Image Processing for Physicists

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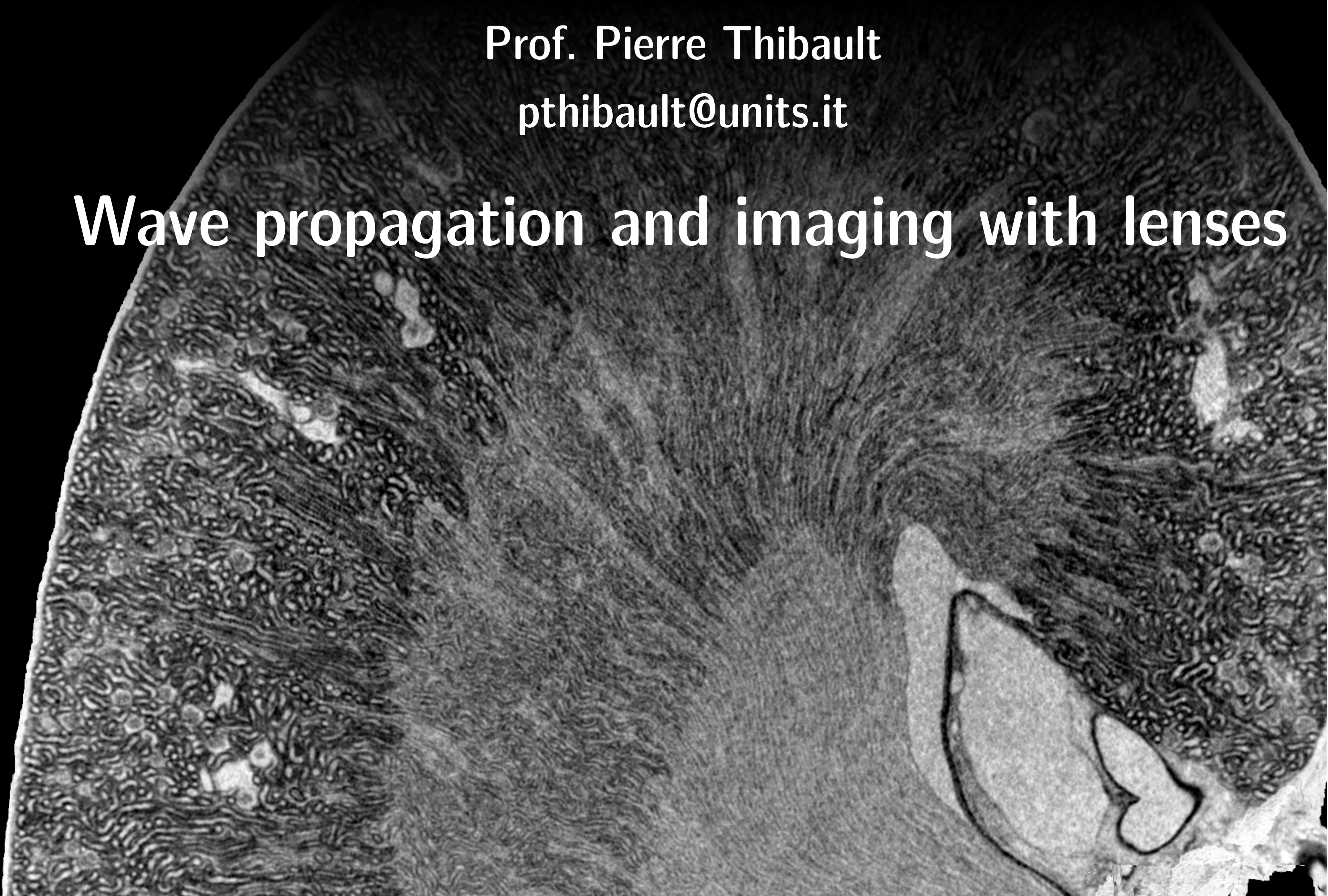
Wave propagation and imaging with lenses



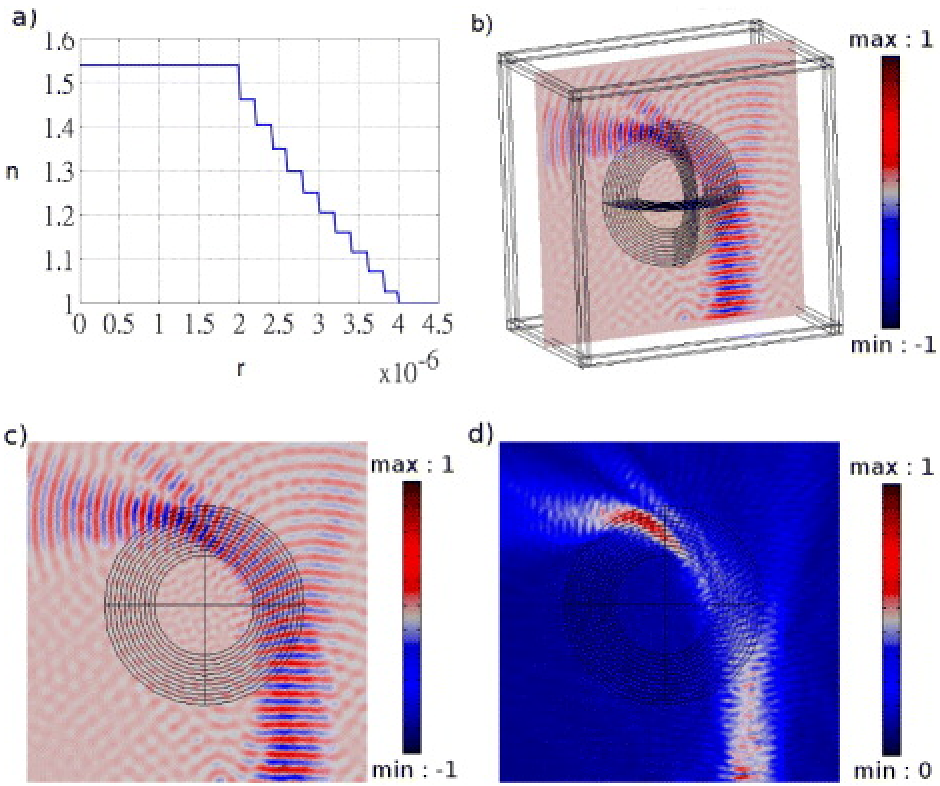
Overview

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

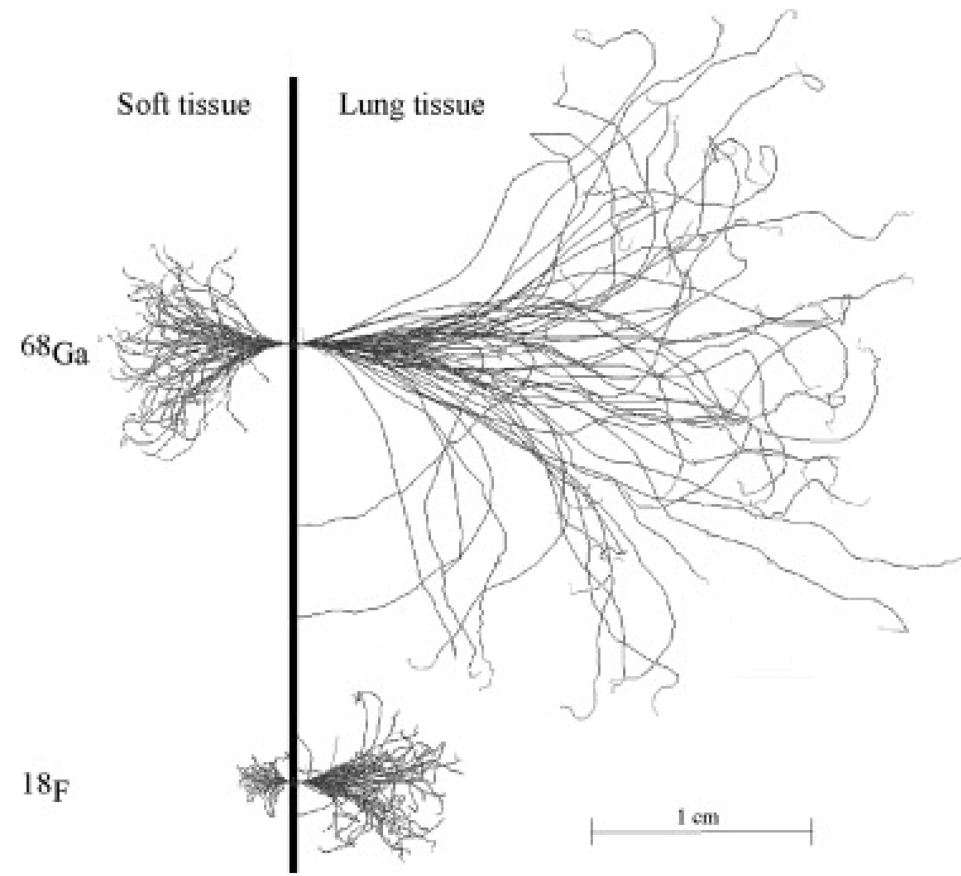
Propagation modeling

- 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.

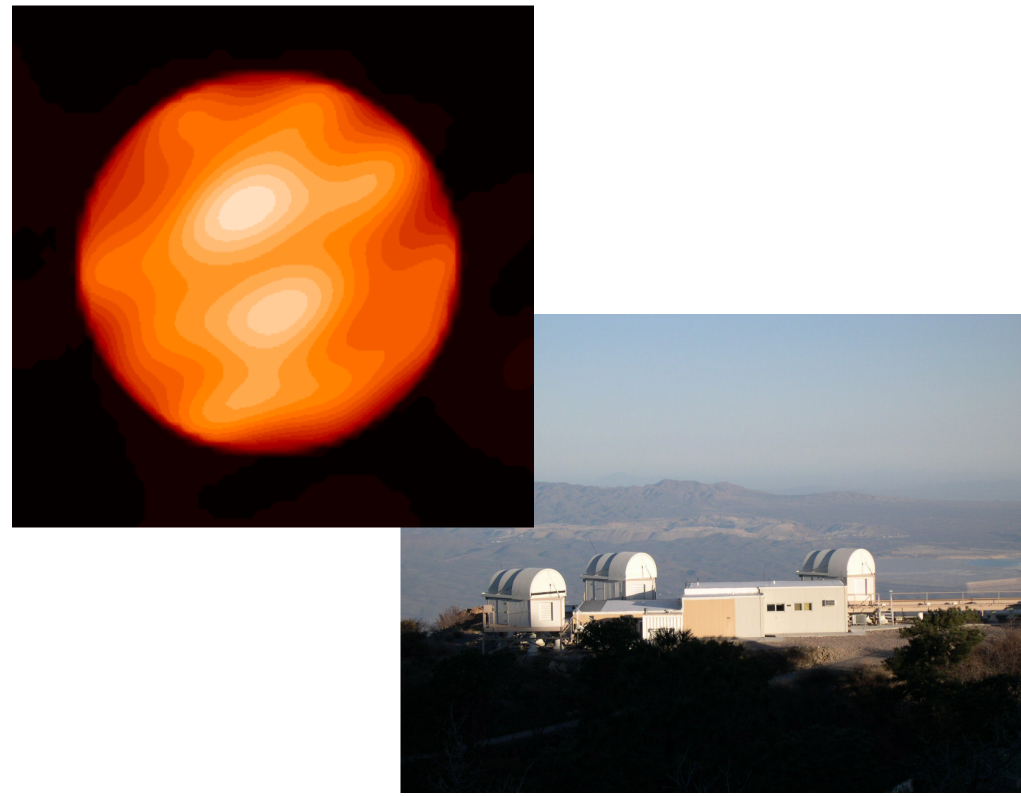
sources: T.M. Chang *et al.* New J. Phys. (2012)
A. Sanchez-Crespo, Appl. Rad. Isotopes (2012)

