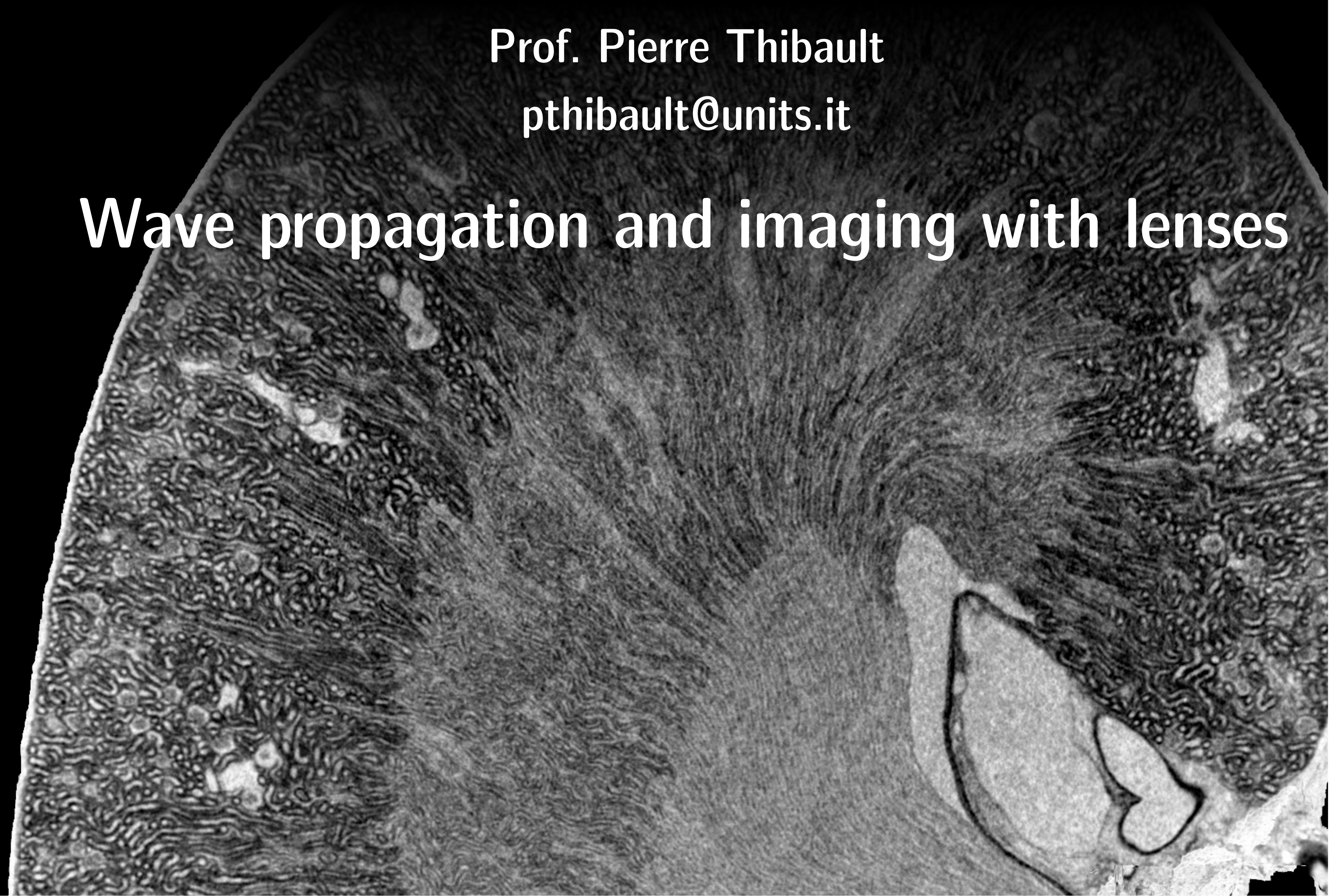
Image Processing for Physicists

Prof. Pierre Thibault
pthibault@units.it

Wave propagation and imaging with lenses



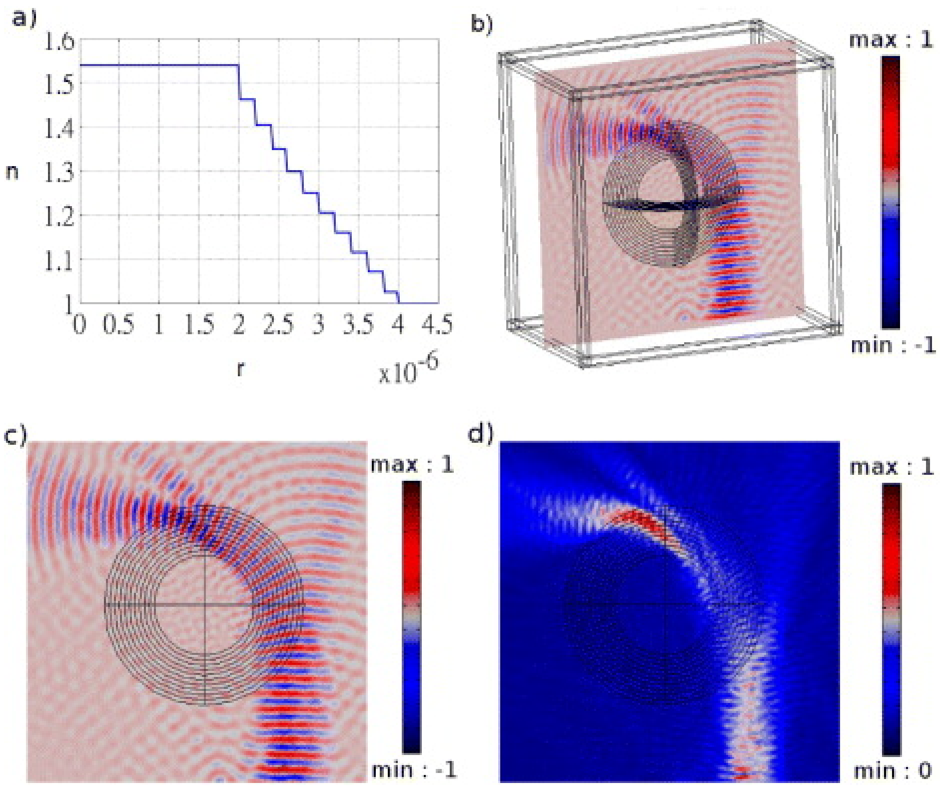
Overview

- Propagation modelization
- Wave propagation:
  - Near-field regime
  - Far-field regime

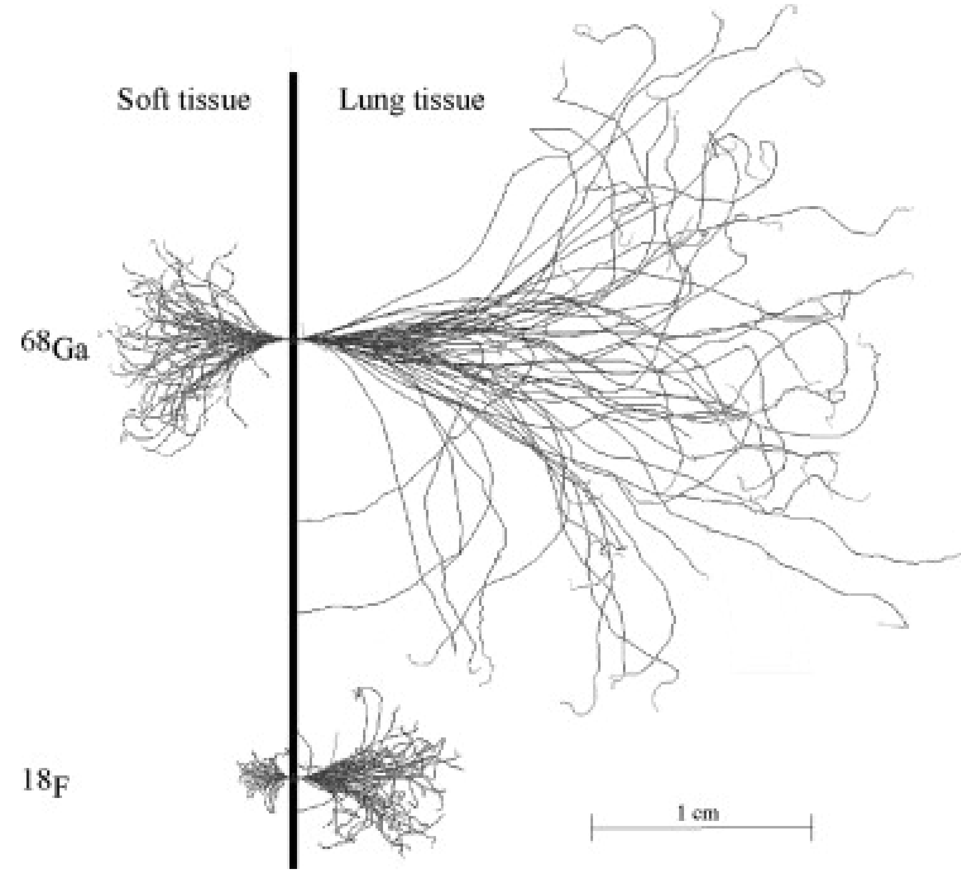
Propagation modeling

- Motivations:

  1. Validation



Finite element simulation of an electro-magnetic field in a dielectric



Monte Carlo simulation of positrons trajectories resulting from ^{68}Ga and ^{18}F decay.

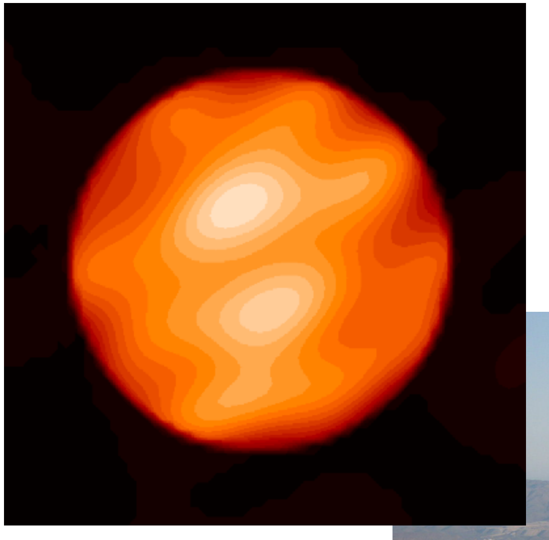
sources: T.M. Chang *et al.* New J. Phys. (2012)
A. Sanchez-Crespo, Appl. Rad. Isotopes (2012)

Propagation modeling

- Motivations:

  2. Inversion

Image reconstruction from sound wave propagation (ultrasonography)



The surface of Betelgeuse reconstructed from interferometric data (IOTA)

sources: wikipedia
Haubois *et al. Astronom. & Astrophys.* (2009)

Propagation modeling

- Particles
  - Model particle tracks (rays) through different media
  - Model may include: refraction, force fields, particle decay and interactions
  - Not included: diffraction
- Wave
  - Model the interaction of a field with a medium
  - Can be very complicated $\rightarrow$ approximations are needed

Propagation modeling

Starting point: Helmholtz equation

- for EM field: neglect polarization (scalar wave approximation) ← Maxwell's equations
- for electron wave, assume high energy electrons

