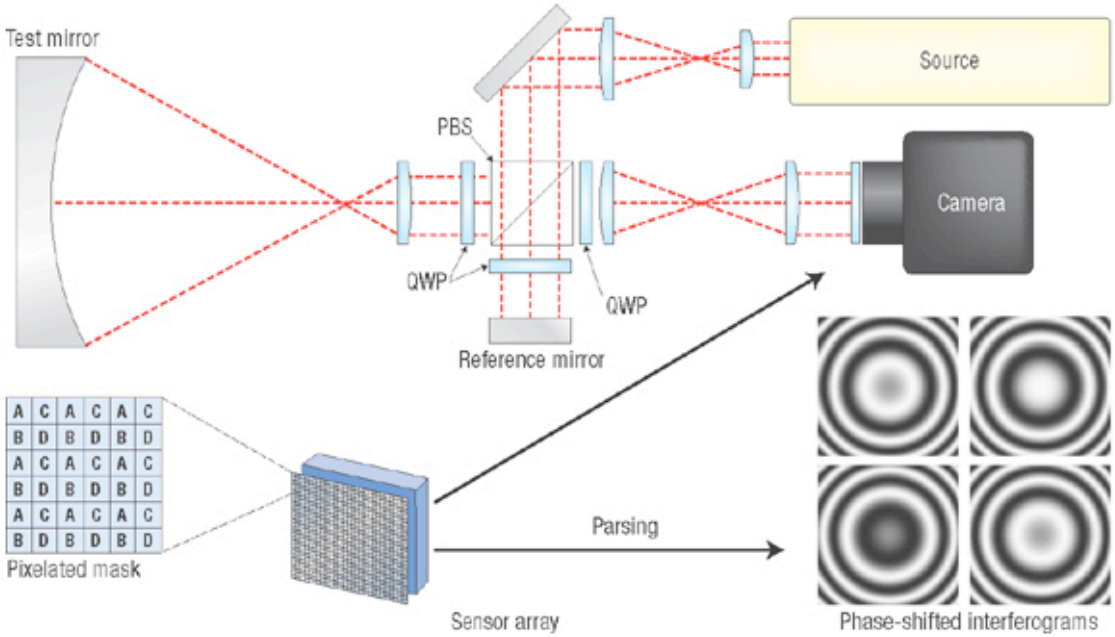
Measuring aberrations

In electron microscopy, contrary to light optics where the wavefront aberrations are measured directly by interferometry, it is necessary to image an object in order to measure the aberrations. There are mainly two possibilities:

1. ronchigram of amorphous or crystalline object (STEM).
2. diffractogram of amorphous object (TEM).

Light optics: Twyman-Green interferometer

Automatic evaluation of optical systems is also performed with the Twyman-Green interferometer.



Examples

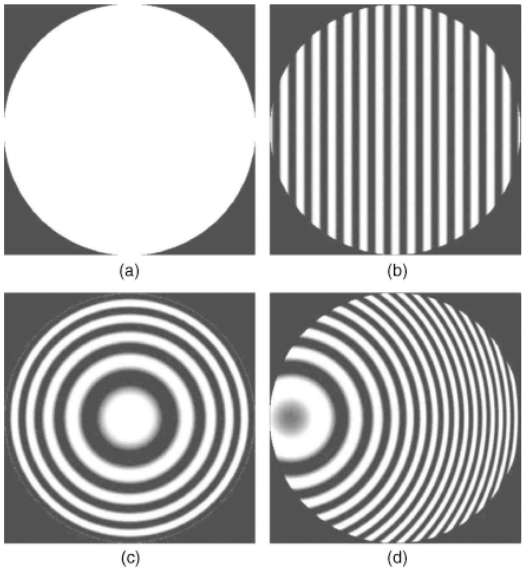


FIGURE 2.42. Interferograms for a perfect lens. (a) With no tilt or defocusing. (b) With tilt. (c) With defocusing. (d) With tilt and defocusing.

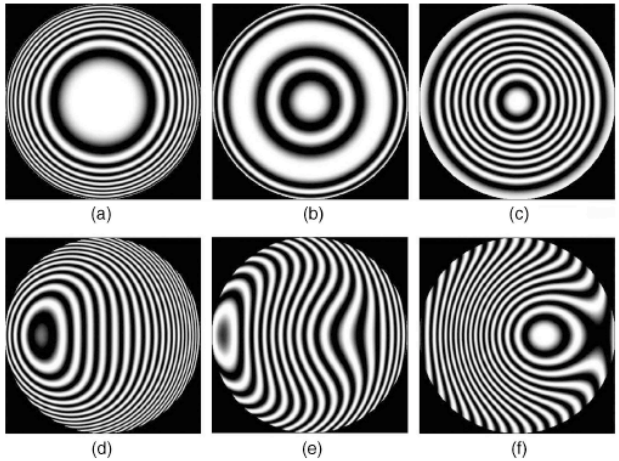


FIGURE 2.43. Interferograms for a lens with spherical aberration at the paraxial, medium, and marginal foci.

References

- W.T. Welford, "Aberrations of the symmetrical optical system", Academic Press, London - New York - San Francisco, 1974.
- J.C. Wyant and K. Creath, "Basic Wavefornt Aberration Theory for Optical Metrology", Academic Press, 1992.