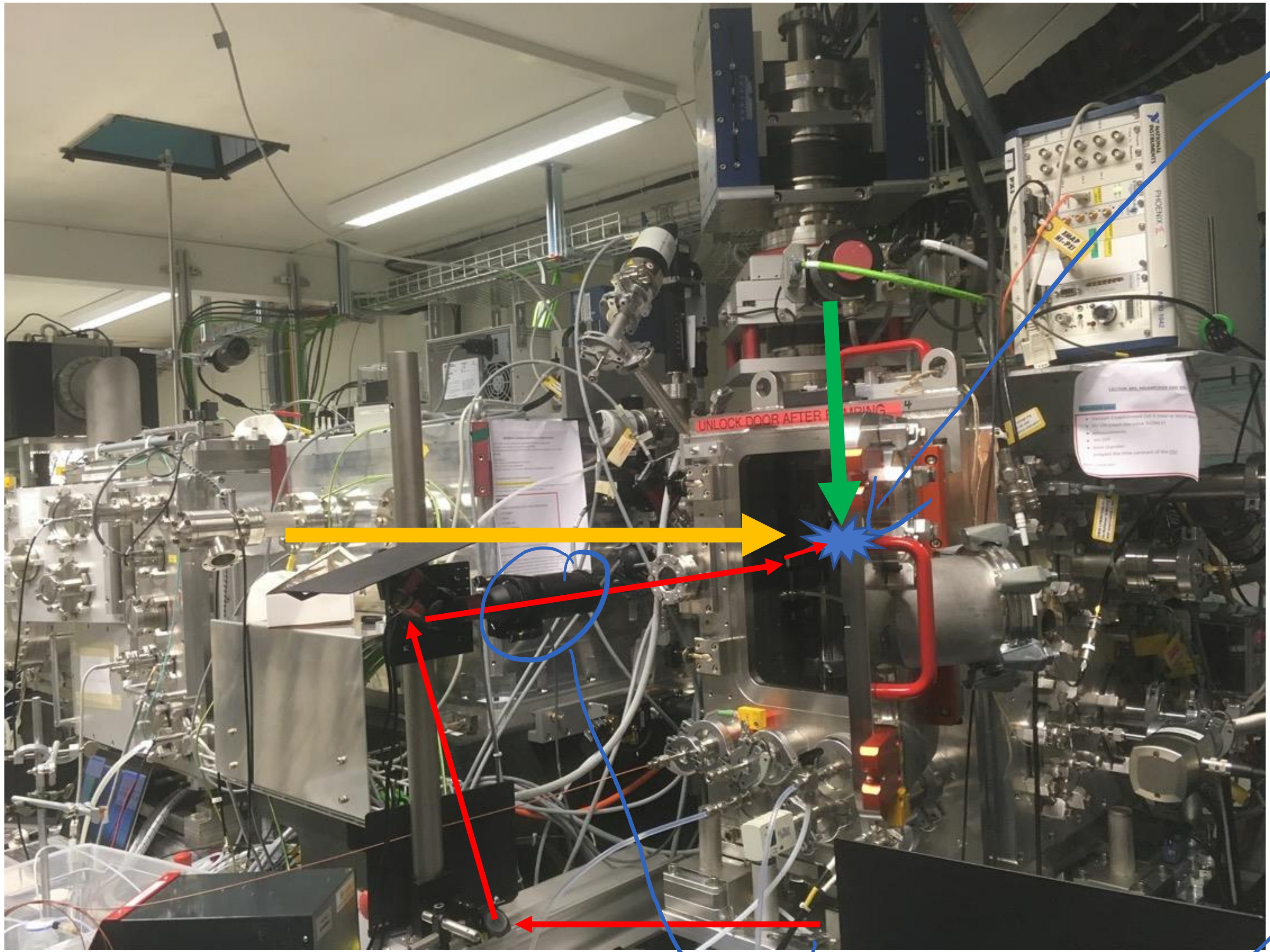
Optical methods in chemistry
or
Photon tools for chemical sciences

Session 6:

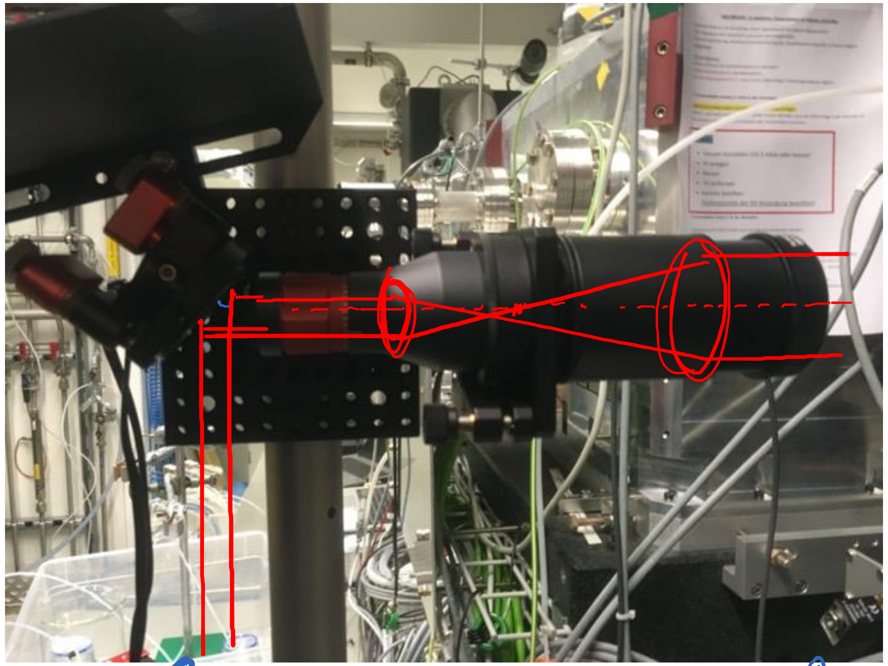
Prologue: Look inside Phoenix beamline for environmental spectroscopy, laser pump – x-ray probe spectroscopy of molecules in solution

Small x-ray focus, $\phi \approx 100 \mu m$



beam expander

Looks familiar? Why is this here?



"small" entrance beam

"large" exit beam

change beam size – focus properties

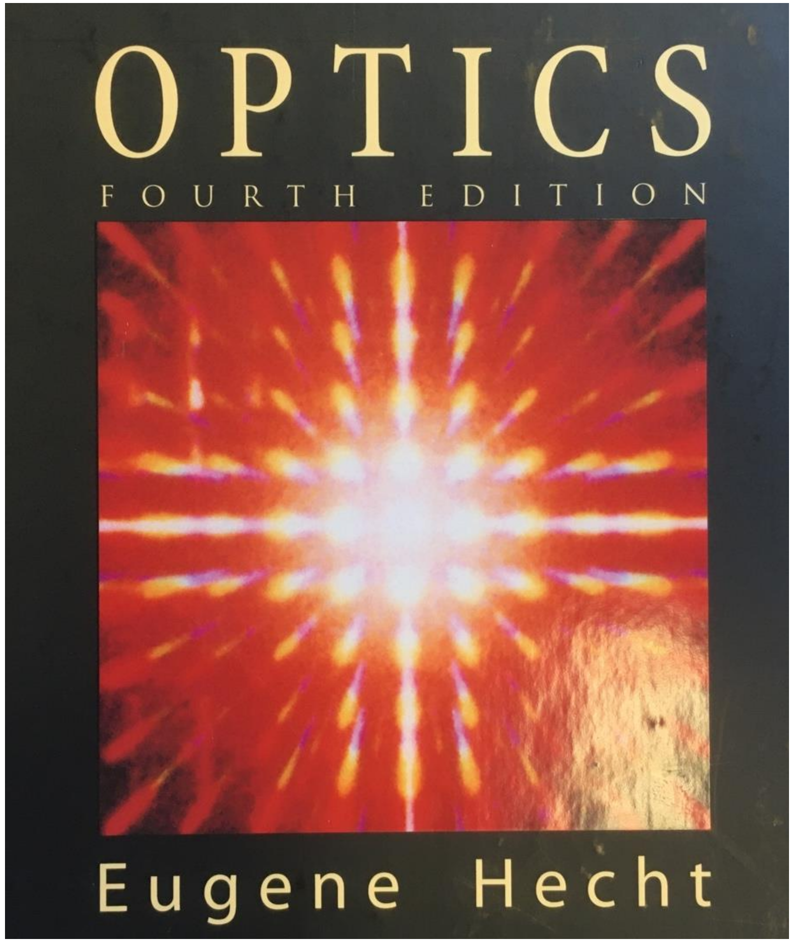
Course layout – contents overview and general structure

- Introduction and ray optics
- Wave optics
- Beams
- From cavities to lasers
- More lasers and optical tweezers
- From diffraction and Fourier optics
- Microscopy
- Spectroscopy
- Electromagnetic optics
- Absorption, dispersion, and non-linear optics
- Ultrafast lasers
- Introduction to x-rays
- X-ray diffraction and spectroscopy
- Summary

This week learning goal:
Change the way you think about diffraction and imaging. Get a different view on optics.