Maxwell approximation as a scalar field:

$\psi \to$ electric field

$$\nabla^2 \psi + \frac{n^2}{c^2} \frac{\partial^2}{\partial t^2} \psi = 0$$

ψ : complex-valued scalar field

n : index of refraction

c : speed of light

For n constant: plane wave solutions

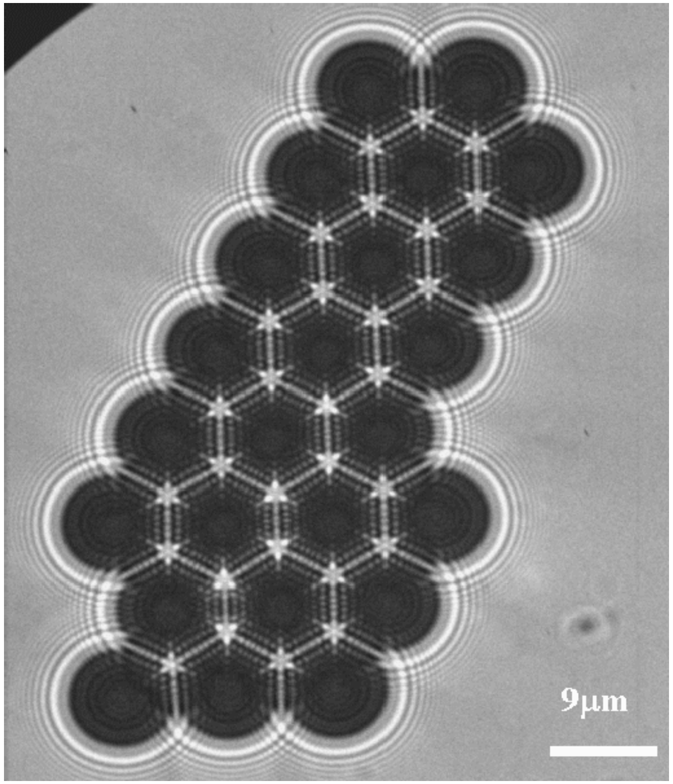
$$\psi(\vec{r}) = \psi_0 e^{i(\vec{k}\cdot\vec{r} - \omega t)}$$

(dispersion relation: $k^2 = \frac{n^2 \omega^2}{c^2}$)

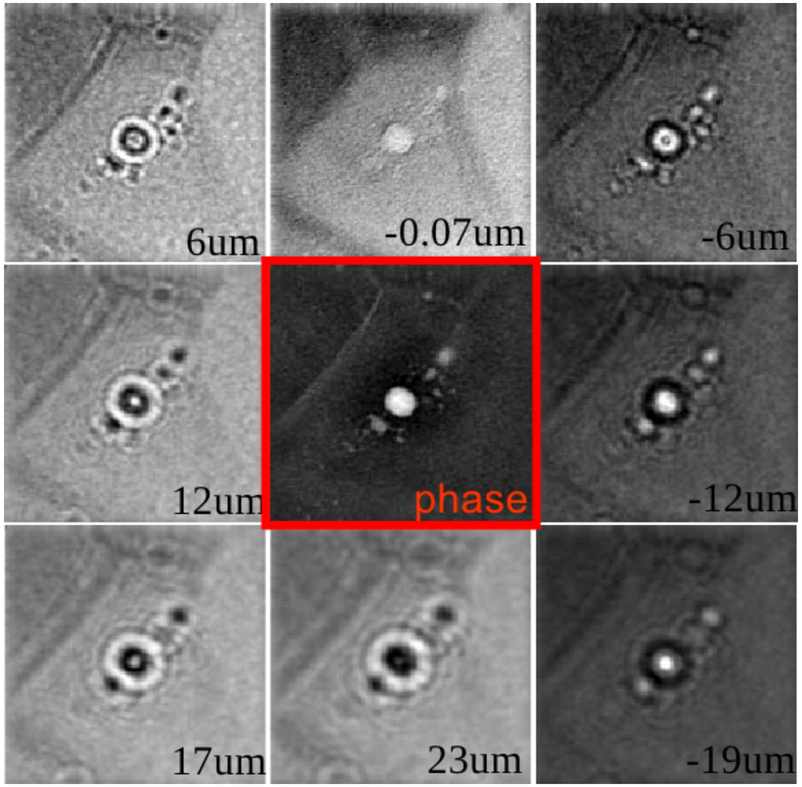
Propagation modeling

- Useful to:
  - better understand optical systems
  - understand diffraction, holography, phase contrast, interferometry, ...

X-ray hologram



TEM through-focus series



sources: Mayo *et al.* Opt. Express (2003)
http://www.christophtkoch.com/Vorlesung/

The physics of propagation

Free space $(n=1)$: General solution is superposition of all plane waves

$$\psi(\vec{r},t) = \sum_{\omega} \sum_{\vec{k}} A_{\omega \vec{k}} e^{i(\vec{k}\cdot\vec{r}-\omega t)}$$

$|k|^2 = \frac{\omega^2}{c^2}$

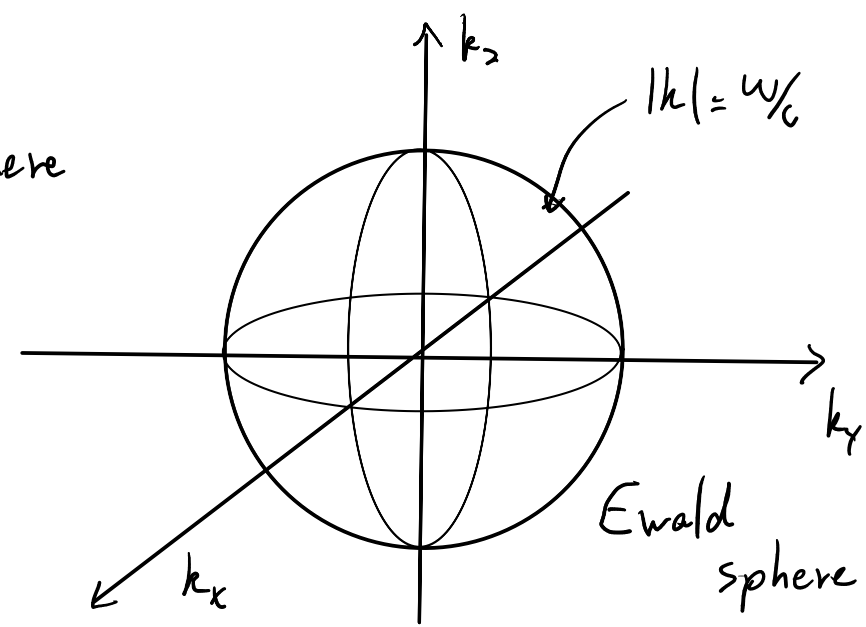
Commonly done: fix ω and solve monochromatic case (removes time)

$$\psi(\vec{r},t) = \psi(\vec{r}) e^{i\omega t} \qquad \psi(\vec{r}) = \sum_{\vec{k}} A_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$$

such that $\boxed{|k| = \omega/c}$

$k_x^2 + k_y^2 + k_z^2 = \frac{\omega^2}{c^2}$ ← surface of a sphere

Only wavevectors lying on the surface of this sphere are part of the solution

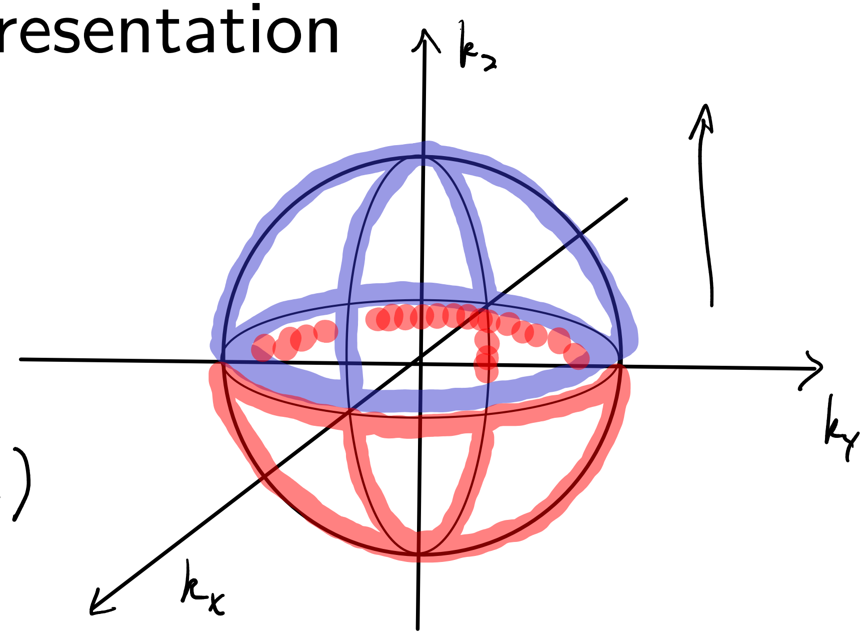


The physics of propagation

Angular spectrum representation

constant

$$k_z = \pm\sqrt{k^2 - k_x^2 - k_y^2}$$



$$\psi(\vec{r}) = \sum_{k_x k_y} A^{+}_{k_x k_y}\, e^{i\left(k_x x + k_y y + \sqrt{k^2 - k_x^2 - k_y^2}\, z\right)} + \sum_{k_x k_y} \cancel{A^{-}_{k_x k_y}}\, e^{i\left(k_x x + k_y y - \sqrt{k^2 - k_x^2 - k_y^2}\, z\right)}$$

0

Consider only propagation towards positive k_z

$$\vec{r}_\perp = (x, y)$$

$$\psi(\vec{r}_\perp ; z) = \sum_{\vec{k}_\perp} A_{\vec{k}_\perp}\, \underbrace{e^{i \vec{k}_\perp \cdot \vec{r}_\perp}}_{\text{2D Fourier transform!}}\, e^{i\sqrt{k^2 - k_\perp^2}\, z}$$

Fourier synthesis equation for <u>any</u> propagating wavefield

Forward propagation

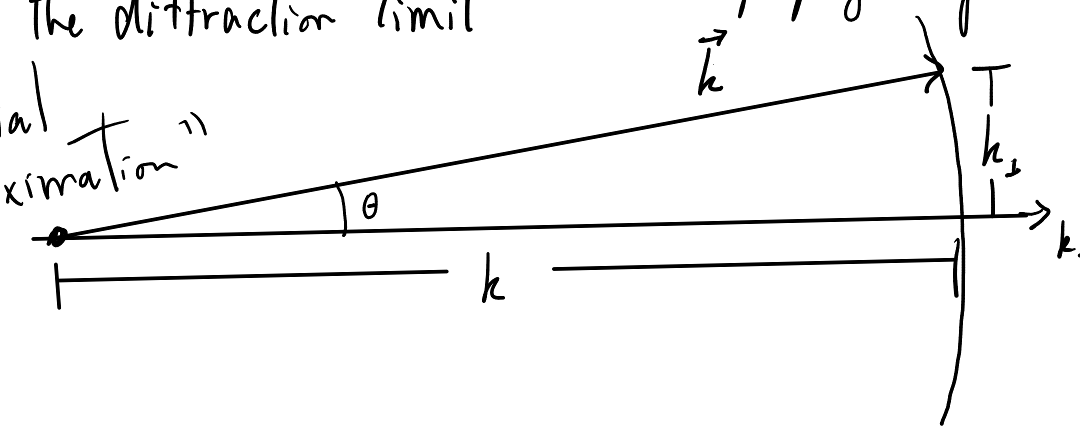
Case $z=0$: $\psi(\vec{r}_\perp; z=0) = \sum_{\vec{k}_\perp} A_{\vec{k}_\perp} \exp(i \vec{k}_\perp \cdot \vec{r}_\perp)$ inverse Fourier transform for ψ