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

↳ Schrödinger's equation

fixed frequency

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

Consider solutions of the form $\psi(\vec{r}, t) \longrightarrow \psi(\vec{r}) e^{i\omega t}$

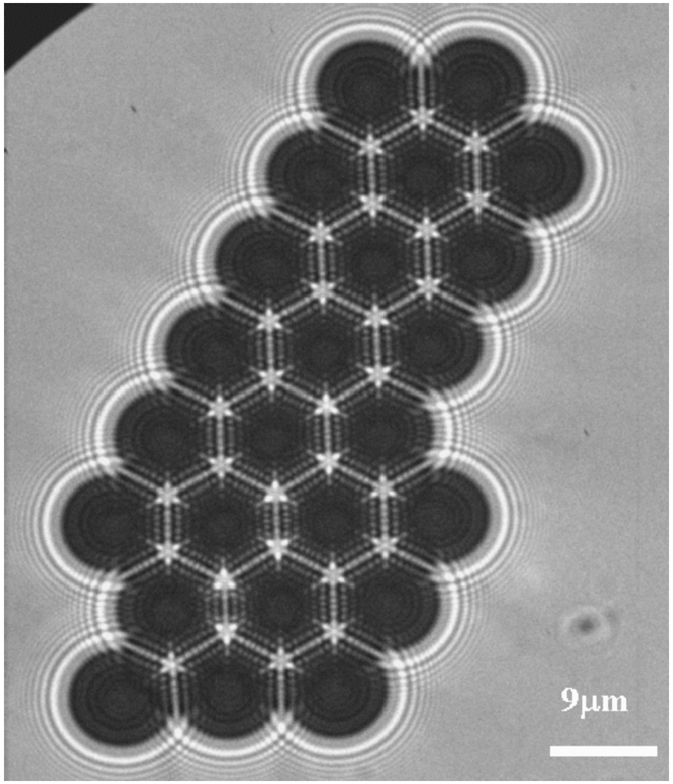
$$\nabla^2 \psi + k^2 n^2 \psi = 0 \qquad k^2 = \frac{\omega^2}{c^2}$$

$k = \frac{2\pi}{\lambda}$ wavenumber

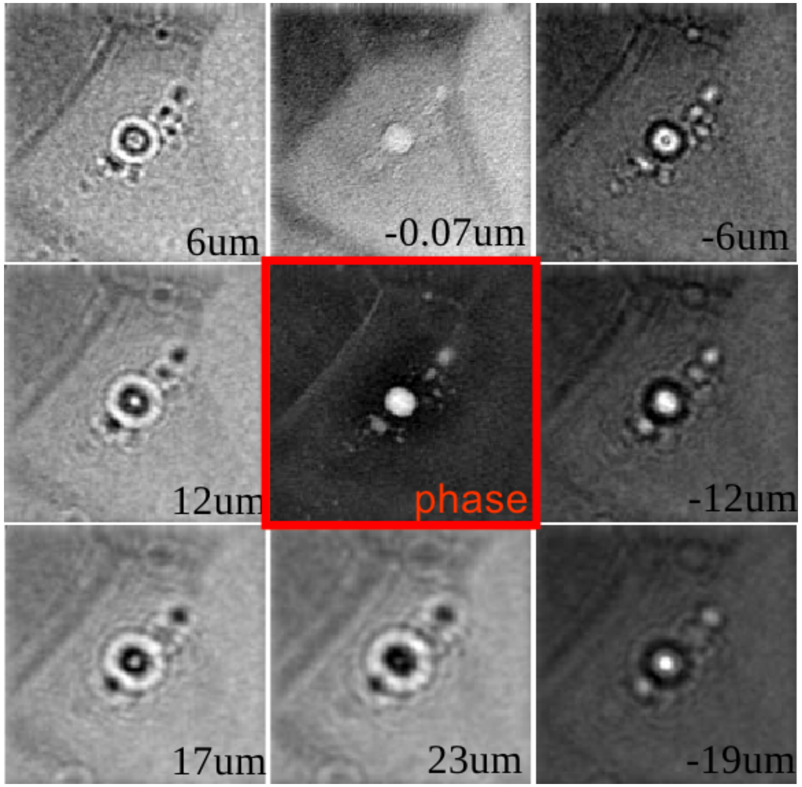
Propagation modeling

- 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 a superposition of plane waves

$$\psi(\vec{r}) = \sum_{\vec{q}} A_{\vec{q}}\, e^{i\vec{q}\cdot\vec{r}} \longleftarrow$$

sum is over $\vec{q}$ such that $|\vec{q}|^2 = k^2$

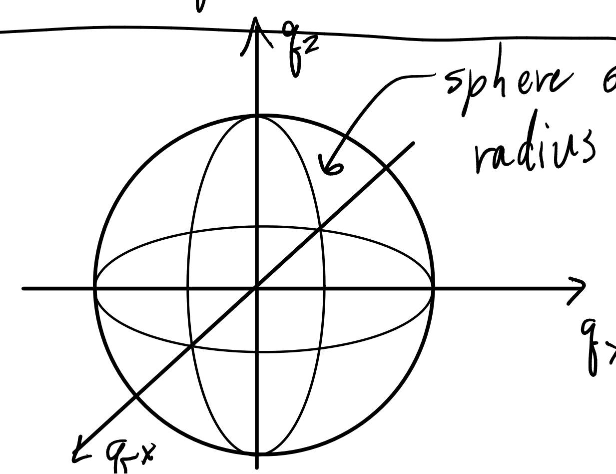
(with time:

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

$$\nabla^2\left(A_{\vec{q}}\, e^{i\vec{q}\cdot\vec{r}}\right) + k^2 A_{\vec{q}}\, e^{i\vec{q}\cdot\vec{r}} = A_{\vec{q}}\, e^{i\vec{q}\cdot\vec{r}}(-q^2) + k^2 A_{\vec{q}}\, e^{i\vec{q}\cdot\vec{r}} = 0$$

$$A_{\vec{q}}\, e^{i\vec{q}\cdot\vec{r}}(k^2 - q^2) = 0$$

$$q_x^2 + q_y^2 + q_z^2 = k^2 \longleftarrow$$ surface of a sphere

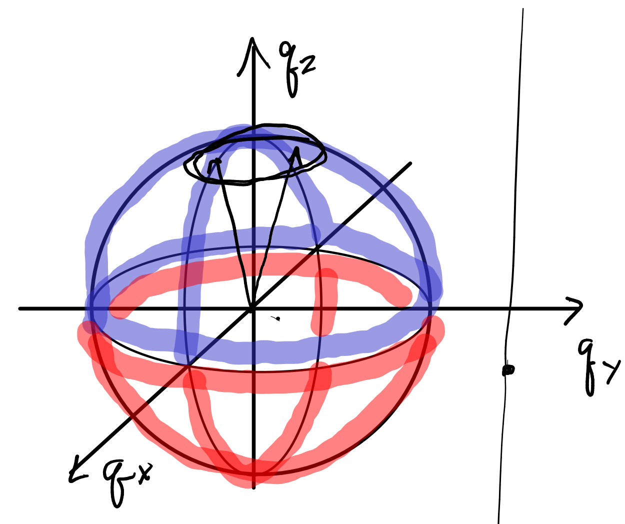


Only wavevectors lying on the surface of this sphere are part of the solution

The physics of propagation

Angular spectrum representation

$$q_z = \pm\sqrt{k^2 - q_x^2 - q_y^2}$$



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

$\cancel{A^{-}_{q_x q_y}} \to 0$ we consider only propagation along positive z

$$\psi(x, y, z) = \underbrace{\sum_{q_x q_y} A_{q_x q_y}\, e^{i(q_x x + q_y y)}}_{\text{2D Fourier transform!}}\, e^{i\sqrt{k^2 - q_x^2 - q_y^2}\, z}$$

Fourier synthesis equation for any propagating wavefield

Forward propagation

Case $z=0$: $\psi(x,y,z=0) = \sum_{q_x q_y} A_{q_x q_y} \exp(i(q_x x + q_y y))$ ← inverse Fourier transform for ψ

$$\Rightarrow \underbrace{A_{q_x q_y} = \mathcal{F}_{2D}\{\psi(x,y,z=0)\}}_{\text{method to compute the amplitudes of each plane wave component in the propagating wavefield}}$$

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

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

Discretization for implementation on a computer:

F.T. $e^{i\vec{q}_\perp \cdot \vec{r}_\perp} \longrightarrow e^{2\pi i \vec{u}\cdot\vec{r}}$ $\qquad \vec{q}_\perp = 2\pi \vec{u}$

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

$x = m_x \Delta x$ ← "pixel size" / "sampling rate"
"sampling pitch"

$u_x = n_x \Delta u$

Forward propagation

$$m_x n_x / N = u_x x = m_x \Delta x \, n_x \Delta u$$

$$\Rightarrow \Delta x \Delta u = 1/N \qquad \Delta u = \frac{1}{N \Delta x}$$

Paraxial approximation: (small angle approximation)

$$\sqrt{k^2 - q_\perp^2} = k\sqrt{1 - q_\perp^2/k^2} \simeq k\left(1 - \frac{q_\perp^2}{2k^2}\right) = k - \frac{q_\perp^2}{2k}$$

$$\Rightarrow \exp\left(iz\sqrt{k^2 - q_\perp^2}\right) \approx \underbrace{\exp(ikz)}_{\text{irrelevant for all purposes}} \exp\left(-\frac{izq_\perp^2}{2k}\right)$$