Literature

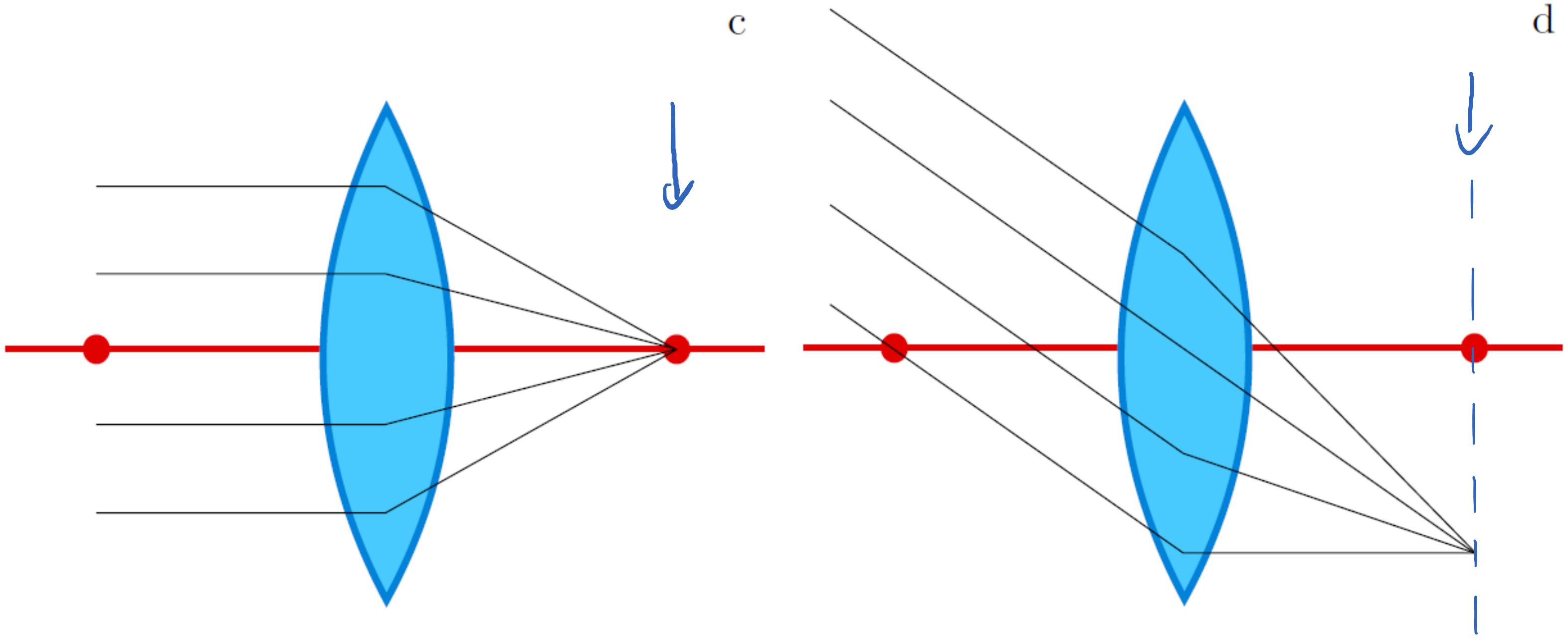
- Todays lecture relies mostly on ”Hecht – Optics”



Recall: Focusing properties of a lens (ray optics)

focal spot

focal spot in focal plane



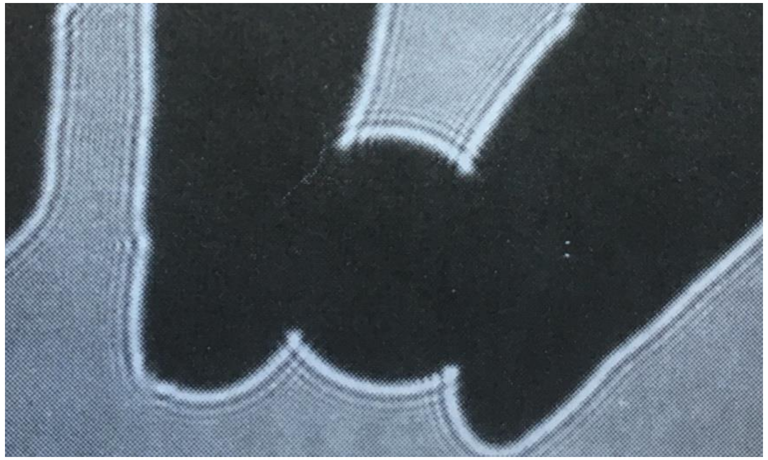
$\Rightarrow$ parallel beams meet at ∞

$\Rightarrow$ lens brings ∞ to focal plane

Diffraction, a short review

https://physicsforme.com/2012/01/04/teaching-waves-with-google-earth/

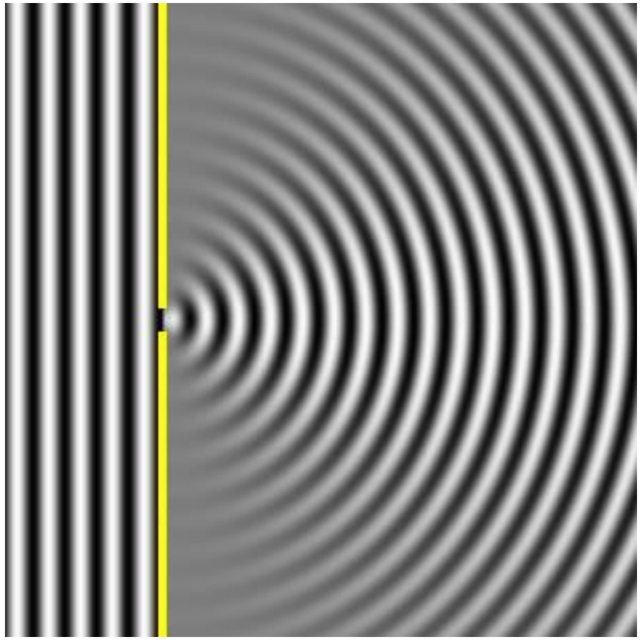
- Should be familiar concept
- A wave encountering an object changes its wavefront. Note that this can also be a density change (later more)
- Fundamental properties of all waves with relevant effects from electron microscopy to shaping coastal landscapes
- In optics most commonly known for limiting resolution in optical setups (microscopes)
- But there is much more!



The Huygens-Fresnel Principle

- Hugens: every point a wave (a luminous disturbance) reaches becomes a source of a spherical wave; the sum of these secondary waves determines the form of the wave at any subsequent time.
- Huygens-Fresnel: every unobstructed point of a wavefront serves as a source of spherical secondary wavelets. The amplitude of the wave beyond is the superposition of all these wavelets. (includes amplitude and relative phase)