$\Longrightarrow A_{\vec{k}_\perp} = \mathcal{F}\{\psi(\vec{r}_\perp; z=0)\}$ ⇐ Formula to compute the amplitude of each plane wave component in the propagating wave field

One last approximation: it is often the case that $|k_\perp| \ll k$
far from the "diffraction limit"

$$\left.\begin{aligned}\Rightarrow \sqrt{k^2 - k_\perp^2} &= k\sqrt{1 - \frac{k_\perp^2}{k^2}} \\ &\simeq k\left(1 - \frac{1}{2}\frac{k_\perp^2}{k^2}\right) \\ &= k - \frac{k_\perp^2}{2k}\end{aligned}\right\}$$

"paraxial approximation"



Since $k = \frac{2\pi}{\lambda}$, we are assuming that the relevant spatial frequencies in $\psi(\vec{r}_\perp; z=0)$ are such that
$|\vec{u}| \ll 1/\lambda$

$$\exp\left(i\sqrt{k^2 - k_\perp^2}\, z\right) = \underbrace{\exp(ikz)}_{\text{irrelevant for us}}\ \underbrace{\exp\left(\frac{-iz k_\perp^2}{2k}\right)}_{\text{"Fresnel propagator"}}$$

Forward propagation

Recipe: $\psi(\vec{r}_\perp; z) = \mathcal{F}^{-1}\left\{\mathcal{F}\{\psi(\vec{r}_\perp; z=0)\}\exp\left(\frac{-izk_\perp^2}{2k}\right)\right\}$

Discretization for implementation on a computer:

Trick #1: F.T. $\quad e^{i\vec{k}_\perp\cdot\vec{r}_\perp} \rightarrow e^{2\pi i\vec{u}\cdot\vec{r}} \qquad \vec{k}_\perp = 2\pi\vec{u}$

$\downarrow$

DFT $\quad e^{2\pi i(m_x n_x/N + m_y n_y/N)} \qquad m_x \frac{n_x}{N} = u_x x$

Trick #2: Discretization $\quad x = m_x \underbrace{\Delta x}_{\text{sampling pitch (space between pixels)}}$

$u_x = n_x \Delta u$

$\frac{\cancel{m_x n_x}}{N} = \cancel{m_x n_x}\Delta x \Delta u$

Put all this together: $\quad \Delta u = \frac{1}{N\Delta x} \leftarrow \boxed{\Delta x \Delta u = \frac{1}{N}}$

$$\exp\left(\frac{-izk_\perp^2}{2k}\right) = \exp\left(-iz\frac{4\pi^2 u^2}{2\left(\frac{2\pi}{\lambda}\right)}\right) = \exp\left(-iz\pi\lambda u^2\right) = \exp\left(-iz\pi\lambda n_x^2 \Delta u^2\right)$$

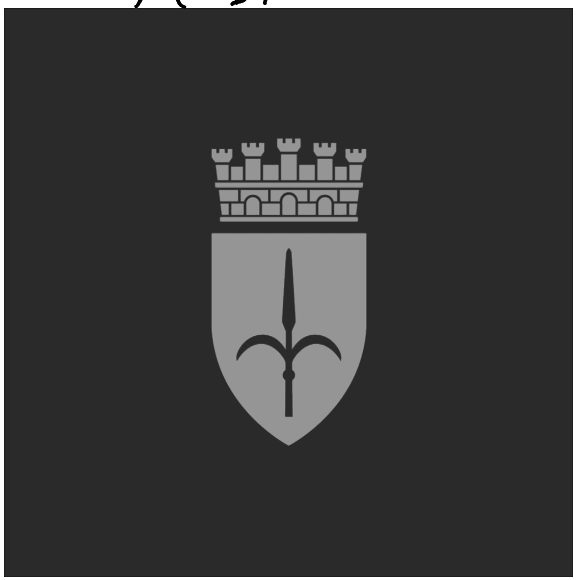
$$= \exp\left(-i\pi\left(\frac{z}{\Delta x}\right)\left(\frac{\lambda}{\Delta x}\right)\left(\frac{n_x}{N}\right)^2\right)$$

Forward propagation

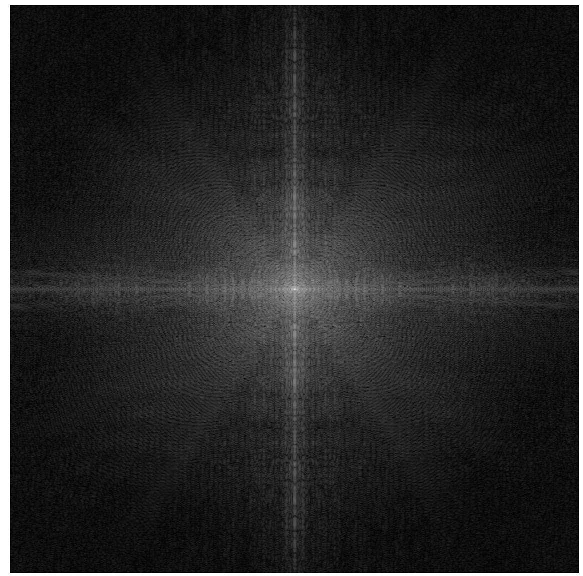
A numerical recipe

$\frac{n_x}{N}$: numpy.fft.fftfreq

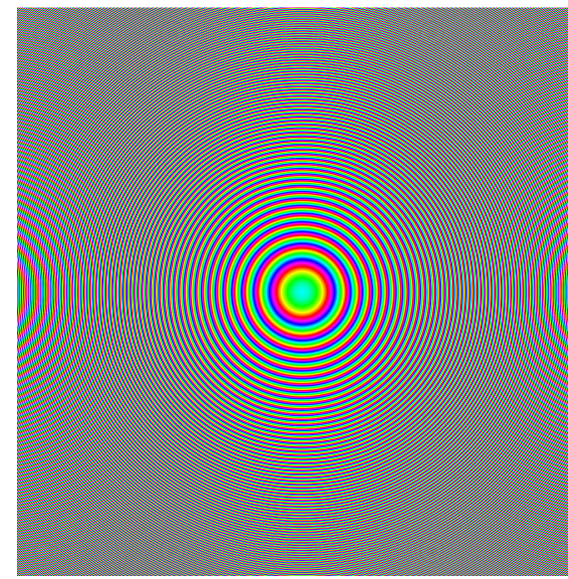
$\psi(\vec{r}_\perp; z=0)$

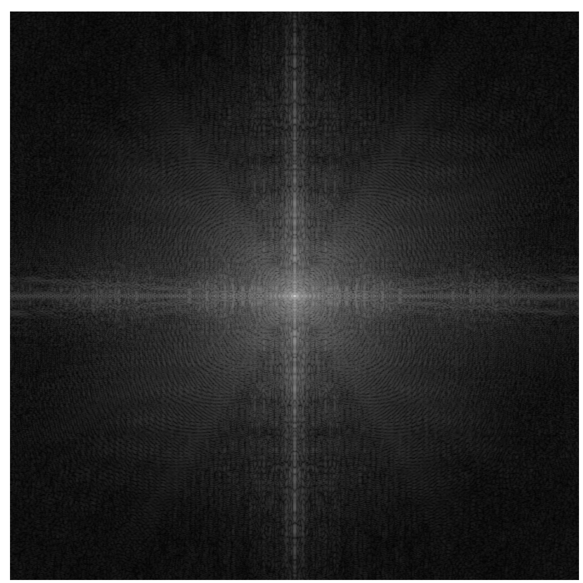


$\mathcal{F}$



$\times \exp\left(\frac{-izk_\perp^2}{2k}\right)$





$\mathcal{F}^{-1}$

Near field, far field

$$\psi(r_\perp; z) = \mathcal{F}^{-1}\left\{ \mathcal{F}\{\psi(r_\perp; z=0)\} \exp\left(\frac{-izk_\perp^2}{2k}\right)\right\}$$

convolution!

$$= \psi(\vec{r}_\perp; z=0) * P_z(\vec{r}_\perp)$$

$$\mathcal{F}^{-1}\left\{\exp(-i\pi\lambda z u^2)\right\}$$

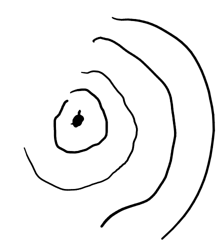
$$\parallel$$

$$\frac{-2\pi i}{\lambda z} \exp\left(i\pi \frac{r^2}{\lambda z}\right)$$

emission from a point source

$$\psi(\vec{r}; z) = \frac{-2\pi i}{\lambda z} \int d^2r' \, \psi(\vec{r}'; z=0) \exp\left(\frac{i\pi(\vec{r}-\vec{r}')^2}{\lambda z}\right)$$

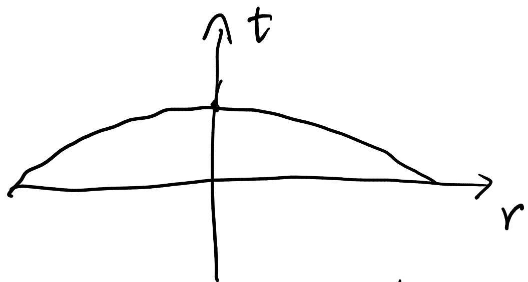
"Fresnel-Huygens integral"



Back focal plane of a lens

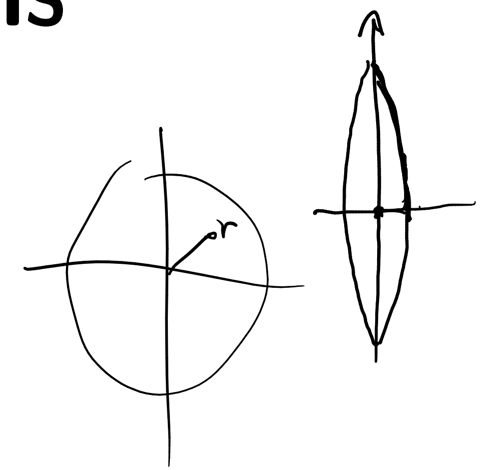
$\alpha > 0$: convergent

* model for a thin lens thickness profile:



$$t(r) = t_0 - \alpha r^2$$

α: curvature of the lens profile



* phase of wavefield passed the lens

$n-1$: phase difference with respect to air

$$(\phi = k(n-1)t) \qquad \phi(\vec{r}_\perp) = \frac{2\pi}{\lambda}(n-1)\,t(\vec{r}_\perp)$$

$$= \underbrace{\frac{2\pi}{\lambda}(n-1)\,t_0}_{\text{doesn't matter}} - \frac{2\pi}{\lambda}(n-1)\,\alpha r_\perp^2$$

* at exit of lens:

$$\psi(\vec{r}_\perp) = \psi_0(\vec{r}_\perp)\cdot \exp\left(-ik(n-1)\,\alpha\, r_\perp^2\right)$$