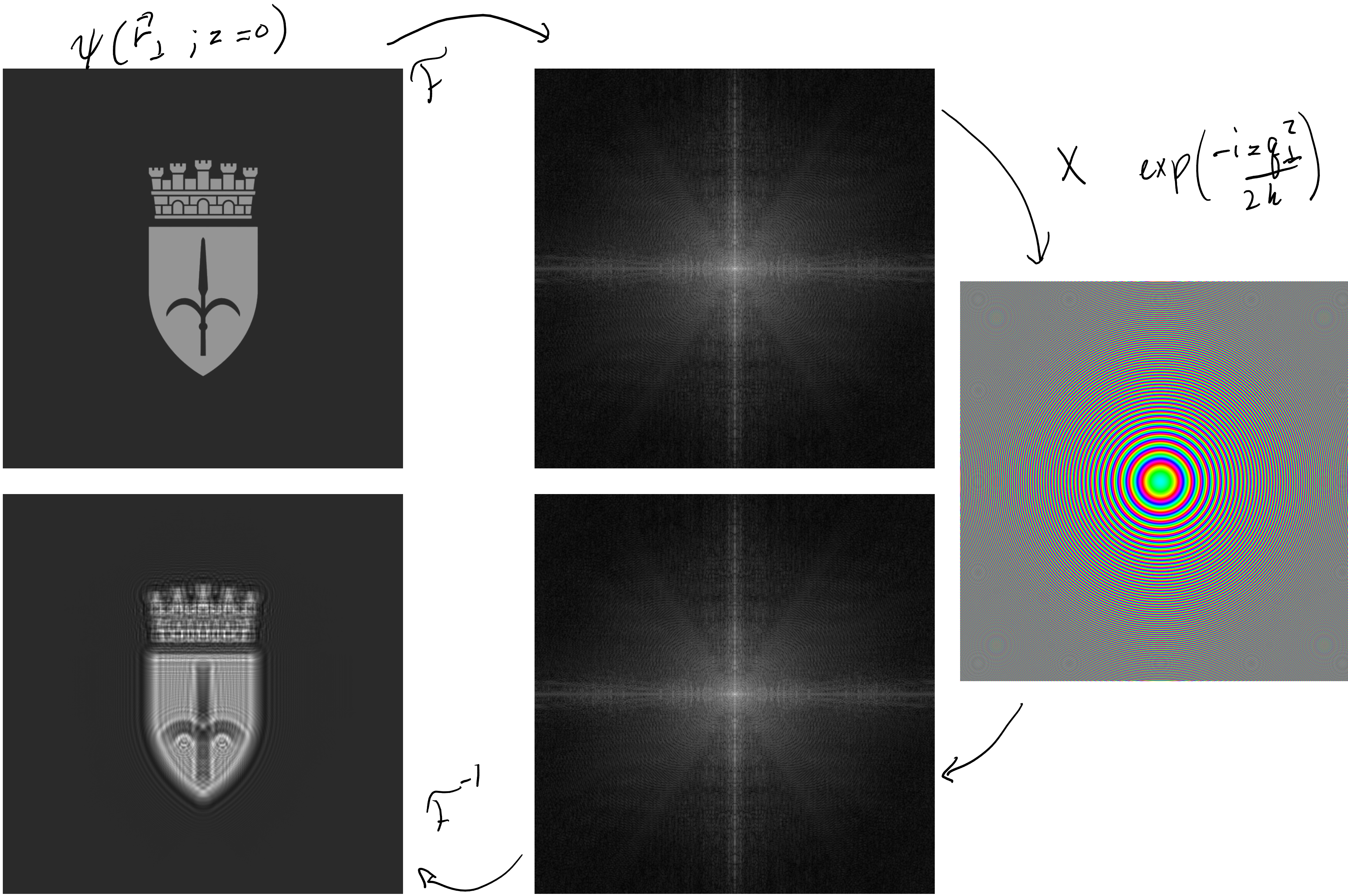
$$\frac{1}{N^2}\frac{1}{\Delta x^2}$$

$$\exp\left(\frac{-izq_\perp^2}{2k}\right) = \exp\left(-iz\frac{4\pi^2 u^2}{2\left(\frac{2\pi}{\lambda}\right)}\right) = \exp\left(-iz\pi\lambda u^2\right) = \exp\left[-iz\pi\lambda(n_x^2 + n_y^2)\Delta u^2\right]$$

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

Forward propagation

A numerical recipe



Near field, far field

$$\psi(\vec{r}_\perp; z) = \mathcal{F}^{-1}\left\{ \mathcal{F}\{\psi(\vec{r}_\perp; z=0)\} \exp(-i\pi z \lambda u^2) \right\} \quad (*)$$

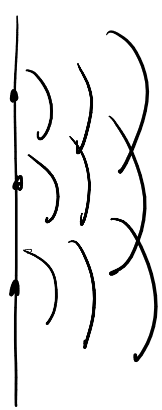
* observation 1: aliasing will occur when λz is too large (exact condition kept as an exercise)

* observation 2: $(*)$ has the form of a convolution!

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

$$\text{where } P_z(\vec{r}_\perp) = \mathcal{F}^{-1}\left\{ \exp(-i\pi z \lambda u^2) \right\}$$

$$= -\frac{2\pi i}{\lambda z} \exp\left(i\pi \frac{r^2}{\lambda z} \right) \quad \text{Fresnel propagator}$$



Huygens construction

Near field, far field

r①

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

Fresnel-Huygens integral

lens could be inserted here

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

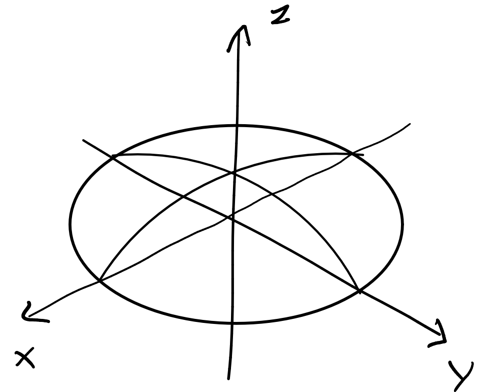
$\vec{u}$

$$= \frac{-2\pi i}{\lambda z}\exp\left(\frac{i\pi r^2}{\lambda z}\right)\underbrace{\int d^2r'\,\psi(\vec{r}'_\perp;z=0)\,\exp\left(\frac{i\pi r'^2}{\lambda z}\right)\exp\left(\frac{-2\pi i\,\vec{r}\cdot\vec{r}'}{\lambda z}\right)}_{\mathcal{F}\left\{\psi(r';z=0)\exp\left(\frac{i\pi r'^2}{\lambda z}\right)\right\}\left(\vec{u}=\frac{\vec{r}}{\lambda z}\right)}$$

$$\Rightarrow \quad \psi(\vec{r};z) = \frac{-2\pi i}{\lambda z}\exp\left(\frac{i\pi r^2}{\lambda z}\right)\mathcal{F}\left\{\psi(r';z=0)\exp\left(\frac{i\pi r'^2}{\lambda z}\right)\right\}\left(\vec{u}=\frac{\vec{r}}{\lambda z}\right)$$

Wave propagation $\Rightarrow z\to\infty \qquad \psi(\vec{r};z\to\infty) \propto \mathcal{F}\{\psi\}\left(\vec{u}=\frac{\vec{r}}{\lambda z}\right)$

Back focal plane of a lens



* thickness profile: $t(r) = \overbrace{t_0}^{\text{irrelevant}} - \underbrace{\alpha}_{\text{curvature}} r^2$

* phase $\phi(\vec{r}_\perp) = k(n-1)\, t(\vec{r}_\perp)$

$$\phi(\vec{r}_\perp) = -\frac{2\pi}{\lambda}(n-1)\,\alpha r_\perp^2$$

* focal length : $(n-1)\alpha = \frac{1}{2f}$

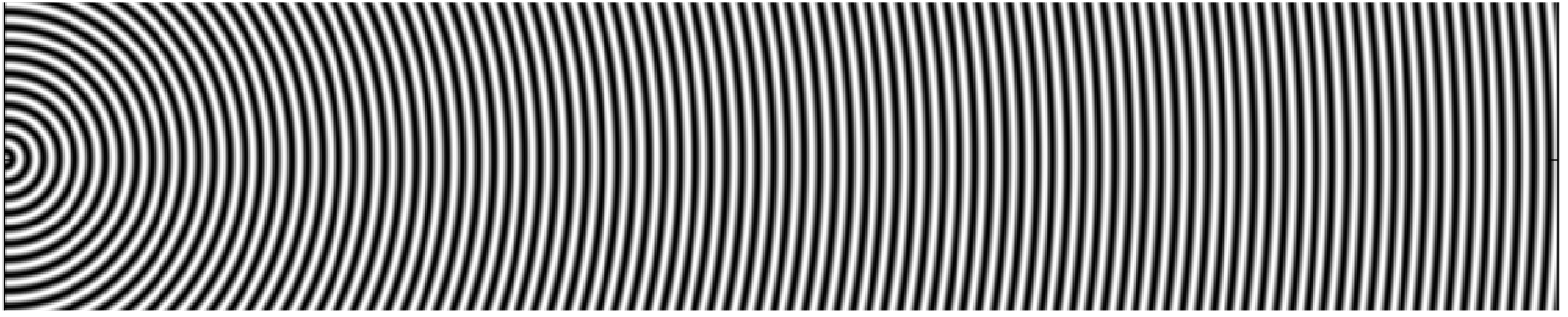
Substitute $\psi(r_\perp; z=0)$ with $\psi(\vec{r}_\perp; z=0)\, \overbrace{\exp\left(-i\frac{\pi r_\perp^2}{2\lambda f}\right)}^{e^{i\phi(\vec{r}_\perp)}}$

$$\Rightarrow \psi(\vec{r}_\perp; z) = \frac{-2\pi i}{\lambda z} \exp\left(\frac{i\pi r^2}{\lambda z}\right) \mathcal{F}\left\{\psi(r_\perp; z=0) \exp\left(\frac{i\pi}{\lambda}\left(\frac{1}{z} - \frac{1}{f}\right) r^2\right)\right\}\left(\vec{u} = \frac{\vec{r}}{\lambda z}\right)$$

* special case : $z = f$ $\Rightarrow$ $\psi(\vec{r}_\perp; z=f)$ = F.T. of $\psi(\vec{r}_\perp; z=0)$

A lens acts as a Fourier transform operator!

Plane waves, point sources

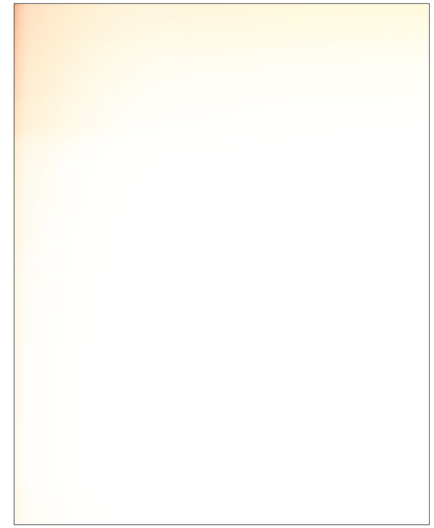


circular waves
evanescent waves
contact region

parabolic waves
near field
Fresnel region

plane waves
far field
Fraunhofer region

Why optical elements?