plane wave



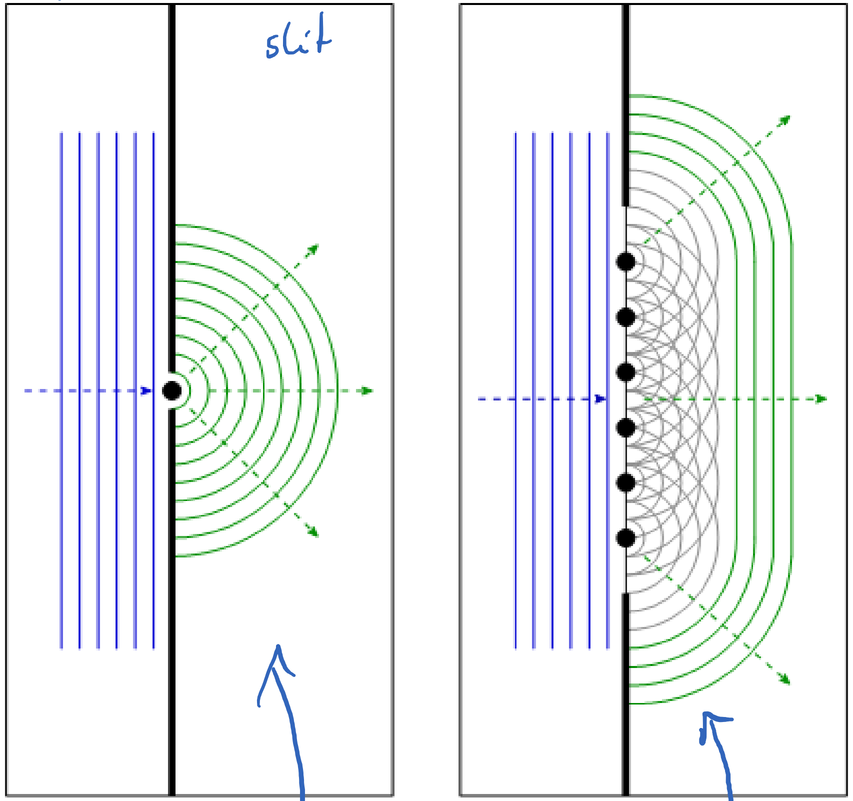
spherical wave

Wavefronts behind slit

Small vs. real slit

infinitesimal small slit

"real" slit



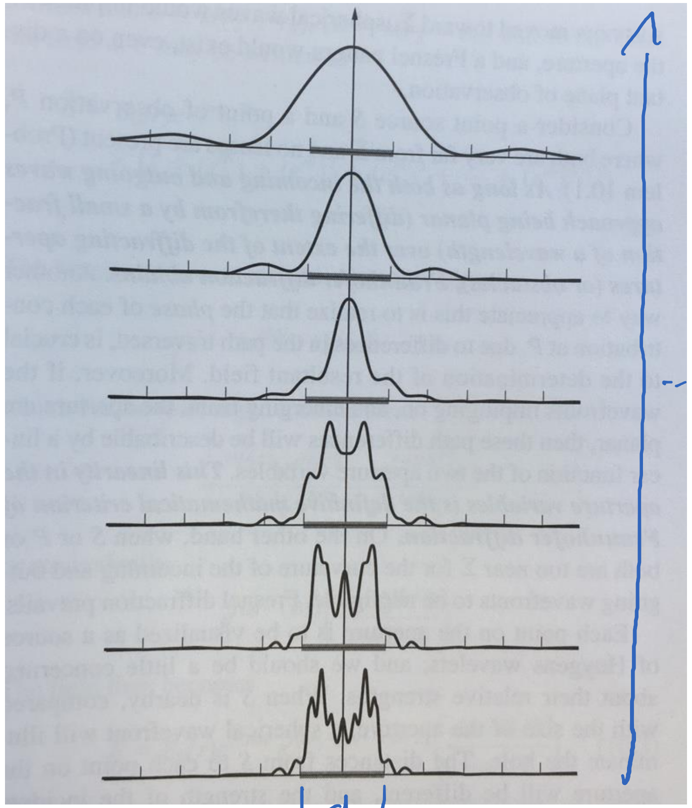
spherical wave

many points of spherical waves

interference / diffraction phenomena with fringes

forward direction essentially plane wave

Fresnel and Fraunhofer regime



D

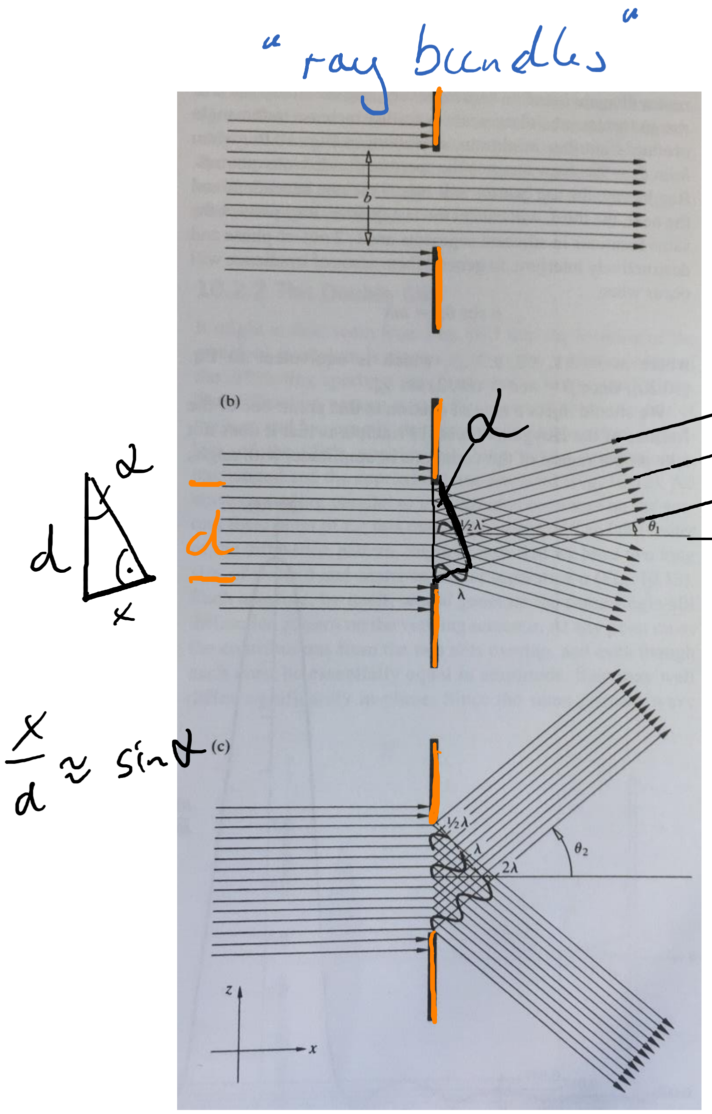
| d |

distance to slit $D \gg d$

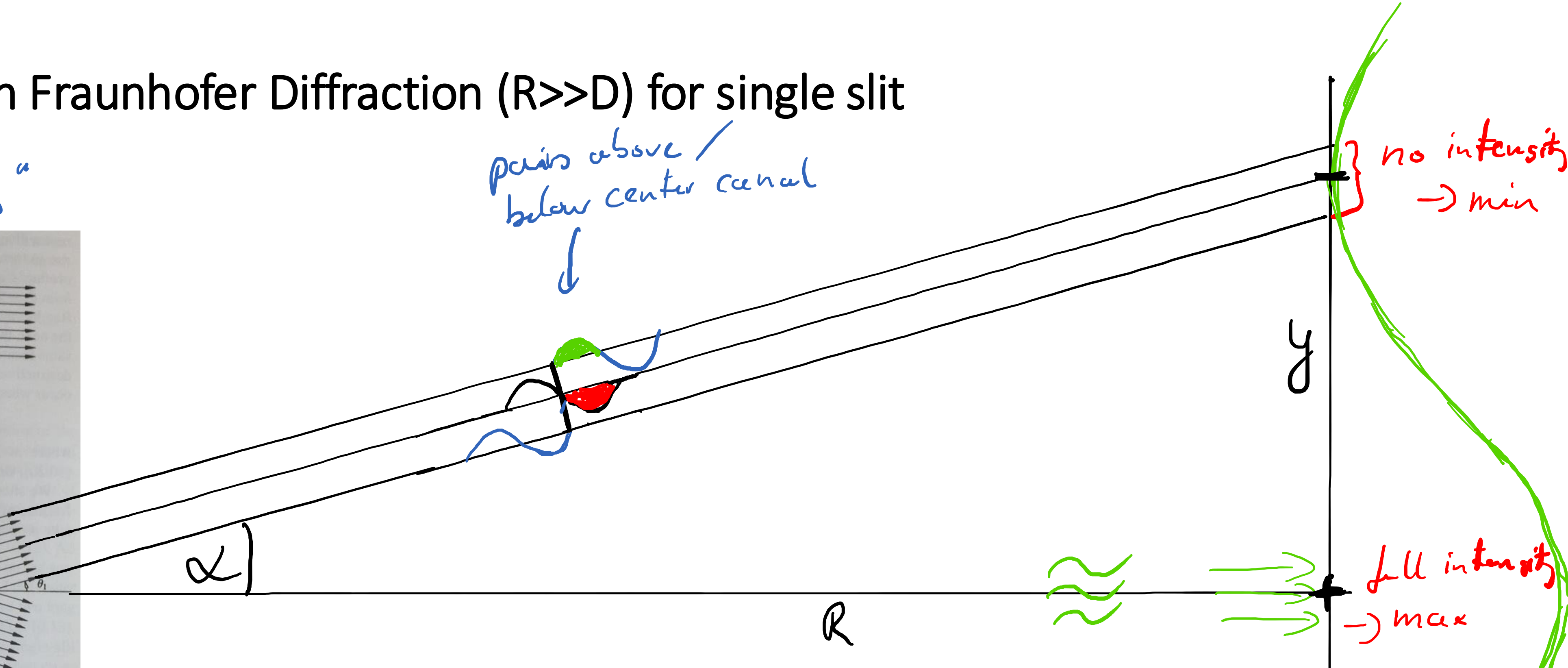
Fraunhofer regime "far field"

Fresnel regime "near field" & details of wavefront are important

Different views on Fraunhofer Diffraction (R>>D) for single slit



$\frac{x}{d} \approx \sin\alpha$



Min is at $\tan\alpha = \frac{y}{R}$

Destructive interference at $\frac{\lambda}{2} \cdot \frac{2}{d} = \frac{\lambda}{d}$

$\sin\alpha = \frac{\lambda}{d}$; $\sin\alpha \approx \tan\alpha$ for small α

$\Rightarrow \boxed{\frac{y}{R} = \frac{\lambda}{d} \Rightarrow y = n\frac{\lambda}{d} \cdot R \text{ for min}}$

$x \rightarrow$ additional path length for lowest ray $\rightarrow$ here choose λ

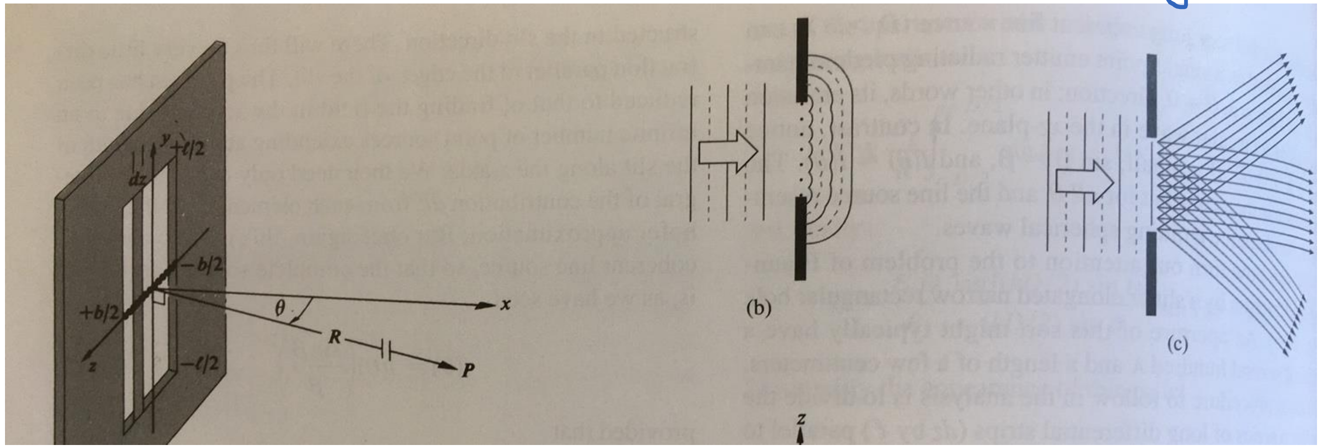
Different views on Fraunhofer Diffraction (R>>D) for single slit