* propagate further:

$$\psi(\vec{r}_\perp; z) = \frac{-2\pi i}{\lambda z}\int d^2r'\, \psi_0(\vec{r}')\, \underbrace{\exp\left(-i\overset{\frac{2\pi}{\lambda}}{k}(n-1)\,\alpha\, \vec{r}'^2\right) \exp\left(\frac{i\pi(\vec{r}-\vec{r}')^2}{\lambda z}\right)}_{*}$$

Back focal plane of a lens

definition $(n-1)\alpha := \frac{1}{2f}$

focal distance

$$* = \exp\left[\frac{2\pi i}{\lambda}\left(-\overbrace{(n-1)\alpha}^{\frac{1}{2f}}\, r'^2 + \frac{\left(r^2 - 2\vec{r}\cdot\vec{r}\,' + r'^2\right)}{2z}\right)\right]$$

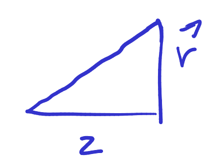
$$= \exp\left(\frac{i\pi r^2}{\lambda z}\right)\exp\left(\frac{i\pi}{\lambda}\left(\frac{1}{z}-\frac{1}{f}\right)r'^2\right)\exp\left(2\pi i\,\frac{\vec{r}\cdot\vec{r}\,'}{\lambda z}\right)$$

$$\psi(\vec{r}_\perp; z) = \frac{-2\pi i}{\lambda z}\exp\left(\frac{i\pi r^2}{\lambda z}\right)\int d^2r'\,\psi_0(\vec{r}\,')\,\underbrace{\exp\left(\frac{i\pi}{\lambda}\left(\frac{1}{z}-\frac{1}{f}\right)r'^2\right)}\,\exp\left(2\pi i\,\vec{r}\,'\cdot\left(\frac{\vec{r}}{\lambda z}\right)\right)$$

* Interesting: $z = f$ $\quad \frac{1}{z} - \frac{1}{f} = 0$

$$\hookrightarrow \psi(\vec{r}_\perp; z=f) = \ldots \int d^2r'\,\psi(\vec{r}\,')\exp\left(2\pi i\,\vec{r}\,'\cdot\overbrace{\left(\frac{\vec{r}}{\lambda z}\right)}^{\vec{u}}\right)$$

$$= \ldots\ \mathcal{F}\{\psi\}\left(\vec{u} = \frac{\vec{r}}{\lambda z}\right)$$



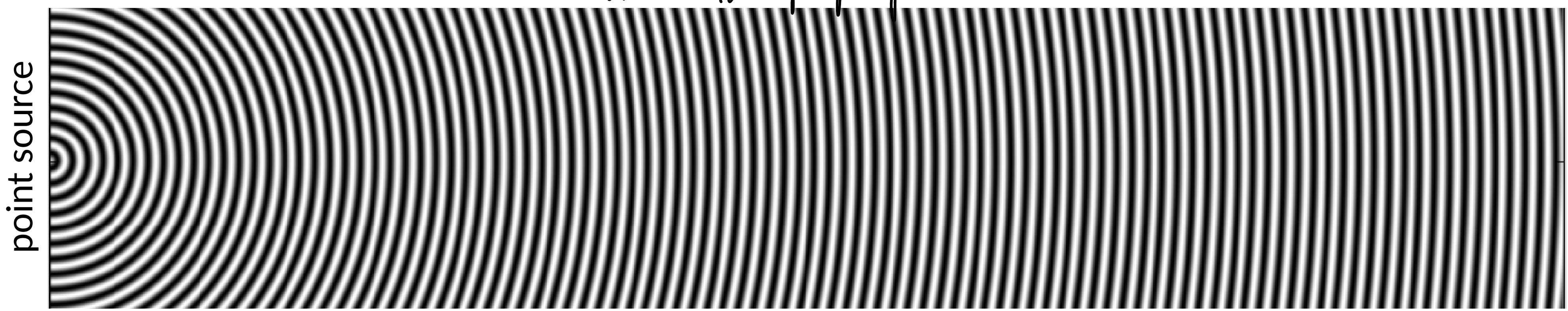
($f=0$: no lens
$z\to\infty$: F.T.
far-field propagation)

A lens acts as a Fourier transform operator!

Plane waves, point sources

$$\psi(\vec{r}_\perp; z \to \infty) = \frac{2\pi i}{\lambda z} \exp\left(\frac{i\pi r^2}{\lambda z}\right) \mathcal{F}\left\{\psi_0(\vec{r})\right\}\left(\vec{u} = \frac{\vec{r}}{\lambda z}\right)$$

Far-field propagation



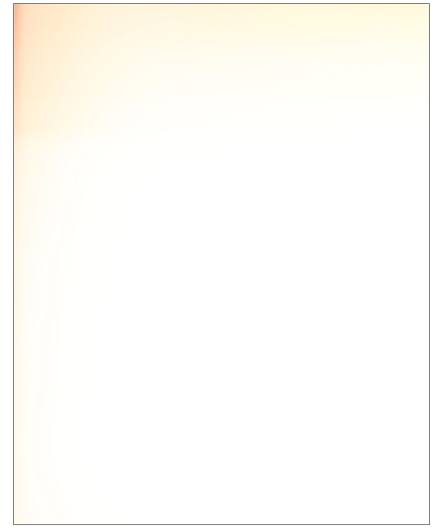
circular waves
evanescent waves
contact region

parabolic waves
near field
Fresnel region

plane waves
far field
Fraunhofer region

Why optical elements?

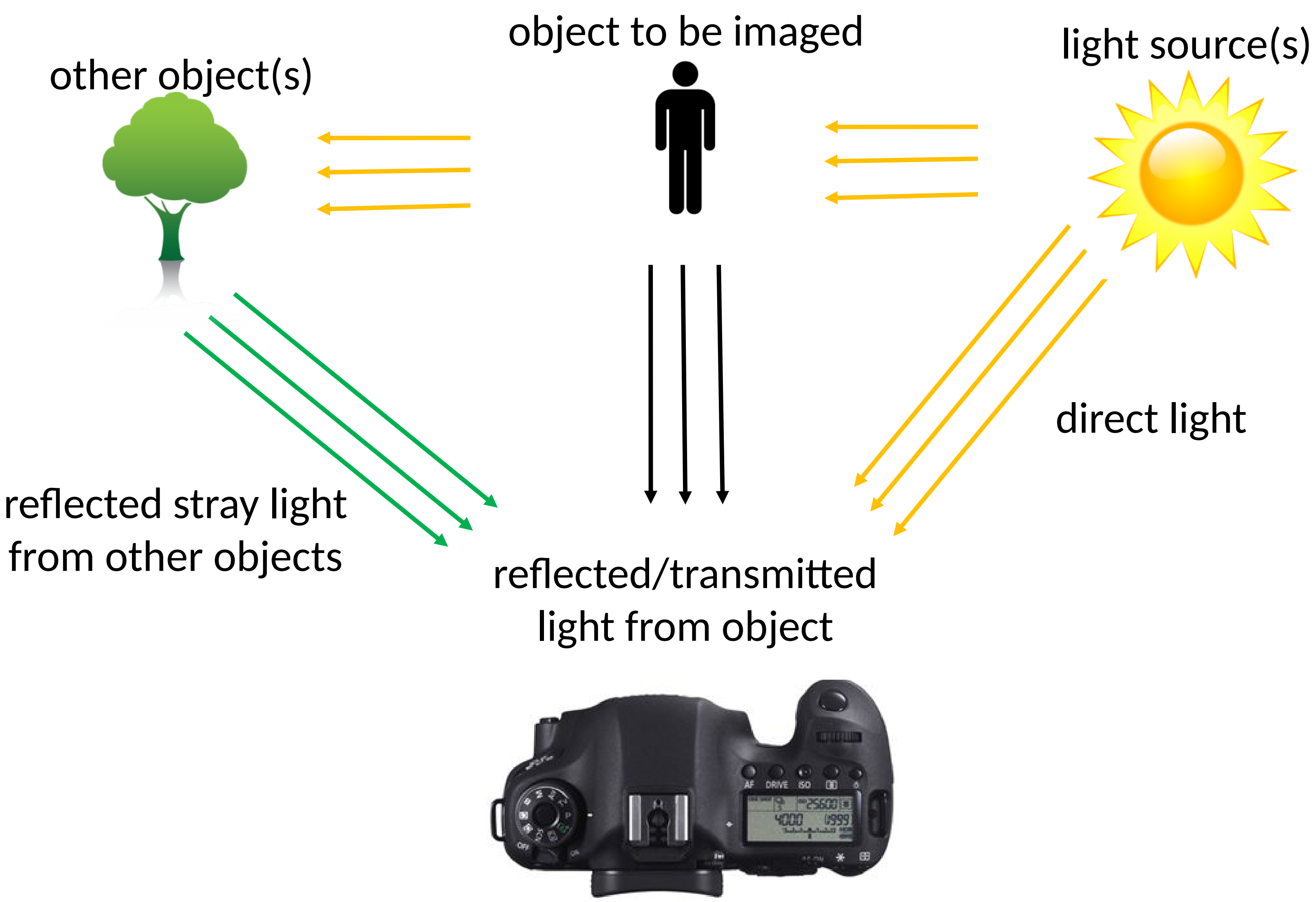
with objective lens



without objective lens

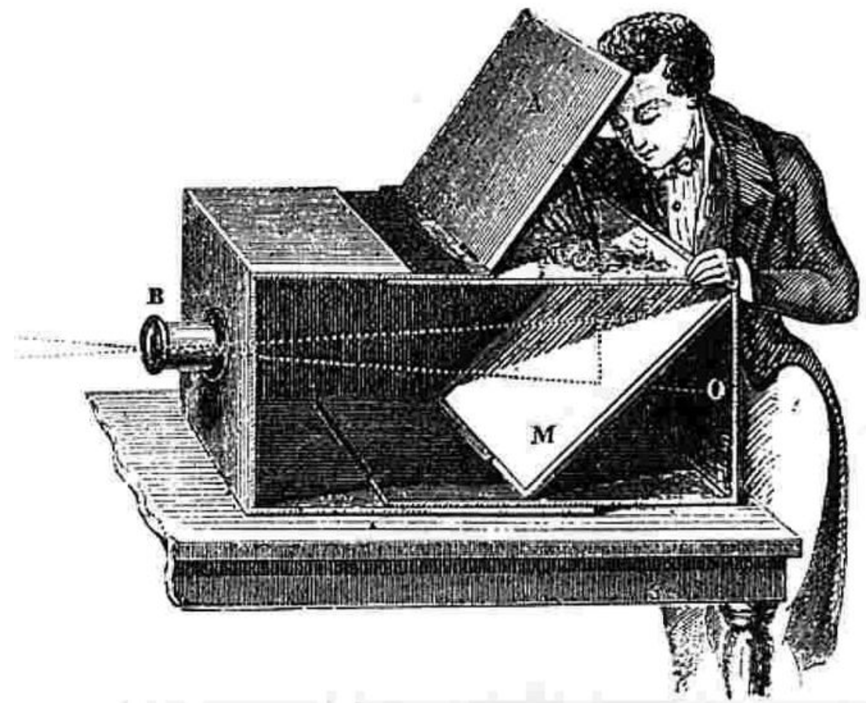
Why optical elements?