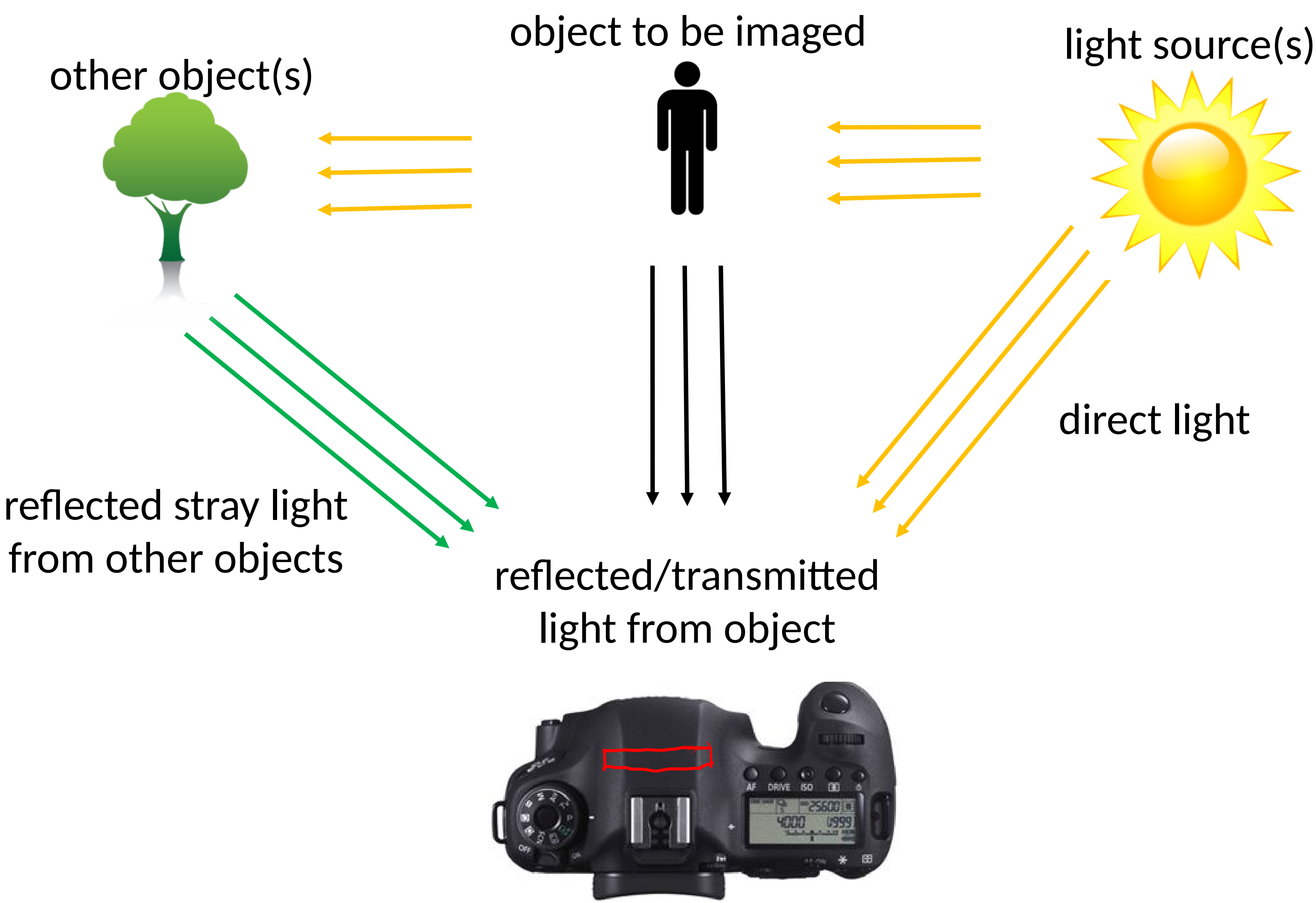


with objective lens

without objective lens

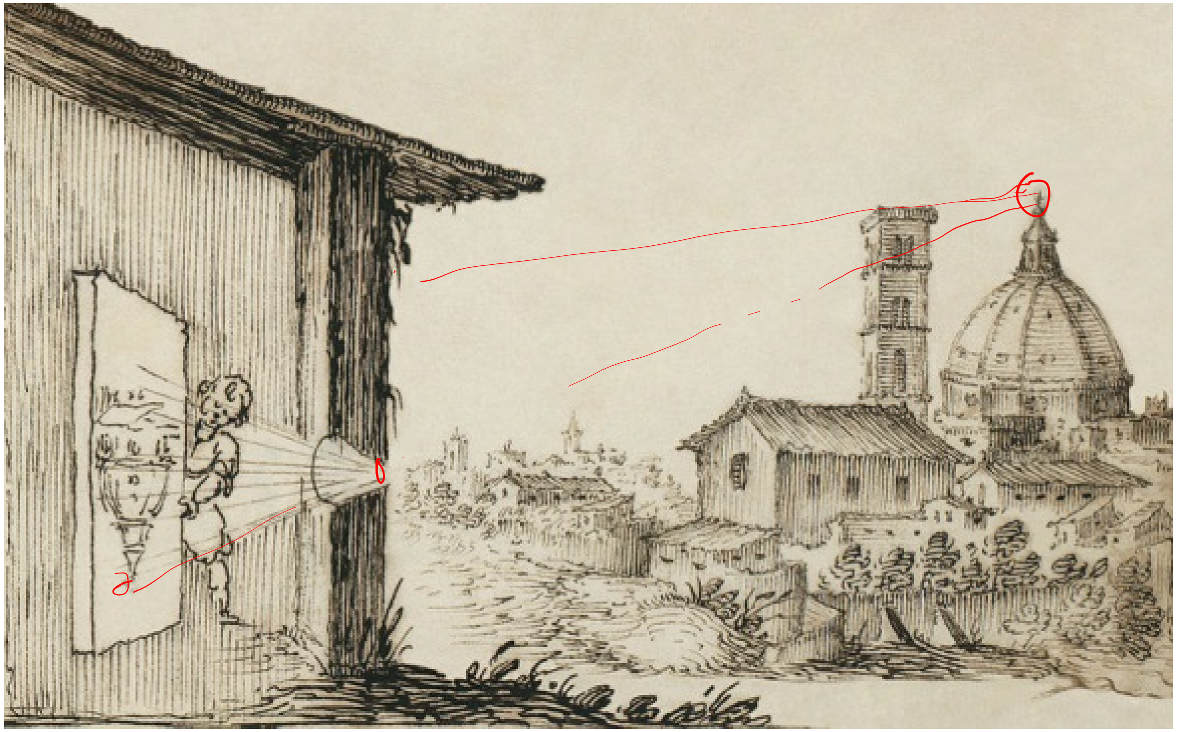
Why optical elements?

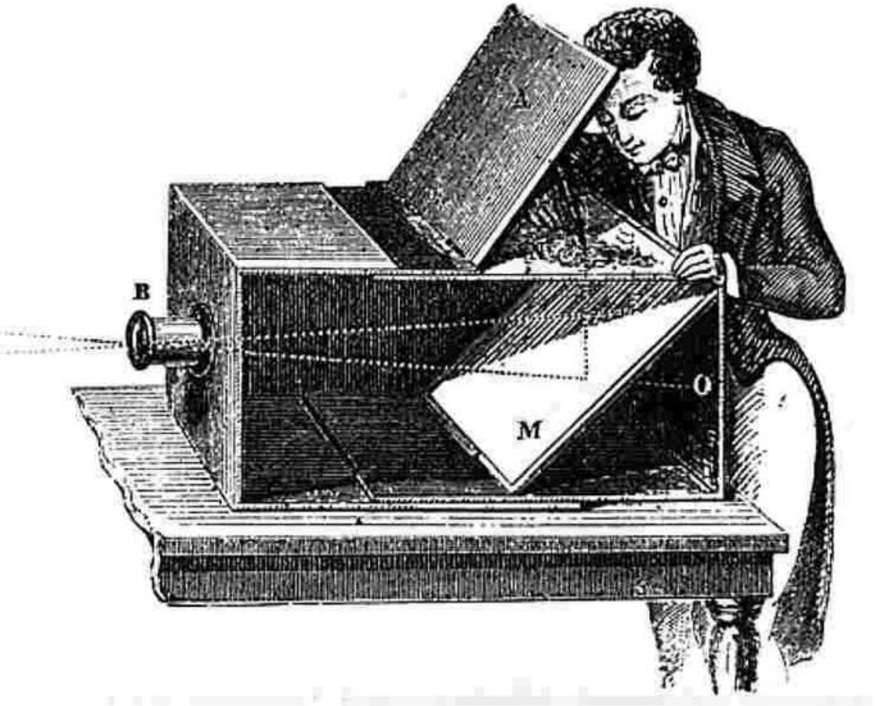
- Information from many sources overlaps in detector plane
- Need models to understand image forming systems