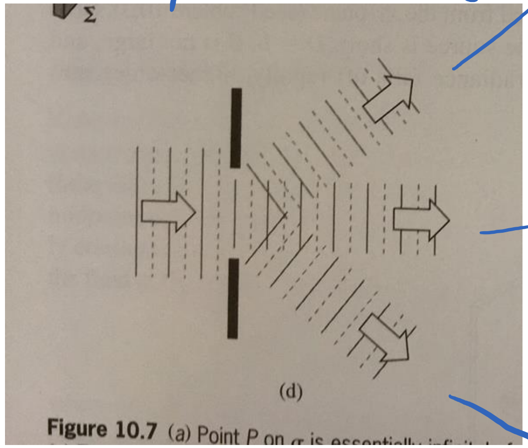
wavelets

rays

plane waves

max





max

max

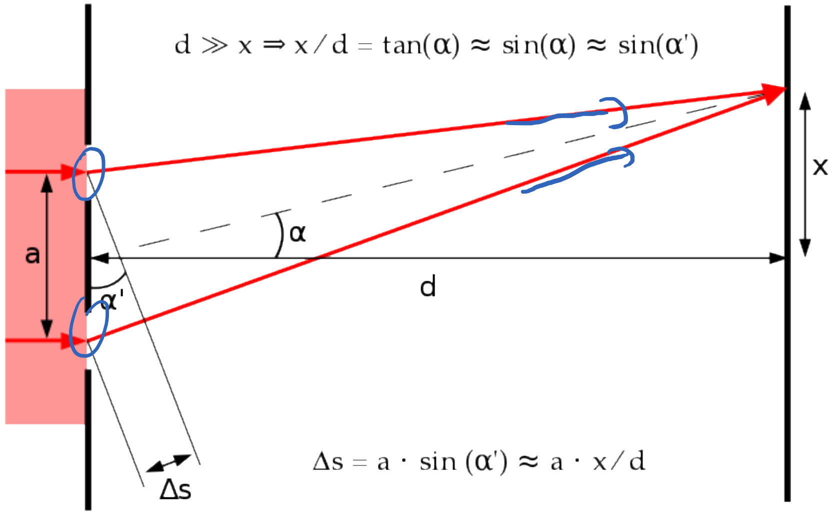
details of wavefront important

interfering rays
↓
geometrical considerations

ray bundles

Now the double slit

→ only hand-waving argument for now



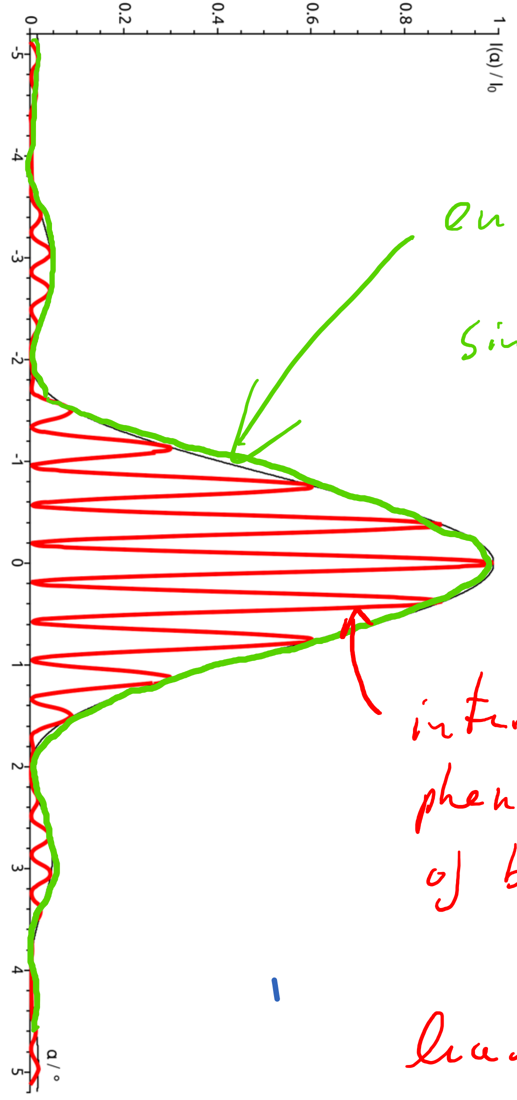
→ interference condition

↓

~ slit distance

↓ two infinites. small slit with distance a

⇒



envelope fct ↕ single slit

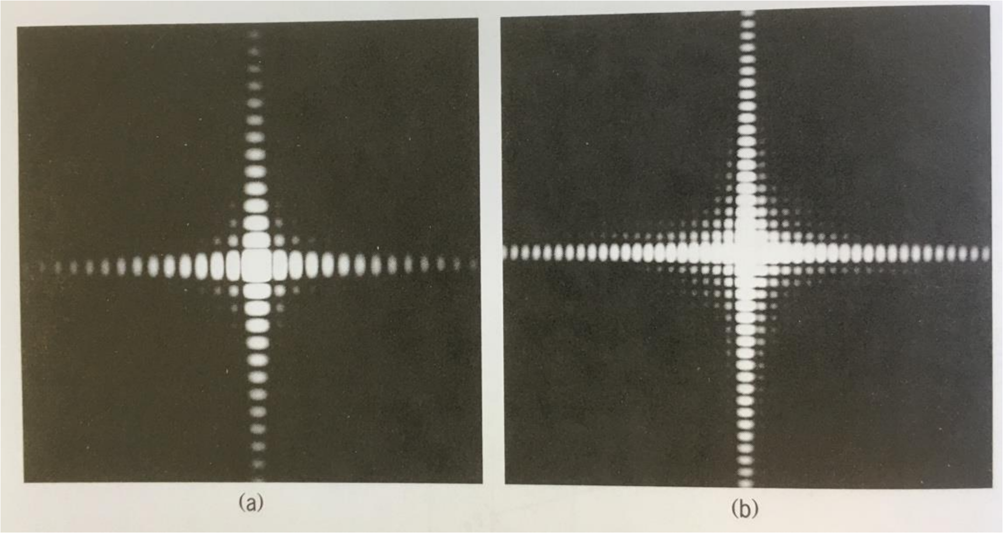
interference phenomena of both slits ↓ leads to fast oscillations

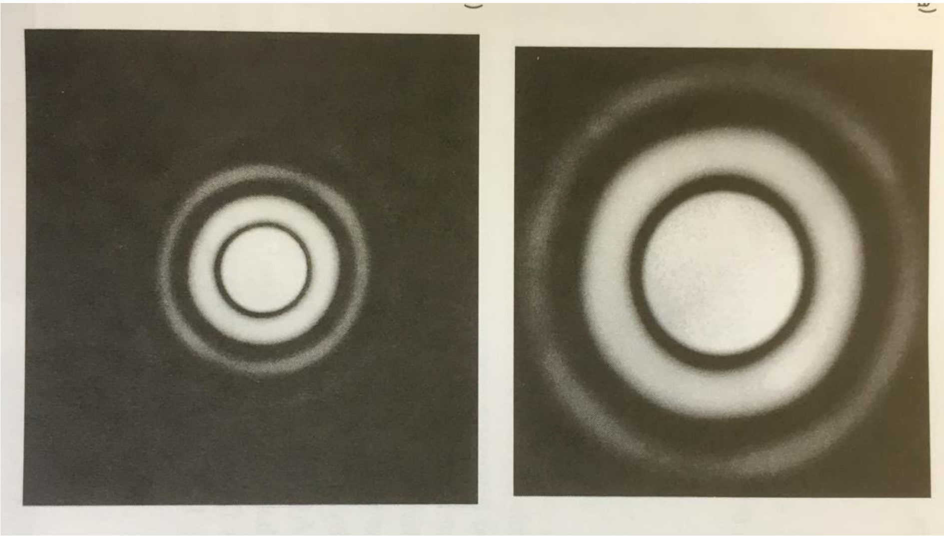
Image source: wikipedia

Diffraction pattern of 2D objects – 2 examples

Square aperture

Round aperture





↳ "cross" with modulations
2D interference pattern

↳ spherical diffraction pattern
can be described with "Bessel" fct

Comment: the diffraction pattern from a spherical aperture is called "Airy pattern". The 0^{th} order is the "Airy disc" with $r = 1.22 \lambda \frac{f}{D}$
→ important in optical setups

Note: Babinets principle

The diffraction pattern of an opaque body is identical to the one of a hole of the same size and shape except in the forward direction.