- Information from many sources overlaps in detector plane
- Need models to understand image forming systems



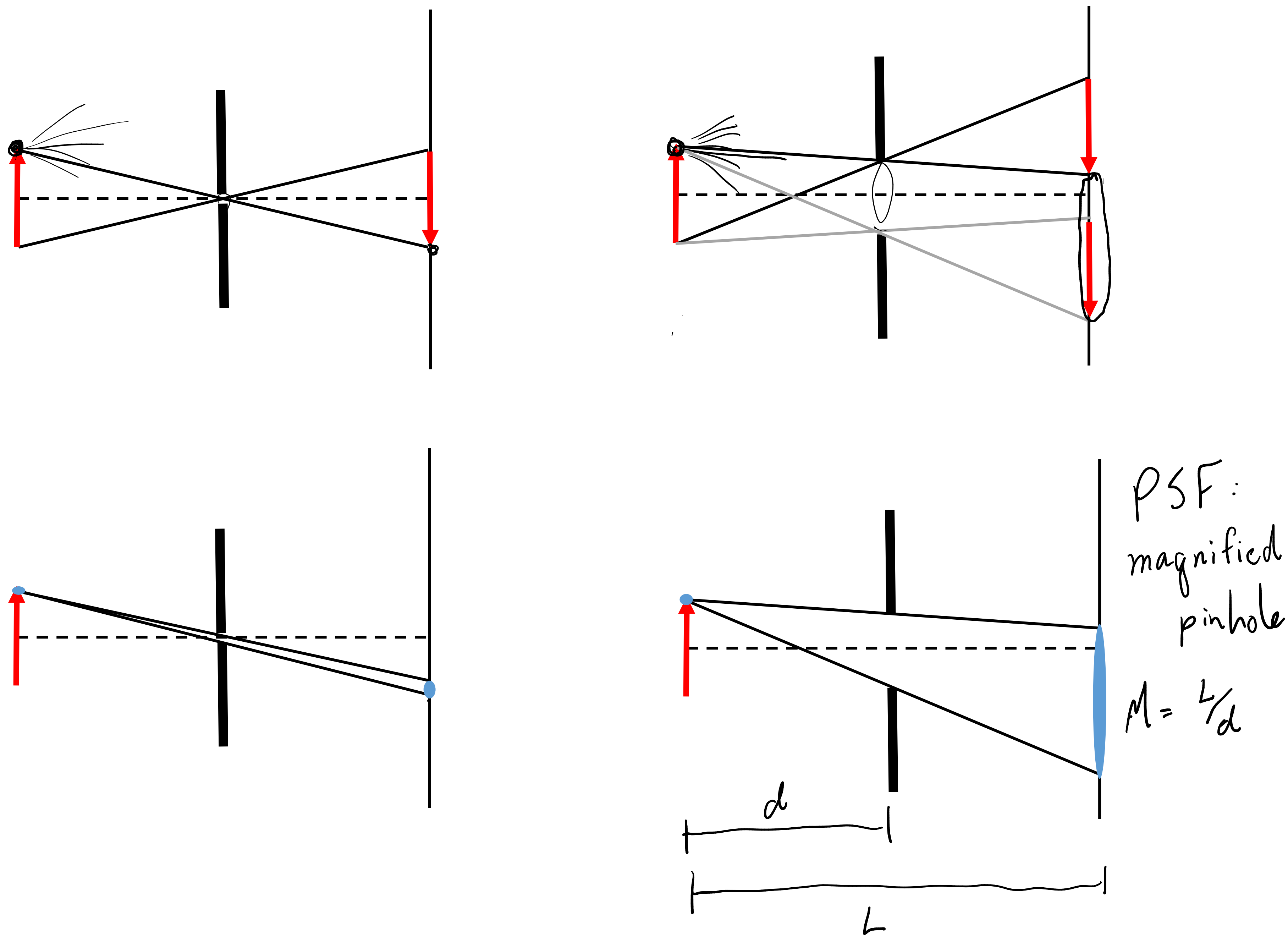
Pinhole camera model

camera obscura



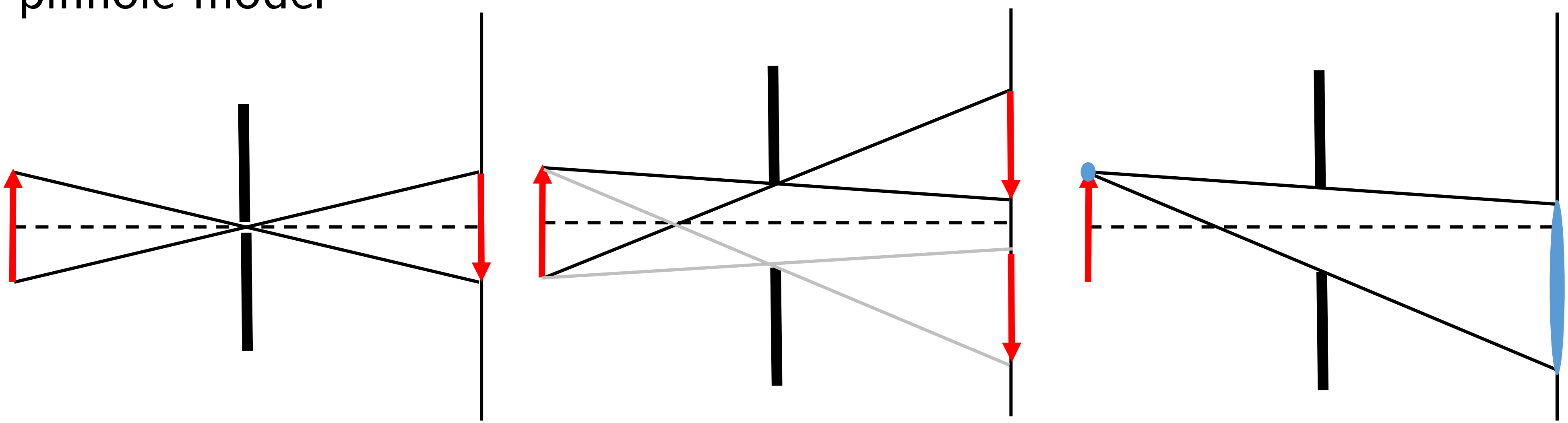
Pinhole camera model

PSF determined by aperture width

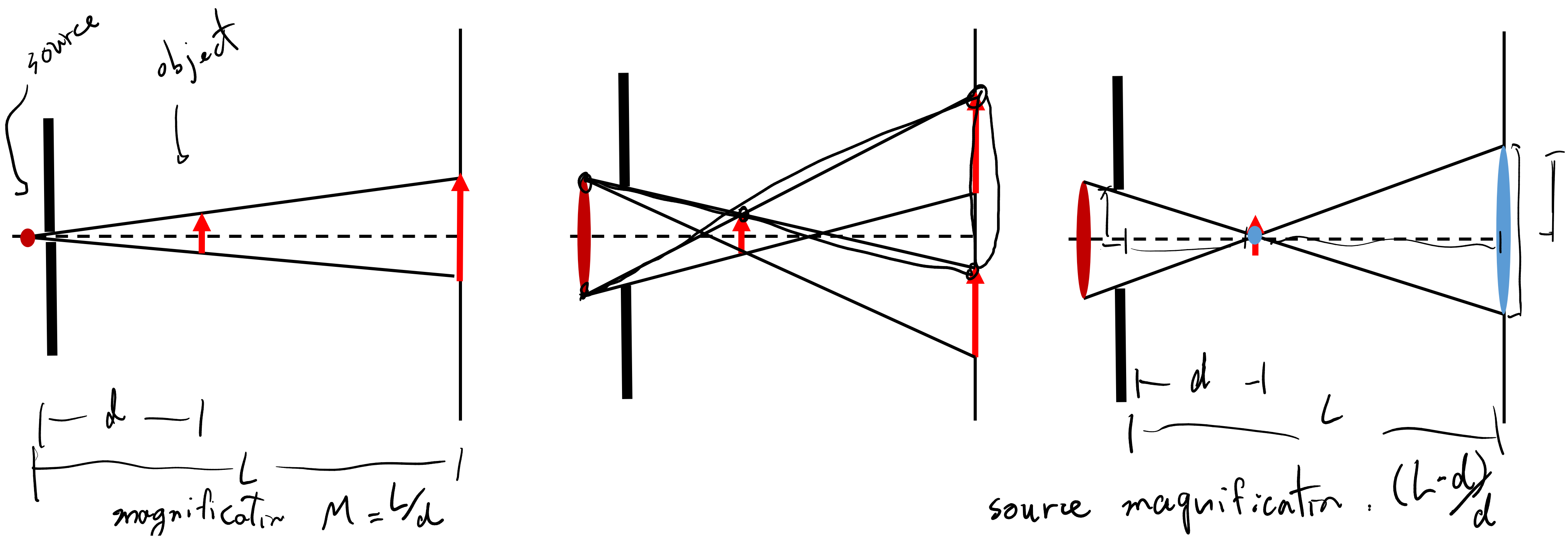


Projection model

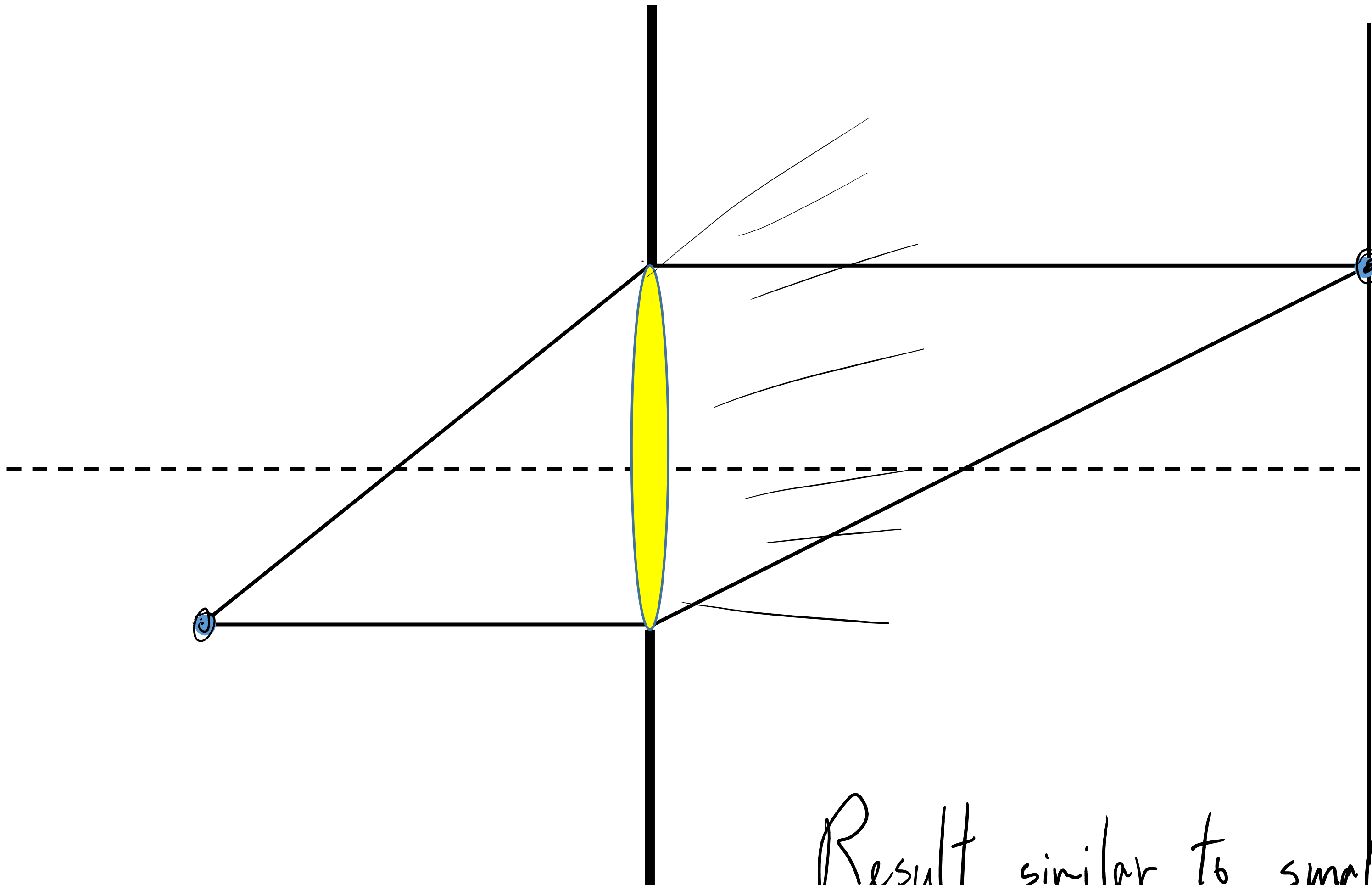
pinhole model



projection model



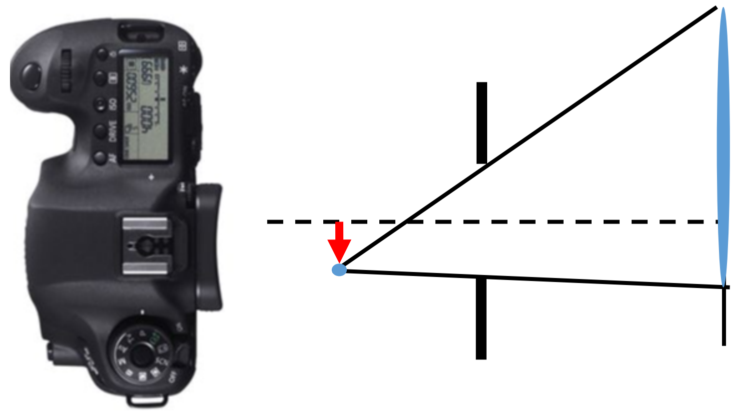
Lens camera model



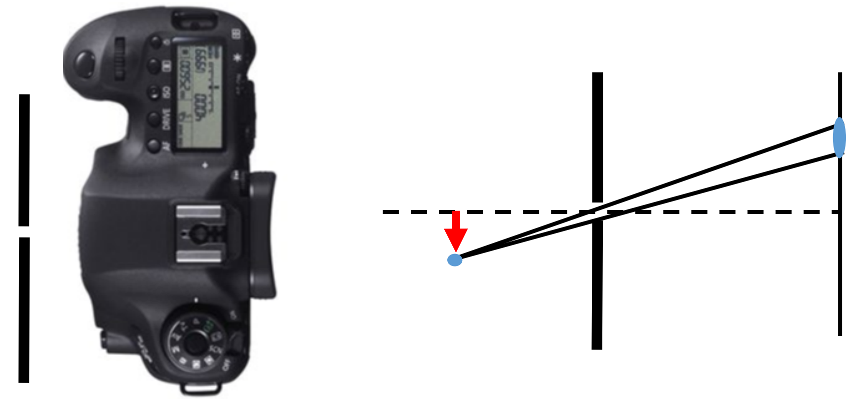
Result similar to small pinhole
but without compromise on intensity