Pinhole camera model

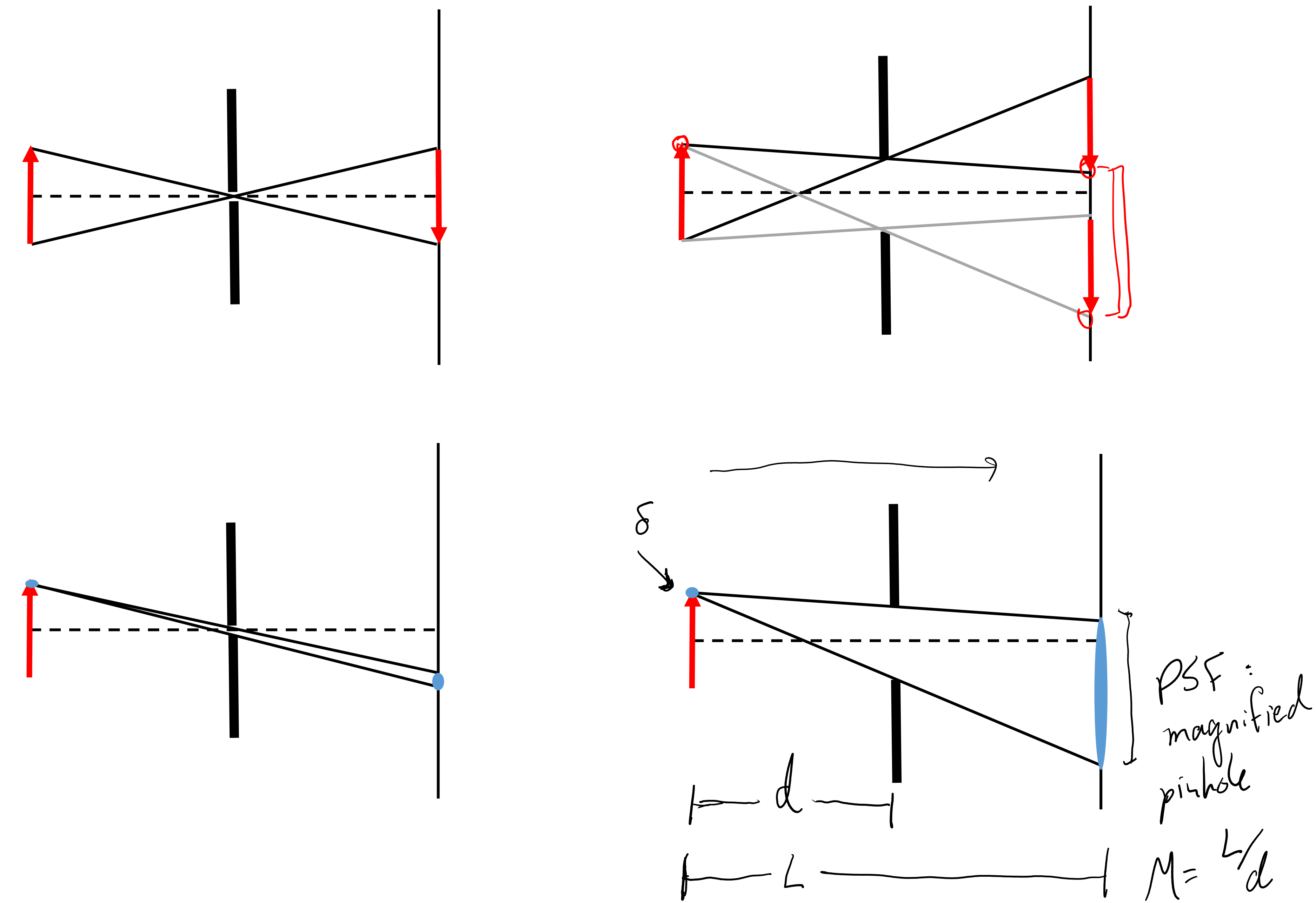
camera obscura





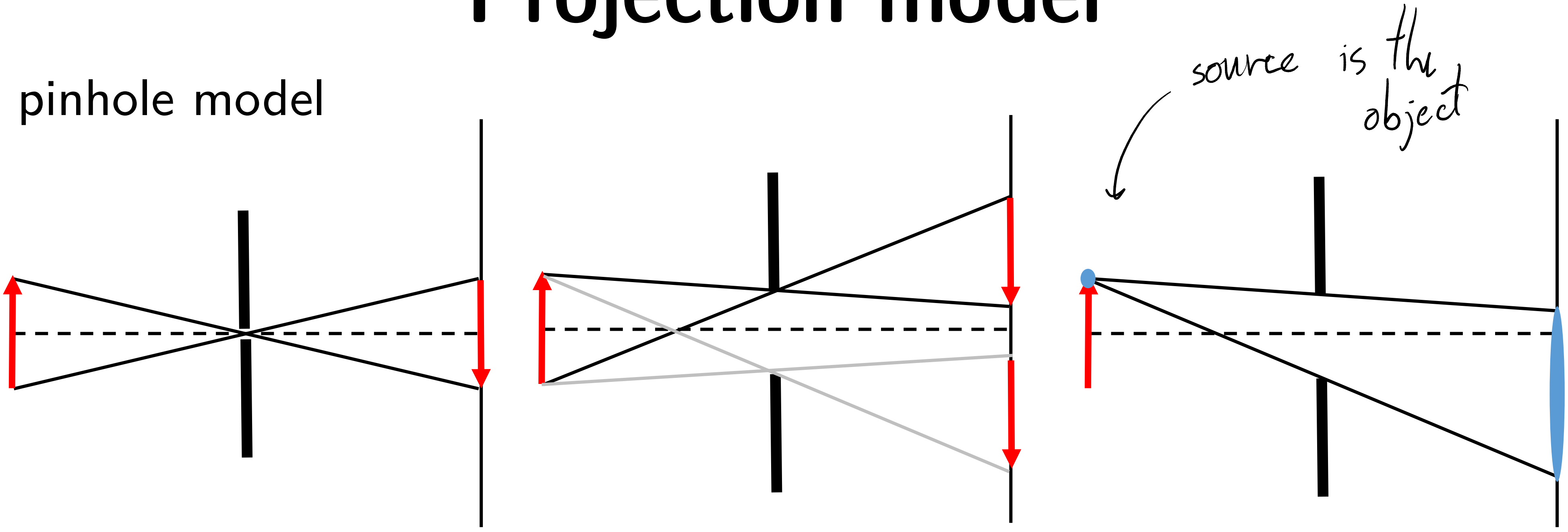
Pinhole camera model

PSF determined by aperture width

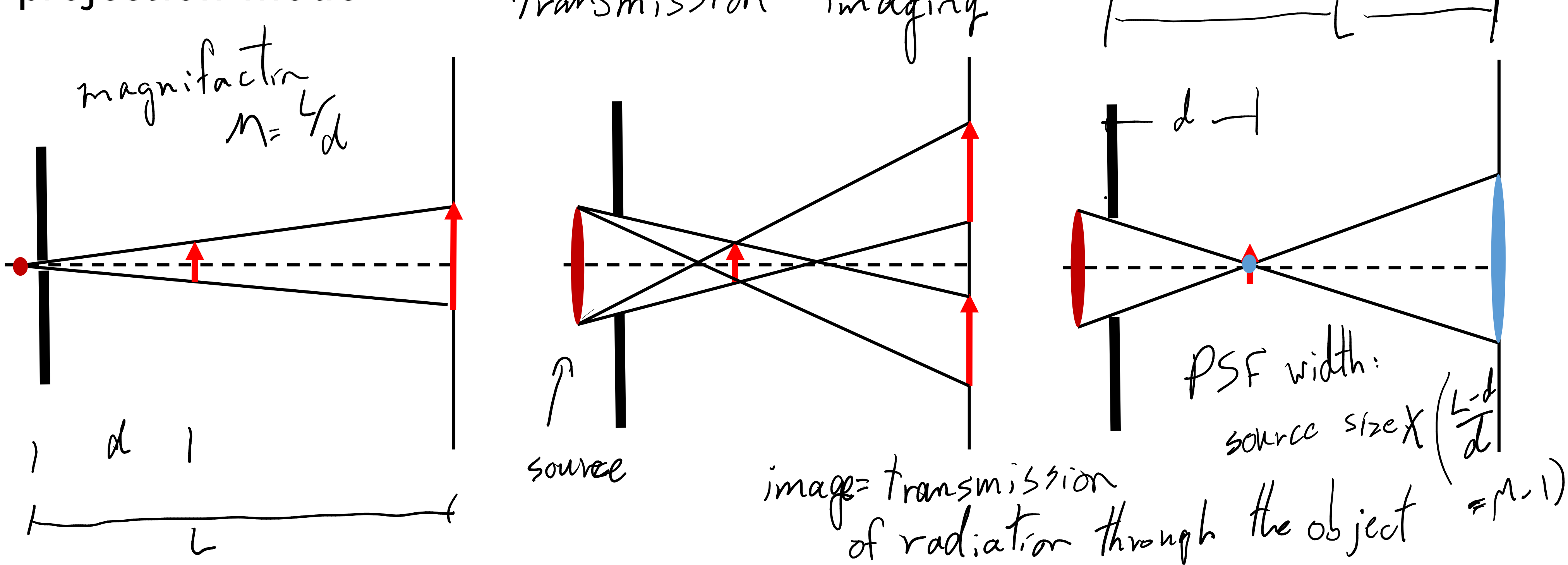


Projection model

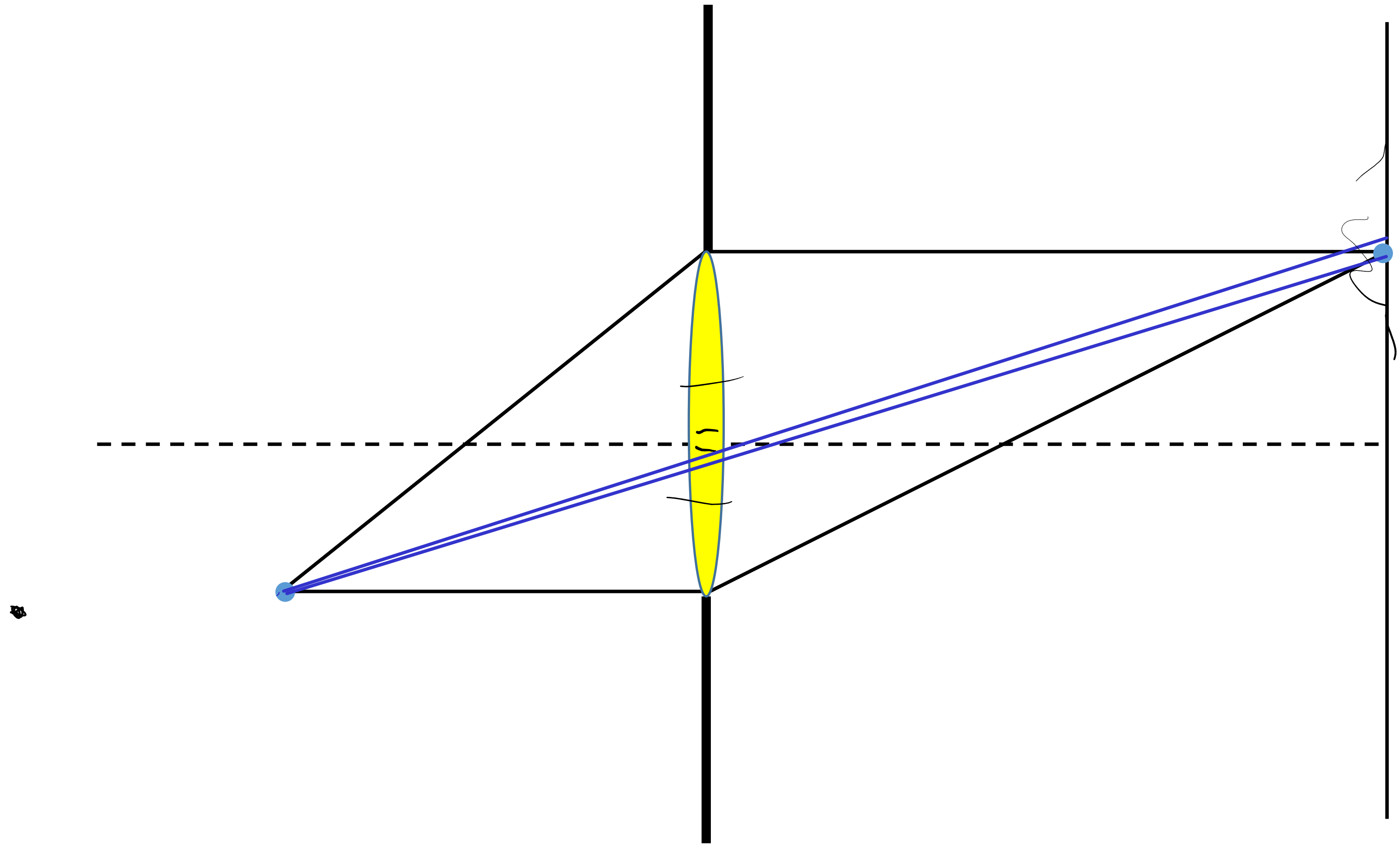
pinhole model



projection model



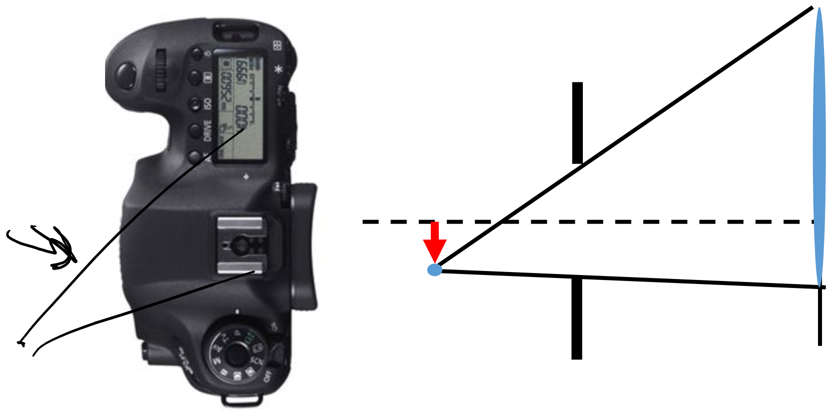
Lens camera model



Result similar to small pinhole but without compromise on intensity

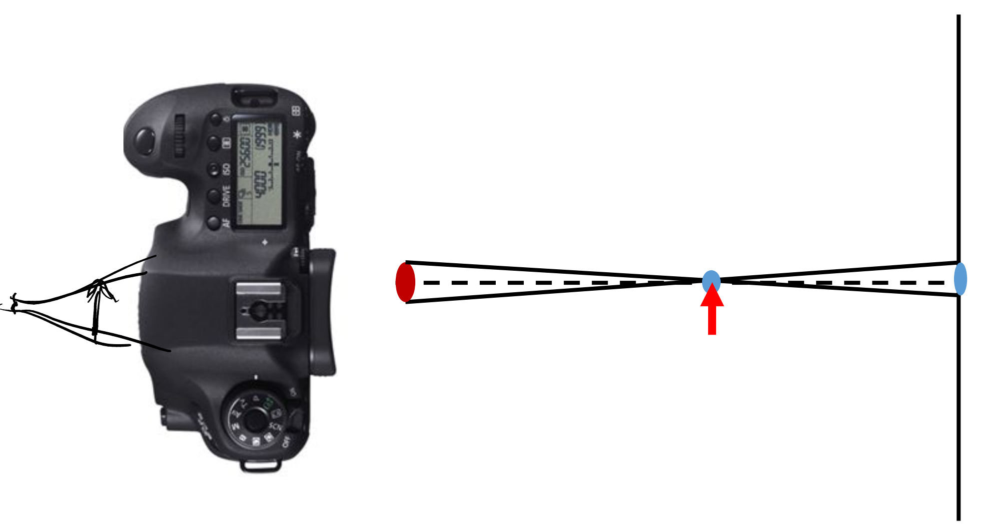
Lens camera model

lensless model

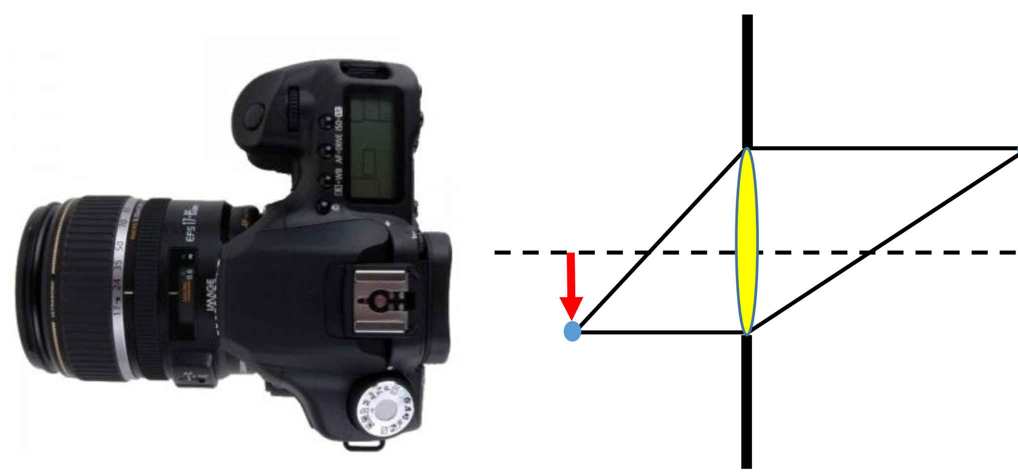


pinhole camera model

projection model

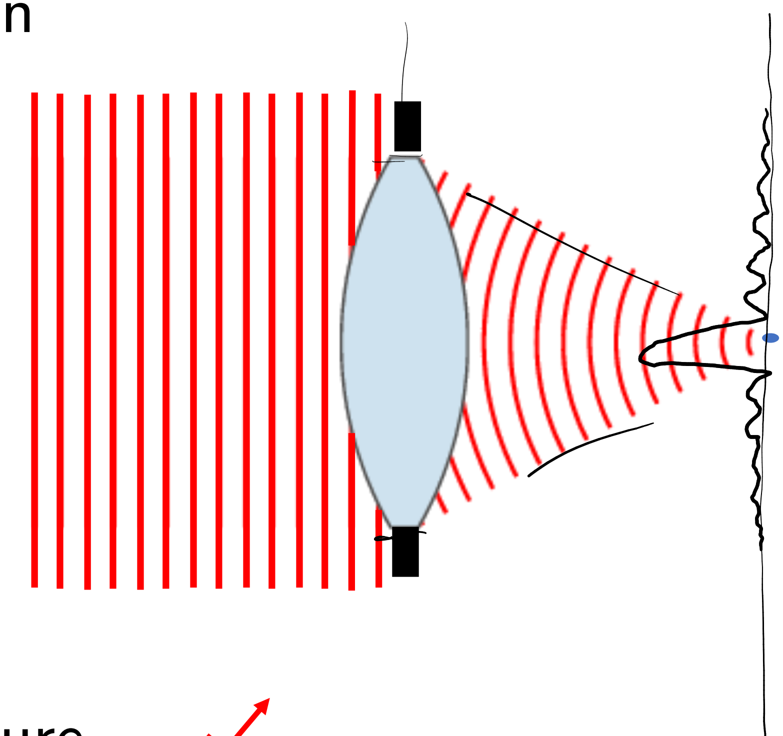


lens camera model



Diffraction-limited imaging systems

- Rayleigh criterion

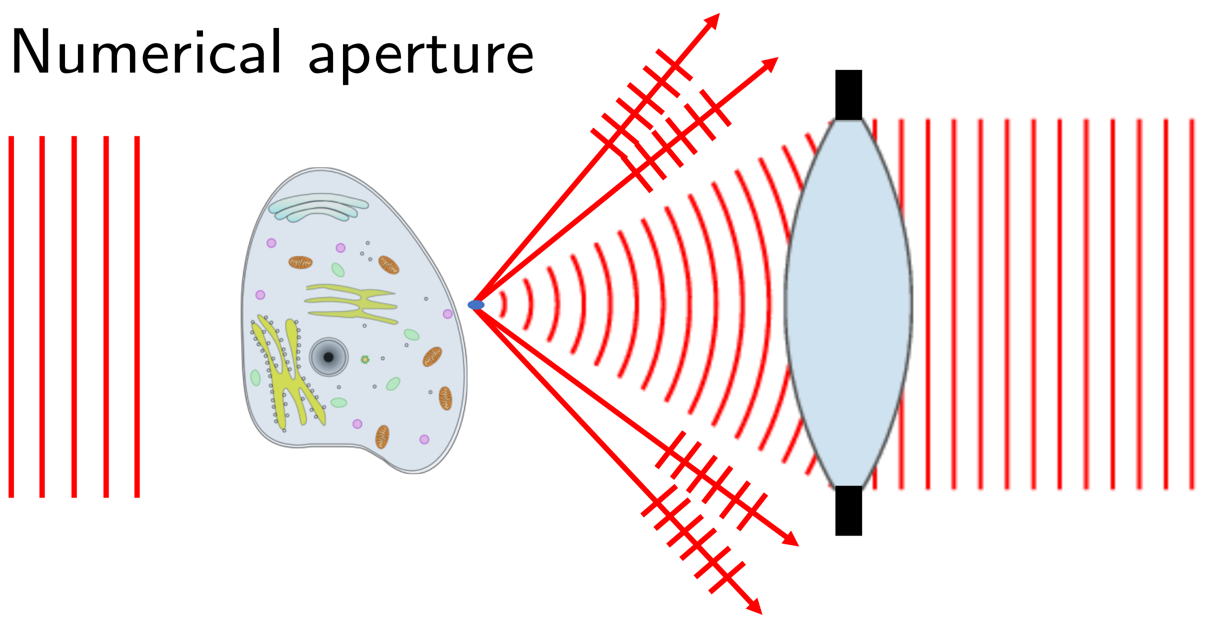


PSF = FT of the pupil

For a disc:

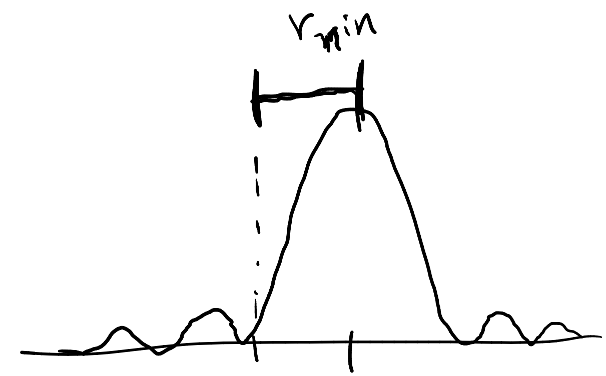
Airy disc
(Bessel function)

- Numerical aperture



inverse Fourier transform of disc of radius $u_{max} \propto \dfrac{J_1(2\pi r u_{max})}{r u_{max}}$

J_1 : First Bessel function



Rayleigh criterion to define resolution: distance from origin to first minimum

$$PSF = \left| \frac{J_1(2\pi r u_{max})}{r u_{max}} \right|^2$$

$$J_1(3.83) = 0$$

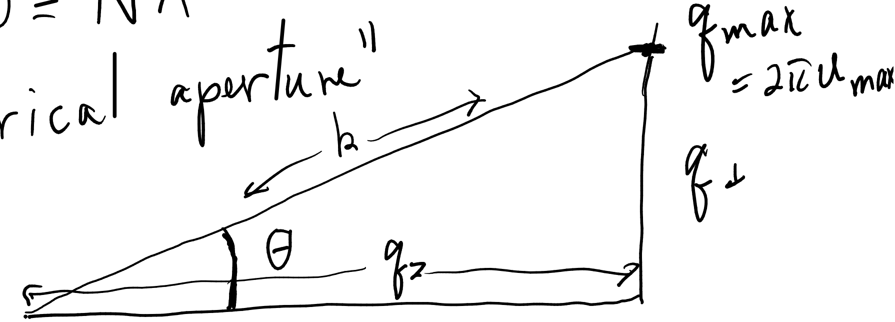
$$J_1(2\pi r_{min} u_{max}) = 0$$

$$2\pi r_{min} u_{max} = 3.83$$

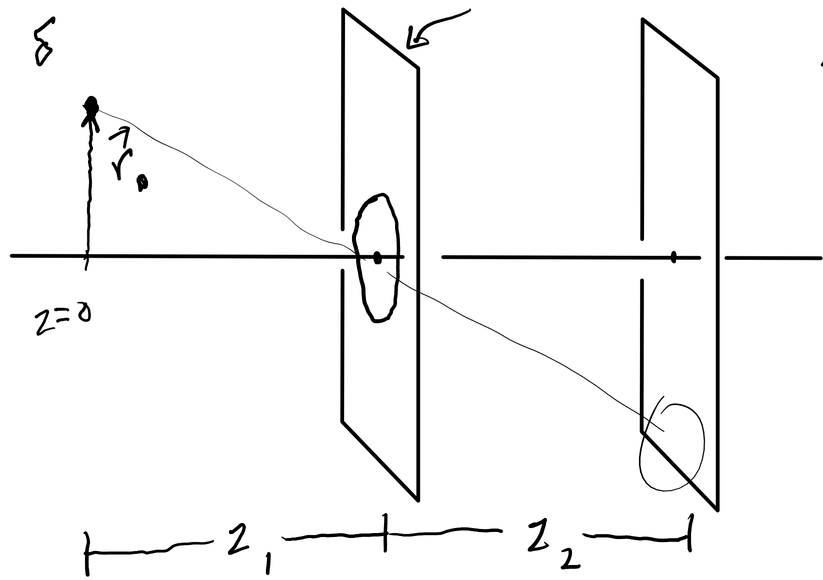
$$2\pi u_{max} = q_{max} = k \sin\theta$$

$\sin\theta = NA$

"numerical aperture"



$$\boxed{r_{min} = \frac{3.83}{k \sin\theta} = \frac{1.22\,\lambda}{2\sin\theta}}$$



1) monochromatic point source at position $\vec{r}_0$ in plane $z=0$

2) propagates to plane z_1

3) multiplied with optical element $\mathcal{O}(\vec{r})$

4) propagate further to plane z_1+z_2

2): $$\psi(\vec{r}\,; z=z_1) = \frac{-2\pi i}{\lambda z_1} \exp\left(\frac{i\pi(\vec{r}-\vec{r}_0)^2}{\lambda z_1}\right)$$