Example:

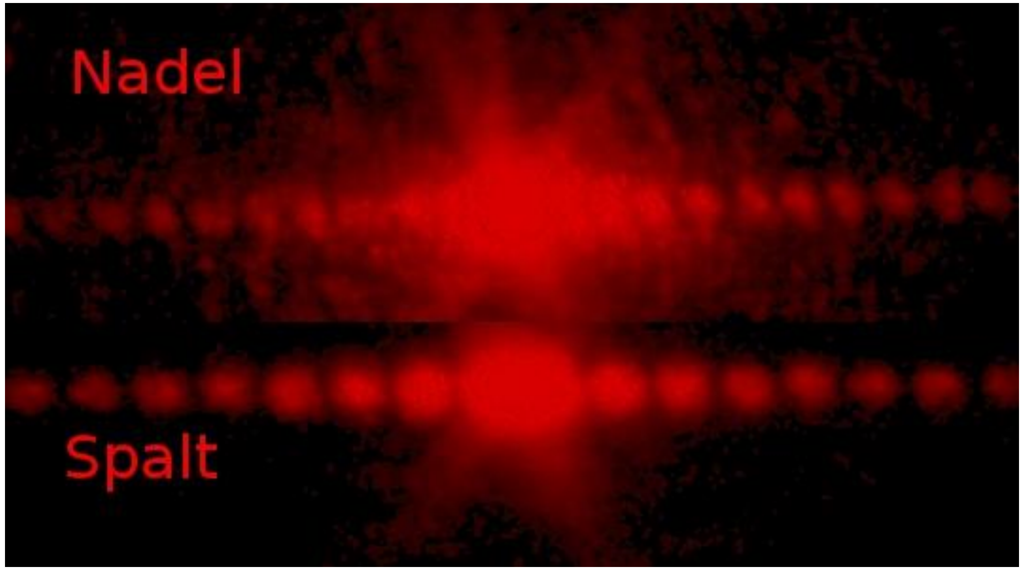


Image: wikipedia

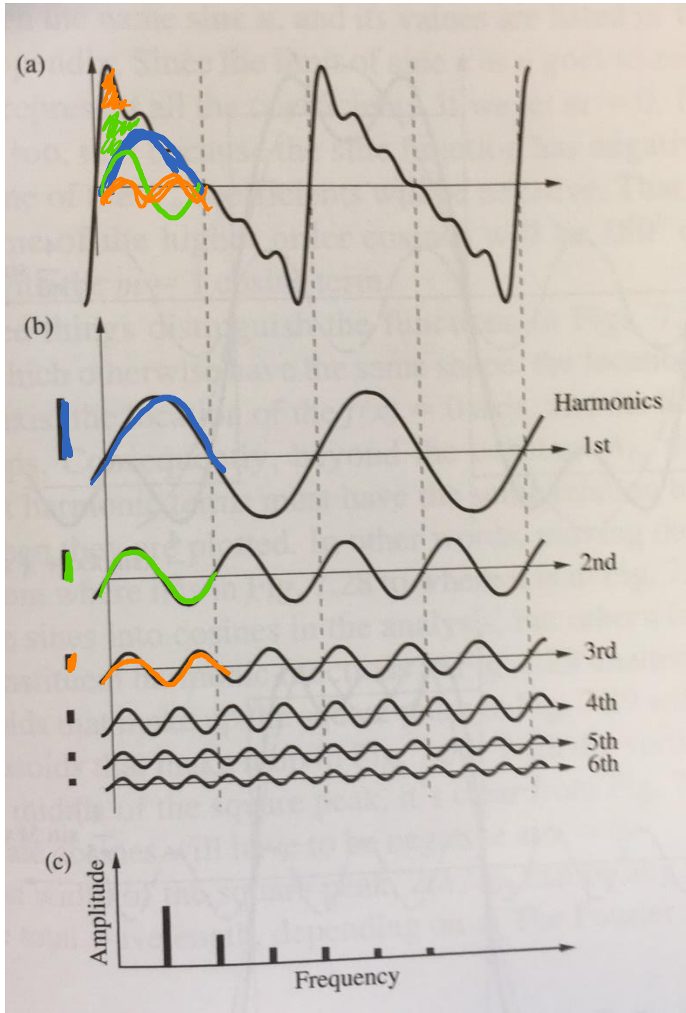
Intermezzo: Fourier Transformation

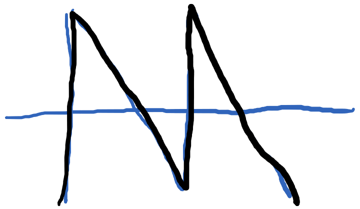
Principle idea → all functions can be represented by a sum of harmonic functions

→ it seems to work

→ it is getting better with more contributions

Principle idea





initial fct

use Σ of harmonic fct

use each harmonic fct with a specific amplitude

Mathematical description

- The principle idea of the Fourier analysis / transformation is that any function can be represented by an (infinite) series of harmonic functions.
- The Fourier transform decomposes a function into its constituent frequencies.

Sum → Integral over all frequencies

Function

Fourier transform describing f(x)

↳ "rule" how amplitudes & frequencies come together

Thus we can write

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} F(k)e^{-ikx}\,dk$$

harmonic fct

provided that

$$F(k) = \int_{-\infty}^{+\infty} f(x)e^{ikx}\,dx$$

↳ Fourier transform

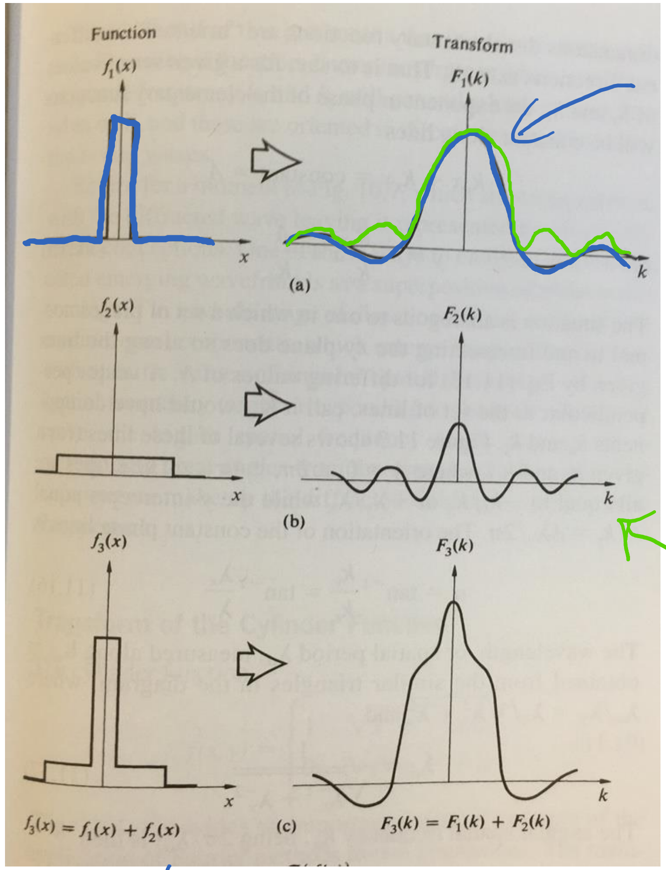
Hecht chapter 11

<u>Note</u> Computers can do this really well (GPU)

Examples

→ Some examples → for everything else there are computers

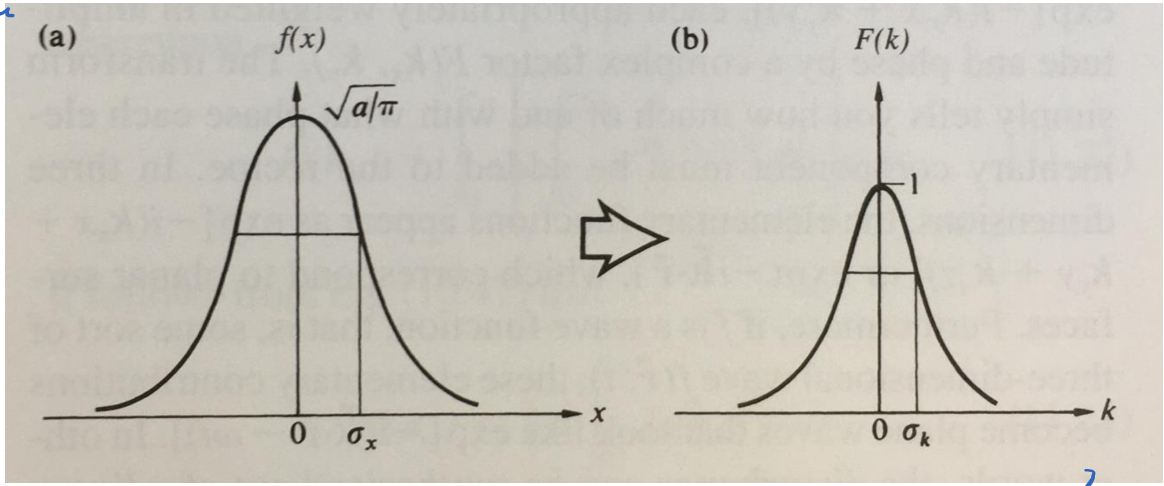
Squares and composite



sinc fct
c.f. interference from a slit
↓
in optics we measure
$I = |A|^2$

↳ composite fct

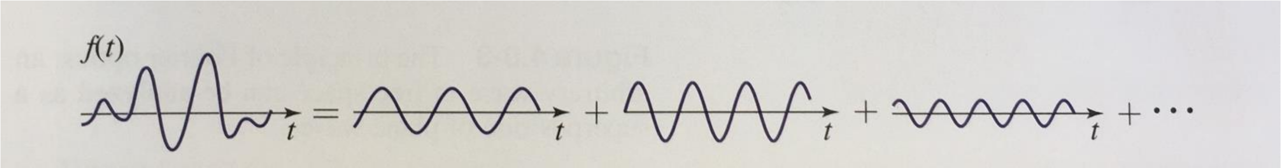
Gauss function



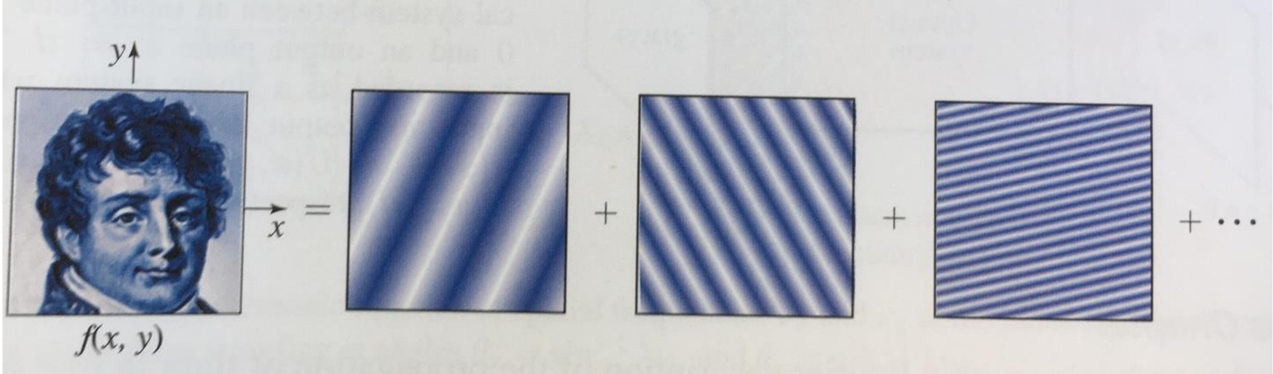
FT(Gauss) → Gaussian

→ Once a Gauss, always a Gauss!