Lens camera model

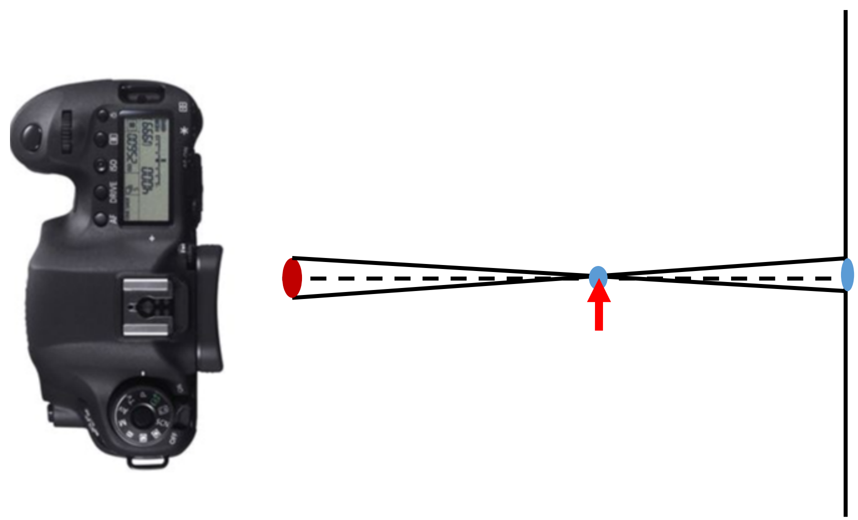
lensless model



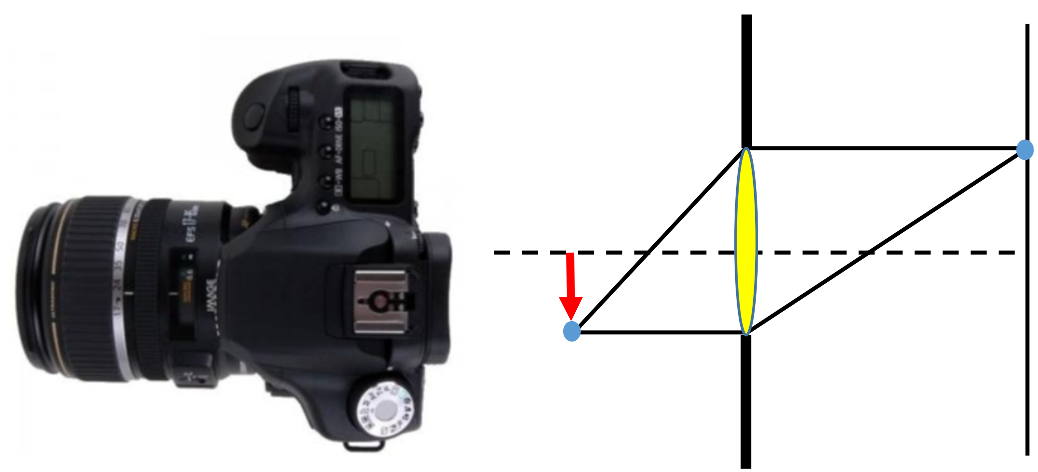
pinhole camera model



projection model

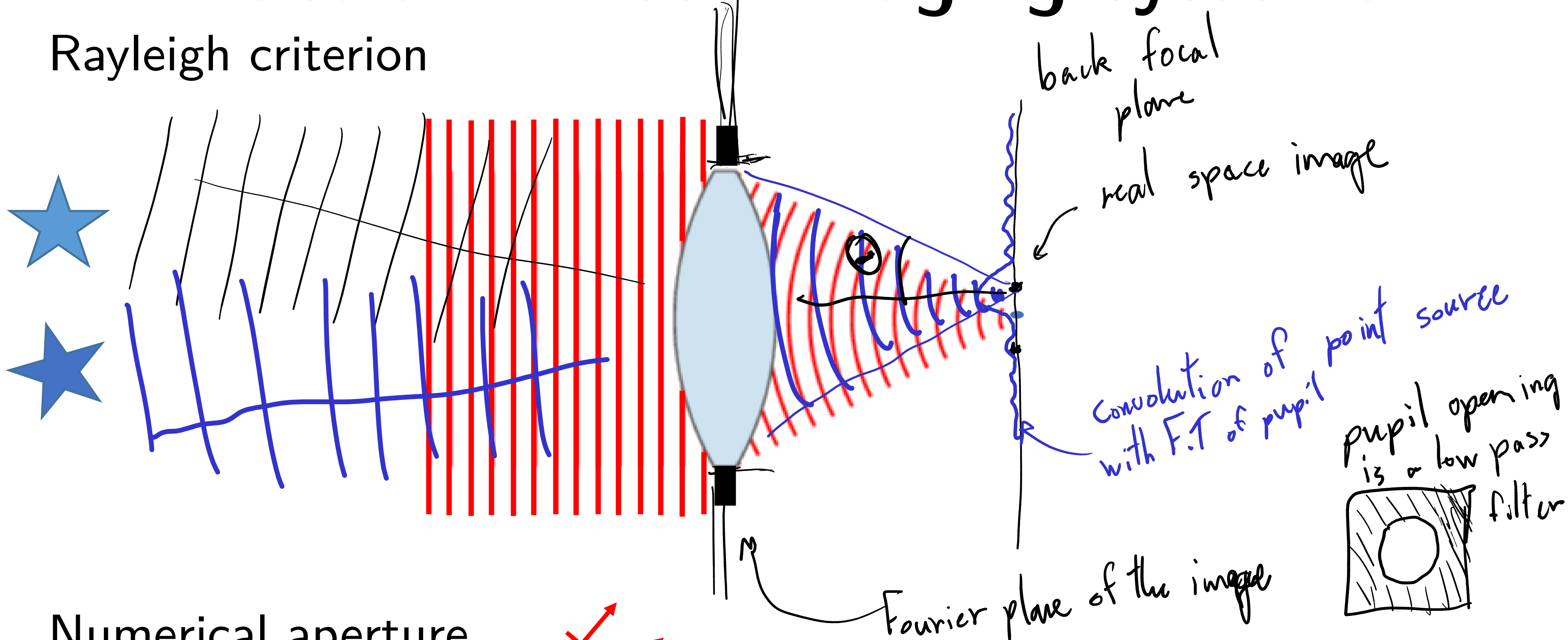


lens camera model

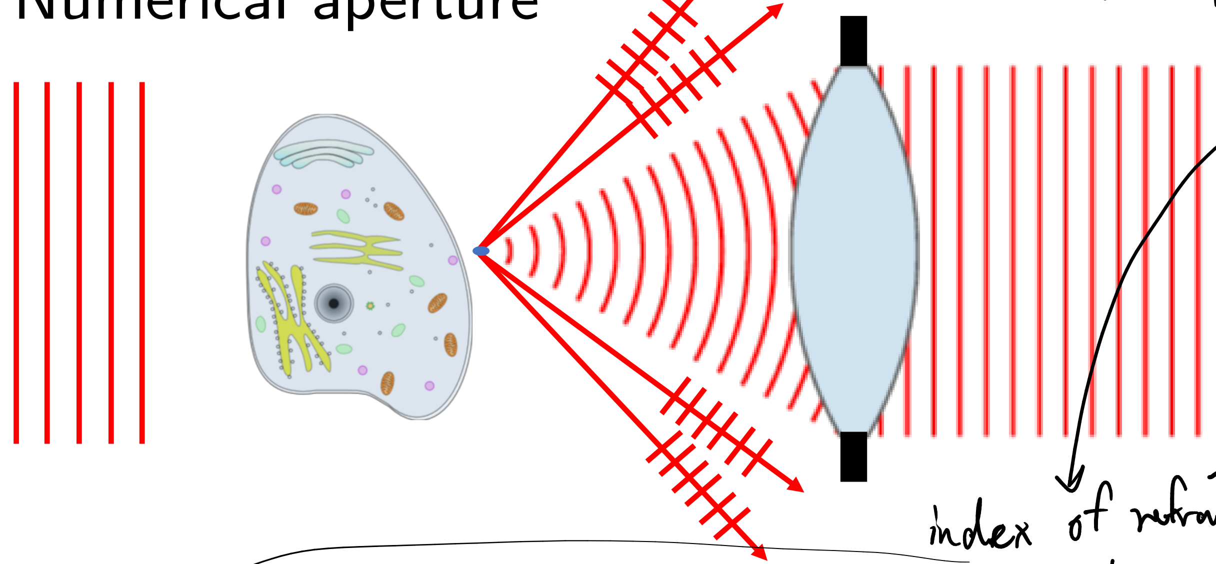


Diffraction-limited imaging systems

- Rayleigh criterion



- Numerical aperture



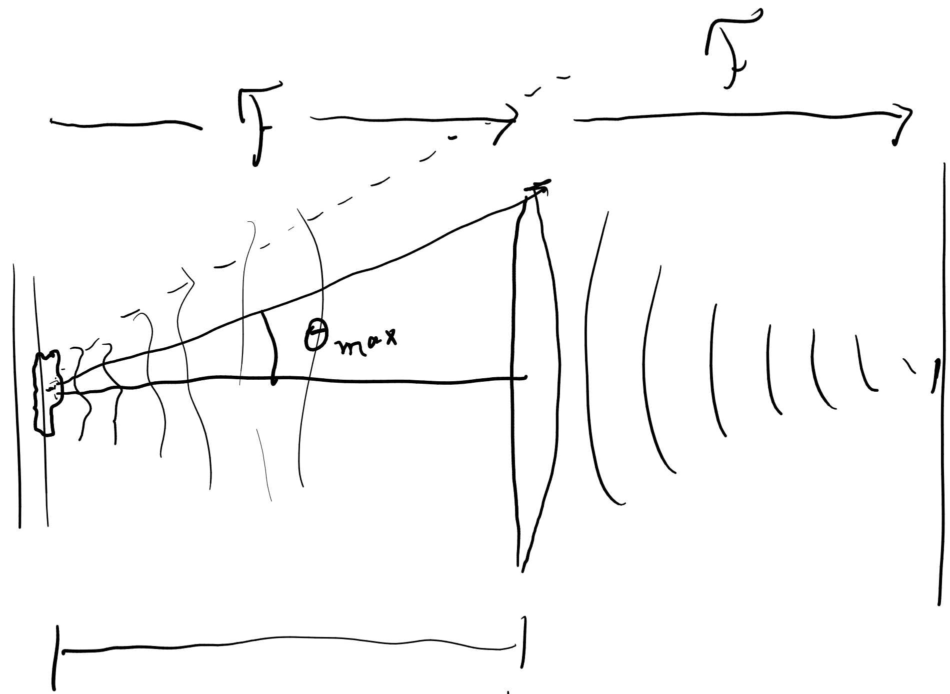
$n \sin\theta = NA$

numerical aperture

resolution

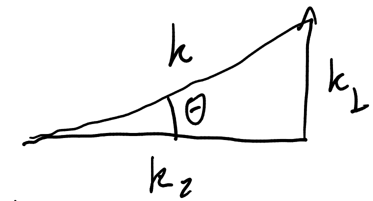
$$\boxed{d_{min} = 1.22 \frac{\lambda}{2NA}}$$

Rayleigh definition for resolution



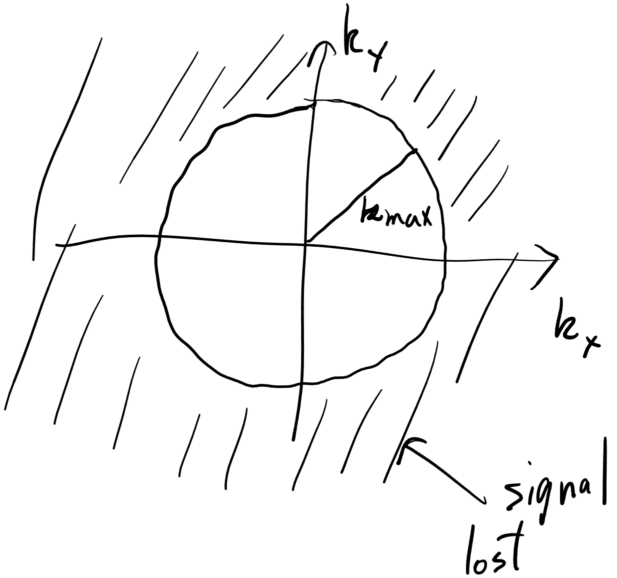
small object ⇒ Fraunhofer regime already in the lens plane

Far field:



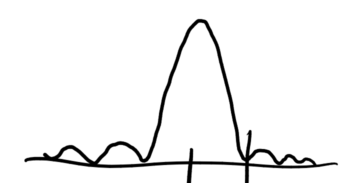
$$\sin\theta_{max} = \frac{k_{max}}{k}$$

maximum spatial frequency captured by a lens with opening given by θ_{max}



F.T. of disc radius k_{max} : $\dfrac{J_1(rk_{max})}{rk_{max}}$