3): $$\psi'(\vec{r}) = \psi(\vec{r}\,; z=z_1)\cdot \mathcal{O}(\vec{r})$$

4): $$\psi(\vec{r}\,; z=z_1+z_2) = \frac{-2\pi i}{\lambda z_2} \underbrace{\exp\left(\frac{i\pi r^2}{\lambda z_2}\right)} \overbrace{\mathcal{F}\left\{\psi'(\vec{r}')\exp\left(\frac{i\pi r'^2}{\lambda z_2}\right)\right\}}^{*}$$

$$\left(\vec{u} = \frac{\vec{r}}{\lambda z_2}\right)$$

$$* = \mathcal{F}\left\{ -\frac{2\pi i}{\lambda z_1} \exp\left[\frac{i\pi}{\lambda z_1}\left[r'^2 - 2\vec{r}'\cdot\vec{r}_0 + r_0^2\right]\right] O(\vec{r}') \exp\left[\frac{i\pi}{\lambda z_2} r'^2\right]\right\}$$

just a shift in Fourier space

$$= -\frac{2\pi i}{\lambda z_1} \exp\left(\frac{i\pi r_0^2}{\lambda z_1}\right) \mathcal{F}\left\{ O(\vec{r}') \underbrace{\exp\left(\frac{i\pi r'^2}{\lambda z^*}\right)} \exp\left(\frac{-2\pi i \vec{r}_0 \cdot \vec{r}'}{\lambda z_1}\right)\right\}$$

will become propagation by distance z^*

$$\left(\frac{1}{z^*} = \frac{1}{z_1} + \frac{1}{z_2}\right)$$

$$= -\frac{2\pi i}{\lambda z_1} \exp\left(\frac{i\pi r_0^2}{\lambda z_1}\right) \mathcal{F}\left\{ O(\vec{r}') \exp\left(\frac{i\pi r'^2}{\lambda z^*}\right)\right\}\left(\vec{u} + \vec{r}_0/\lambda z_1\right)$$

observation: $\frac{1}{z^*} = \frac{1}{z_1} + \frac{1}{z_2} \rightarrow z^* = \frac{z_1 z_2}{z_1 + z_2} \Rightarrow \frac{1}{z_1 z_2} = \frac{1}{z^*(z_1+z_2)}$

$$\frac{1}{z_2} = \frac{1}{z^*} - \frac{1}{z_1}$$

$$\psi(\vec{r}; z = z_1 + z_2) = \left(\frac{-2\pi i}{\lambda(z_1+z_2)}\right)\left(\frac{-2\pi i}{\lambda z^*}\right) \exp\left[\frac{i\pi r^2}{\lambda z^*}\right] \exp\left[\frac{-i\pi r^2}{\lambda z_1}\right] \exp\left[\frac{i\pi r_0^2}{\lambda z_1}\right]$$

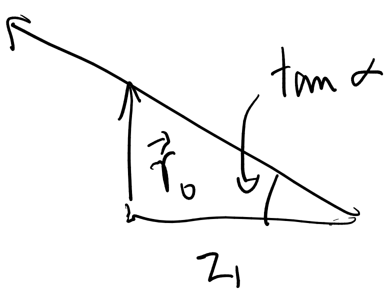
$$\mathcal{F}\left\{ O(\vec{r}) \exp\left(\frac{i\pi r'^2}{\lambda z^*}\right)\right\}\left(\vec{u} = \frac{\vec{r}}{\lambda z_2} - \frac{\vec{r}_0}{\lambda z_1}\right)$$