Expansion 2D



← 1D → ok



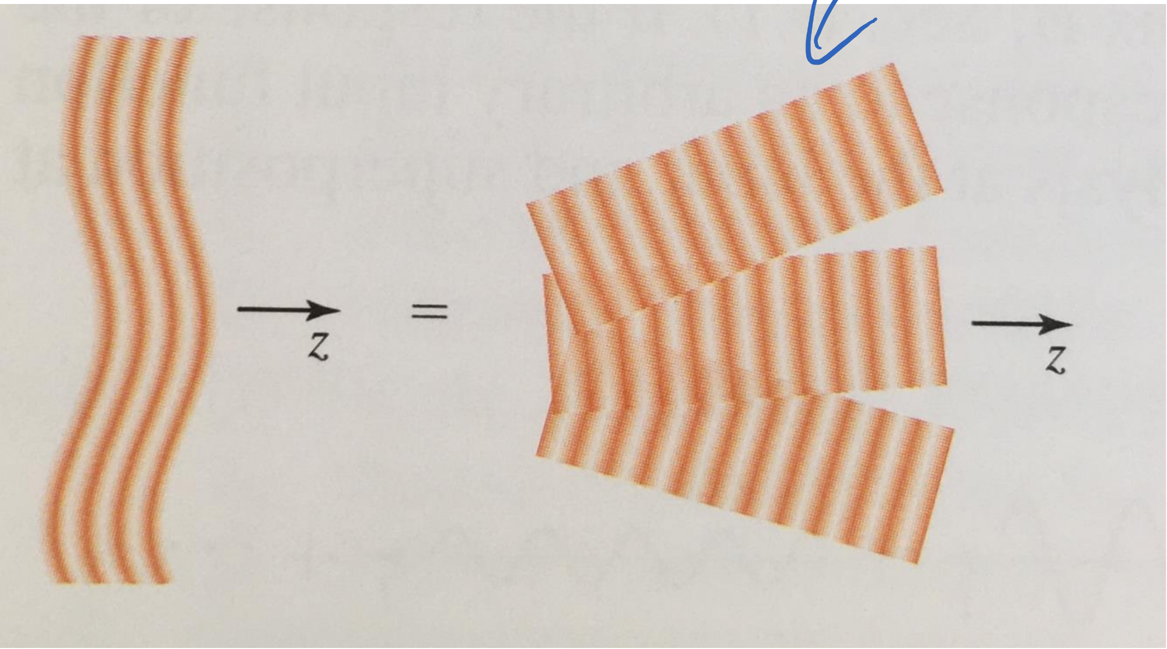
← also possible in 2D

⇓

anything can be constructed out of a sum of plane waves!

Principle of Fourier Optics: Any wavefront can be analyzed as superposition of plane waves

c.f. slide 10: "ray bundles"

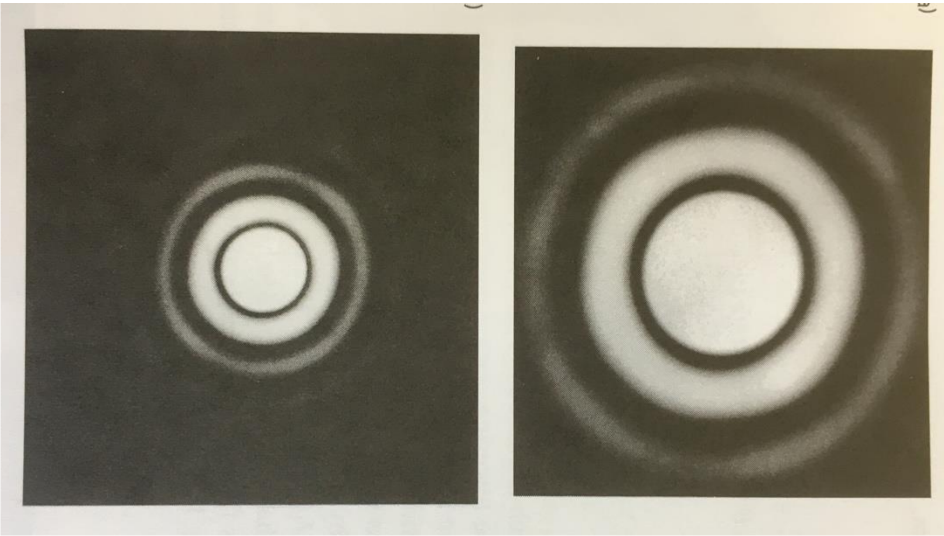


WF = Σ plane waves

Implications

Fourier transform of round aperture and airy pattern

Experiment: Diffraction pattern of circular aperture, Airy pattern

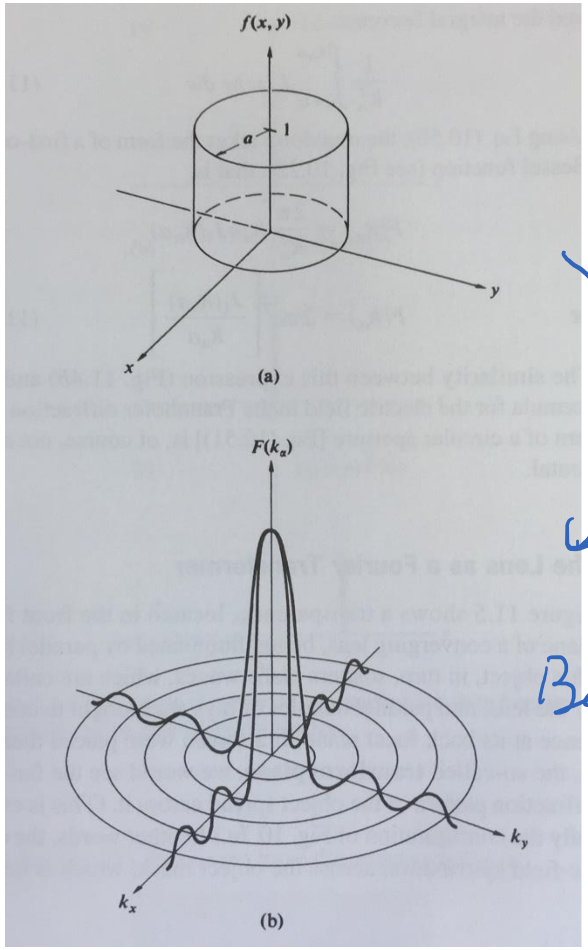


Diffraction pattern ⇒ Bessel fct

That is not a coincidence!

Generally The diffraction pattern of an object is described by its FT

Theory: Fourier transform of cylinder or "top-hat" function



Bessel fct

Diffraction as Fourier transform:

With this: double slit again

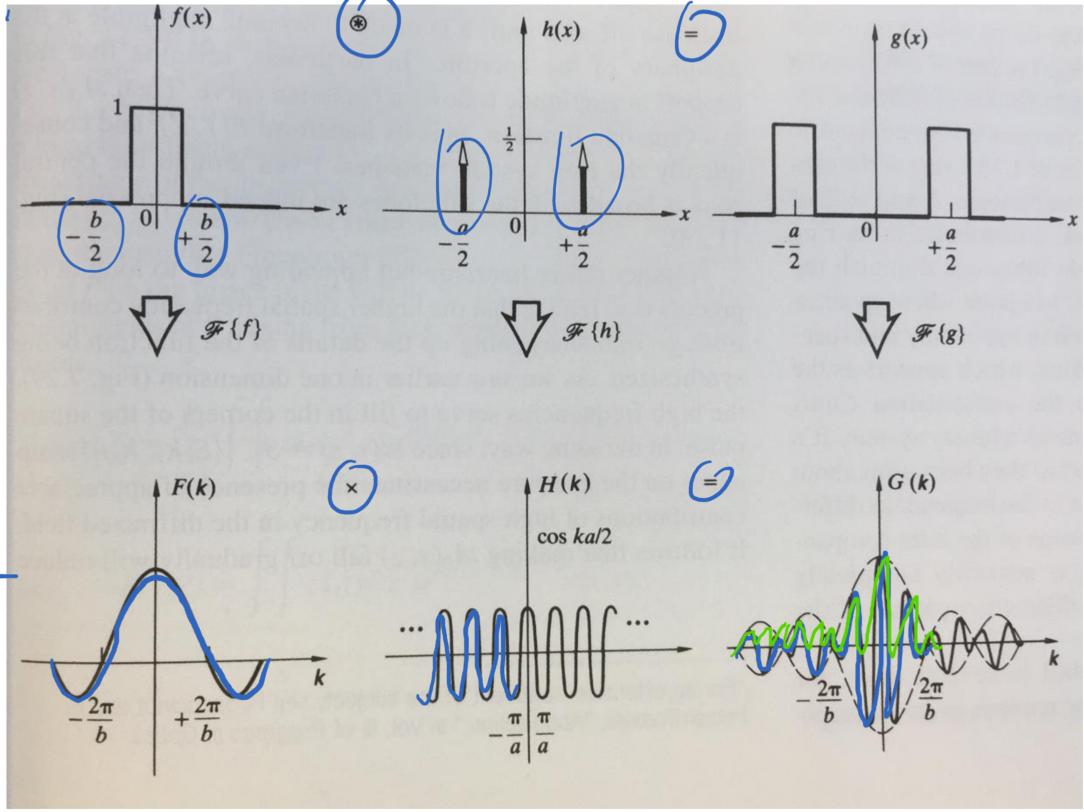
Maths

Convolution theorem

$$F(f * g) = F(f) \cdot F(g)$$

FT of convolution of two functions is point product of their FT

"double slit"