J_1 : First Bessel function



$\boxed{\text{Rayleigh: resolution = distance of first 0 from origin } J_1(3.83) = 0}$

$r_{min} k_{max} = 3.83$

$$PSF = \left| \frac{J_1(rk_{max})}{rk_{max}} \right|^2$$ PSF!

Scanning systems

$$r_{min} = \frac{3.83}{k \sin\theta_{max}}$$

$$\frac{3.83}{\pi} = 1.22 \qquad = \frac{1.22\,\lambda}{2 \sin\theta_{max}}$$

$$NA = \sin\theta_{max}$$

$$\Rightarrow d \approx r_{min} = 1.22 \frac{\lambda}{2NA}$$

Transmission

- **S**canning **T**ransmission **E**lectron **M**icroscopy
- **S**canning **T**ransmission **X**-ray **M**icroscopy
- …

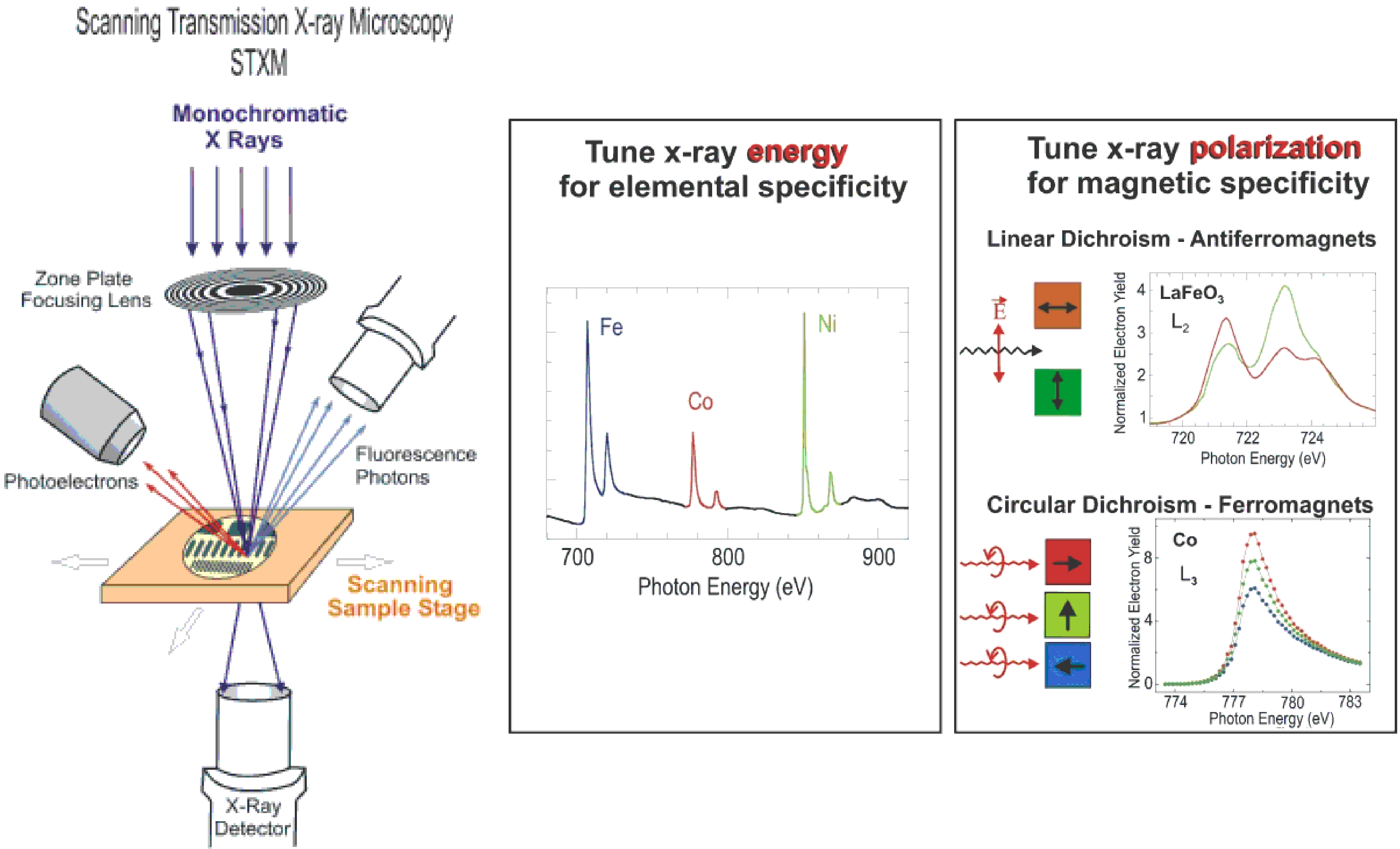
Indirect (reflection, scattering, fluorescence, …)

- **L**aser **S**canning **C**onfocal **M**icropsopy
- **S**canning **E**lectron **M**icroscopy
- **X**-ray **F**luorescence **M**icroscopy
- **P**hoto**E**mission **E**lectron **M**icroscopy
- ...