$\rightarrow O(?; z = z^*)$

$$O(\vec{R}; z=z^*) = \frac{-2\pi i}{\lambda z^*} \exp\left(\frac{i\pi R^2}{\lambda z^*}\right) \mathcal{F}\left\{ O(\vec{r}\,') \exp\left(\frac{i\pi r'^2}{\lambda z^*}\right)\right\}\left(u = \frac{\vec{R}}{\lambda z^*}\right)$$

$$\frac{\vec{R}}{\lambda z^*} = \frac{\vec{r}}{\lambda z_2} - \frac{\vec{r}_0}{\lambda z_1} \qquad \vec{R} = \vec{r}\,\frac{z^*}{z_2} - \vec{r}_0\,\frac{z^*}{z_1} = \vec{r}\,\frac{z_1}{z_1+z_2} - \vec{r}_0\,\frac{z_2}{z_1+z_2}$$

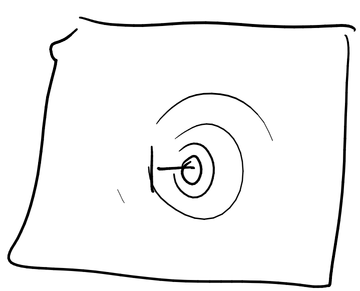
$$\psi(\vec{r}; z = z_1+z_2) = \frac{-2\pi i}{\lambda(z_1+z_2)} \exp\left[\frac{i\pi(r_0^2 - r^2)}{\lambda z_1}\right] O\left(\frac{z_1}{z_1+z_2}\vec{r} - \frac{z_2}{z_1+z_2}\vec{r}_0 ; z = z^*\right)$$



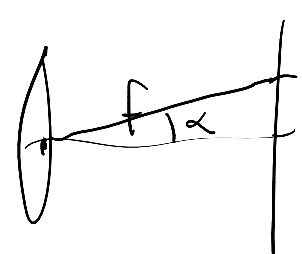
$O(\vec{r})$: lens of focal length f

$$O\left(\vec{r} - f \underbrace{\frac{r_0}{z_1}}_{\tan\alpha} ; \underbrace{z = f}\right)$$

$\rightarrow$ F.T of pupil function

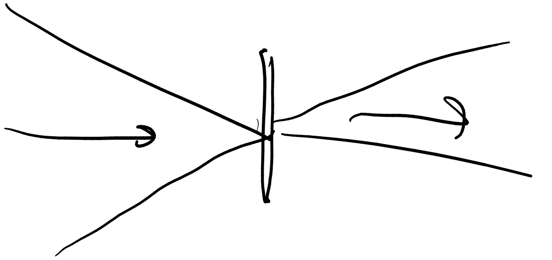


$f \tan\alpha$



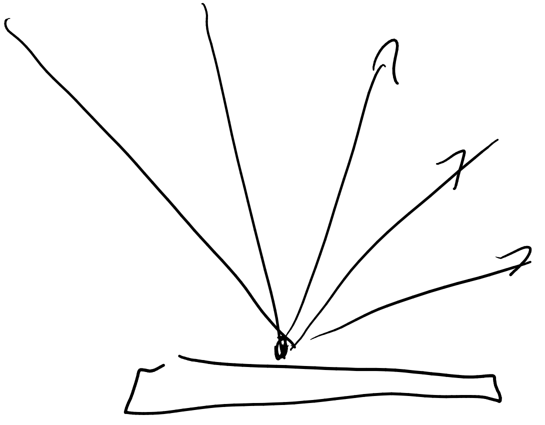
Scanning systems

Transmission



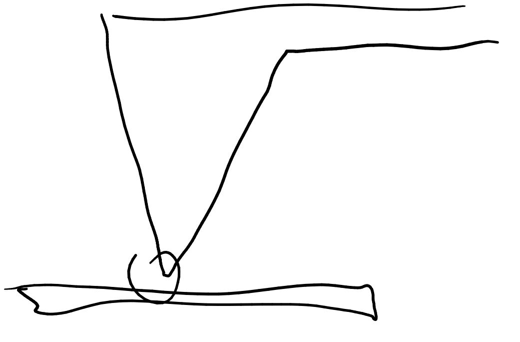
- **S**canning **T**ransmission **E**lectron **M**icroscopy
- **S**canning **T**ransmission **X**-ray **M**icroscopy
- …

Indirect (reflection, scattering, fluorescence, …)



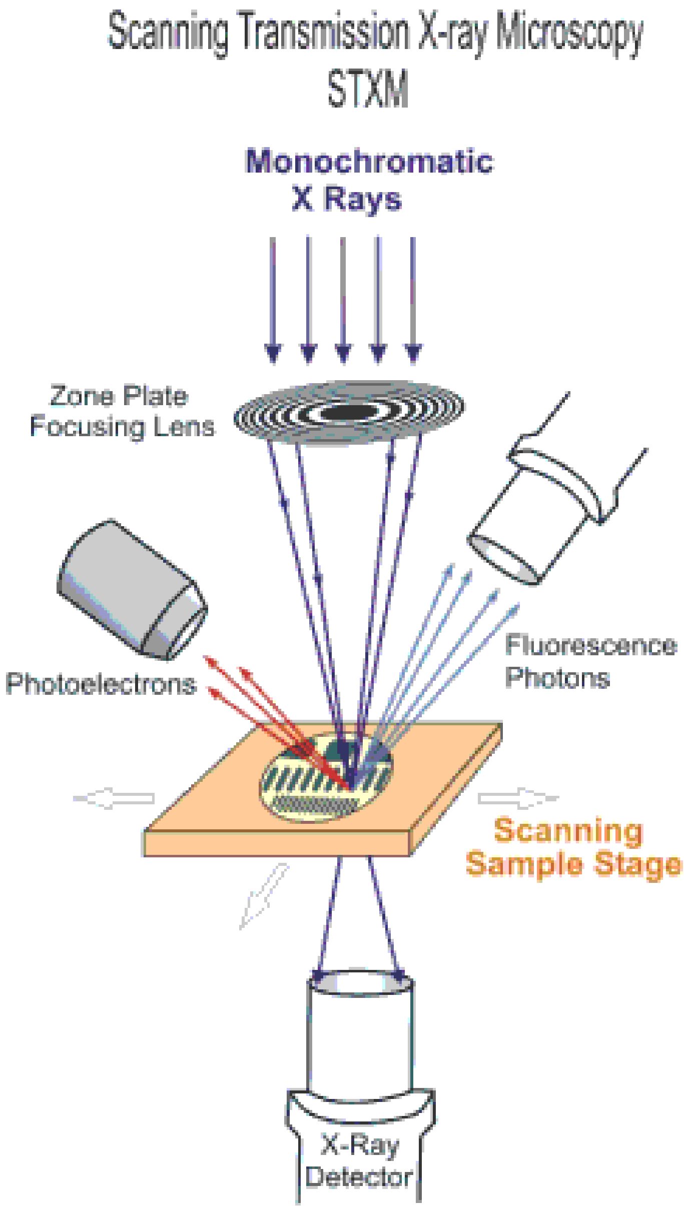
- **L**aser **S**canning **C**onfocal **M**icropsopy
- **S**canning **E**lectron **M**icroscopy
- **X**-ray **F**luorescence **M**icroscopy
- **P**hoto**E**mission **E**lectron **M**icroscopy
- ...

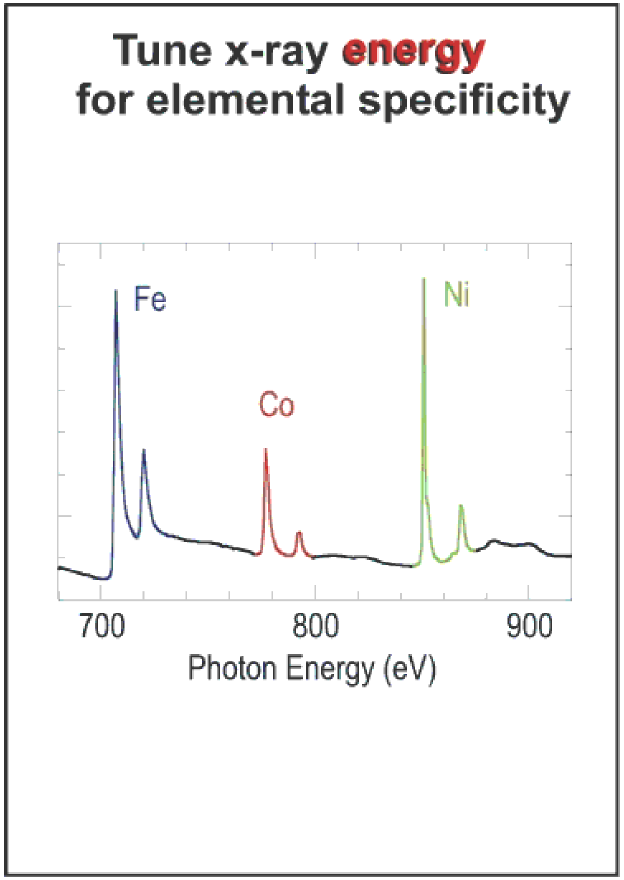
Physical probe

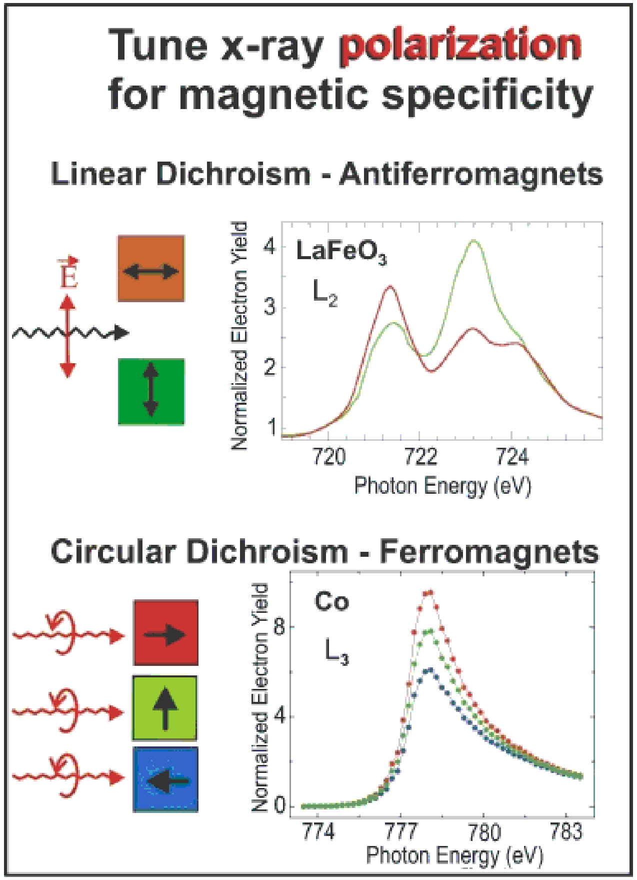


- **A**tomic **F**orce **M**icroscopy
- **S**canning **T**unneling **M**icroscopy
- ...