← real space

FT

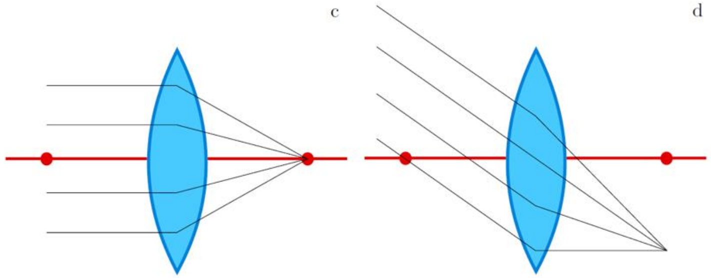
← diffraction pattern

slit / aperture

cos / δ fct

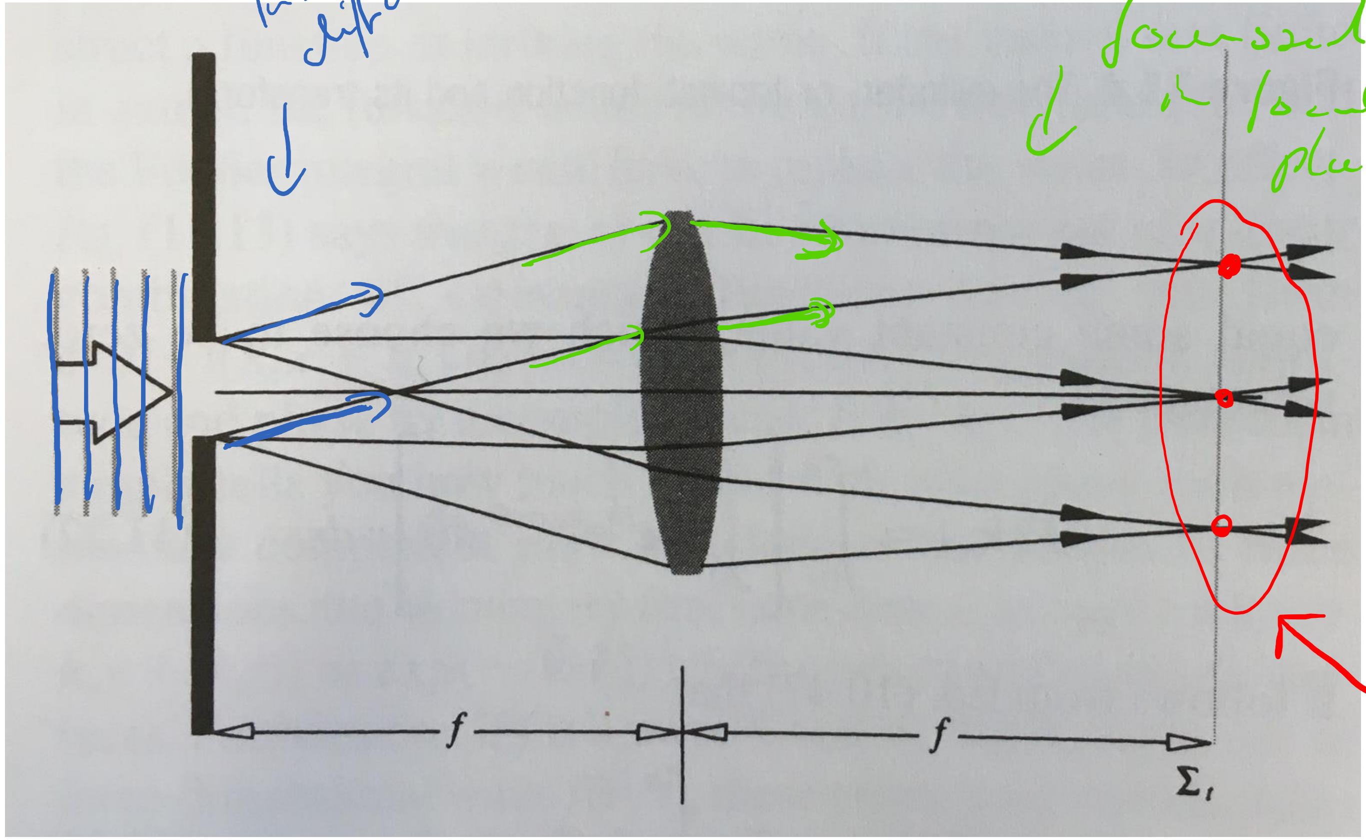
$I = |\text{Amplitude}|^2$

Lens as Fourier transformer



interference / diffraction

focussed in focal plane



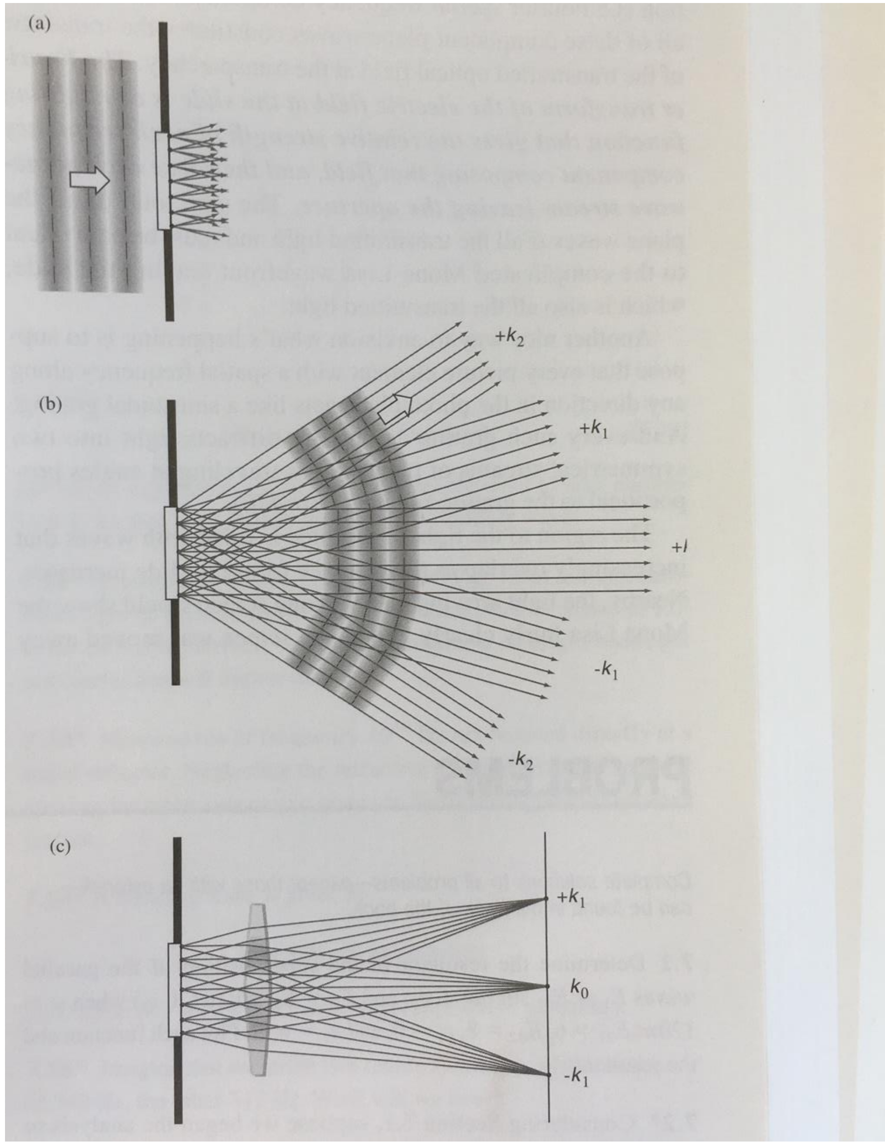
Lens pulls diffraction pattern (FT of object) into focal plane

FT of our slit!