Physical probe

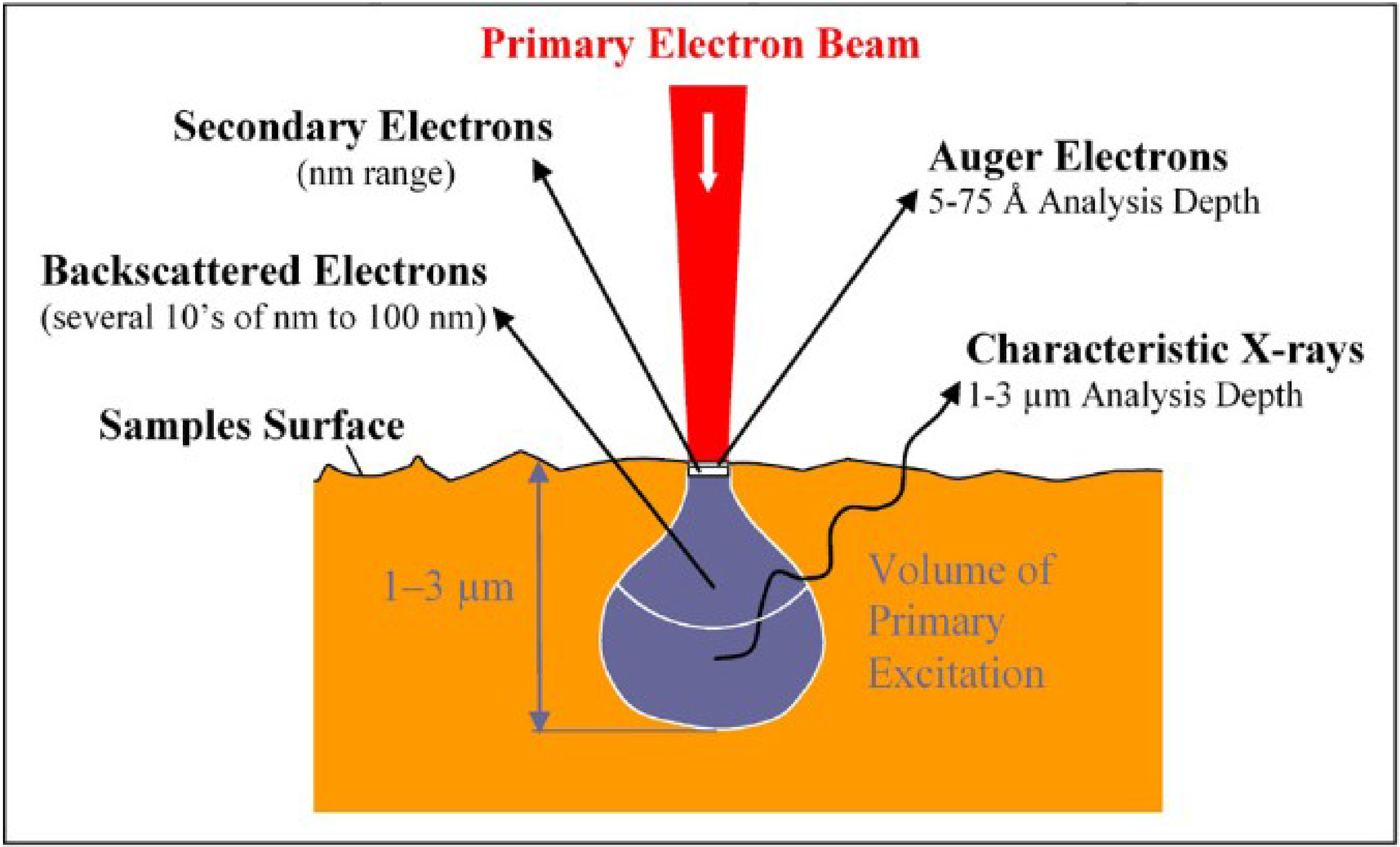
- **A**tomic **F**orce **M**icroscopy
- **S**canning **T**unneling **M**icroscopy
- ...

Scanning transmission X-ray microscopy

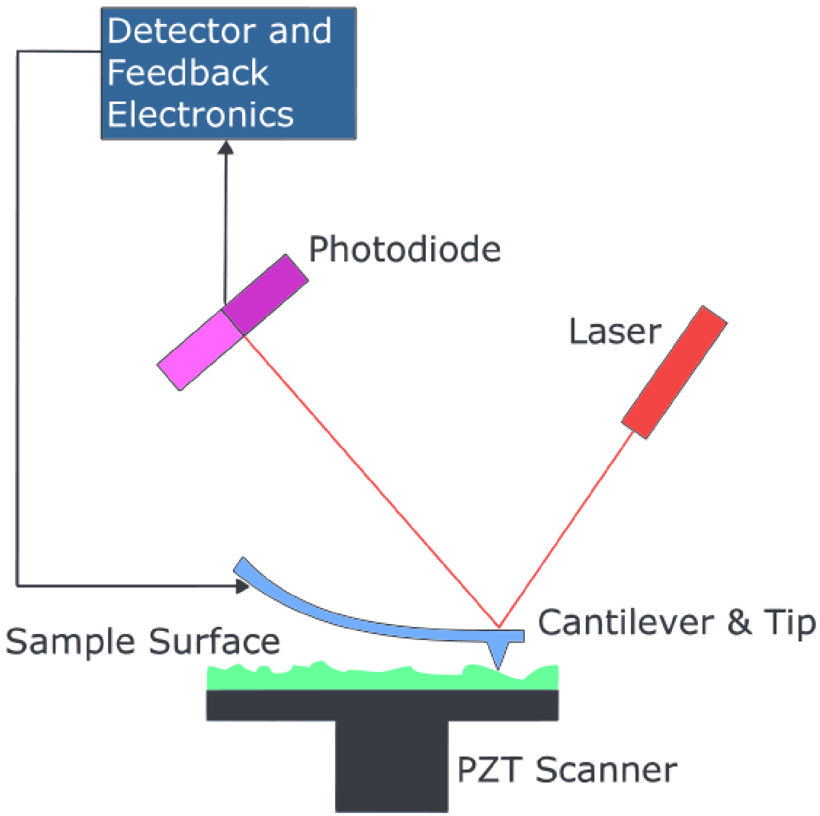


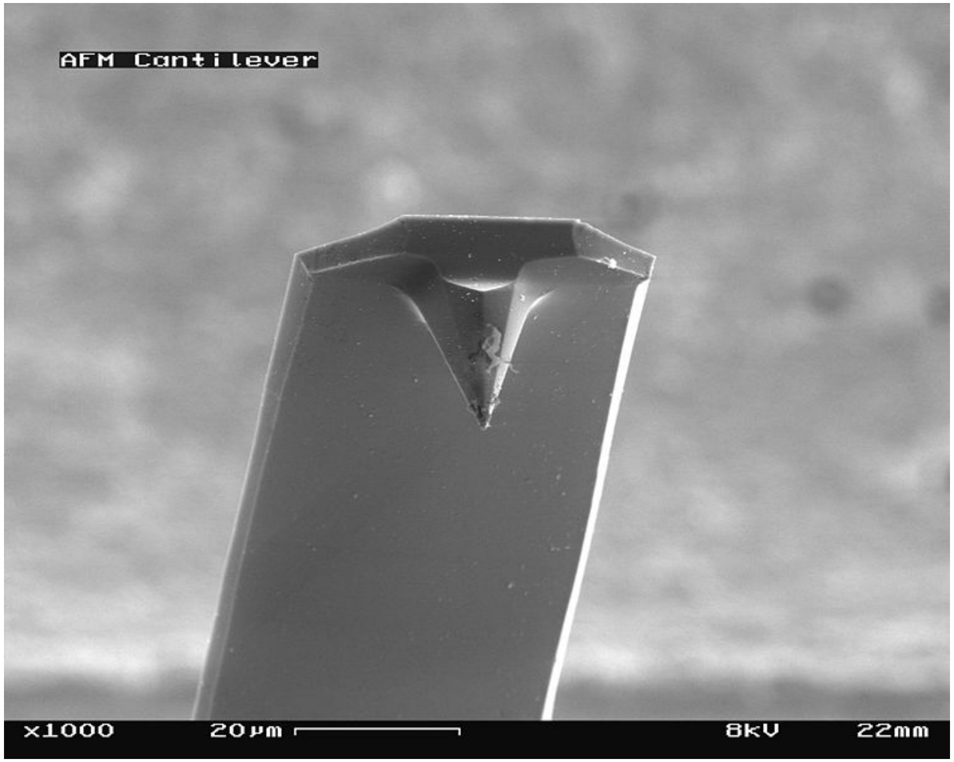
source: http://www-ssrl.slac.stanford.edu

Scanning electron microscopy



Atomic force microscopy





Resolution in scanning systems

Resolution mainly limited by probe size, interaction region

e.g. $\frac{J_1(x)}{x}$

Note: coherent vs incoherent imaging

coherent:

Image: $I = |PSF * \psi|^2$

propagated wavefield

incoherent:

Image: $I = |PSF|^2 * |\psi|^2$

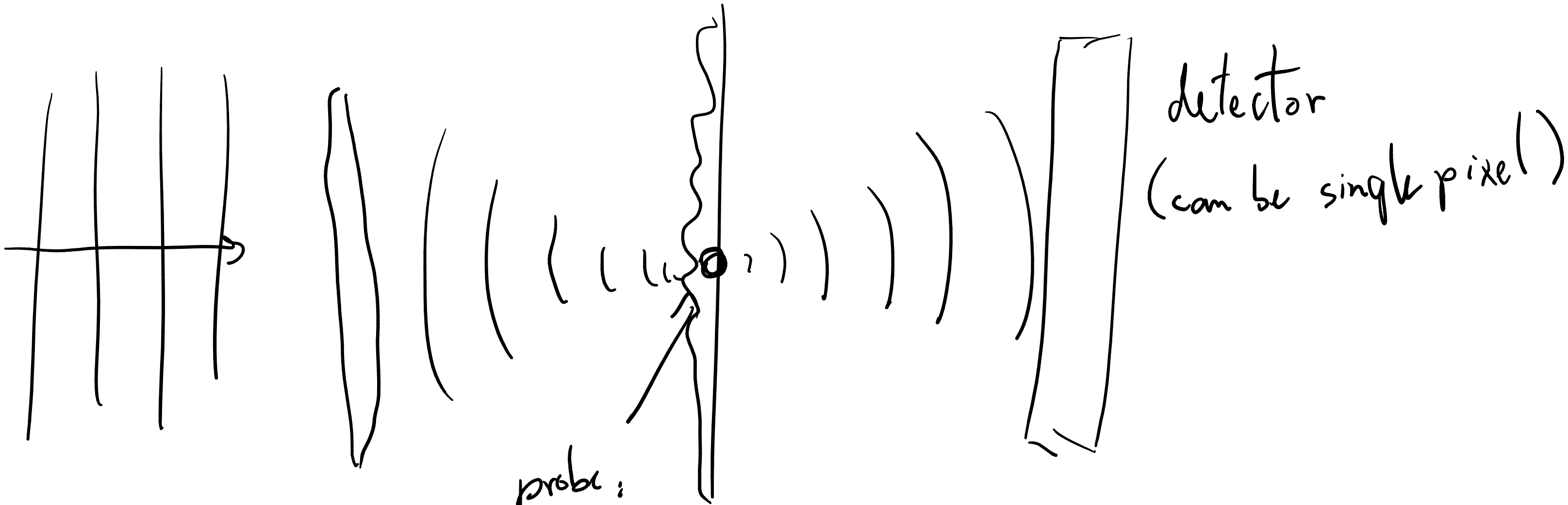
coherent vs incoherent

can interfere vs cannot interfere

scanning system = incoherent transmission

Scanning vs. full field systems

Transmission probe: the reciprocity theorem



PSF given by lens NA

$\Rightarrow$ resolution in a scanning system : $1.22 \dfrac{\lambda}{2NA}$

focusing lens

transmission system : objective lens