Scanning transmission X-ray microscopy

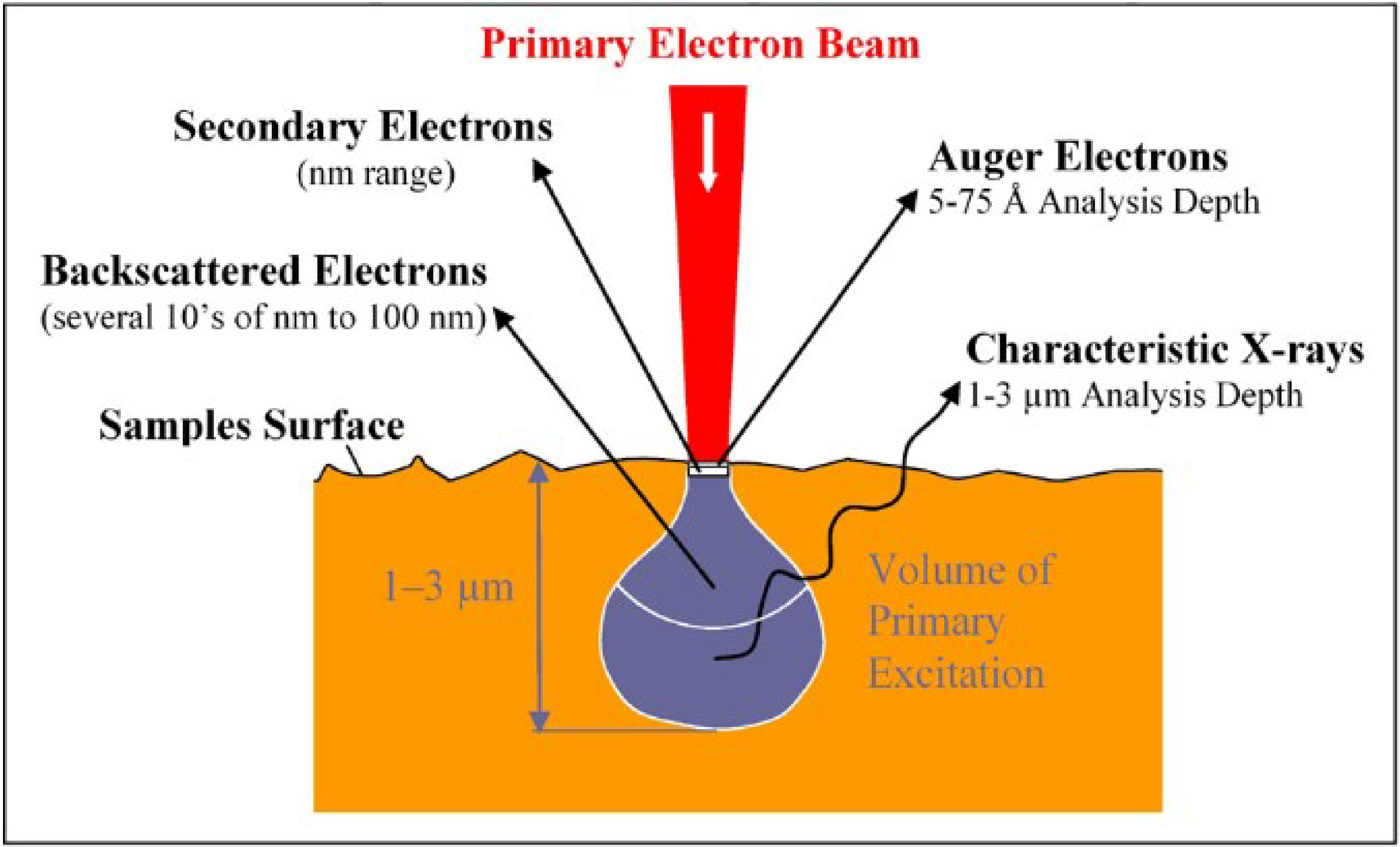




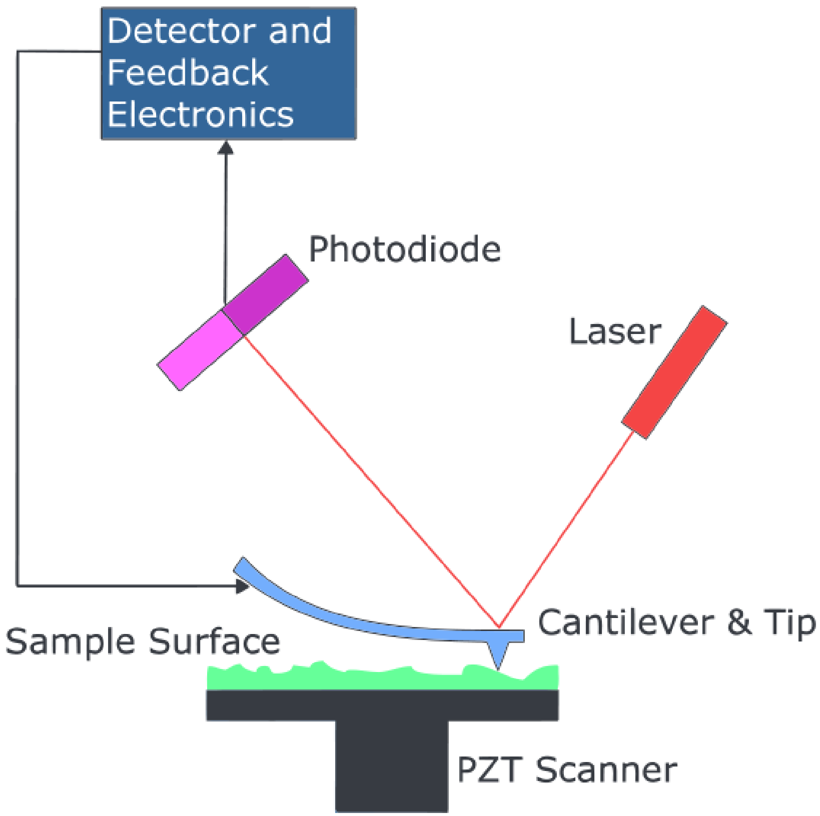


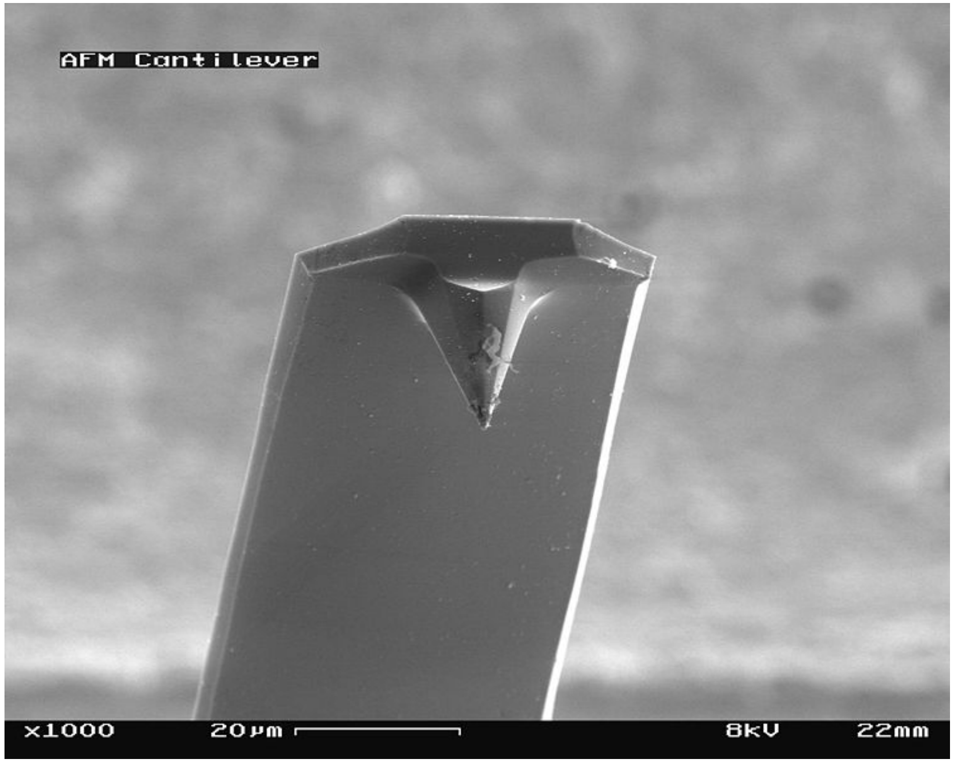
source: http://www-ssrl.slac.stanford.edu

Scanning electron microscopy



Atomic force microscopy

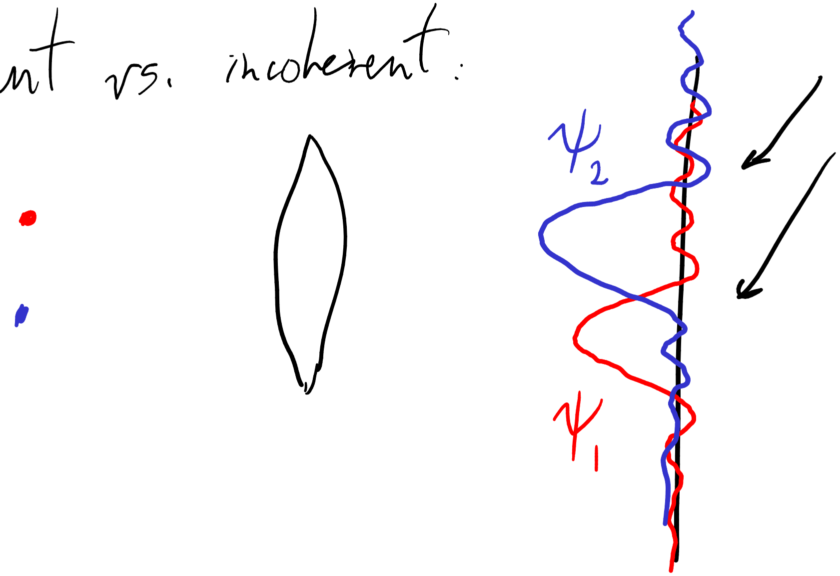




Resolution in scanning systems

Resolution mainly limited by probe size

coherent vs. incoherent:



Two images of point sources.

What is measured:

1) if the two sources are perfectly coherent → they interfere

↳ same frequency, same phase

$$|\psi_1 + \psi_2|^2$$

2) if the two sources are completely incoherent: their intensities add up

$$|\psi_1|^2 + |\psi_2|^2$$

PSF for a scanning system is the intensity of the image of a point source $|\psi|^2$

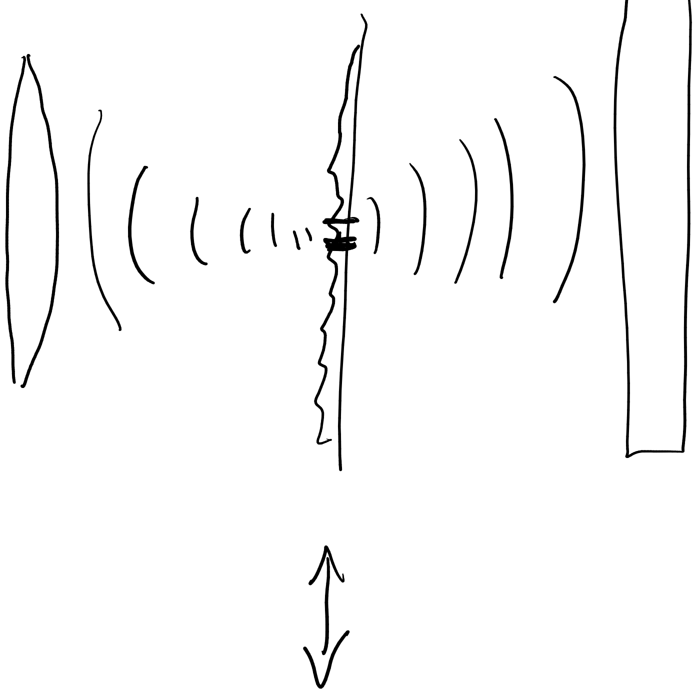
e.g. $$\left| \frac{J_1(2\pi r u_{max})}{r u_{max}} \right|^2$$

In general $I = PSF_{inc} * |\psi|^2$

Scanning vs. full field systems

Transmission probe: the reciprocity theorem

Incoherent system



equivalent
if using
same lens