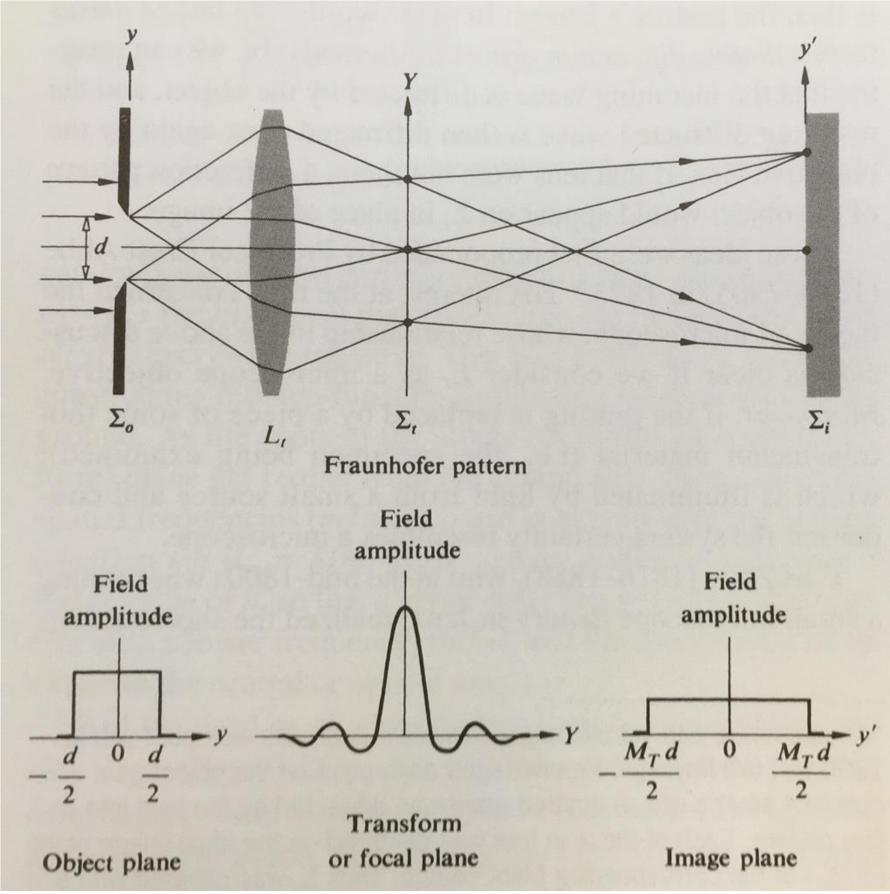
diffraction pattern @ ∞

focussed in focal plane

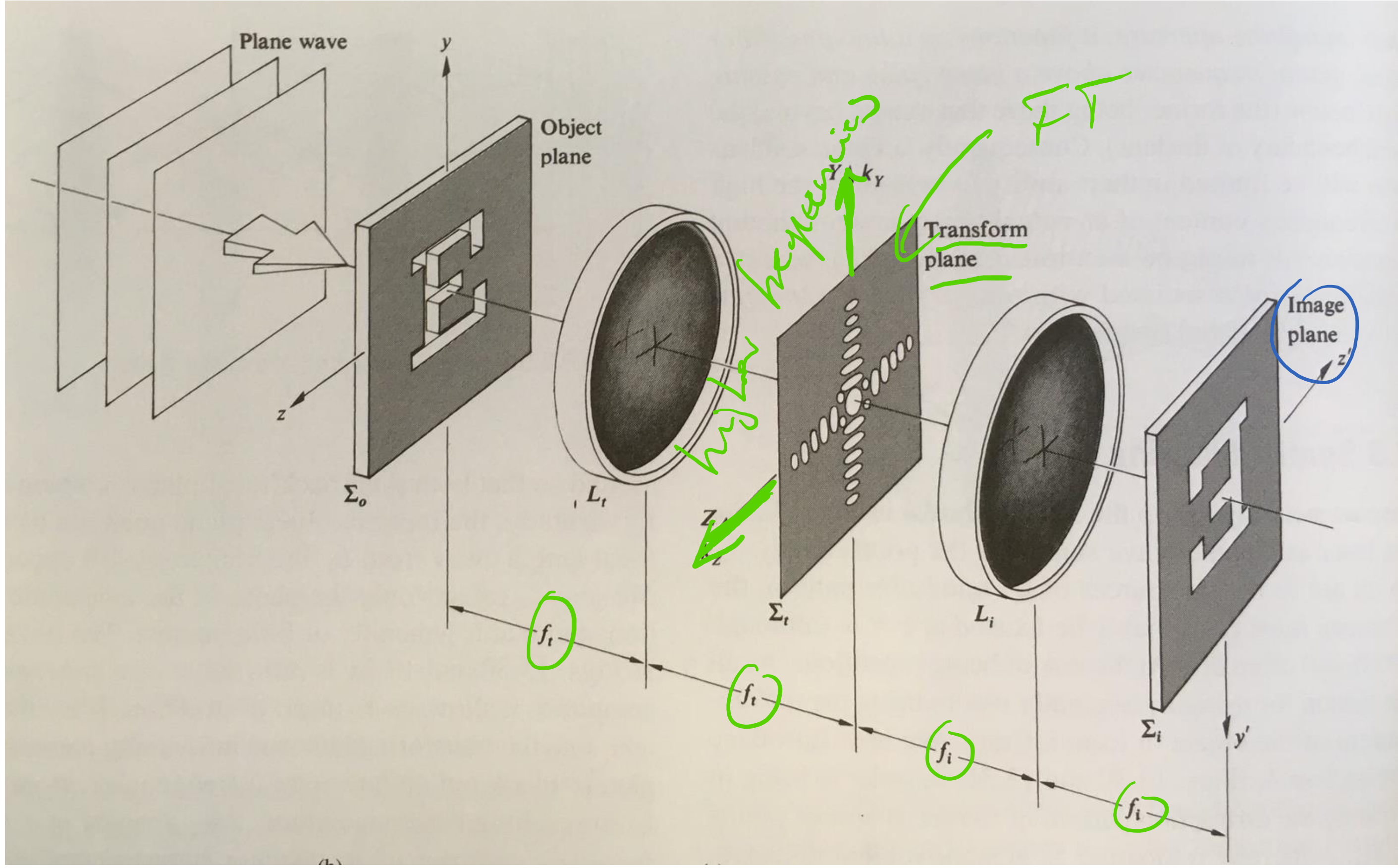
Gedankenexperiment for imaging:



Abbe image formation



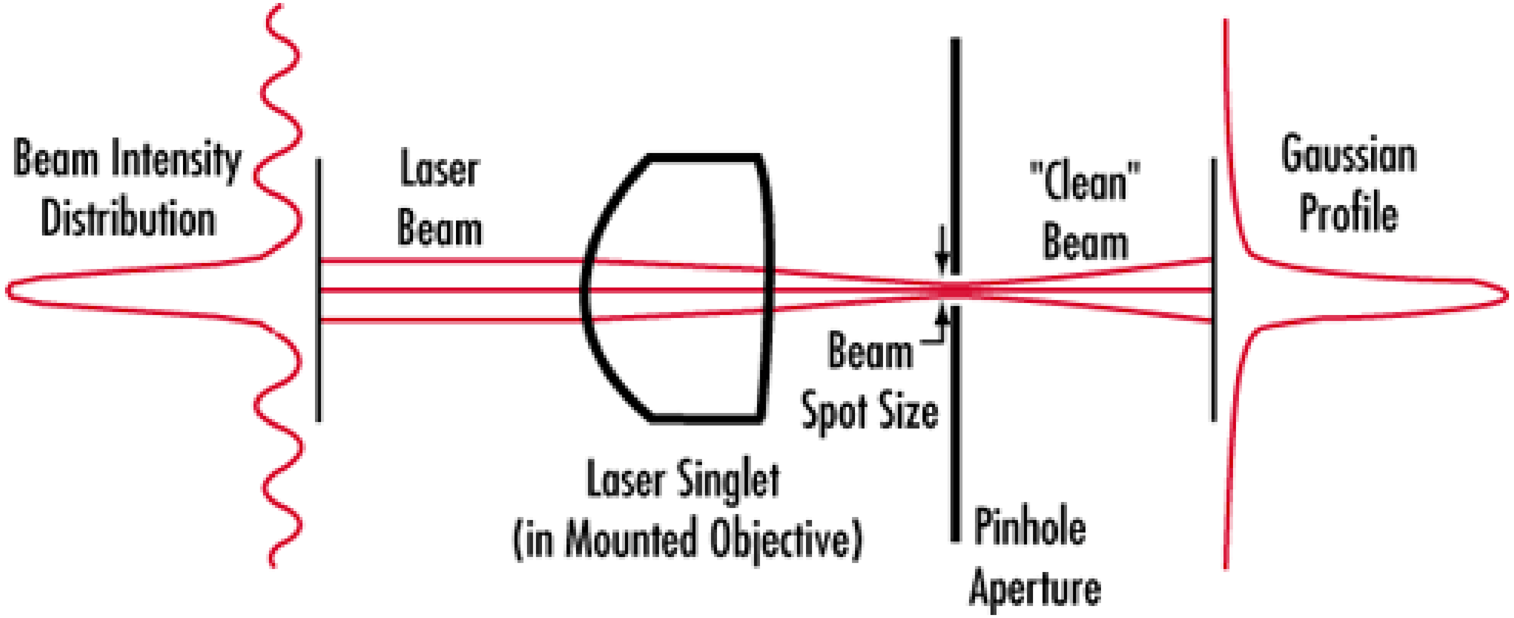
4f imaging setup



Remember

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \underbrace{F(k)\, e^{-ikx}\, dk}_{\text{Frequencies}}$$

Note on optical tricks: How to make a Gaussian beam or “Spatial Filtering”



https://www.edmundoptics.com/resources/application-notes/lasers/understanding-spatial-filters/

Summary

- From familiar diffraction
- To Fourier transform in diffraction
- Learned that lens can do FT transform

- Concept maybe overwhelming BUT it has tremendous applications
    - Microscopy
    - TEM
    - X-ray techniques

- Image filtering

The end.